

for multiple regression

https://andyigg.com/spa3-1/

Software

• R: http://cran.r-project.org/

• RStudio:

https://www.rstudio.com/products/rstudio/download/#download

Assessment of residuals

- Outliers
- Influential observations
- Normality of residuals
- Equal variance of residuals
- Independence of residuals

Multiple Linear Regression Example

```
set.seed(108); n= 100; beta0 = array(c(3,2,1,1), c(1,4))

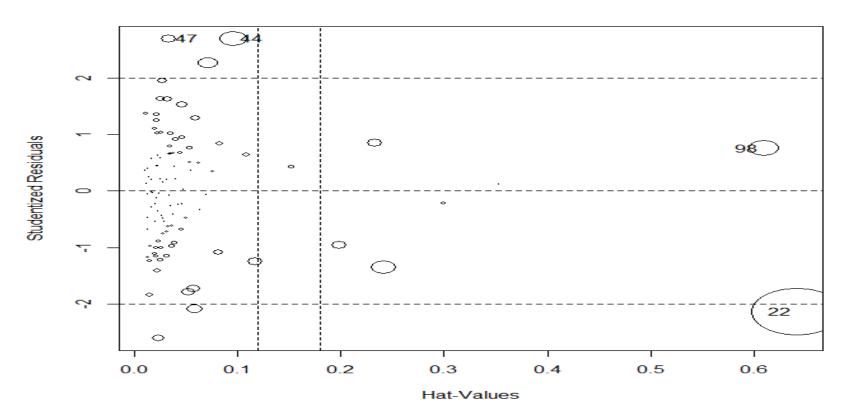
x1=rgamma(n, 1, 1/10); x2=rchisq(n, df = 3); x3=rexp(n)

X= cbind(x1, x2, x3)

y= beta0[,1] + beta0[,2]*x1 + beta0[,3]*x2 + beta0[,4]*x1*x2 + rnorm(n,sd=1.5)
```

```
Call:
                                      lm(formula = y \sim x1 + x2 + x3 + x1:x2 + x1:x3)
                                      Residuals:
                                          Min
                                                  10 Median
                                                                        Max
                                                                 30
                                      -3.7979 -1.0429 -0.0360 0.9585 3.8980
                                      Coefficients:
• summary(mlm)
                                                  Estimate Std. Error t value Pr(>|t|)
                                      (Intercept) 2.770501
                                                            0.392648 7.056 2.89e-10 ***
                                                            0.031253 65.406 < 2e-16 ***
                                                  2.044134
                                      x2
                                                  1.075617
                                                            0.092715 11.601 < 2e-16 ***
                                                 -0.225363 0.229452 -0.982
                                      x1:x2
                                                 0.991471 0.008786 112.846 < 2e-16 ***
                                      x1:x3
                                                 -0.003571 0.024526 -0.146
                                                                               0.885
                                      Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
                                      Residual standard error: 1.52 on 94 degrees of freedom
                                      Multiple R-squared: 0.9989,
                                                                   Adjusted R-squared: 0.9989
                                      F-statistic: 1.731e+04 on 5 and 94 DF, p-value: < 2.2e-16
                                                           > confint(mlm, level=0.95)
                                                                           2.5 %
                                                                                     97.5 %
                                                            (Intercept) 1.9908882 3.55011356
• confint(mlm, level=0.95)
                                                                        1.9820801 2.10618759
                                                           x2
                                                                        0.8915291 1.25970485
                                                           x3
                                                                       -0.6809452 0.23021915
                                                           x1:x2
                                                                       0.9740257 1.00891550
                                                           x1:x3
                                                                       -0.0522689 0.04512595
                             > anova (mlm)
                             Analysis of Variance Table
anova(mlm)
                             Response: y
                                       Df Sum Sq Mean Sq
                                                          F value Pr(>F)
                                        1 132044 132044 57176.0092 <2e-16 ***
                             x2
                                        1 36281
                                                  36281 15709.9284 <2e-16 ***
                             x3
                                                      0
                                                           0.1101 0.7408
                                        1 31555
                                                  31555 13663.6479 <2e-16 ***
                             x1:x2
                             xl:x3
                                              0
                                                      0
                                                           0.0212 0.8845
                                            217
                                                                                            5
                             Residuals 94
                             Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Outliers?



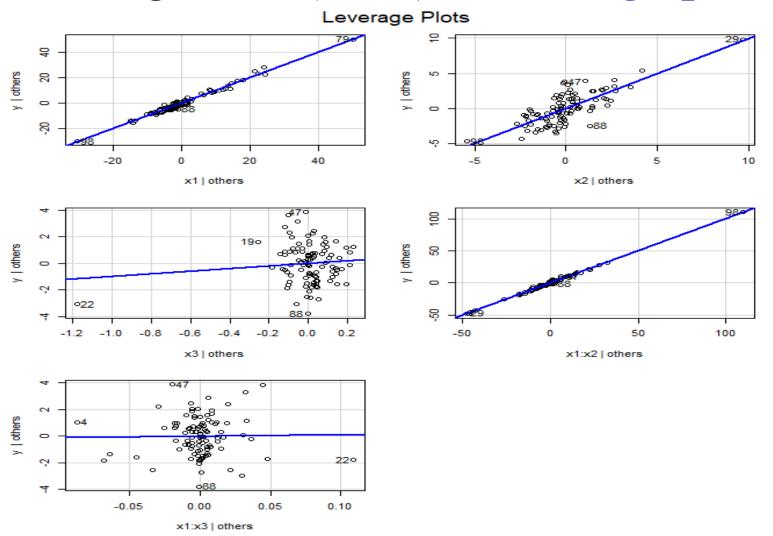
#install.packages("car"); library(car)influencePlot(mlm)

Assessing outliers

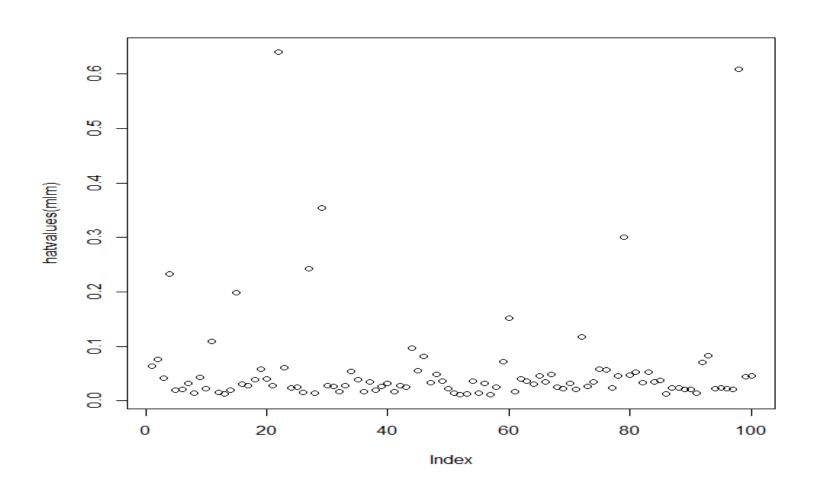
outlierTest(mlm) # Bonferonni p-value

Now, Bonferroni: $1-\frac{\alpha}{k} = \alpha'$, where k is the number of test e.g. $1-(1-\text{pnorm}(-2.696387))/6 = 1-\text{pnorm}(2.696387)/6 \approx 0.832$

leveragePlots(mlm) # leverage plots

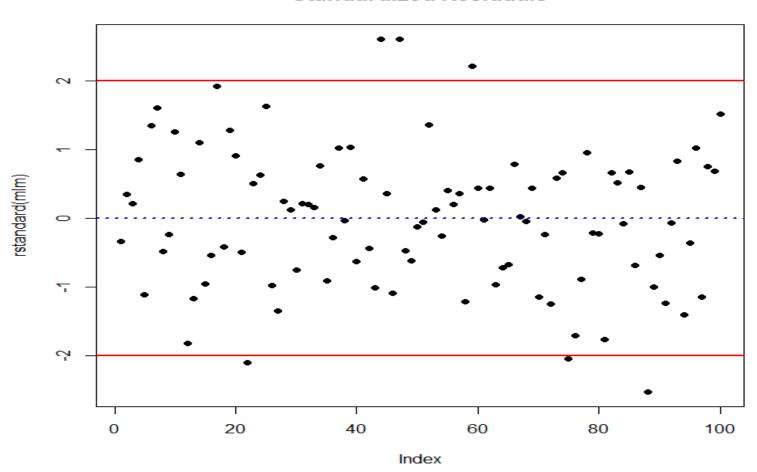


plot(hatvalues(mlm)) # leverage plots



Standardized residuals plot

Standardized Residuals



```
plot(rstandard(mlm), type = "p",main = "Standardized Residuals")
points( 1:n, rstandard(mlm), pch = 19)
```

Influential observations: cook's distance

```
# Cook's D plot

# Identify D values > 4/(n-p-1)

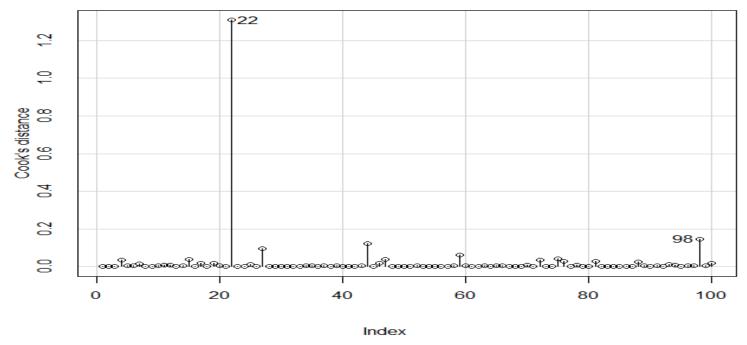
cooks=cooks.distance(mlm)

cooks_mlm=cooks[cooks > 4/( n - length(mlm$coefficients ) )]

cooks_mlm
```

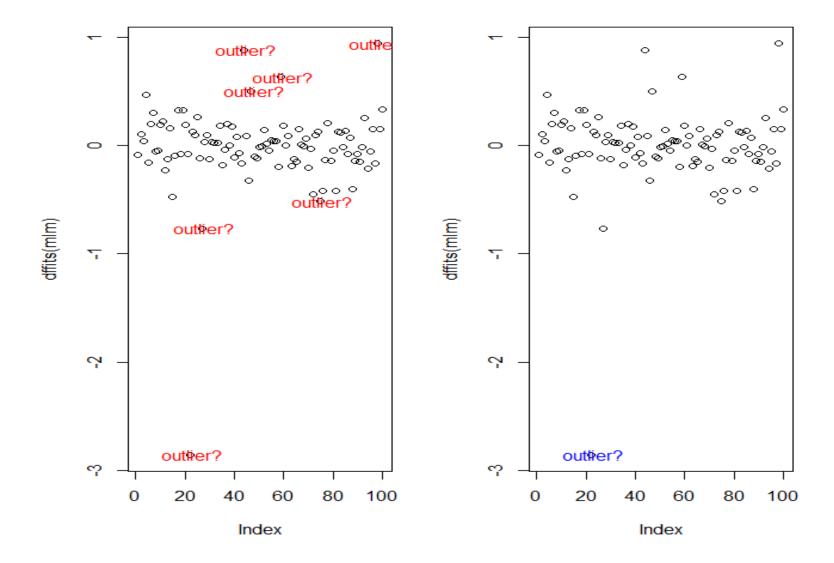
influenceIndexPlot(mlm, vars="Cook", id.n=length(cooks_out))



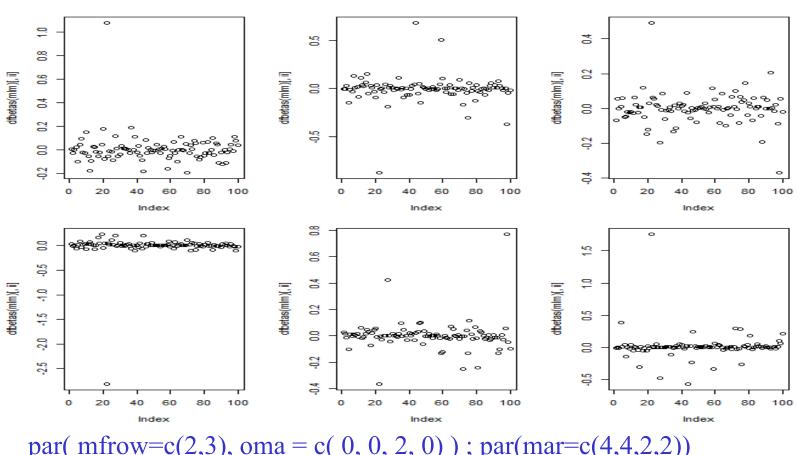


Influential observations: dffits

```
# dffits
par( mfrow=c(1,2), oma = c(0,0,2,0) ); par(mar=c(4,4,2,2))
plot(dffits(mlm)); # now, p=5
# dffits > sqrt((p+1)/n)
text(x=1:length(dffits(mlm))+1, y=dffits(mlm),
labels=ifelse(abs(dffits(mlm))>2*sqrt((5+1)/n), "outlier?",""),
col="red")
\# dffits > 1)
plot(dffits(mlm)); # now, p=5
text(x=1:length(dffits(mlm))+1, y=dffits(mlm),
labels=ifelse(abs(dffits(mlm))>1, "outlier?",""), col="blue")<sub>14</sub>
```

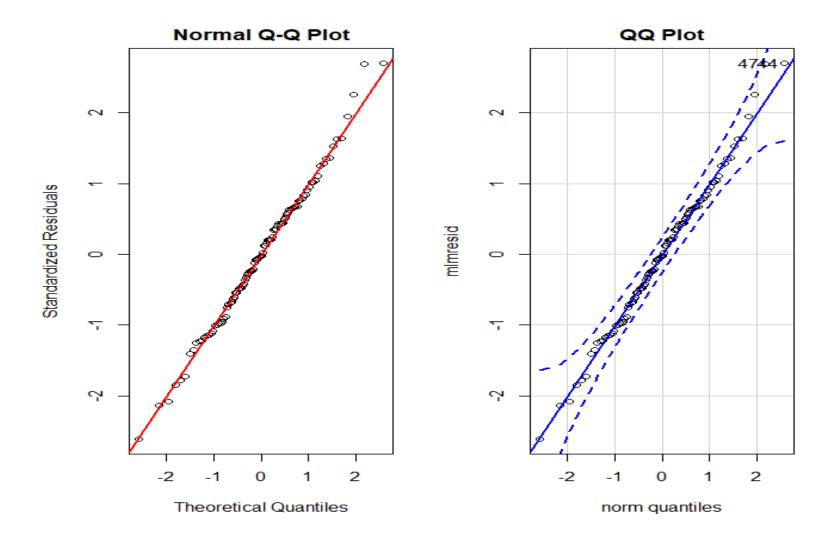


Influential observations: dfbetas



par(mfrow=c(2,3), oma = c(0,0,2,0)); par(mar=c(4,4,2,2)) for(ii in 1:length(mlm\$coefficients)){ plot(dfbetas(mlm)[,ii]) }

Normality of residuals



17

```
# library(MASS)
mlmresid=studres(mlm)
par( mfrow=c(1,2), oma = c( 0, 0, 2, 0) );
par(mar=c(4,4,2,2))
qqnorm(mlmresid, ylab ="Standardized Residuals")
qqline(mlmresid, lty=1, lwd=2,col="red" )
```

qqPlot(mlmresid, main="QQ Plot") # QQ plot for studentized residual

Formal Tests for normality

- shapiro.test(mlmresid)
- ks.test(mlmresid, "pnorm", mean(mlmresid), sd(mlmresid))
- #require(nortest)lillie.test(mlmresid)

• ...

```
> shapiro.test(mlmresid) # Shapiro-Wilks normality test
        Shapiro-Wilk normality test
data: mlmresid
W = 0.99349, p-value = 0.9155
> ks.test(mlmresid, "pnorm", mean(mlmresid), sd(mlmresid)) # Kolmogorov-Smirnov normality test
        One-sample Kolmogorov-Smirnov test
data: mlmresid
D = 0.035714, p-value = 0.9996
alternative hypothesis: two-sided
> require (nortest)
> lillie.test(mlmresid) # Lilliefors (Kolomorov-Smirnov) normality test
       Lilliefors (Kolmogorov-Smirnov) normality test
data: mlmresid
D = 0.035714, p-value = 0.9895
```

Which Normality Test Should I Use?

• Kolmogorov-Smirnov test

It is more sensitive near the center of the density than at the tails than other tests; large n

Shapiro-Wilks test

Doesn't work well if several values in the data set are the same. Works best for data sets with small n, but can be used with larger data sets.

• Lillie test (adjusted Kolmogorov-Smirnov test)

More powerful than Kolmogorov-Smirnov test

http://www.hmwu.idv.tw/web/R_AI/v2/hmwu_StatR-05-2_NonParametric_adv.pdf https://www.nrc.gov/docs/ML1714/ML17143A100.pdf

Parametric Test (normality)

- T-test
- Anova
- Pearson correlation test

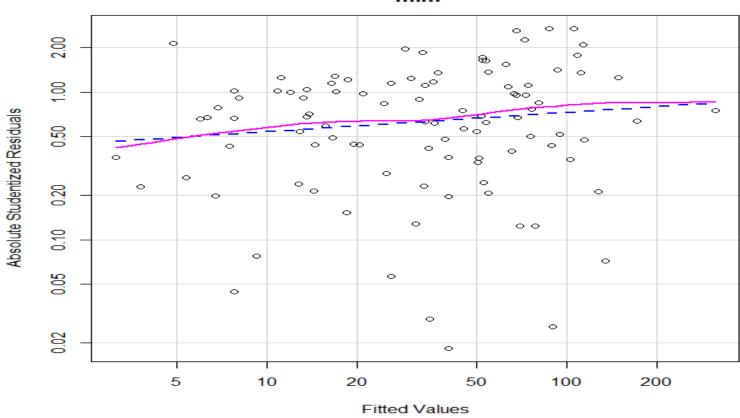
•

Which Normality Test Should I Use?

- It is preferable that normality be assessed both visually and through normality tests, of which the **Shapiro-Wilk test** is recommended.
- The KS or Lillie test should be "carefully" used owing to its low power.

Evaluate homoscedasticity

Spread-Level Plot for mlm



spreadLevelPlot(mlm)

Test for homoscedasticity

- ncvTest(mlm) # Non-constant Variance
 Score Test
- Computes a score test of the hypothesis of constant error variance against the alternative that the error variance changes with the level of the response (fitted values), or with a linear combination of predictors.

```
> ncvTest(mlm) # non-constant error variance test
Non-constant Variance Score Test
Variance formula: ~ fitted.values
Chisquare = 2.617584, Df = 1, p = 0.10569
```

Introduce some test homogeneity of variances

- leveneTest # package{car}
- **fligner.test**: (nonparametric) k-sample test
- **mood.test**: two-sample test for a difference in scale parameters
- **ansari.test**: two-sample test for a difference in scale parameters. (testing for equal variance for non-normal samples)
- **bartlett.test**: a parametric test of the null that the variances in each of the groups (samples) are the same.
- **var.test**: an F test to compare the variances of two samples from normal populations.

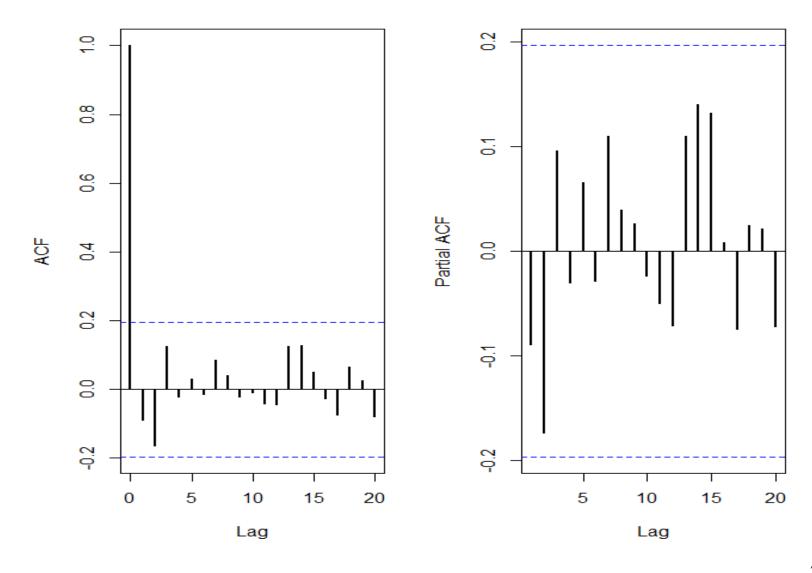
• ...

Test for independence

 durbinWatsonTest(mlm) # test for autocorrelated errors

```
> durbinWatsonTest(mlm) # test for autocorrelated errors
lag Autocorrelation D-W Statistic p-value
    1   -0.09174254     2.158922     0.462
Alternative hypothesis: rho != 0
>
> |
```

Residuals: dependence diagnosis



Multi-collinearity: variance inflation factors

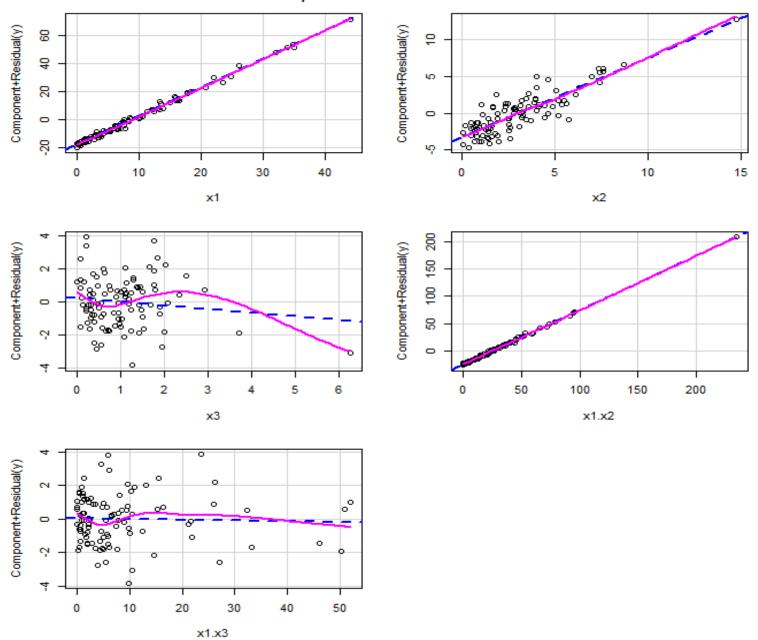
- vif >10: multi-collinearity
- Cohen, J, Cohen, P, West, S. G., and Aiken, L. S. 2003. Applied Multiple Regression/Correlation Analysis for the Behavioral Sciences (3rd ed.). Hillsdale, NJ: Lawrence Erlbaum.
- Kutner, Nachtsheim, and Neter, 2004, Applied Linear Regression Models, Fourth Edition, McGraw-Hill Irwin.)

```
> vif(mlm)
             x2 x3 x1:x2 x1:x3
3.296571 1.971189 1.703740 3.188911 3.233037
> set.seed(108); n= 100; beta0 = array(c(3, 2, 1, 1), c(1,4))
> x1=rgamma( n, 1, 1/10 ) ; x2= 1.5*x1 + rnorm( n, sd= 0.5 ) ; x3=rexp( n )
> X= cbind( x1, x2, x3 )
> y= beta0[,1] + beta0[,2]*x1 + beta0[,3]*x2 + beta0[,4]*x1*x2 + rnorm( n, sd=1.5 )
> mlm2 = lm(y \sim x1 + x2 + x3 + x1:x2 + x1:x3)
> vif(mlm2)
                x2
                      x3 x1:x2 x1:x3
732.252036 753.418106 2.266356 7.620066 3.559061
```

(Non-) Linearity

- These functions construct component+residual plots, also called partial-residual plots, for linear and generalized linear models.
- df = data.frame(y,x1,x2,x3,x1.x2=x1*x2, x1.x3=x1*x3)
 lm.fit1 = lm(y ~ ., df); crPlots(lm.fit1)

Component + Residual Plots



Global Validation of Linear Model Assumptions

- Pena, EA and Slate, EH (2006). Global validation of linear model assumptions, *J. Am. Stat. Assoc.*, **101**(473):341-354.
- library(gvlma)summary(gvlma(mlm))

```
Call:
lm(formula = y \sim x1 + x2 + x3 + x1:x2 + x1:x3)
Residuals:
   Min
         10 Median 30
                                  Max
-3.7979 -1.0429 -0.0360 0.9585 3.8980
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 2.770501 0.392648 7.056 2.89e-10 ***
\times 1
            2.044134 0.031253 65.406 < 2e-16 ***
x2
            1.075617 0.092715 11.601 < 2e-16 ***
           -0.225363 0.229452 -0.982 0.329
×3
           0.991471 0.008786 112.846 < 2e-16 ***
x1:x2
x1:x3
          -0.003571 0.024526 -0.146 0.885
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Residual standard error: 1.52 on 94 degrees of freedom
Multiple R-squared: 0.9989, Adjusted R-squared: 0.9989
F-statistic: 1.731e+04 on 5 and 94 DF, p-value: < 2.2e-16
ASSESSMENT OF THE LINEAR MODEL ASSUMPTIONS
USING THE GLOBAL TEST ON 4 DEGREES-OF-FREEDOM:
Level of Significance = 0.05
Call:
gvlma(x = mlm)
                    Value p-value
                                                Decision
Global Stat
                0.90519 0.9238 Assumptions acceptable.
                 0.37302 0.5414 Assumptions acceptable.
Skewness
Kurtosis
                  0.00225 0.9622 Assumptions acceptable.
Link Function
                 0.49035 0.4838 Assumptions acceptable.
```

Heteroscedasticity 0.03957 0.8423 Assumptions acceptable.

Comparing models: ANOVA

```
> mlm mainterms = lm( y~x1+x2+x3)
> anova(mlm, mlm mainterms )
Analysis of Variance Table
Model 1: y \sim x1 + x2 + x3 + x1:x2 + x1:x3
Model 2: y \sim x1 + x2 + x3
 Res.Df RSS Df Sum of Sq F Pr(>F)
1 94 217
2 96 31772 -2 -31555 6831.8 < 2.2e-16 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
> mlm = lm(y \sim x1 + x2 + x3 + x1:x2 + x1:x3)
> mlm correct = lm( y~x1+x2+x1:x2)
>
> anova(mlm, mlm correct)
Analysis of Variance Table
Model 1: y \sim x1 + x2 + x3 + x1:x2 + x1:x3
Model 2: y \sim x1 + x2 + x1:x2
 Res.Df RSS Df Sum of Sq F Pr(>F)
1 94 217.09
2 96 221.49 -2 -4.4042 0.9535 0.3891
```

Model selection

```
require(MASS)  \begin{aligned} &\text{mlm\_all=lm}(y\sim x1+x2+x3+x1:x2+x1:x3+x2:x3\;)\\ &\text{data.input} = \text{data.frame}(\;y,\;x1,\;x2,\;x3,\;x1*x2,\;x1*x3,\;x2*x3\;) \end{aligned}   &\text{fit.full} = \text{lm}(y\sim .,\;\text{data.input})\;;\; \text{fit.null} = \text{lm}(y\sim 1,\;\text{data.input})\;;
```

data.input)

```
Start: AIC=762.14
          Df Sum of Sq
                          RSS AIC
+ x1...x2 1 182385 17712 521.68
                132044 68054 656.29
+ ×1
+ x1...x3 1 8
+ x2 1 2
+ x2...x3 1
<none>
+ x3 1
                86219 113879 707.77
                 21689 178408 752.67
                  9107 190990 759.48
                        200097 762.14
                    27 200070 764.13
Step: AIC=521.68
y ~ x1...x2
          Df Sum of Sq
                            RSS AIC
           1 17176.8 535.4 173.79
+ x1...x3 1 4219.1 13493.1 496.48
+ x2 1 3624.1 14088.1 500.79
+ x2...x3 1 1664.1 16048.2 513.82
                         17712.2 521.68
<none>
        1 336.2 17376.0 521.77
+ x3
Step: AIC=173.79
y \sim x1...x2 + x1
          Df Sum of Sq RSS AIC
           1 313.921 221.49 87.521
+ x2...x3 1 128.132 407.28 148.433
+ x1...x3 1 4.181 531.23 175.003
+ x3 1 0.032 525 00
Step: AIC=87.52
y \sim x1...x2 + x1 + x2
          Df Sum of Sq
                          RSS AIC
                        221.49 87.521
                 4.3552 217.13 87.535
+ x3
+ x1...x3 1
                2.1763 219.31 88.533
+ x2...x3 1
                0.4981 220.99 89.296
Call:
lm(formula = y \sim xl...x2 + xl + x2, data = data.input)
Coefficients:
(Intercept)
                 x1...x2
                                 2.043
      2.571
                    0.991
                                                1.062
```

stepAIC(fit.null,direction="forward",scope=list(upper=fit.full,lower=fit.null)) # lm(formula = y ~ x1...x2 + x1 + x2, data = data.input)

```
Start: AIC=89.28
y \sim x1 + x2 + x3 + x1...x2 + x1...x3 + x2...x3
         Df Sum of Sa
                       RSS
                               AIC
                 0.0
                       212.3 87.28
- x1...x3 1
<none>
                       212.3 89.28
- x2...x3 1
                4.8 217.1 89.51
                7.0 219.3 90.53
- x3
         1
- x2
          1
              60.3 272.6 112.29
             9404.1 9616.4 468.61
- x1
- x1...x2 1 28938.4 29150.7 579.51
Step: AIC=87.28
y \sim x1 + x2 + x3 + x1...x2 + x2...x3
         Df Sum of Sq
                       RSS
                              AIC
<none>
                       212.3 87.28
- x2...x3 1
                4.8 217.1 87.53
- x3
         1
                8.7 221.0 89.30
- x2
         1
               60.4 272.7 110.31
- x1
         1 13364.8 13577.1 501.10
- x1...x2 1 30734.8 30947.1 583.49
Call:
lm(formula = y \sim x1 + x2 + x3 + x1...x2 + x2...x3, data = data.input)
Coefficients:
(Intercept)
                    x1
                                x2
                                            x3
                                                   x1...x2
    3.3680
                2.0354
                          0.8701
                                      -0.6948
                                                    0.9933
   x2...x3
    0.1460
```

```
Start: AIC=762.14
v ~ 1
         Df Sum of Sq
                         RSS
                              AIC
+ x1...x2 1 182385 17712 521.68
200097 762.14
<none>
              27 200070 764.13
+ ×3
Step: AIC=521.68
y ~ x1...x2
         Df Sum of Sq RSS AIC
1 17177 535 173.79
          1 17177
+ >:1
+ x1...x3 1 4219 13493 496.48
+ x2 1 3624 14088 500.79
+ x2...x3 1 1664 16048 513.82
Step: AIC=173.79
y \sim x1...x2 + x1
          Df Sum of Sq
                        RSS
+ x2
          1 314
1 128
                        221 87.52
+ x2...x3
                        407 148.43
                        535 173.79
+ x1...x3 1 4 531 173.79
+ x3 1 0 535 175.78
- x1 1 17177 17712 521.68
- x1...x2 1 67518 68054 656.29
<none>
Step: AIC=87.52
y \sim x1...x2 + x1 + x2
         Df Sum of Sq
                        RSS
                               AIC
221 87.52
<none>
lm(formula = y \sim x1...x2 + x1 + x2, data = data.input)
Coefficients:
(Intercept)
                 x1...x2
                                   \sim 1
                               2.043
                                            1.062
      2.571
                   0.991
```

stepAIC(fit.null,direction="both" ,scope=list(upper=fit.full,lower=fit.null)) # lm(formula = y ~ x1...x2 + x1 + x2, data = data.input)

```
Start: AIC=762.14
v ~ 1
         Df Sum of Sq
                          RSS AIC
+ x1...x2 1 182385 17712 521.68

+ x1 1 132044 68054 656.29

+ x1...x3 1 86219 113879 707.77

+ x2 1 21689 178408 752.67

+ x2...x3 1 9107 190990 759.48

<none>
                        200097 762.14
<none>
           1 27 200070 764.13
+ ×3
Step: AIC=521.68
y ~ x1...x2
          Df Sum of Sq RSS AIC
1 17177 535 173.79
+ ×1
          1 17177
+ x1...x3 1 4219 13493 496.48
+ x2 1 3624 14088 500.79
+ x2...x3 1 1664 16048 513.82
Step: AIC=173.79
y \sim x1...x2 + x1
          Df Sum of Sq
                          RSS
+ x2
           1 314
1 128
                          221 87.52
+ x2...x3 1
                          407 148.43
535 173.79
Step: AIC=87.52
y \sim x1...x2 + x1 + x2
          Df Sum of Sq
                          RSS
                                 AIC
221 87.52
<none>
lm(formula = y \sim x1...x2 + x1 + x2, data = data.input)
Coefficients:
(Intercept)
                 x1...x2
                                     \sim 1
                                 2.043
                    0.991
                                               1.062
      2.571
```

stepAIC(fit.null,direction="forward",scope=list(upper=fit.full,lower=fit.null), $\mathbf{k=log(n)}$ # lm(formula = y ~ x1...x2 + x1 + x2, data = data.input)

```
Start: AIC=762.14
v ~ 1
          Df Sum of Sq
                          RSS AIC
+ x1...x2 1 182385 17712 521.68
+ x1 1 132044 68054 656.29
27 200070 764.13
+ ×3
Step: AIC=521.68
y ~ x1...x2
          Df Sum of Sq RSS AIC
1 17177 535 173.79
+ x1 17177
+ x1...x3 1 4219
+ x2 1 3624
+ x2...x3 1 1664
                        13493 496.48
                         14088 500.79
                        16048 513.82
Step: AIC=173.79
y ~ x1...x2 + x1
          Df Sum of Sq
                        RSS
                         221 87.52
+ x2
           1 314
                   128
                          407 148.43
+ x2...x3
                          535 173.79
<none>
             4
                        531 175.00
535 175.78
+ x1...x3
+ *3
                 17177 17712 521.68
- \times 1
 - x1...x2 1
                  67518 68054 656.29
Step: AIC=87.52
y \sim x1...x2 + x1 + x2
          Df Sum of Sq
                         RSS
                                AIC
<none>
                         221 87.52
                         217 87.53
+ x3
                   4.4
                         219
          1
1
1
 + x1...x3
                   2.2
                               88.53
 + x2...x3
                          221
                               89.30
               313.9
                        535 173.79
- x2
- x 1
               13866.6 14088 500.79
 - x1...x2 1 31551.1 31773 582.12
Call:
lm(formula = y \sim x1...x2 + x1 + x2, data = data.input)
Coefficients:
 (Intercept)
                 x1...x2
                                    \sim 1
                                                  ×2
                                2.043
                                              1.062
       2.571
                    0.991
stepAIC(fit.full,direction="backward", k=log(n))
      lm(formula = y \sim x1...x2 + x1 + x2, data = data.input)
                                                       42
```

```
Start: AIC=762.14
v ~ 1
         Df Sum of Sq
                          RSS
                               AIC
+ x1...x2 1 182385 17712 521.68
200097 762.14
<none>
                   27 200070 764.13
+ ×3
Step: AIC=521.68
y ~ x1...x2
          Df Sum of Sq RSS AIC
1 17177 535 173.79
          1 17177
+ >:1
+ x1
+ x1...x3 1 4219 13493 496.48
+ x2 1 3624 14088 500.79
+ x2...x3 1 1664 16048 513.82
17712 521.68
Step: AIC=173.79
y \sim x1...x2 + x1
          Df Sum of Sq
                         RSS
+ x2
          1 314
1 128
                         221 87.52
+ x2...x3 1
                         407 148.43
535 173.79
+ x1...x3 1 4 531 175.00
+ x3 1 0 535 175.78
- x1 1 17177 17712 521.68
- x1...x2 1 67518 68054 656.29
                          535 173.79
Step: AIC=87.52
y \sim x1...x2 + x1 + x2
          Df Sum of Sq
                         RSS
                                AIC
221 87.52
<none>
lm(formula = y \sim x1...x2 + x1 + x2, data = data.input)
Coefficients:
(Intercept)
                 x1...x2
                                    >< 1
                                2.043
                   0.991
                                              1.062
      2.571
```

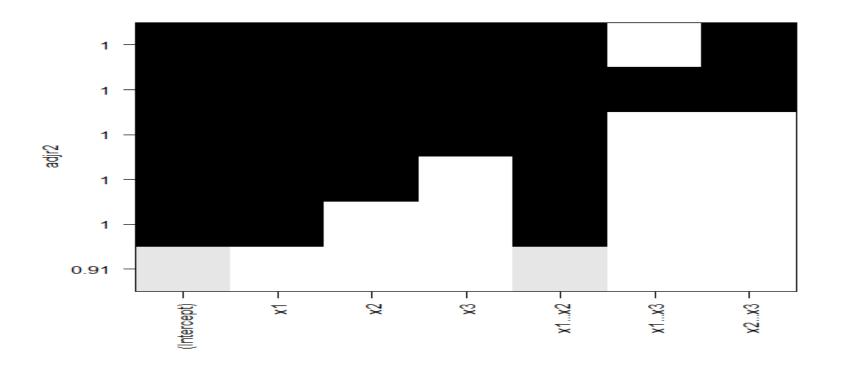
stepAIC(fit.null,direction="both", scope=list(upper=fit.full,lower=fit.null), k=log(n) # lm(formula = $y \sim x1...x2 + x1 + x2$, data = data.input)

Select on all subsets

```
library(leaps)
data.input = data.frame(y, x1, x2, x3, x1*x2,
x1*x3, x2*x3)
model.com = regsubsets(y\sim., nvmax=30,
data=data.input)
model.sum = summary(model.com)
names(model.sum) # "which" "rsq" "rss"
"adjr2" "cp" "bic" "outmat" "obj"
```

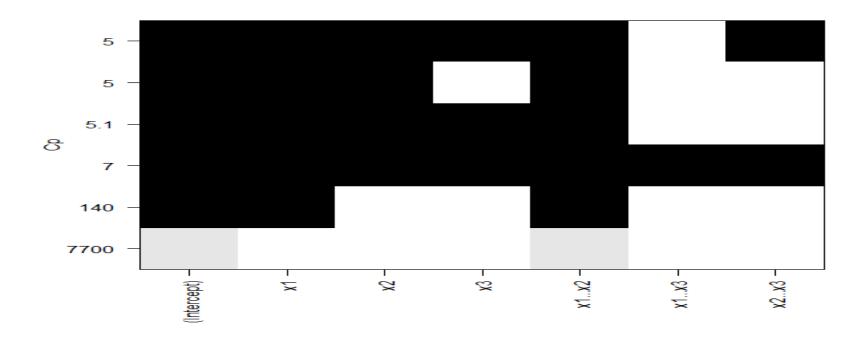
which.min(model.sum\$rss) # 6 which.min(model.sum\$adjr2) # 1 which.min(model.sum\$cp) # 5 which.min(model.sum\$bic) # 3

Adjusted R-squared



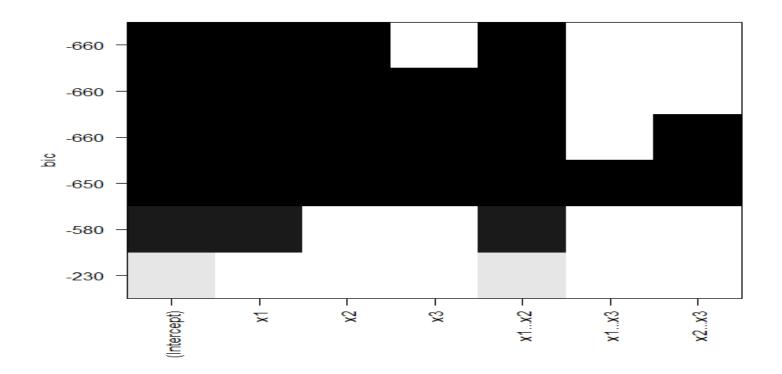
plot(model.com,scale="adjr2")₄₆

Cp (AIC)



plot(model.com,scale="Cp") 47

BIC



plot(model.com,scale="bic")