Statistics 206

Homework 7 Solution

Due : November 23, 2015, In Class

1. Tell true or false of the following statements.

   (a) With many potential X variables, we can first fit a model with all these variables, and then drop those having non-significant regression coefficients by t-tests.

   FALSE. This would not work in presence of multicollinearity since then important X variables could be all dropped. This is because, with multicollinearity, T-tests for individual X variables could be all non-significant, yet there is a significant regression relation between the response variable and the set of X variables.

   (b) A correct model must be a good model.

   FALSE. A correct model is one has little bias, but it may have large variance.

   (c) With too many nuisance X variables, the model tends to have a large model bias.

   FALSE. A model with too many nuisance X variables tends to have large variance.

   (d) With the R_p^2 criterion, we aim to select the model with the largest R_p^2.

   FALSE. The model with the largest R_p^2 is the full model. We should choose the model(s) starting from where adding additional X variables won't increase R_p^2 much anymore.

   (e) For models of the same size, their $Press_p$ values are monotonically decreasing with the decreasing of SSE_p.

   FALSE. $Press_p$ values are not monotone with respect to SSE_p.

   (f) For models of the same size, their C_p, AIC_p, BIC_p values are monotonically decreasing with the decreasing of SSE_p.

   TRUE.

   (g) For a given model, its SSE_p is always no greater than its $Press_p$.

   TRUE. The fitted value for the ith case when this case is deleted while fitting the regression model can never be better than the fitted value when the ith case is included in regression model fitting.

   (h) Compared with AIC_p, BIC_p criterion tends to select smaller models because it puts more penalty on model size.

   TRUE. $AIC_p = n \log \frac{SSE_p}{n} + 2p$, $BIC_p = n \log \frac{SSE_p}{n} + \log(n)p$. And when $n \geq 8$, then $\log(n) > 2$.

   (i) The stepwise procedures are guaranteed to find the best model according to a given criterion.

   FALSE. They may end up with suboptimal models rather than the global optimal.

Problems 2 to 6. Model Selection, Validation and Diagnostic. *Diabetes data. This data consist of* 19 *variables on* 403 *subjects from* 1046 *subjects who were interviewed in a study to understand the prevalence of obesity, diabetes, and other cardiovascular risk factors in central Virginia for African Americans. We will consider building regression models with* `glyhb` *as the response variable as Glycosolated Hemoglobin* $>$ 70 *is often taken as a positive diagnostics of diabetes. The data set and description are under Resources/Homework. Please attach your R codes and plots.*

2. **Processing of the data.**

   (a) Read the data into R. Replace the missing values in the variable `frame` (indicated by an empty string “) by ’NA’ and drop the old class “.

   ```
   > diabetes = read.table('diabetes.txt', header=TRUE)  #read data
   > is.na(diabetes$frame)=which(diabetes$frame=='')  #repalce '' with NA
   > diabetes$frame=droplevels(diabetes$frame) #takes away the old class ''
   > summary(diabetes$frame)
   large medium  small   NA's
   103    184    104     12
   ```

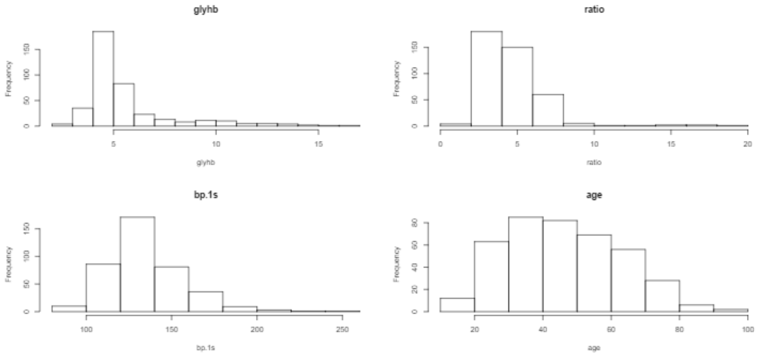
   (b) Drop `id, bp.2s, bp.2d` from the data. The column `id` are patient IDs and thus is not a meaningful predictor. The variables `bp.2s, bp.2d` have many missing values. You may use the code:

   ```
   > drops=c("id","bp.2s", "bp.2d")
   > data=diabetes[,!(names(diabetes)%in%drops)]
   ```

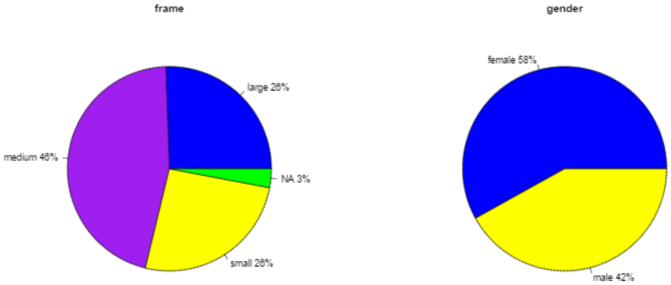
   (c) Which of the (remaining) variables are quantitative variables and which are qualitative variables? Draw histogram for `glyhb` and comment on its distribution. Draw histograms for the rest quantitative variables and draw pie charts for qualitative variables.

   ```
   > sapply(diabetes,class)
   id        chol  stab.glu        hdl      ratio      glyhb  location
   "integer" "integer" "integer" "integer" "numeric" "numeric"  "factor"
   age     gender     height     weight      frame     bp.1s     bp.1d
   "integer"  "factor" "integer" "integer"  "factor" "integer" "integer"
   bp.2s     bp.2d     waist       hip  time.ppn
   "integer" "integer" "integer" "integer" "integer"
   ```

   `glyhb`,`ratio`,`bp.1s` and `age` are quantitative variables (either `numeric` or `integer`). `gender` and `frame` are qualitative variables (`factor`).

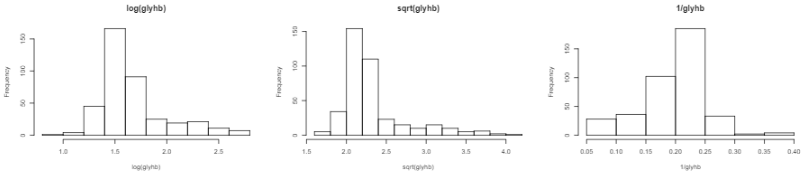


All four variables appear more or less right skewed.



`frame` has nearly half (46%) medium, one quarter (26%) large and one quarter (26%) small. `gender` has 58% female and 42% male.

(d) It turns out that the distribution of `glyhb` is severely right-skewed. Thus, you want to consider some transformations. Draw histogram for $\log(glyhb)$, $\sqrt{glyhb}$ and $\frac{1}{glyhb}$, respectively. Which distribution appears to be the most Normal like among the three? Denote it by `glyhb*`.



The third one, $\frac{1}{glyhb}$ appears to be the most normal like. Denote `glyhb*` $= \frac{1}{glyhb}$.

```
> glyhbs=1/diabetes$glyhb
> diabetes=cbind(glyhbs,diabetes)
```

(e) Replace the column `glyhb` in `data` by `glyhb*` and refer to `glyhb*` as `glyhb` hereafter and use it as the response variable.

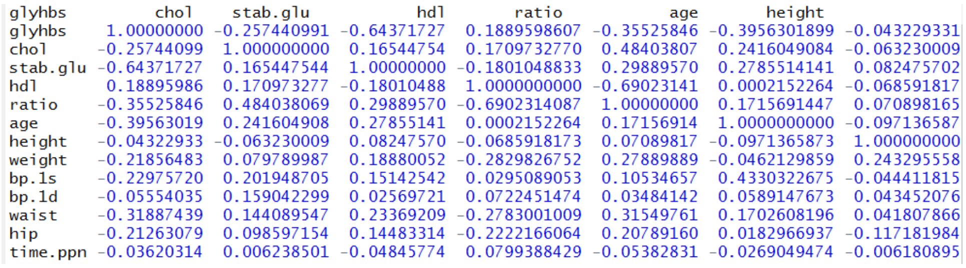
(f) Drop all the cases having missing value. You may use the code:

```
> index.na=apply(is.na(data), 1, any)
                                ## identify cases with missing value.
> data.s=data[index.na==FALSE,]  ##drop cases with missing value.
> any(is.na(data.s)) ## this should return FALSE -- no NA in data.s
> dim(data.s)  ##this should return 366 16: 366 cases, 16 variables.
> table(data.s$frame)  ## this should show three classes.
```

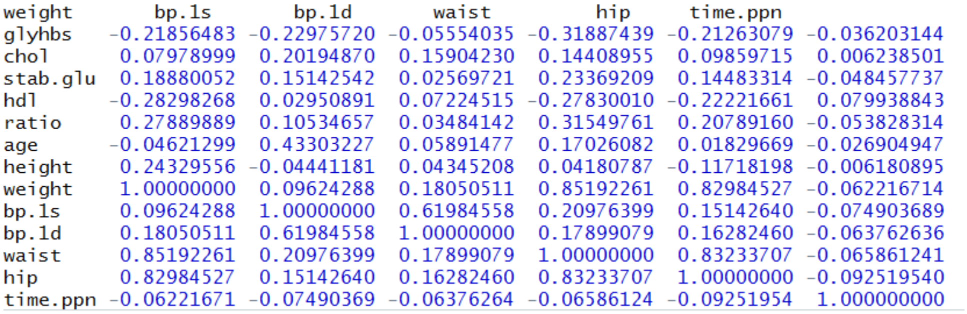
(g) Draw scatterplot matrix and obtain the pairwise correlation matrix for all quantitative variables. Do you observe nonlinearity?

The pairwise correlations are as follows:

Figure 1: Pairwise Correlations



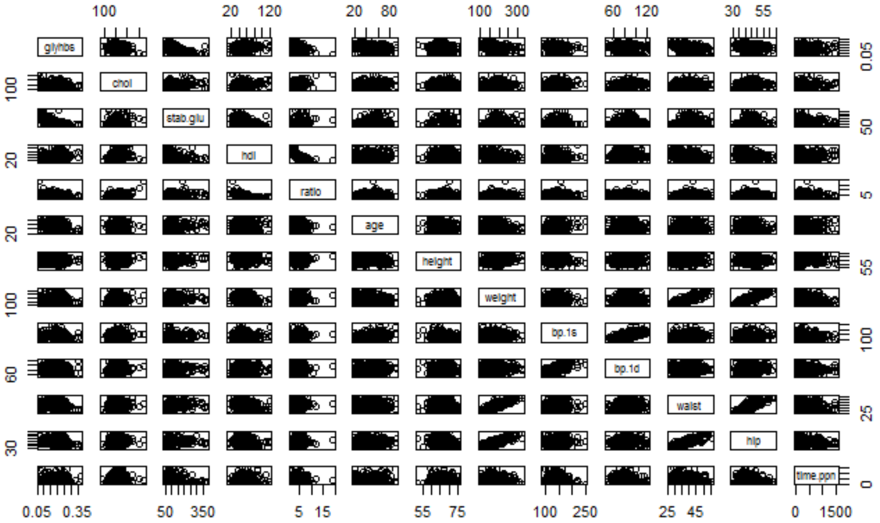
```
glyhbs          chol    stab.glu           hdl        ratio          age       height
glyhbs    1.00000000 -0.257440991 -0.64371727  0.1889598607 -0.35525846 -0.3956301899 -0.043229331
chol     -0.25744099  1.000000000  0.16544754  0.1709732770  0.48403807  0.2416049084 -0.063230009
stab.glu -0.64371727  0.165447544  1.00000000 -0.1801048833  0.29889570  0.2785514141  0.082475702
hdl       0.18895986  0.170973277 -0.18010488  1.0000000000 -0.69023141  0.0002152264 -0.068591817
ratio    -0.35525846  0.484038069  0.29889570 -0.6902314087  1.00000000  0.1715691447  0.070898165
age      -0.39563019  0.241604908  0.27855141  0.0002152264  0.17156914  1.0000000000 -0.097136587
height   -0.04322933 -0.063230009  0.08247570 -0.0685918173  0.07089817 -0.0971365873  1.000000000
weight   -0.21856483  0.079789987  0.18880052 -0.2829826752  0.27889889 -0.0462129859  0.243295558
bp.1s    -0.22975720  0.201948705  0.15142542  0.0295089053  0.10534657  0.4330322675 -0.044411815
bp.1d    -0.05554035  0.159042299  0.02569721  0.0722451474  0.03484142  0.0589147673  0.043452076
waist    -0.31887439  0.144089547  0.23369209 -0.2783001009  0.31549761  0.1702608196  0.041807866
hip      -0.21263079  0.098597154  0.14483314 -0.2222166064  0.20789160  0.0182966937 -0.117181984
time.ppn -0.03620314  0.006238501 -0.04845774  0.0799388429 -0.05382831 -0.0269049474 -0.006180895
```



```
weight        bp.1s       bp.1d       waist         hip       time.ppn
glyhbs   -0.21856483 -0.22975720 -0.05554035 -0.31887439 -0.21263079 -0.036203144
chol      0.07978999  0.20194870  0.15904230  0.14408955  0.09859715  0.006238501
stab.glu  0.18880052  0.15142542  0.02569721  0.23369209  0.14483314 -0.048457737
hdl      -0.28298268  0.02950891  0.07224515 -0.27830010 -0.22221661  0.079938843
ratio     0.27889889  0.10534657  0.03484142  0.31549761  0.20789160 -0.053828314
age      -0.04621299  0.43303227  0.05891477  0.17026082  0.01829669 -0.026904947
height    0.24329556 -0.04441181  0.04345208  0.04180787 -0.11718198 -0.006180895
weight    1.00000000  0.09624288  0.18050511  0.85192261  0.82984527 -0.062216714
bp.1s     0.09624288  1.00000000  0.61984558  0.20976399  0.15142640 -0.074903689
bp.1d     0.18050511  0.61984558  1.00000000  0.17899079  0.16282460 -0.063762636
waist     0.85192261  0.20976399  0.17899079  1.00000000  0.83233707 -0.065861241
hip       0.82984527  0.15142640  0.16282460  0.83233707  1.00000000 -0.092519540
time.ppn -0.06221671 -0.07490369 -0.06376264 -0.06586124 -0.09251954  1.000000000
```

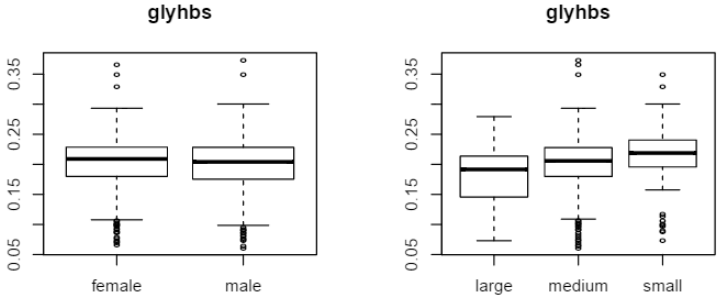
The scatterplot matrix is as follows:

Figure 2: Scatter Plot Matrix for Quantitative Variables



There is no obvious nonlinearity between `glyhb` with the other variables. There are positive linear relationships between weight and waist, weight and hip, bp.1s and bp.1d, waist and hip. We can see the correlation between these pairs are high.

(h) Draw side-by-side box plots to show how `glyhb` is distributed in male and female, and how it is distributed in the three `frame` classes.



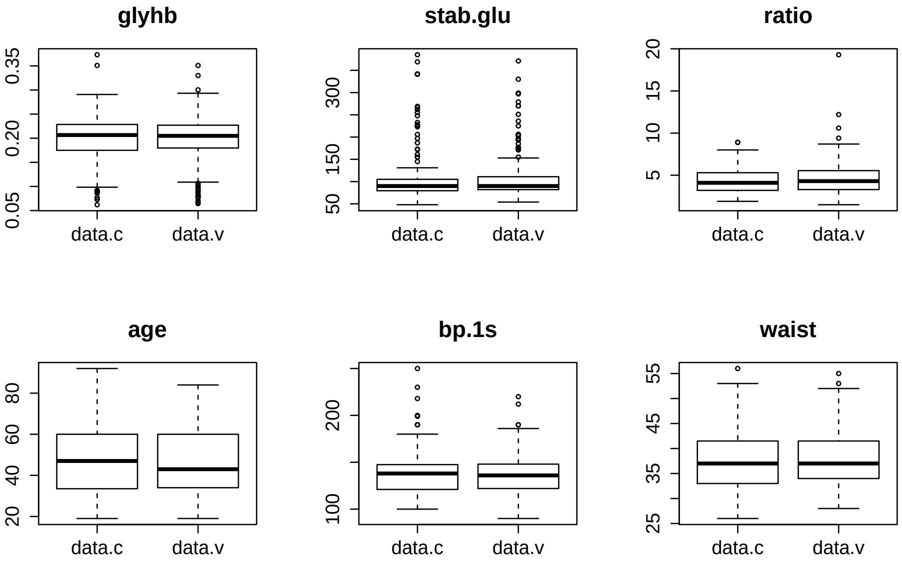
The distribution of `glyhb` is more symmetric in within each class. Also `glyhb` appears to decrease from small to large frame.

(i) Randomly split data into two equal halves: a training data set and a validation data set. You may use the code:

```
> set.seed(10) ## set seed for random number generator
               ##so everyone gets the same split of the data.
> n.s=nrow(data.s) ## number of cases in data.s (366)
> index.s=sample(1: n.s, size=366/2, replace=FALSE)
               ## randomly sample 183 cases to form the training data.
> data.c=data.s[index.s,]  ## get the training data set.
> data.v=data.s[-index.s,]
               ## the remaining 183 cases form the validation set.
```

(j) Examine whether the training data and validation data look alike. Draw side-by-side boxplots for `glyhb`, `stab.glu`, `ratio`, `age`, `bp.1s` and `waist`, in training data and validation data, respectively. Are these variables having similar distributions in these two sets?

```
> par(mfrow=c(2,3))
> boxplot(data.c$glyhb,data.v$glyhb,main=’glyhb’,names=c(’data.c’,’data.v’))
> boxplot(data.c$stab.glu,data.v$stab.glu,main=’stab.glu’,names=c(’data.c’,
+                                                                   ’data.v’))
> boxplot(data.c$ratio,data.v$ratio,main=’ratio’,names=c(’data.c’,’data.v’))
> boxplot(data.c$age,data.v$age,main=’age’,names=c(’data.c’,’data.v’))
> boxplot(data.c$bp.1s,data.v$bp.1s,main=’bp.1s’,names=c(’data.c’,’data.v’))
> boxplot(data.c$waist,data.v$waist,main=’waist’,names=c(’data.c’,’data.v’))
```



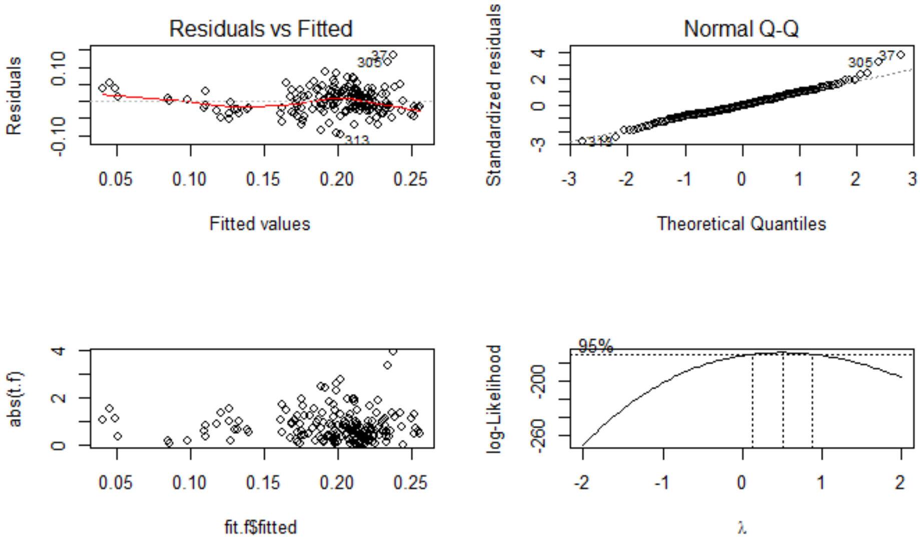
Yes, they have similar distributions.

3. **Selection of first-order effects.** We now consider subsets selection from the pool of all first-order effects of the 15 predictors.

   (a) Fit a model with all first-order effects (Model 1). How many regression coefficients are there in this model? What is the *MSE* from this model? Apply box-cox procedure on this model. Does it appear that any transformation of the response variable is still needed?

```
lm(glyhb ˜., data=data.c) ## data.c denotes the training data
Call:
lm(formula = glyhbs ˜ ., data = data.c)

Residuals:
Min        1Q    Median        3Q       Max
-0.097813 -0.022472 -0.002034  0.021097  0.134611

Coefficients:
Estimate Std. Error t value Pr(>|t|)
(Intercept)     4.819e-01  8.499e-02   5.670 6.19e-08 ***
chol           -6.857e-05  1.695e-04  -0.405   0.6863
stab.glu       -5.314e-04  5.418e-05  -9.807  < 2e-16 ***
hdl             1.211e-04  5.492e-04   0.220   0.8258
ratio          -2.414e-03  6.588e-03  -0.366   0.7145
locationLouisa -1.808e-03  5.969e-03  -0.303   0.7623
age            -5.487e-04  2.199e-04  -2.495   0.0136 *
gendermale     -7.422e-04  1.018e-02  -0.073   0.9420
height         -1.212e-03  1.123e-03  -1.079   0.2820
weight          2.210e-04  2.034e-04   1.087   0.2788
framemedium     1.417e-03  7.861e-03   0.180   0.8572
framesmall     -1.062e-02  9.596e-03  -1.107   0.2699
bp.1s          -1.214e-04  1.708e-04  -0.711   0.4782
bp.1d           3.198e-05  2.505e-04   0.128   0.8986
waist          -1.893e-03  1.148e-03  -1.649   0.1010
hip            -1.177e-03  1.352e-03  -0.870   0.3854
time.ppn       -1.444e-05  9.881e-06  -1.461   0.1459
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 0.0372 on 166 degrees of freedom
Multiple R-squared:  0.5547,  Adjusted R-squared:  0.5118
F-statistic: 12.92 on 16 and 166 DF,  p-value: < 2.2e-16


> fit1=lm(glyhb˜.,data=data.c)
> length(fit1$coefficients)   #17 regression coefficients
[1] 17
> anova(fit1)['Residuals',3]   #MSE
[1] 0.001383855
```

Figure 3: Model Diagnostics



The box-cox plot suggests no further transformation on the response variable is needed.

(b) Consider best subsets selection using the R function `regsubsets()` from the `leaps` library with Model 1 as the full model. Return the top 1 best subset of all subset sizes up to 16. Get SSE_p,R^2_p, $R^2_{a,p}$, C_p, AIC_p,BIC_p for each of these models. Identify the best model according to each criterion. For the best model according to C_p criterion, what do you observe about its C_p value? Do you have a possible explanation?

```
> library(leaps)
> sub_set=regsubsets(glyhb˜.,data=data.c,nbest=1,nvmax=16,method="exhaustive")
> sum_sub=summary(sub_set)
> n=nrow(data.c)
> ## number of coefficients in each model: p
> p.m=as.integer(as.numeric(rownames(sum_sub$which))+1)
> sse=sum_sub$rss
> aic=n*log(sse/n)+2*p.m
> bic=n*log(sse/n)+log(n)*p.m
> res_sub=cbind(sum_sub$which,sse,sum_sub$rsq,sum_sub$adjr2,sum_sub$cp,
+               aic, bic)
> fit0=lm(glyhb~1,data=data.c) ##fit the model with only intercept
> sse1=sum(fit0$residuals^2)
> p=1
> c1=sse1/0.001384-(n-2*p)
> aic1=n*log(sse1/n)+2*p
> bic1=n*log(sse1/n)+log(n)*p
> none=c(1,rep(0,16),sse1,0,0,c1,bic1,aic1)
> res_sub=rbind(none,res_sub) ##combine the results with other models
> colnames(res_sub)=c(colnames(sum_sub$which),"sse", "R^2", "R^2_a", "Cp",
+                      "aic", "bic")
> res_sub
(Intercept) chol stab.glu hdl ratio locationLouisa age gendermale height
none           1    0        0   0     0              0   0          0      0
1              1    0        1   0     0              0   0          0      0
2              1    0        1   0     0              0   1          0      0
3              1    0        1   0     0              0   1          0      0
4              1    0        1   0     1              0   1          0      0
5              1    0        1   0     1              0   1          0      0
6              1    0        1   0     1              0   1          0      0
7              1    0        1   0     1              0   1          0      0
8              1    0        1   0     1              0   1          0      1
9              1    0        1   0     1              0   1          0      1
10             1    0        1   0     1              0   1          0      1
11             1    1        1   0     1              0   1          0      1
12             1    1        1   0     1              1   1          0      1
13             1    1        1   1     1              1   1          0      1
14             1    1        1   1     1              1   1          0      1
15             1    1        1   1     1              1   1          0      1
16             1    1        1   1     1              1   1          1      1
weight framemedium framesmall bp.1s bp.1d waist hip time.ppn       sse
none      0           0          0     0     0     1   0        0 0.5158646
1         0           0          0     0     0     0   0        0 0.2864076
2         0           0          0     0     0     0   0        0 0.2574112
3         0           0          0     0     0     1   0        0 0.2428890
4         0           0          0     0     0     1   0        0 0.2401432
5         0           0          1     0     0     1   0        0 0.2367131
6         0           0          1     0     0     1   0        1 0.2343460
7         0           0          1     1     0     1   0        1 0.2331725
8         0           0          1     1     0     1   0        1 0.2326634
9         1           0          1     0     0     1   1        1 0.2314193
10        1           0          1     1     0     1   1        1 0.2303187
11        1           0          1     1     0     1   1        1 0.2300477
```

```
12        1           0          1     1     0     1   1        1 0.2299216
13        1           0          1     1     0     1   1        1 0.2298166
14        1           1          1     1     0     1   1        1 0.2297510
15        1           1          1     1     1     1   1        1 0.2297274
16        1           1          1     1     1     1   1        1 0.2297200
R^2     R^2_a           Cp       aic       bic
none 0.0000000 0.0000000 191.73453170 -1069.256 -1072.466
1    0.4448009 0.4417335  27.96351331 -1178.148 -1171.729
2    0.5010102 0.4954659   9.01014928 -1195.682 -1186.053
3    0.5291612 0.5212701   0.51619889 -1204.309 -1191.471
4    0.5344840 0.5240230   0.53201659 -1204.389 -1188.342
5    0.5411332 0.5281708   0.05337754 -1205.022 -1185.765
6    0.5457220 0.5302352   0.34280455 -1204.861 -1182.395
7    0.5479966 0.5299165   1.49487219 -1203.780 -1178.104
8    0.5489836 0.5282473   3.12693590 -1202.180 -1173.294
9    0.5513952 0.5280574   4.22797088 -1201.161 -1169.066
10   0.5535287 0.5275711   5.43265348 -1200.033 -1164.729
11   0.5540541 0.5253676   7.23678869 -1198.249 -1159.735
12   0.5542986 0.5228374   9.14564365 -1196.349 -1154.626
13   0.5545020 0.5202329  11.06983181 -1194.433 -1149.500
14   0.5546292 0.5175150  13.02241521 -1192.485 -1144.343
15   0.5546751 0.5146758  15.00531267 -1190.504 -1139.152
16   0.5546893 0.5117678  17.00000000 -1188.510 -1133.948
```

Best model:

SSE, R^2: Model 16 (full model)
R^2_a: Model 6 (glu, ratio, age, frame, waist, time)
C_p, AIC: Model 5 (glu, ratio, age, frame, waist)
BIC: Model 3 (glu, age, waist)

For the model with the smallest C_p statistic (Model 5), its C_p value is 0.053 which is much smaller than $p (= 6)$ of this model. Here all the models being considered are submodels of the full model, so their $SSE \geq SSE_f$ and thus the C_p statistic of a submodel satisfies $C_p \geq (n - P) - (n - 2p) = 2p - P$. If SSF_f is not much smaller than SSE of a submodel (i.e., the additional variables in the full model have not much additional contribution in explaining Y), then the C_p of the submodel could be quite small.

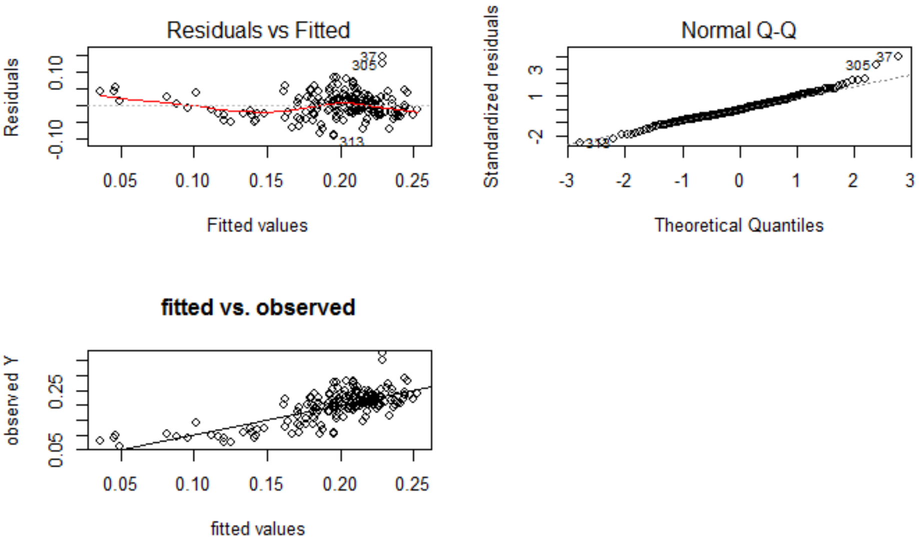
(c) We now explore stepwise procedures. Apply the `forward stepwise procedure` using R function `stepAIC()`, starting from the null-model and using the AIC_p criterion. What is the model being selected? Denote this model by Model fs1. Is it the "best" model according to AIC_p criterion identified in the previous question? If not, how its AIC value compare with AIC of the "best" model?

```
> library(MASS)
> step.f=stepAIC(fit0,scope=list(upper=fit1, lower=~1), direction="both",
+                  k=2)
> step.f$anova
Stepwise Model Path
Analysis of Deviance Table

Initial Model:
glyhb ~ 1

Final Model:
glyhb ~ stab.glu + age + waist + ratio


Step Df    Deviance Resid. Df Resid. Dev       AIC
1                                182  0.5158646 -1072.466
2 + stab.glu  1 0.229457010       181  0.2864076 -1178.148
3      + age  1 0.028996427       180  0.2574112 -1195.682
4    + waist  1 0.014522110       179  0.2428890 -1204.309
5    + ratio  1 0.002745821       178  0.2401432 -1204.389
```

The final model contains glu, age, waist and ratio. It's not the best model according to AIC_p criterion identified in part (i) and it's AIC of -1204.389 is slightly larger, indicating a slightly suboptimal model.

(d) Comment on the residual vs. fitted value plot and the residual Q-Q plot of Model fs1. Does this model appear to be adequate?

Figure 4: Model Diagnostics for Model fs1



The residual vs. fitted plot shows non-constant error variance. The QQ plot indicates slight right skewness. Otherwise, the model seems reasonable.

4. **Selection of first- and second- order effects.** We now consider subsets selection from the pool of first-order effects as well as 2-way interaction effects of the 15 predictors.

   (a) Fit a model with all first-order and 2-way interaction effects (Model 2). How many regression coefficients are there in this model? What is the MSE from this model? Do you have any concern about the fitting of this model and why?

   ```
   > fit2=lm(glyhb~.^2,data=data.c)
   > length(fit2$coefficients) #number of coefficients
   [1] 136
   > anova(fit2)["Residuals",3] #MSE
   [1] 0.001036088
   ```

   Relative to the sample size, there are too many X variables (136) in the model.

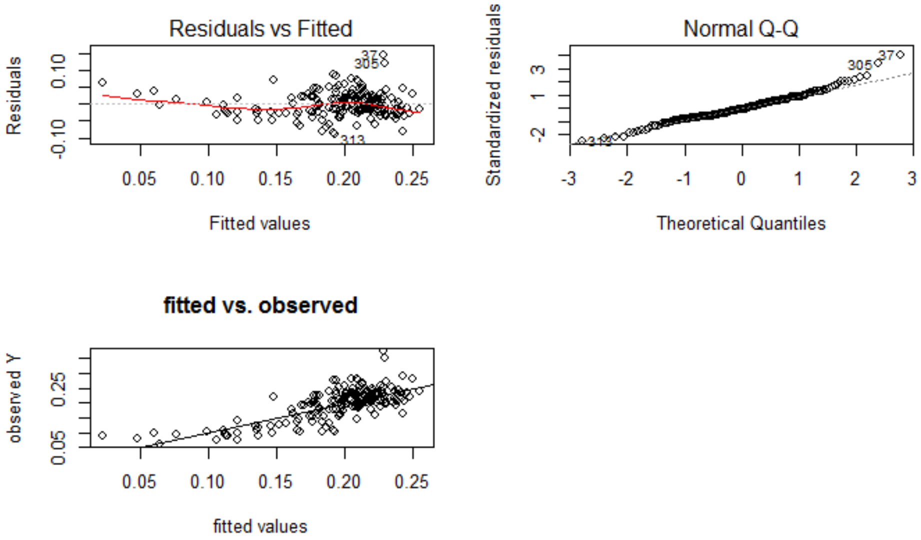
   (b) Apply the `forward stepwise procedure` using R function `stepAIC()`, starting from the null-model and using the AIC_p criterion. What is the model being selected? Denote this model by Model fs2. Compare its AIC value with that of Model fs1. What do you find?

   ```
   > step.f2=stepAIC(fit0,scope=list(upper=fit2, lower=~1), direction="both",
   + k=2)
   > step.f2$anova
   Stepwise Model Path
   Analysis of Deviance Table

   Initial Model:
   glyhb ~ 1

   Final Model:
   glyhb ~ stab.glu + age + waist + ratio + stab.glu:ratio + age:ratio


   Step Df    Deviance Resid. Df Resid. Dev       AIC
   1                                    182  0.5158646 -1072.466
   2       + stab.glu  1 0.229457010       181  0.2864076 -1178.148
   3            + age  1 0.028996427       180  0.2574112 -1195.682
   4          + waist  1 0.014522110       179  0.2428890 -1204.309
   5          + ratio  1 0.002745821       178  0.2401432 -1204.389
   6 + stab.glu:ratio  1 0.003550630       177  0.2365926 -1205.115
   7      + ratio:age  1 0.002608308       176  0.2339843 -1205.144
   ```

   The final model contains glu, age, waist, ratio, glu:ratio and age:ratio. Its AIC is -1205.144, which is slightly smaller than that of Model.fs1.

(c) Comment on the residual vs. fitted value plot and the residual Q-Q plot of Model fs2. Does this model appear to be adequate?

Figure 5: Model Diagnostics for Model fs2



The residual vs. fitted plot still shows non-constant error variance. The QQ plot indicates slight right skewness. Otherwise, the model seems reasonable.

(d) Apply the `forward selection procedure`. What model do you end up with?

Notes: You could try best subsets selection using the R function `regsubsets()` from the `leaps` library, e.g. return the top 1 best subset of all subset sizes up to 16 with the full model being Model 2. However, be careful, you may have to stop the R session due to the slowness of this procedure! So save all that you want to save before you try this.

```
> step.f3=stepAIC(fit0,scope=list(upper=fit2, lower=~1), direction="forward",
+                    k=2)
> step.f3$anova
Stepwise Model Path
Analysis of Deviance Table

Initial Model:
glyhb ~ 1

Final Model:
glyhb ~ stab.glu + age + waist + ratio + stab.glu:ratio + age:ratio
```

```
Step Df    Deviance Resid. Df Resid. Dev       AIC
1                                   182  0.5158646 -1072.466
2       + stab.glu  1 0.229457010       181  0.2864076 -1178.148
3            + age  1 0.028996427       180  0.2574112 -1195.682
4          + waist  1 0.014522110       179  0.2428890 -1204.309
5          + ratio  1 0.002745821       178  0.2401432 -1204.389
6 + stab.glu:ratio  1 0.003550630       177  0.2365926 -1205.115
7      + ratio:age  1 0.002608308       176  0.2339843 -1205.144
```

We end up with Model.fs2, the same model obtained by forward stepwise procedure.

5. **Model validation.** We now consider validation of the two models fs1 and fs2 selected by the forward stepwise procedure.

   (a) **Internal validation of Models fs1 and fs2**. For this purpose, we need to compute C_p and $Press_p$ for these models. For C_p, we need an unbiased estimator of the error variance σ^2. The largest model we have considered so far is Model 2. However, this model has a very large number of regression coefficients (relative to the sample size), making its parameter estimation unreliable due to large sampling variability. Therefore, we decided to use a smaller model consisting of all predictors identified by Model fs1 (the forward stepwise selected first-order model), as well all the 2-way interaction terms among these predictors. Denote this model by Model 3. Note that, Model fs2 is also a sub-model of Model 3. How many regression coefficients are there in Model 3 ? What is MSE from Model 3? Calculate SSE_p, MSE_p, C_p and $Press_p$ for Models fs1 and fs2 and briefly comment on the results, e.g., does it appear to be substantial model bias in these two models? Should overfitting be a concern?

```
> data.cc=data.c[, c("glyhb", "stab.glu", "age", "waist", "ratio")]
> fit3=lm(glyhb~.^2, data=data.cc)
> length(fit3$coefficients) #number of coeffiicents in Model 3
[1] 11
> mse3= anova(fit3)["Residuals",3] #MSE for Model 3
> mse3
[1] 0.001346963
> sse.fs1=anova(step.f)["Residuals",2] #first order selected
> sse.fs1
[1] 0.2401432
> sse.fs2=anova(step.f2)["Residuals",2] #second order selected
> sse.fs2
[1] 0.2339843
> mse.fs1=anova(step.f)["Residuals",3] #MSE for Model fs1
> mse.fs1
[1] 0.001349119
> mse.fs2=anova(step.f2)["Residuals",3] #MSE for Model fs2
> mse.fs2
[1] 0.001329456
> p.fs1=length(step.f$coefficients) #5
> p.fs1
[1] 5
> p.fs2=length(step.f2$coefficients) #7
> p.fs2
[1] 7
> cp.fs1=sse.fs1/mse3-(n-2*p.fs1) #C_p for Model fs1
> cp.fs1
[1] 5.284958
> cp.fs2=sse.fs2/mse3-(n-2*p.fs2) #C_p for Model fs2
> cp.fs2
[1] 4.712495
> press.fs1=sum(step.f$residuals^2/(1-influence(step.f)$hat)^2)
> press.fs1
[1] 0.2535404
> press.fs2=sum(step.f2$residuals^2/(1-influence(step.f2)$hat)^2)
> press.fs2
[1] 0.2534834
```

For both Model fs1 and Model fs2, $C_p \approx p$ and $Press_p$ and SSE_p are reasonably close, supporting their validity: little bias and not much overfitting.

(b) **External validation using the validation set**. We now fit Models fs1 and fs2 on the validation data set. Compare the fitted regression coefficients from the training data and those from the validation data. Are the two sets of estimated regression coefficients having the same sign? Are their values similar? How about the two sets of standard errors? Does it appear that Models fs1 and fs2 have consistent estimates on the training data and validation data? Calculate the mean squared prediction error (MSPE) using the validation data for each of the two models. How do these $MSPE_v$ compare with the respective $Press_p/n$ and SSE_p/n (Note here n is the sample size of the training data, i.e., 183)? Which model among the two has a smaller $MSPE_v$?

```
### Model fs1
> fit.fs1.v=lm(step.f,data=data.v) #Model fs1 on validation data
> summary(step.f) #summary on training data

Call:
lm(formula = glyhb ~ stab.glu + age + waist + ratio, data = data.c)

Residuals:
Min        1Q    Median        3Q       Max
-0.091989 -0.022720 -0.001251  0.020707  0.144356
```

```
Coefficients:
Estimate Std. Error t value Pr(>|t|)
(Intercept)  3.490e-01  1.843e-02  18.932  < 2e-16 ***
stab.glu    -5.368e-04  5.219e-05 -10.287  < 2e-16 ***
age         -6.412e-04  1.698e-04  -3.776 0.000217 ***
waist       -1.398e-03  5.075e-04  -2.756 0.006465 **
ratio       -2.848e-03  1.997e-03  -1.427 0.155439
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 0.03673 on 178 degrees of freedom
Multiple R-squared: 0.5345,Adjusted R-squared: 0.524
F-statistic: 51.09 on 4 and 178 DF,  p-value: < 2.2e-16

> summary(fit.fs1.v) #summary on validation data

Call:
lm(formula = step.f, data = data.v)

Residuals:
Min        1Q    Median        3Q       Max
-0.151518 -0.018954  0.000226  0.017982  0.133835

Coefficients:
Estimate Std. Error t value Pr(>|t|)
(Intercept)  0.3287126  0.0187828  17.501  < 2e-16 ***
stab.glu    -0.0004436  0.0000575  -7.715 8.31e-13 ***
age         -0.0006694  0.0001815  -3.687 0.000301 ***
waist       -0.0008451  0.0004945  -1.709 0.089243 .
ratio       -0.0042812  0.0014718  -2.909 0.004089 **
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 0.03633 on 178 degrees of freedom
Multiple R-squared:  0.47,Adjusted R-squared: 0.4581
F-statistic: 39.46 on 4 and 178 DF,  p-value: < 2.2e-16

#percent change in parameter estimation
> round(abs(coef(step.f)-coef(fit.fs1.v))/abs(coef(step.f))*100,3)
(Intercept)    stab.glu         age       waist       ratio
5.813       17.359       4.402      39.573      50.310
> sd.fs1= summary(step.f)$coefficients[,"Std. Error"]
> sd.fs1.v= summary(fit.fs1.v)$coefficients[,"Std. Error"]
#percent change in standard errors
```

```
> round(abs(sd.fs1-sd.fs1.v)/sd.fs1*100,3)
(Intercept)    stab.glu         age       waist       ratio
1.889      10.190       6.925       2.545      26.283
```

ANS. Consistency for Model fs1: reasonable. Signs for parameter estimates are all the same, but percent change can be as big as 50%.

```
##mean squared prediction error
> newdata=data.v[,-5]
> pred.fs1=predict.lm(step.f, newdata)
> mspe.fs1=mean((pred.fs1-data.v[,5])^2)
> mspe.fs1
[1] 0.001329283
> press.fs1/n
[1] 0.001385467
> mse.fs1
[1] 0.001349119

### Model fs2
> fit.fs2.v=lm(step.f2,data=data.v) #Model fs1 on validation data
> summary(step.f2) #summary on training data

Call:
lm(formula = glyhb ~ stab.glu + age + waist + ratio + stab.glu:ratio +
age:ratio, data = data.c)

Residuals:
Min        1Q    Median        3Q       Max
-0.089202 -0.022258 -0.003599  0.021182  0.145324

Coefficients:
Estimate Std. Error t value Pr(>|t|)
(Intercept)     3.527e-01  3.162e-02  11.152  < 2e-16 ***
stab.glu       -9.522e-04  2.186e-04  -4.355 2.25e-05 ***
age             7.247e-05  5.277e-04   0.137   0.8909
waist          -1.305e-03  5.079e-04  -2.570   0.0110 *
ratio          -2.158e-03  6.565e-03  -0.329   0.7427
stab.glu:ratio  7.507e-05  3.775e-05   1.988   0.0483 *
age:ratio      -1.724e-04  1.231e-04  -1.401   0.1631
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 0.03646 on 176 degrees of freedom
Multiple R-squared: 0.5464,Adjusted R-squared: 0.531
F-statistic: 35.34 on 6 and 176 DF,  p-value: < 2.2e-16
```

```
> summary(fit.fs2.v) #summary on validation data

Call:
lm(formula = step.f2, data = data.v)

Residuals:
Min        1Q    Median        3Q       Max
-0.148870 -0.017817 -0.000883  0.018924  0.125159

Coefficients:
Estimate Std. Error t value Pr(>|t|)
(Intercept)     3.122e-01  3.031e-02  10.302   <2e-16 ***
stab.glu       -2.435e-04  1.413e-04  -1.724   0.0865 .
age            -8.409e-04  5.465e-04  -1.539   0.1257
waist          -9.390e-04  4.991e-04  -1.881   0.0616 .
ratio           7.797e-05  6.220e-03   0.013   0.9900
stab.glu:ratio -3.984e-05  2.581e-05  -1.544   0.1245
age:ratio       3.366e-05  1.201e-04   0.280   0.7796
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 0.03629 on 176 degrees of freedom
Multiple R-squared: 0.4772,Adjusted R-squared: 0.4594
F-statistic: 26.78 on 6 and 176 DF,  p-value: < 2.2e-16

> #percent change in parameter estimation
> round(abs(coef(step.f2)-coef(fit.fs2.v))/abs(coef(step.f2))*100,3)
(Intercept)       stab.glu            age          waist          ratio
11.465         74.424       1260.423         28.060        103.612
stab.glu:ratio      age:ratio
153.071        119.518
> sd.fs2= summary(step.f2)$coefficients[,"Std. Error"]
> sd.fs2.v= summary(fit.fs2.v)$coefficients[,"Std. Error"]
> #percent change in standard errors
> round(abs(sd.fs2-sd.fs2.v)/sd.fs2*100,3)
(Intercept)       stab.glu            age          waist          ratio
4.157         35.370          3.571          1.731          5.248
stab.glu:ratio      age:ratio
31.637          2.436
```

ANS. Consistency for Model fs2: Both sign and magnitude changed.

```
#mean squared prediction error
> newdata=data.v[,-5]
> pred.fs2=predict.lm(step.f2, newdata)
> mspe.fs2=mean((pred.fs2-data.v[,5])^2)
> mspe.fs2 #larger than mspe.fs1
[1] 0.00152642
> press.fs2/n
[1] 0.001385155
> mse.fs2
[1] 0.001329456
```

ANS. For both models, $MSPE_v$ is not much bigger than $Press_p/n$ and SSE_p/n, though $MSPE_v$ is closer to $Press_p/n$ and SSE_p/n in Model fs1. Moreover, Model fs1 has smaller $MSPE_v$.

(c) Based on both internal and external validation, which model you would choose as the final model? Fit the final model using the entire data set (training and validation combined). Write down the fitted regression function and report the R summary() and anova() output.

ANS. Model fs1 is preferred based on smaller $MSPE_v$ and more consistent parameter estimation in training and validation data sets.

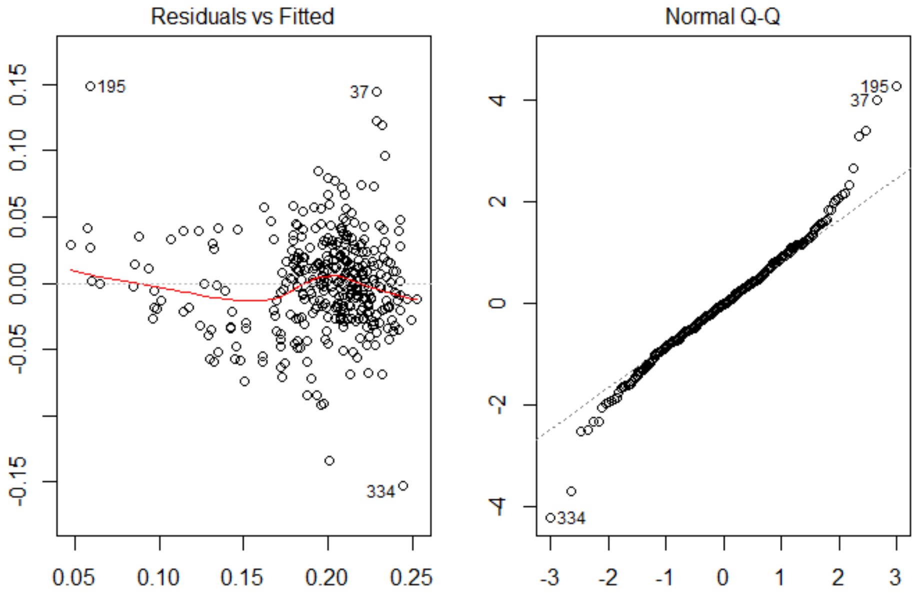
```
> fit.fs1.final=lm(step.f, data=data.s) #fit Model fs1 on whole data
> summary(fit.fs1.final)

Call:
lm(formula = step.f, data = data.s)

Residuals:
Min        1Q    Median        3Q       Max
-0.152555 -0.020528 -0.000382  0.019560  0.148412

Coefficients:
Estimate Std. Error t value Pr(>|t|)
(Intercept)  3.380e-01  1.306e-02  25.881  < 2e-16 ***
stab.glu    -4.922e-04  3.838e-05 -12.825  < 2e-16 ***
age         -6.561e-04  1.229e-04  -5.338 1.67e-07 ***
waist       -1.080e-03  3.516e-04  -3.071  0.00229 **
ratio       -3.661e-03  1.181e-03  -3.100  0.00209 **
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 0.03643 on 361 degrees of freedom
Multiple R-squared: 0.5005,Adjusted R-squared: 0.495
F-statistic: 90.45 on 4 and 361 DF,  p-value: < 2.2e-16

> anova(fit.fs1.final)
```

```
Analysis of Variance Table

Response: glyhb
Df  Sum Sq Mean Sq  F value    Pr(>F)
stab.glu    1 0.39753 0.39753 299.5043 < 2.2e-16 ***
age         1 0.04867 0.04867  36.6682 3.515e-09 ***
waist       1 0.02125 0.02125  16.0081 7.655e-05 ***
ratio       1 0.01276 0.01276   9.6103  0.002087 **
Residuals 361 0.47915 0.00133
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1
```

6. **Model diagnostic: Outlying and influential cases.** Conduct model diagnostic for the final model from the previous problem.

   (a) Draw residual vs. fitted value plot and residual Q-Q plot and comment on these plots.

Figure 6: Model Diagnostics for final model



ANS. The residual plot shows non-constancy in error variance. The Normal QQ plot shows heavy tails probably due to outliers.

   (b) Obtain the studentized deleted residuals and identify any outlying Y observations. Use the Bonferroni outlier test procedure at $\alpha = 0.1$.

The studentized deleted residuals are calculated through this equation:

$$t_i = e_i \sqrt{\frac{n-p-1}{SSE(1-h_{ii}) - e_i^2}}$$

To identify the outlying Y observations, we use the Bonferroni outlier test procedure at $\alpha = 0.1$. The Bonferronis threshold is

$$t(1 - \frac{\alpha}{2n}; n-p-1) = 3.676928$$

The Y observations corresponding to those studentized deleted residuals which are greater than the Bonferroni's threshold can be deemed as significant outlying observations. They are as follows:

```
> idx.Y ##  outliers
[1]  34 176 303 330
```

The code is as follows:

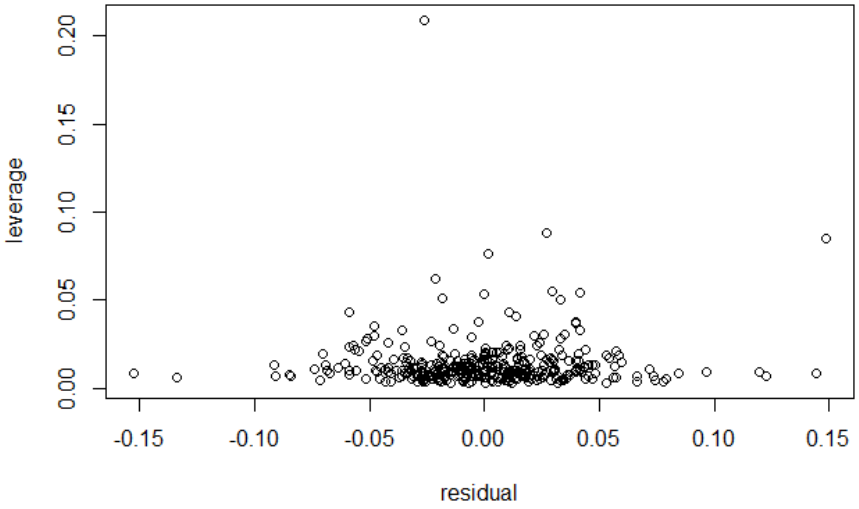
```
## check outliers in Y
res=residuals(fit.fs1.full)# residuals of the final model
n = nrow(data.s)
p = ncol(data.s)
h1 = influence(fit.fs1.full)$hat
d.res.std=studres(fit.fs1.full) #studentized deleted residuals

max(abs(d.res.std))
sort(abs(d.res.std),decreasing=T)
qt(1-0.1/(2*n),n-p-1) # bonferronis thresh hold
idx.Y = as.vector(which(abs(d.res.std)>=qt(1-0.1/(2*n),n-p-1)))
idx.Y ## outliers
```

(c) Obtain the leverage and identify any outlying X observations. Draw residual vs. leverage plot.

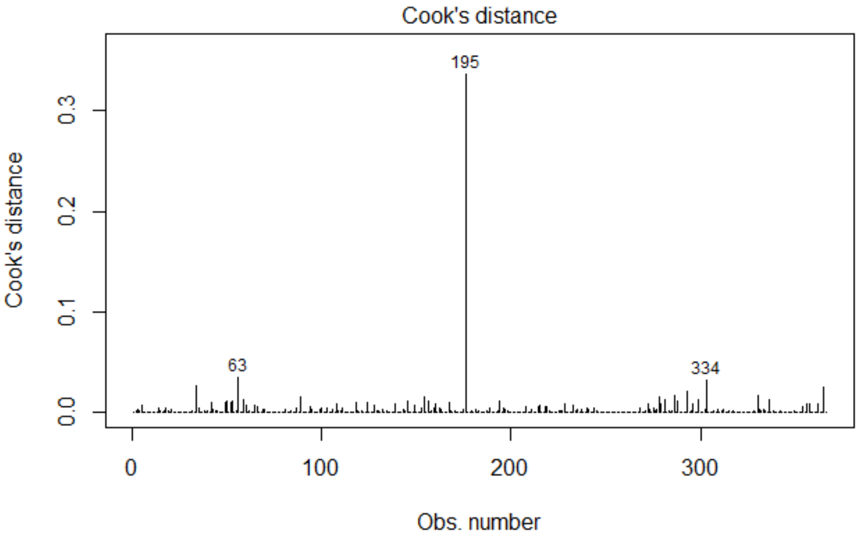
```
idx.X = as.vector(which(h1>(2*p/n)))
idx.X ## two outliers
plot(h1,res,xlab="leverage",ylab="residuals")


> idx.X ## outliers
[1]  56 156
```

The leverages are obtained and compared with the value of $\frac{2p}{n} = 0.08743169$. The cases with $h_{ii} > \frac{2p}{n}$ are defined as outlying X observations. There are 2 cases defined as outlying X observations, their indexes are shown above.

Figure 7: Residuals vs. Leverage Plot



(d) Draw an influence index plot using Cook's distance. Are there any influential cases according to this measure?



```
cook.d = res^2*h1/(p*1.293*(1-h1)^2)
cook.max = cook.d[which(cook.d==max(cook.d))]
```

```
pf(cook.max,p,n-p)

idx = c(idx.X,idx.Y)
cook.d[idx]
pf(cook.d[idx],p,n-p)
```

According to the Cook's distance plot, case 195 has the biggest Cook's distance.

$$D_{195} = \frac{e_i^2}{p * MSE} \frac{h_{ii}}{(1 - h_{ii})^2} = 0.0001079778$$

$$p_{195} = P(F_{16,350} < 0.0001079778) = 8.99587e - 30$$

Therefore, even case 195 has little aggregated influence on all the fitted values. Hence there is no influential cases according to this measure.

(e) Calculate the average absolute percent difference in the fitted values with and without the most influential case identified from the previous question. What does this measure indicate the influence of this case?

The potential influential case identified previously is the 195th case,
we fit the model without 195th case and calculate the average absolute percent difference in the fitted values as 0.03163563. For 195th case, the percentage change on the fitted value with or without the case is very small. Therefore, no case have an unduly large influence on prediction and thus all cases may be retained.

```
fit.fs1.full2=lm(fit.fs1, data=data.s[-195,])
f1=fitted(fit.fs1.full)
f2=fitted(fit.fs1.full2)
f1=f1[-195]
f=f1-f2
sum=0
for(i in 1:length(f1))
{
sum=sum+abs(f[i]/f1[i]);
}
yhat_195=fitted(fit.fs1.full)[195]
beta_new=as.vector(fit.fs1.full2$coefficients)
x_195=c(1,data.s$stab.glu[195],data.s$age[195],
data.s$waist[195],data.s$ratio[195])
y_195=t(beta_new)%*%x_195
sum=sum+abs((yhat_195-y_195)/yhat_195)
per.average=sum*100/366
```

7. **Studentized deleted residuals.** In the following, no assumption is made on the data or the model unless it is explicitly stated.

(a) Assume the observed response vector $\mathbf{Y} \in \mathbb{R}^n$ has $Var(\mathbf{Y}) = \sigma^2 \mathbf{I}_n$. Show that, the ith deleted residual $d_i = Y_i - \widehat{Y}_{i(i)}$ has

$$Var(d_i) = \frac{\sigma^2}{1 - h_{ii}}.$$

ANS For the ith deleted residual:

$$d_i = Y_i - \hat{Y}_{i,(i)} = \frac{e_i}{1 - h_{ii}}$$

Therefore:

$$Var(d_i) = Var\left(\frac{e_i}{1 - h_{ii}}\right) = \frac{1}{(1 - h_{ii})^2} Var(e_i) = \frac{1}{(1 - h_{ii})^2} \times \sigma^2 \times (1 - h_{ii}) = \frac{\sigma^2}{(1 - h_{ii})}$$

(b) Let

$$SSE_{(i)} = \sum_{j:j \neq i} (Y_j - \widehat{Y}_{j(i)})^2, \quad MSE_{(i)} = \frac{SSE_{(i)}}{n - p - 1},$$

i.e., $SSE_{(i)}$ and $MSE_{(i)}$ are the SSE and MSE of the regression fit excluding case i, respectively. Show that

$$SSE_{(i)} = SSE - \frac{e_i^2}{1 - h_{ii}}.$$

Hints: Recall that

$$SSE_{(i)} = \tilde{\mathbf{Y}}^T (\mathbf{I} - \mathbf{H}) \tilde{\mathbf{Y}},$$

where

$$\tilde{\mathbf{Y}} = \mathbf{Y} - \mathbf{d}_{(i)}, \quad where, \quad \mathbf{d}_{(i)} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ d_i \\ 0 \\ \vdots \\ 0 \end{bmatrix},$$

i.e., $\tilde{\mathbf{Y}}$ *is the same as* $\mathbf{Y}$ *except for the* i*th element, where it is* $\widehat{Y}_{i(i)}$.

ANS Denote

$$\mathbf{D}' = \begin{bmatrix} 0 & ... & 0 & d_i & 0 & ... & 0 \end{bmatrix}$$

Where $d_i = \frac{e_i}{1-h_{ii}}$. Therefore:

$$\begin{aligned}
SSE_{(i)} &= \tilde{\mathbf{Y}}'(\mathbf{I_n} - \mathbf{H})\tilde{\mathbf{Y}} = (\mathbf{Y} - \mathbf{D})'(\mathbf{I_n} - \mathbf{H})(\mathbf{Y} - \mathbf{D})' \\
&= \mathbf{Y}'(\mathbf{I_n} - \mathbf{H})\mathbf{Y} - \mathbf{D}'(\mathbf{I_n} - \mathbf{H})\mathbf{Y} - \mathbf{Y}'(\mathbf{I_n} - \mathbf{H})\mathbf{D} + \mathbf{D}'(\mathbf{I_n} - \mathbf{H})\mathbf{D} \\
&= SSE - \mathbf{D}'\mathbf{e} - \mathbf{e}'\mathbf{D} + \mathbf{D}'(\mathbf{I_n} - \mathbf{H})\mathbf{D} \text{ since } (\mathbf{I_n} - \mathbf{H})\mathbf{Y} = \mathbf{e} \\
&= SSE - \frac{e_i^2}{1-h_{ii}} - \frac{e_i^2}{1-h_{ii}} + (1-h_{ii})d_i^2 \\
&= SSE - \frac{e_i^2}{1-h_{ii}} - \frac{e_i^2}{1-h_{ii}} + (1-h_{ii})\frac{e_i^2}{(1-h_{ii})^2} \\
&= SSE - \frac{e_i^2}{1-h_{ii}} - \frac{e_i^2}{1-h_{ii}} + \frac{e_i^2}{1-h_{ii}} = SSE - \frac{e_i^2}{1-h_{ii}}
\end{aligned}$$

(c) Show that the studentized deleted residual

$$t_i = \frac{d_i}{s\{d_i\}} = \frac{d_i}{\sqrt{MSE_{(i)}/(1-h_{ii})}}$$

can be computed by:

$$t_i = e_i\sqrt{\frac{n-p-1}{SSE(1-h_{ii}) - e_i^2}}.$$

ANS

$$\begin{aligned}
t_i = \frac{d_i}{s\{d_i\}} &= \sqrt{1-h_{ii}}\frac{d_i}{\sqrt{MSE_{(i)}}} = \sqrt{1-h_{ii}}\frac{1}{\sqrt{MSE_{(i)}}} \times \frac{e_i}{1-h_{ii}} \\
&= \frac{e_i}{\sqrt{MSE_{(i)} \times (1-h_{ii})}} = e_i\sqrt{\frac{n-p-1}{SSE_{(i)} \times (1-h_{ii})}} \\
&= e_i\sqrt{\frac{n-p-1}{(SSE - \frac{e_i^2}{1-h_{ii}}) \times (1-h_{ii})}} \\
&= e_i\sqrt{\frac{n-p-1}{SSE(1-h_{ii}) - e_i^2}}
\end{aligned}$$

(d) **(Optional Problem).** Under the Normality assumption, i.e., $\mathbf{Y}$ is an n-dimensional Normal random vector with $Var(\mathbf{Y}) = \sigma^2\mathbf{I}_n$, show that $SSE_{(i)}$ is independent with Y_i and $\widehat{Y}_{i(i)}$. Therefore, $SSE_{(i)}$ is independent with d_i. If we further assume that the model is correct, then the deleted residual d_i has mean zero and the studentized deleted residual t_i follows a $t_{(n-p-1)}$ distribution.

ANS For any given regression model, its SSE is always independent with a fitted value based on this model, so $SSE_{(i)}$ is independent with $\widehat{Y}_{i(i)}$. Also $SSE_{(i)}$ only involve Y_{-i} which are all independent with Y_i, therefore $SSE_{(i)}$ is also independent with Y_i.

8. **Cook's distance.** Show that the Cook's distance

$$D_i := \frac{\sum_{j=1}^{n}(\widehat{Y}_j - \widehat{Y}_{j(i)})^2}{p \times MSE}, \quad i = 1, \cdots, n$$

can be computed by:

$$D_i = \frac{e_i^2}{p \times MSE}\frac{h_{ii}}{(1-h_{ii})^2}.$$

Hints: Note that

$$\sum_{j=1}^{n}(\widehat{Y}_j - \widehat{Y}_{j(i)})^2 = (\mathbf{Y} - \tilde{\mathbf{Y}})^T \mathbf{H}(\mathbf{Y} - \tilde{\mathbf{Y}}).$$

ANS

$$\sum_{j=1}^{n}\left(\hat{Y}_j - \hat{Y}_{j,(i)}\right)^2 = (\mathbf{Y} - \tilde{\mathbf{Y}})'\mathbf{H}(\mathbf{Y} - \tilde{\mathbf{Y}}) = \mathbf{D}'\mathbf{H}\mathbf{D} = d_i^2 h_{ii}$$

Therefore:

$$Di = \frac{\sum_{j=1}^{n}\left(\hat{Y}_j - \hat{Y}_{j,(i)}\right)^2}{p \times MSE} = \frac{d_i^2 h_{ii}}{p \times MSE} = \frac{e_i^2}{p \times MSE}\frac{h_{ii}}{(1-h_{ii})^2}$$