ST518 - Multiple linear regression module

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Multiple linear regression(MLR)

Toy example: A random sample of students taking the same exam:

X_1 X_2 Y

IQ	Study TIME	GRADE
105	10	75
110	12	79
120	6	68
116	13	85
122	16	91
130	8	79
114	20 X_{72}	98 $= y_7$
102	15	76

$X \ (8 \times 3)$

$E(Y | X_1, X_2)$

Consider a regression model for the GRADE of subject i, Y_i, in which the mean of Y_i is a linear function of two predictor variables X_{i1} = IQ and X_{i2} = Study TIME for subjects $i = 1, \ldots, 8$:

$$Y = \beta_0 + \beta_1 \text{IQ} + \beta_2 \text{TIME} + \text{error}$$

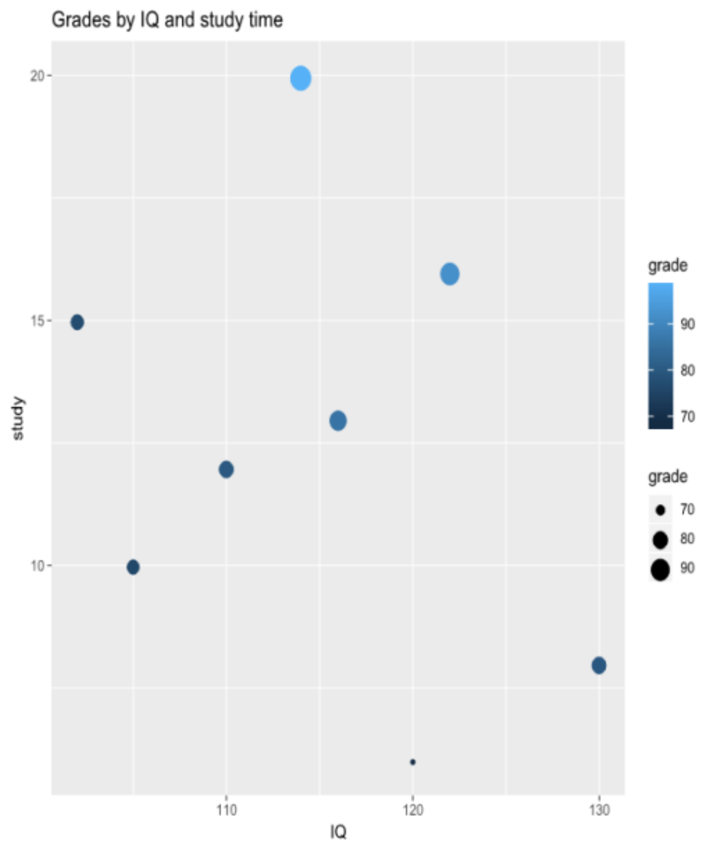
or

$j=1$ $j=2$

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + E_i \quad \text{for} \quad i = 1, \ldots, 8$$

```
> library(ggplot2)
> iqstudy.plot <- ggplot(iqstudy.dat,aes(IQ,study))
> iqstudy.plot  + geom_point(aes(color=grade, size=grade))
+ ggtitle("Grades by IQ and study time")
```

layered graphics



MLR model w/ p independent variables

- Observed values of p independent/predictor variables for i^{th} subject from sample denoted by $x_{i\cdot} = (x_{i1}, x_{i2}, \ldots, x_{ip})$
- response variable for i^{th} subject denoted by Y_i
- For $i = 1, \ldots, n$, MLR model for Y_i :

$$Y_i = \overbrace{\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip}}^{\mu\{x_{i1}, \ldots, x_{in}\}} + E_i .$$

linear combo of $x_{i1}, x_{i2}, \ldots, x_{in}$

- As in SLR, $E_1, \ldots, E_n \overset{iid}{\sim} N(0, \sigma^2)$, or at least $IND(0, \sigma^2)$.

Least squares estimates of regression parameters (β_i) minimize $SS[E]$:
coefficients

$$SS[E] = \sum_{i=1}^{n} (y_i - (\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip}))^2$$

$$MS(E) = \boxed{\hat{\sigma}^2 = \frac{SS[E]}{n-p-1}} \qquad E(\hat{\sigma}^2) = \sigma^2$$

Interpretations of regression parameters:

- σ^2 is unknown error variance parameter.
- $\beta_0, \beta_1, \dots, \beta_p$ are $p+1$ unknown regression parameters:
  - β_0 : average response when $x_1 = x_2 = \ldots = x_p = 0$ intercept
  - β_i is called a partial slope for x_i. Represents mean change in y per unit increase in x_i **with all other independent variables held fixed**.

For the IQ/study time example, with $p = 2$ and $n = 8$,

IQ TIME

$$\hat{\beta}_0 = 0.74, \ \hat{\beta}_1 = 0.47, \ \hat{\beta}_2 = 2.1$$

$$\begin{pmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \hat{\beta}_2 \end{pmatrix} = \begin{pmatrix} .74 \\ .47 \\ 2.1 \end{pmatrix} = \hat{\beta}.$$

What is the uncertainty associated with these parameter estimates? → BR
Is $\beta_1 = 0$ and/or $\beta_2 = 0$ consistent with data?
(Statistical inference.)

$ → $Y_i = \beta_0 + \beta_1 X_{i1} + \epsilon_i$

$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \epsilon_i$

SQFT

Matrix formulation of MLR

Let $x_{i\cdot}$ be a row vector for p observed independent variables for individual i

$$x_{i\cdot} = (1, x_{i1}, x_{i2}, x_{i3}, \ldots, x_{ip}) \quad (1 \times (p+1)).$$

$X\beta = \begin{pmatrix} 1 \; x_{11} \; x_{12} \\ \vdots \end{pmatrix} \begin{pmatrix} \beta_0 \\ \vdots \\ \beta_p \end{pmatrix}$

MLR model for $Y_1, \ldots, Y_n$ given by

$$\begin{aligned}
Y_1 &= \beta_0 + \beta_1 x_{11} + \beta_2 x_{12} + \cdots + \beta_p x_{1p} + E_1 \\
Y_2 &= \beta_0 + \beta_1 X_{21} + \beta_2 X_{22} + \cdots + \beta_p X_{2p} + E_2 \text{ (fill this in!)} \\
\vdots &= \vdots \\
Y_n &= \beta_0 + \beta_1 x_{n1} + \beta_2 x_{n2} + \cdots + \beta_p x_{np} + E_n
\end{aligned}$$

$\mathrm{var}(E) = \begin{pmatrix} \sigma^2 & & 0 \\ & \sigma^2 & \\ 0 & & \sigma^2 \end{pmatrix} = \sigma^2 \cdot I_n$

System of n equations can be expressed using matrices: $\boxed{Y = X\beta + E}$

$(n \times (p+1))$

- Y denotes a response vector $(n \times 1)$
- X denotes a design matrix $(n \times (p+1))$
- β denotes a vector of regression parameters $((p+1) \times 1)$
- E denotes an error vector $(n \times 1)$, assumed $MVN(0, \sigma^2 I_n)$.

$\begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{pmatrix} = \beta$

To obtain matrix expressions for the LS estimates of β, take partial derivatives of the sum of squares function,

objective fcn.

dim(Y) = n×1

$$\begin{aligned} Q(\beta) &= \sum\left(Y_i - (\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip})\right)^2 \\ &= (Y - X\beta)'(Y - X\beta) \\ &= Y'Y - Y'X\beta - (X\beta)'Y + (X\beta)'X\beta \in \mathbb{R} \\ &\quad Y'Y - Y'X\beta - \beta'X'Y + \beta'X'X\beta = Y'Y - 2Y'X\beta + \beta'X'X\beta \end{aligned}$$

Note that if b is $p \times 1$ and A is $(p \times p)$, then $\frac{\partial b'Ab}{\partial b} = (A + A')b$.

$$\frac{\partial Q}{\partial \beta} = -2X'Y + (X'X + (X'X)')\beta = -2X'Y + 2(X'X)\beta \overset{set}{=} 0$$

The $p+1$ equations with $p+1$ unknowns obtained by setting this vector of partial derivatives are called the **normal equations**.

$$(X'X)\beta = X'Y$$

$$(X'X)^{-1}(X'X)\beta = (X'X)^{-1}X'Y$$

$$I\beta = (X'X)^{-1}X'Y$$

$$\boxed{\hat\beta = (X'X)^{-1}X'Y}$$

Recall from SLR

$$\beta_1 = \frac{\sum(x_i - \bar x)Y_i}{\sum(x_i - \bar x)^2}$$

$$[\sum(x_i - \bar x)^2]^{-1}\sum(x_i - \bar x)Y_i$$

$$\frac{\partial Q}{\partial \beta} = 0 \Longrightarrow \hat\beta = (X'X)^{-1}X'Y$$

$$Var(\hat\beta_1 | X) = \frac{\sigma^2}{\sum(x_i - \bar x)^2} = [\sum(x_i - \bar x)^2]^{-1}\sigma^2$$

Moments of linear combinations of random vectors

Let Y denote a $p \times 1$ random vector with mean μ and covariance matrix Σ. Suppose a is a $p \times 1$ (fixed) vector of coefficients. Then

$$\boxed{\begin{aligned} E(a'Y) &= a'\mu \\ \mathrm{Var}(a'Y) &= a'\Sigma a. \end{aligned}}$$

So, let's derive $\mathrm{Var}(\widehat{\beta}|X)$:

$$\begin{aligned}
\mathrm{Var}(\widehat{\beta}|X) &= V[\overbrace{(X'X)^{-1}X'}^{A}Y|X] \\
&= ((X'X)^{-1}X')\mathrm{Var}(Y|X)((X'X)^{-1}X')' \\
&= ((X'X)^{-1}X')\sigma^2 I_n((X'X)^{-1}X')' \\
&= \sigma^2((X'X)^{-1}X')((X'X)^{-1}X')' \\
&= \sigma^2(X'X)^{-1}\underbrace{X'X(X'X)^{-1}}_{I}\text{(untranspose RHS)} \\
&= \sigma^2 \; (X'X)^{-1}
\end{aligned}$$

The variance-covariance matrix of the vector of estimated regression coefficients.

$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^{-1} = \frac{1}{|ad-bc|}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$

$$
\begin{aligned}
\hat{\beta} &= (X'X)^{-1}X'Y \\
\mathrm{Var}(\hat{\beta}) &= \sigma^2(X'X)^{-1} \\
&= \Sigma \\
\widehat{\mathrm{Var}}(\hat{\beta}) &= MS[E](X'X)^{-1} \\
&= \widehat{\Sigma} \\
\widehat{\mathrm{Var}}(a'\hat{\beta}) &= a'\widehat{\Sigma}a
\end{aligned}
$$

— exercise: verify for $p=1$

$\hat\beta = \begin{pmatrix} \hat\beta_0 \\ \hat\beta_1 \end{pmatrix} = \begin{pmatrix} \bar Y - \hat\beta_1 \bar X \\ \frac{\sum (X_i - \bar X) Y_i}{\sum (X_i - \bar X)^2} \end{pmatrix}$

$\hat\mu(1,13,14) = \hat\beta_0 + \hat\beta_1 13 + \hat\beta_2 14 = (1,13,14)\hat\beta = a'\hat\beta$

- $(X'X)^{-1}$ verbalized as "x prime x inverse"
- X assumed to be of full *rank*

$$
\begin{aligned}
\hat{Y} &= X\hat{\beta} = X(X'X)^{-1}X'Y = HY \\
e &= Y - \hat{Y} = Y - X\hat{\beta} = (I-H)Y \\
e'e &= (Y-\hat{Y})'(Y-\hat{Y}) = Y'(I-H)'(I-H)Y = Y'(I-H)Y
\end{aligned}
$$

$= SS(E)$

- $\hat{Y}$ is called the vector of fitted or predicted values
- $H = X(X'X)^{-1}X'$ is called the hat matrix. It is *idempotent*.
- e is the vector of residuals

IQ, Study TIME example, $p = 2$ predictors and $n = 8$ observations, consider $X, Y, (X'X)^{-1}, (X'X)^{-1}X; Y, X(X'X)^{-1}X'Y$.

$$X = \begin{pmatrix} 1 & 105 & 10 \\ 1 & 110 & 12 \\ 1 & 120 & 6 \\ 1 & 116 & 13 \\ 1 & 122 & 16 \\ 1 & 130 & 8 \\ 1 & 114 & 20 \\ 1 & 102 & 15 \end{pmatrix}, \quad X'X = \begin{pmatrix} n = 8 & 919 & 100 \\ 919 & 106165 & 11400 \\ 100 & 11400 & 1394 \end{pmatrix}$$

$\sum X_{i2}$ hrs

$\sum X_{i1} X_{i2}$

$\sum X_{i2}^2$ hrs^2

$$(X'X)^{-1} = \begin{pmatrix} 28.90 & -0.23 & -0.22 \\ -0.23 & 0.0018 & 0.0011 \\ -0.22 & 0.0011 & 0.0076 \end{pmatrix}$$

$$\hat{\beta} = (X'X)^{-1}X'Y = \begin{pmatrix} 0.74 \\ 0.47 \\ 2.10 \end{pmatrix} =? \begin{pmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \hat{\beta}_2 \end{pmatrix}$$

$$SS[E] = e'e = (Y - \hat{Y})'(Y - \hat{Y}) = 45.8, \quad e'e/df = 9.15 =? \quad MS(E) = \hat{\sigma}^2$$

$$\widehat{\Sigma} = MS[E](X'X)^{-1} = \begin{pmatrix} 264.45 & -2.07 & -2.05 \\ -2.07 & 0.017 & 0.010 \\ -2.05 & 0.010 & 0.070 \end{pmatrix}$$

Distribution of parameter estimators,

- If $E \sim N(0, \sigma^2 I)$, then the LS estimator, $\widehat{\beta} \sim N(\beta, \Sigma)$. and
- the t-statistics formed from $t = (\widehat{\beta}_j - \beta_j)/\sqrt{\widehat{\Sigma}_{jj}}$ follow t-distributions with $df = n - p - 1$.
- If $E \sim IND(0, \sigma^2)$, the normality of $\widehat{\beta}$ is approximate.

Some questions - use preceding pages

1. What is the estimate for β_1? Interpretation? $\hat{\beta}_1 = .417$ (SE = .13)
2. What is the standard error of $\hat{\beta}_1$?
3. Is $\beta_1 = 0$ plausible, while controlling for possible linear associations between Test Score and Study time? $(t(0.025, 5) = 2.57)$
4. Estimate the mean grade among the population of ALL students with $IQ = 113$ who study $TIME = 14$ hours.
5. Report a standard error for the estimate in 4
6. Report a 95% confidence interval for the quantity being estimated in 4
7. Report a 95% prediction interval for an individual student with $IQ = 113$, $TIME = 14$.
8. Estimate the std. deviation among students whose mean estimated in 4

Some answers

1. $\hat{\beta}_1 = 0.47$ (second element of $(X'X)^{-1}X'Y$, exam points per IQ point for students studying the same amount)
2. $\sqrt{0.017} = 0.13$ (square root of middle element of $\widehat{\Sigma}$)
3. $H_0 : \beta_1 = 0$, T-statistic: $t = (\hat{\beta}_1 - 0)/SE(\hat{\beta}_1)$
   Observed value is $t = .47/\sqrt{.017} = .47/.13 = 3.6 > 2.57$,
   ("$\hat{\beta}_1$ differs significantly from 0.")
4. Unknown population mean: $\theta = \beta_0 + \beta_1(113) + \beta_1(14)$
   Estimate : $\hat{\theta} = (1, 113, 14) * \hat{\beta} = 83.6$
5. $\text{Var}((1, 113, 14) * \hat{\beta}) = (1, 113, 14)\widehat{\text{Var}}(\hat{\beta})(1, 113, 14)'$
   or $(1, 113, 14)\widehat{\Sigma}(1, 113, 14)' = 1.3$ or $SE(\hat{\theta}) = \sqrt{1.3} = 1.14$ (on $df =$ ________)
6. $\hat{\theta} \pm t(0.025, 5)SE(\hat{\theta})$ or $83.6 \pm 2.57(1.14)$ or $(80.7, 86.6)$
7. $\hat{Y} \pm t(0.025, 5)\sqrt{MS(E) + SE(\hat{\theta})^2}$ or $83.6 \pm 2.57\sqrt{(9.15 + 1.14^2)}$ or $(75.3, 91.9)$
8. $\sqrt{MS(E)} = \sqrt{9.15} = 3.0$ (points)

```
DATA GRADES; INPUT IQ STUDY GRADE @@;  CARDS;
105 10 75 110 12 79 120 6 68 116 13 85 122 16 91 130 8 79 114 20 98 102 15 76
DATA EXTRA; INPUT IQ STUDY GRADE; CARDS;
113 14 .
DATA BOTH; SET GRADES EXTRA;
PROC REG; MODEL GRADE = IQ STUDY/P CLM XPX INV COVB;
```

```
                          The SAS System
                         The REG Procedure

                  Model Crossproducts X'X X'Y Y'Y

Variable          Intercept              IQ           STUDY           GRADE
Intercept                 8             919             100             651
IQ                      919          106165           11400           74881
STUDY                   100           11400            1394            8399
GRADE                   651           74881            8399           53617

              X'X Inverse, Parameter Estimates, and SSE

Variable          Intercept              IQ           STUDY           GRADE
Intercept      28.898526711    -0.226082693    -0.224182192    0.7365546771
IQ             -0.226082693    0.0018460178    0.0011217122     0.473083715
STUDY          -0.224182192    0.0011217122    0.0076260404    2.1034362851
GRADE          0.7365546771     0.473083715    2.1034362851    45.759884688

                       Analysis of Variance

                                  Sum of          Mean
Source                   DF      Squares        Square    F Value    Pr > F
Model                     2    596.11512     298.05756      32.57    0.0014
Error                     5     45.75988       9.15198
Corrected Total           7    641.87500

(Output continued next page)
```

Variable	DF	Parameter Estimate	Standard Error	t Value	Pr > |t|
Intercept	1	0.73655	16.26280	0.05	0.9656
IQ	1	0.47308	0.12998	3.64	0.0149
STUDY	1	2.10344	0.26418	7.96	0.0005

Covariance of Estimates

Variable	Intercept	IQ	STUDY
Intercept	264.47864999	-2.069103589	-2.051710248
IQ	-2.069103589	0.016894712	0.010265884
STUDY	-2.051710248	0.010265884	0.0697933458

$\hat{\Sigma} = MS(E)(X'X)^{-1}$

Output Statistics

Obs	Dependent Variable	Predicted Value	Std Error Mean Predict	95% CL Mean		95% CL Predict		Residual
1	75	71.4447	1.9325	66.4770	76.4124	62.2169	80.6725	3.5553
(abbreviated)								
8	76	80.5426	1.9287	75.5847	85.5005	71.3201	89.7652	-4.5426
9	.	83.6431	1.1414	80.7092	86.5771	75.3315	91.9548	.

Sum of Residuals	0
Sum of Squared Residuals	45.75988
Predicted Residual SS (PRESS)	125.73575

(This 9^{th} "observation" in the output data set is an illustration of the "missing y" trick to get software to generate prediction limits.)

```
> # lm() in R
> iqstudy.dat
   IQ study grade
1 105    10    75
2 110    12    79
(abbreviated)
7 114    20    98
8 102    15    76
> iqstudy.out <- lm(iqstudy.dat$grade ~ iqstudy.dat$IQ + iqstudy.dat$study)
> coef(iqstudy.out)
      (Intercept)    iqstudy.dat$IQ iqstudy.dat$study
        0.7365547         0.4730837         2.1034363
> vcov(iqstudy.out)
                  (Intercept) iqstudy.dat$IQ iqstudy.dat$study
(Intercept)        264.478650    -2.06910359       -2.05171025
iqstudy.dat$IQ      -2.069104     0.01689471        0.01026588
iqstudy.dat$study   -2.051710     0.01026588        0.06979335
> summary(iqstudy.out)
Call: lm(formula = iqstudy.dat$grade ~ iqstudy.dat$IQ + iqstudy.dat$study)

Residuals:
       1        2        3        4        5        6        7        8
 3.55529  0.98300 -2.12722  2.04106 -1.10775 -0.06493  1.26318 -4.54264

Coefficients:
                  Estimate Std. Error t value Pr(>|t|)
(Intercept)         0.7366    16.2628   0.045 0.965629
iqstudy.dat$IQ      0.4731     0.1300   3.640 0.014909 *
iqstudy.dat$study   2.1034     0.2642   7.962 0.000504 ***

Residual standard error: 3.025 on 5 degrees of freedom
Multiple R-squared:  0.9287,    Adjusted R-squared:  0.9002
F-statistic: 32.57 on 2 and 5 DF,  p-value: 0.001357
```

Variable Selection

x_1, x_2, x_3 denote p independent variables. Consider several models:

1. $\mu(x_1, x_2, x_3) = E(Y|x_1, x_2, x_3) = \beta_0 + \beta_1 x_1$
2. $\mu(x_1, x_2, x_3) = E(Y|x_1, x_2, x_3) = \beta_0 + \beta_2 x_2$
3. $\mu(x_1, x_2, x_3) = E(Y|x_1, x_2, x_3) = \beta_0 + \beta_3 x_3$
4. $\mu(x_1, x_2, x_3) = E(Y|x_1, x_2, x_3) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3$
5. $\mu(x_1, x_2, x_3) = E(Y|x_1, x_2, x_3) = \beta_0 + \beta_1 x_1 + \beta_3 x_3$
6. $\mu(x_1, x_2, x_3) = E(Y|x_1, x_2, x_3) = \beta_0 + \beta_1 x_1 + \beta_2 x_2$
7. $\mu(x_1, x_2, x_3) = E(Y|x_1, x_2, x_3) = \beta_0 + \beta_2 x_2 + \beta_3 x_3$

Language

A is nested in B means model A can be obtained by placing linear restrictions on parameter values in model B (e.g. $\beta_1 = \beta_2$)

True or false:

- Model 1 nested in Model 4
- Model 2 nested in Model 4
- Model 3 nested in Model 4
- Model 1 nested in Model 5
- Model 4 nested in Model 1
- Model 5 nested in Model 4

A nested in $B \longrightarrow A$ called *reduced*, B called *full*.
p - number of regression parameters in full model
q - number of regression parameters in reduced model
$p - q$ - number of regression parameters being tested.

$$\begin{aligned} SS[Tot] &= SS[R] + SS[E] \\ \sum(Y_i - \overline{Y})^2 &= \sum(\widehat{Y}_i - \overline{Y})^2 + \sum(\widehat{Y}_i - Y_i)^2 \end{aligned}$$

Variable/model Selection - concepts

In comparing two models, suppose
$\beta_1, \ldots, \beta_q$ in reduced (r) model (A)
$\beta_1, \ldots, \beta_q, \beta_{q+1}, \ldots, \beta_p$ in full (f) model (B).
Comparison of models A and B amounts to testing

$H_0 : \beta_{q+1} = \beta_{q+2} = \cdots = \beta_p = 0$ (model A ok)
$H_1 : \beta_{q+1}, \beta_{q+2}, \cdots, \beta_p$ not all 0 (need model B)

$$\text{Let} \quad F = \frac{(SS[E]_r - SS[E]_f)/(p-q)}{MS[E]_f} = \frac{MS[H_0]}{MS[E]}$$

Difference in the numerator called an *extra regression sum of squares*:

$$R(\beta_{q+1}, \beta_{q+2}, \ldots, \beta_p | \beta_0, \beta_1, \beta_2, \ldots, \beta_q) = SS[R]_f - SS[R]_r = \underline{\hspace{4cm}}.$$

(ok to suppress β_0 in these extra SS terms.)

Theory gives that if H_0 holds (model A appropriate), F behaves according to F distribution with $p-q$ numerator, $n-p-1$ denominator degrees of freedom. (Write $\sim F_{p-q,n-p-1}$)

Extra SS terms for comparing some nested models on preceding page:

- Model 1 in model 4: $R(\beta_2, \beta_3|\beta_1)$
- Model 2 in model 4 ?
- Model 3 in model 4 ?
- Model 1 in model 5: $R(\beta_3|\beta_1)$
- Model 5 in model 4: ?

To compare Models 1 and 4, compute $F = (R(\beta_2, \beta_3|\beta_1)/2)/MSE_4$ on $df = 2, n-3-1$ If observed F sufficiently large, models said to differ significantly, reduced model rejected in favor of full model. If F small, reduced model plausible.

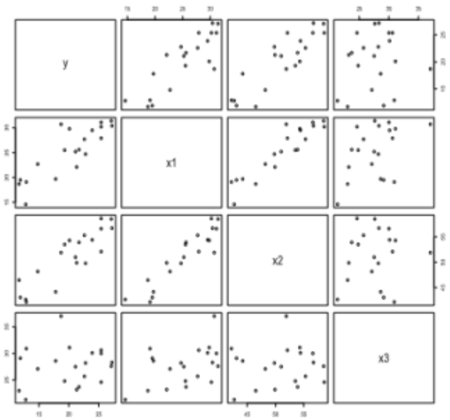
An example: How to measure body fat?

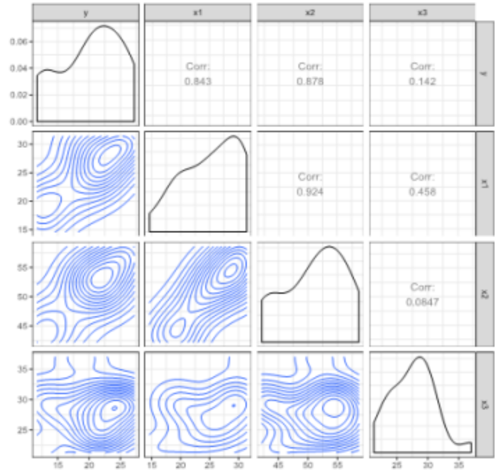
For each of $n = 20$ healthy individuals, the following measurements were made: bodyfat percentage y_i, triceps skinfold thickness, x_1, thigh circumference x_2, midarm circumference x_3. (See "bodyfat.txt")

```
x1     x2     x3     y
19.5   43.1   29.1   11.9
24.7   49.8   28.2   22.8
(abbreviated)
22.7   48.2   27.1   14.8
25.2   51.0   27.5   21.1
```

Summary statistics:

Symbol	Variable	mean	st. dev.
y	Body fat	20.2	5.1
x1	Triceps	25.3	5.0
x2	Thigh Circ.	51.2	5.2
x3	Midarm Circ.	27.6	3.6






```
> pairs(bodyfat.df[,c(4,1:3)])
> scatterplot(bodyfat.df,lower=list(continuous="density"),data.var=c(4,1:3),diag=list(continuous=
  + "densityDiag"))
```

```
               Pearson Correlation Coefficients, N = 20
                       Prob > |r| under H0: Rho=0

                       y              x1              x2              x3

     y           1.00000         0.84327         0.87809         0.14244
                                  <.0001          <.0001          0.5491

     x1          0.84327         1.00000         0.92384         0.45778
                  <.0001                          <.0001          0.0424

     x2          0.87809         0.92384         1.00000         0.08467
                  <.0001          <.0001                          0.7227

     x3          0.14244         0.45778         0.08467         1.00000
                  0.5491          0.0424          0.7227
```

Marginal associations between y and x_1 and between y and x_2 are highly significant, providing evidence of a strong $r \approx 0.85$ linear association between bodyfat and triceps skinfold and between bodyfat and thigh circumference.

Multicollinearity: linear associations among the independent variables; causes problems such as inflated sampling variances for $\hat{\beta}$.

x_1 and x_2 are particularly problematic. Imagine trying to balance a planar table top in the third dimension over "legs" that arise from the (x_1, x_2) coordinates. Highly unstable.

```
data bodyfat;
   input x1 x2 x3 y;         cards;
  19.5  43.1  29.1  11.9
  24.7  49.8  28.2  22.8
   (data abbreviated)
  22.7  48.2  27.1  14.8
  25.2  51.0  27.5  21.1
;
proc reg data=bodyfat;
   model y=x1 x2 x3; model y=x1; model y=x2; model y=x3;  *usually use 4 lines of code;
```

```
                          Parameter       Standard
    Variable      DF       Estimate          Error    t Value    Pr > |t|
    Intercept      1      117.08469       99.78240       1.17      0.2578
    x1             1        4.33409        3.01551       1.44      0.1699
    x2             1       -2.85685        2.58202      -1.11      0.2849
    x3             1       -2.18606        1.59550      -1.37      0.1896

                          Parameter       Standard
    Variable      DF       Estimate          Error    t Value    Pr > |t|
    Intercept      1       -1.49610        3.31923      -0.45      0.6576
    x1             1        0.85719        0.12878       6.66      <.0001

                          Parameter       Standard
    Variable      DF       Estimate          Error    t Value    Pr > |t|
    Intercept      1      -23.63449        5.65741      -4.18      0.0006
    x2             1        0.85655        0.11002       7.79      <.0001

                          Parameter       Standard
    Variable      DF       Estimate          Error    t Value    Pr > |t|
    Intercept      1       14.68678        9.09593       1.61      0.1238
    x3             1        0.19943        0.32663       0.61      0.5491
```

Model Selection - examples

In bodyfat data, consider comparing SLR of Y on x_1 with full additive model.

$$\begin{aligned} \text{Model } A : \mu(x_1, x_2, x_3) &= \beta_0 + \beta_1 x_1 \\ \text{Model } B : \mu(x_1, x_2, x_3) &= \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 \end{aligned}$$

or the null hypothesis

$$H_0 : \beta_2 = \beta_3 = 0 \quad \text{vs} \quad H_1 : \beta_2, \beta_3 \text{ not both } 0$$

after accounting for x_1.

$$F = \frac{(396.9 - 352.3)/2}{6.15} = \frac{22.3}{6.15} = 3.64$$

How many df? The 95^{th} percentile is $F(0.05, \ , \ ) = 3.63$.

Q: Conclusion from this comparison of nested models?

After accounting for effect of x_1, the (partial) association between y and the pair x_2 and/or x_3 may be declared ________________ at $\alpha =$ ______.

```
* To get this $F$-ratio in SAS, try ;
proc reg data=bodyfat;
   model y=x1 x2 x3;
   test x2=0,x3=0;
run;
```

```
proc reg;
   model y=x1 x2 x3 / ss1 ss2;
run;
```

```
The SAS System
The REG Procedure
                      Analysis of Variance

                               Sum of            Mean
Source                 DF     Squares          Square    F Value    Pr > F
Model                   3   396.98461       132.32820      21.52    <.0001
Error                  16    98.40489         6.15031
Corrected Total        19   495.38950

Root MSE           2.47998    R-Square     0.8014
Dependent Mean    20.19500    Adj R-Sq     0.7641
Coeff Var         12.28017

                 Parameter     Standard
Variable    DF    Estimate        Error  t Value  Pr > |t|    Type I SS    Type II SS
Intercept    1   117.08469     99.78240     1.17    0.2578   8156.76050      8.46816
x1           1     4.33409      3.01551     1.44    0.1699    352.26980     12.70489
x2           1    -2.85685      2.58202    -1.11    0.2849     33.16891      7.52928
x3           1    -2.18606      1.59550    -1.37    0.1896     11.54590     11.54590
```

Type I - ________________. Type II - ________________ p-values are *partial*
Note agreement between p−values from Type II F tests and p−values from t tests from parameter estimates from MLR.

Type I sums of squares - sequential (order of selection matters)
Type II sums of squares - partial (Δ SSE due to adding term A to model with all other terms not 'containing' A)
Type III sums of squares - partial

$$\begin{aligned} R(\beta_1|\beta_0) &= 352.3 \\ R(\beta_2|\beta_0,\beta_1) &= \underline{\hspace{4cm}} \\ R(\beta_3|\beta_0,\beta_1,\beta_2) &= \underline{\hspace{4cm}} \\ R(\beta_1|\beta_0,\beta_2,\beta_3) &= 12.7 \\ R(\beta_2|\beta_0,\beta_1,\beta_3) &= \underline{\hspace{4cm}} \end{aligned}$$

Type II test for β_j - test of partial association between y and x_j $\boxed{\text{after accounting for all other } x_i}$

Type II F-ratios from bodyfat data for x_1, x_2, x_3, respectively:

$$F = \frac{12.7/1}{6.15} = 2.07, \quad F = \frac{7.5/1}{6.15} = 1.22, \quad F = \frac{11.5/1}{6.15} = 1.88.$$

(Partial) effects significant ? (Use $F(0.95, 1, 16) = 4.49$.)

Exercise: Carry out the corresponding F-tests to compare models.

In PROC REG output, which models are the type I tests comparing?

1. Type I SS for x_1 appropriate for SLR of y on x_1.
2. Type I SS for x_2 appropriate for test of association between y and x_2 after accounting for x_1.
3. Type I test for x_3 same as type II test for x_3.

In all three of these tests, $MS[E]$ computed from full model (#4).

Some model comparison examples

1. Compare models 1 and 6
2. Compare models 2 and 6

For 1. use $R(\beta_2|\beta_0, \beta_1)$ in the F ratio:

$$\begin{aligned} F &= \frac{R(\beta_2|\beta_0, \beta_1)}{MS[E]_6} \\ &= \frac{33.2}{(SS[Tot] - R(\beta_1, \beta_2|\beta_0)/(20-2-1)} \\ &= \frac{33.2}{(495.4 - 352.3 - 33.2)/(20-2-1)} \\ &= \frac{33.2}{109.9/17} = 5.1 \end{aligned}$$

Note that $SS[E]_f = (SS[Tot] - SS[R]_f)$ and $SS[R]_f = SS[R]_r + R(\beta_2|\beta_0, \beta_1)$

$F(0.05, 1, 17) = 4.45$: model 1 rejected in favor of model 6: there is evidence ($p = 0.037$) of association between y and x_2 after accounting for dependence on x_1.

To compare models 2 and 6, we need $SS[R]_r = R(\beta_2|\beta_0) = 382.0$ which cannot be gleaned from preceding output. You could also get it from $r^2_{yx_2} \times SS[Tot]$ or from running something like

```
proc reg;
   model y=x1 x2/ss1 ss2;
run;
                            The REG Procedure

                                  Sum of           Mean
Source                  DF       Squares         Square    F Value    Pr > F
Model                    2     385.43871      192.71935      29.80    <.0001
Error                   17     109.95079        6.46769
Corrected Total         19     495.38950

                   Parameter   Standard
Variable     DF     Estimate      Error  t Value   Pr > |t|     Type I SS   Type II SS
Intercept     1    -19.17425    8.36064    -2.29     0.0348    8156.76050     34.01785
x1            1      0.22235    0.30344     0.73     0.4737     352.26980      3.47289
x2            1      0.65942    0.29119     2.26     0.0369      33.16891     33.16891
```

$$F = \frac{R(\beta_1|\beta_0,\beta_2)/(\Delta df)}{MS[E]_f} = \frac{(SS[R]_f - SS[R]_r)/1}{6.5} = \frac{352.3 + 33.2 - 382.0}{6.5} = \frac{3.4}{6.5} \approx 0.5$$

Conclusions?

- x_2 gives you a little when you add it to model with x_1
- x_1 gives you nothing when you add it to model with x_2
- Take model with x_2. (Has higher r^2 too.)
- these comparisons of nested models easy to carry out using TEST statement in PROC REG.

Another example, revisiting test scores and study times

Consider this sequence of analyses:

1. Regress GRADE on IQ.
2. Regress GRADE on IQ and TIME.
3. Regress GRADE on TIME IQ TI where TI = TIME*IQ.

ANOVA (Grade on IQ)

SOURCE	DF	SS	MS	F	p-value
IQ	1	15.9393	15.9393	0.153	0.71
Error	6	625.935	104.32		

No evidence that IQ has anything to do with grade, but we did not look at study time. Looking at the *multiple* regression we get

```
                          The REG Procedure

                         Analysis of Variance

                                     Sum of           Mean
Source                    DF        Squares         Square    F Value    Pr > F
Model                      2      596.11512      298.05756      32.57    0.0014
Error                      5       45.75988        9.15198
Corrected Total            7      641.87500

                               Parameter       Standard
     Variable       DF          Estimate          Error    t Value    Pr > |t|
     Intercept       1           0.73655       16.26280       0.05      0.9656
     IQ              1           0.47308        0.12998       3.64      0.0149
     study           1           2.10344        0.26418       7.96      0.0005
```

Now the test for dependence on IQ is significant $p = 0.0149$. Why?

The interaction model

```
                          The REG Procedure
                         Analysis of Variance

                                      Sum of           Mean
   Source                    DF      Squares         Square    F Value    Pr > F
   Model                      3    610.81033      203.60344      26.22    0.0043
   Error                      4     31.06467        7.76617
   Corrected Total            7    641.87500
                         Parameter Estimates

                   Parameter     Standard
Variable     DF     Estimate        Error   t Value   Pr > |t|     Type I SS    Type II SS
Intercept     1     72.20608     54.07278      1.34     0.2527         52975      13.84832
IQ            1     -0.13117      0.45530     -0.29     0.7876      15.93930       0.64459
study         1     -4.11107      4.52430     -0.91     0.4149     580.17582       6.41230
IQ_study      1      0.05307      0.03858      1.38     0.2410      14.69521      14.69521
```

Model discussion. We call the product I*S = IQ*STUDY an "interaction" term.

$$\hat{G} = 72.21 - 0.13 * I - 4.11 * S + 0.0531(I * S)$$

Now if IQ = 100 we get

$$\hat{G} = (72.21 - 13.1) + (-4.11 + 5.31)S$$

and if IQ 120 we get

$$\hat{G} = (72.21 - 15.7) + (-4.11 + 6.37)S.$$

With interaction model, one extra hour of study increases expected grade by 1.20 points for someone with IQ = 100 and by 2.26 points for someone with IQ = 120. Since interaction not significant, we might go back to simpler "additive" model. (*example taken from Dickey's ST512 notes.*)

Some questions about design matrices

Recall three models under consideration for the bodyfat data

$$\begin{aligned} M_1: \quad \mu(x_1, x_2, x_3) &= \beta_0 + \beta_1 x_1 \\ M_2: \quad \mu(x_1, x_2, x_3) &= \beta_0 + \beta_2 x_2 \\ M_6: \quad \mu(x_1, x_2, x_3) &= \beta_0 + \beta_1 x_1 + \beta_2 x_2 \end{aligned}$$

Q: $MS[E]_{M_6} < MS[E]_{M_1}$ and $MS[E]_{M_6} < MS[E]_{M_2}$ but the partial slopes have larger standard errors in M_6. Why? ________________

Design matrices

$$X_{M6} = \begin{pmatrix} 1 & 19.5 & 43.1 \\ 1 & 24.7 & 49.8 \\ \vdots & \vdots & \vdots \\ 1 & 25.2 & 51.0 \end{pmatrix} \qquad X_{M1} = \begin{pmatrix} 1 & 19.5 \\ 1 & 24.7 \\ \vdots & \vdots \\ 1 & 25.2 \end{pmatrix}$$

$$(X'X)_{M6} = \begin{pmatrix} ? & 506.1 & 1023.4 \\ & 13386.3 & 26358.7 \\ & & 52888.0 \end{pmatrix}$$

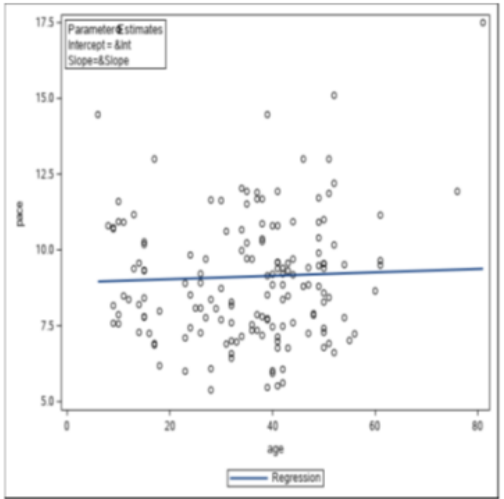
$$(X'X)_{M1} = \begin{pmatrix} ? & ? \\ & ? \end{pmatrix} \qquad (X'X)^{-1}_{M1} = \begin{pmatrix} 1.39 & -0.053 \\ & 0.002 \end{pmatrix}$$

$$(X'X)_{M2} = \begin{pmatrix} ? & ? \\ & ? \end{pmatrix} \qquad (X'X)^{-1}_{M2} = \begin{pmatrix} 5.08 & -0.098 \\ & 0.0019 \end{pmatrix}$$

$$(X'X)^{-1}_{M6} = \begin{pmatrix} 10.8 & 0.29 & -0.35 \\ & 0.014 & -0.012 \\ & & 0.013 \end{pmatrix}$$

Q: Why is $\mathrm{Var}(\hat{\beta}_0)$ bigger in M_2 than in M_1?

```
  pace      age     sex

5.38333      28      M
5.46667      39      M
    (abbreviated)
17.2667      10      F
17.5000      81      M
```



Resolution 5k run, Centennial campus

Symbol	Variable	mean	st. dev.	variance
y	Pace	9.1	2.2	5.0
x	Age	35.1	14.7	216.5

```
                         Parameter      Standard
Variable       DF         Estimate         Error     t Value     Pr > |t|

Intercept       1          8.92271       0.45724       19.51       <.0001
age             1          0.00564       0.01203        0.47       0.6396
```

Let $E_i \stackrel{iid}{\sim} N(0, \sigma^2)$. Quadratic model for pace (Y) as a function of age (x):

$$Y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + E_i \quad \text{for } i = 1, \ldots, 160$$

- $\beta = (\beta_0, \beta_1, \beta_2)'$ is a vector of unknown regression parameters
- σ^2 is the unknown error variance of paces given age x.

Compare this model with the (previously discarded) SLR model

$$Y_i = \beta_0 + \beta_1 x_i + E_i \text{ for } i = 1, \ldots, 160$$

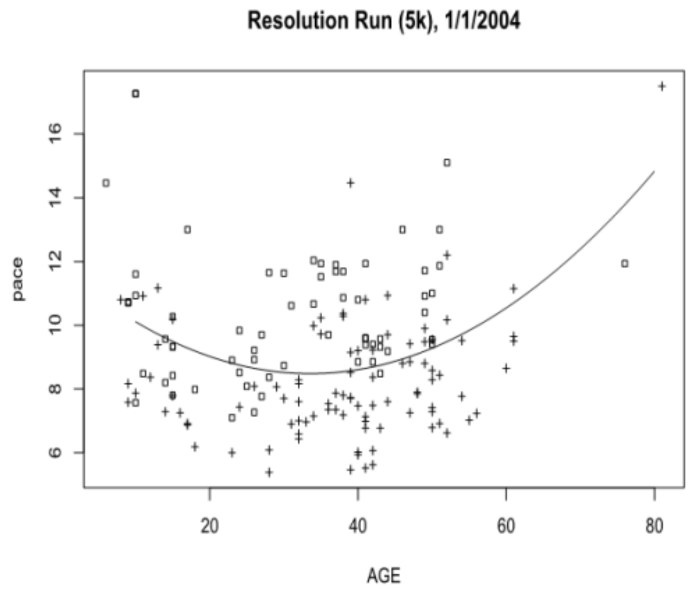
Q1: Does β_1 have the same interpretation in both models?
Q2: How can we compare the two models?
A2: Using F-ratios to compare nested models (see output next page).

$$\begin{aligned} F &= \frac{R(\beta_2|\beta_0, \beta_1)}{MS[E]_{full}} \\ &= \frac{(SS[R]_{full} - SS[R]_{red})/1}{MS[E]_{full}} = \frac{(SS[E]_{red} - SS[E]_{full})/1}{MS[E]_{full}} \\ &= \frac{(113.6 - 1.1)/1}{4.3} = \frac{(787.0 - 674.4)/1}{4.3} \\ &= 26.2 \\ &= \left(\frac{\hat{\beta}_2}{SE}\right)^2 \end{aligned}$$

with $F(0.05, 1, 157) = 3.90$. Since $26.2 >> 3.9$, the linear model is implausible when compared to the quadratic model. Also, $R(\beta_1, \beta_2|\beta_0) = 113.6$, $F = (113.6/2)/4.3 = 26.4/2 = 13.2$ so that $H_0 : \beta_1 = \beta_2 = 0$ can be rejected.

```
PROC REG DATA=one;  /* age2 defined in data step as age*age */
   MODEL pace=age;  /* not necessary in light of MODEL2 statement */
   MODEL pace=age age2/ss1;  /* ss1 generates sequential sums of squares */
RUN;
```

```
                              The REG Procedure
                                Model: MODEL1

                            Analysis of Variance

                                        Sum of           Mean
 Source                    DF          Squares          Square    F Value    Pr > F
 Model                      1          1.09650         1.09650       0.22    0.6396
 Error                    158        786.99821         4.98100
 Corrected Total          159        788.09472

                              Parameter        Standard
   Variable       DF           Estimate           Error     t Value     Pr > |t|
   Intercept       1            8.92271         0.45724       19.51       <.0001
   age             1            0.00564         0.01203        0.47       0.6396

                                Model: MODEL2

                            Analysis of Variance

                                        Sum of           Mean
 Source                    DF          Squares          Square    F Value    Pr > F
 Model                      2        113.64500        56.82250      13.23    <.0001
 Error                    157        674.44972         4.29586
 Corrected Total          159        788.09472

                      Parameter       Standard
  Variable     DF      Estimate          Error   t Value   Pr > |t|     Type I SS
  Intercept     1      11.78503        0.70216     16.78     <.0001         13310
  age           1      -0.19699        0.04113     -4.79     <.0001       1.09650
  age2          1       0.00294     0.00057380      5.12     <.0001     112.54850
```



Fitted model is

$$\hat{\mu}(x) = 11.785 - 0.197\ x + 0.00294\ x^2$$

or

$$\hat{\mu}(age) = 11.785 - 0.197\ age + 0.00294\ age^2.$$

Inference for response Y given predictor x_i.

Random sample of $n = 31$ trees drawn from population of trees. $p = 3$ variables measured on each:

- x_{i1}: "girth", tree diameter in inches
- x_{i2}: "height" (in feet)
- Y_i: volume of timber, in cubic feet.

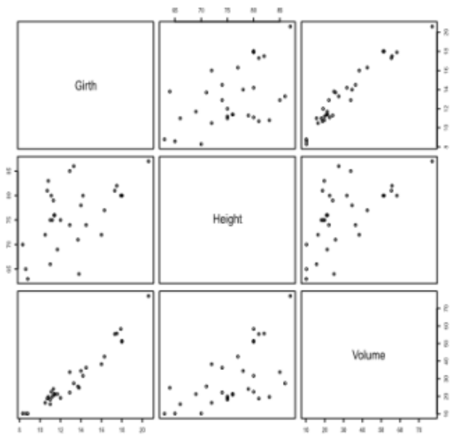
Given x_1 and x_2, a MLR model for these data given by

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + E_i \text{ for } i = 1, \ldots, n$$

For trees with x_1, x_2 the model for mean volume is

$$\mu(x_1, x_2) = E(Y|x_1, x_2) = \beta_0 + \beta_1 x_1 + \beta_2 x_2.$$

A scatterplot matrix



Some questions involving linear combinations of regression coefficients

Consider all trees with girth $x_{01} = 15$ *in* and height $x_{02} = 80$ *ft* .

- Estimate the mean volume among these trees, along with a standard error and 95% confidence interval.
- Obtain a 95% prediction interval of y_0, the volume from an individual tree sampled from this population of 80 footers, with girth 15 inches.

SAS generates $\hat{\beta}$ and $\widehat{Var}(\hat{\beta}) = MSE * (X'X)^{-1}$

Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	2	7684.16251	3842.08126	254.97	<.0001
Error	28	421.92136	15.06862		
Corrected Total	30	8106.08387			

Root MSE	3.88183	R-Square	0.9480
Dependent Mean	30.17097	Adj R-Sq	0.9442
Coeff Var	12.86612		

Parameter Estimates

Variable	DF	Parameter Estimate	Standard Error	t Value	Pr > |t|
Intercept	1	-57.98766	8.63823	-6.71	<.0001
Girth	1	4.70816	0.26426	17.82	<.0001
Height	1	0.33925	0.13015	2.61	0.0145

Covariance of Estimates

Variable	Intercept	Girth	Height
Intercept	74.6189461	0.4321713812	-1.050768886
Girth	0.4321713812	0.0698357838	-0.017860301
Height	-1.050768886	-0.017860301	0.0169393298

Inference for the mean response in MLR Recall that if Y a $p \times 1$ random vector with mean μ and covariance matrix Σ. and a a $p \times 1$ (fixed) vector of coefficients.

$$\boxed{\begin{array}{rcl} E(a'Y) & = & a'\mu \\ \mathrm{Var}(a'Y) & = & a'\Sigma a. \end{array}}$$

Consider subpopulation of trees with Girth 15 and Height 80. To estimate mean volume among these trees, with estimated std. error, take $x_0' = (1, 15, 80)$ and consider $\boxed{\widehat{\mu}(x_0) = x_0'\widehat{\beta}.}$

$$\boxed{\begin{array}{rcl} E(x_0'\widehat{\beta}) & = & x_0'\beta \\ \mathrm{Var}(x_0'\widehat{\beta}) & = & x_0'\widehat{\Sigma}x_0 \end{array}}$$

Substitution of $\widehat{\beta}$ and $\widehat{\Sigma} = MSE(X'X)^{-1}$ gives the estimates:

$$\begin{array}{rcl} \widehat{\mu}(x_0) & = & (1, 15, 80)\begin{pmatrix} -58.0 \\ 4.71 \\ 0.34 \end{pmatrix} = 39.8 \\ \widehat{\mathrm{Var}}(\widehat{\mu}(x_0)) & = & (1, 15, 80)\begin{pmatrix} 74.62 & 0.43 & -1.05 \\ 0.43 & 0.070 & -0.018 \\ -1.05 & -0.018 & 0.017 \end{pmatrix}\begin{pmatrix} 1 \\ 15 \\ 80 \end{pmatrix} = 0.72 \\ \widehat{SE}(\widehat{\mu}(x_0)) & = & \sqrt{.72} = 0.849 \end{array}$$

which can be obtained using PROC REG and the missing y trick:

Obs	treenumber	Girth	Height	Volume	p	sepred
32	100	15	80	.	39.7748	0.84918

95% Prediction limits? Use $\pm t(.025, 28)\sqrt{.72 + MS(E)}$.

Partial correlations

The partial correlation coefficient for x_1 in the MLR

$$E(Y|x_1, x_2, \dots, x_p) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p$$

is defined as the correlation coefficient between the residuals computed from the two regressions below:

$$\begin{aligned} Y &= \beta_0 + \beta_2 x_2 + \cdots + \beta_p x_p + E \\ X_1 &= \beta_0 + \beta_2 x_2 + \cdots + \beta_p x_p + E \end{aligned}$$

Call these sets of residuals $e_{y\cdot 2,3,\dots,p}$ and $e_{1\cdot 2,3,\dots,p}$ respectively. The *partial correlation* between y and x_1 after accounting for the linear association between y and $x_2, x_3, \dots, x_p$ is defined as

$$r_{y1\cdot 2,3,\cdots,p} = \text{correlation between } e_{y\cdot 2,3,\dots,p} \text{ and } e_{1\cdot 2,3,\dots,p}.$$

The *partial coeff. of determination* is $r^2_{y1\cdot 2,3,\cdots,p}$.

Note also that

$$r^2_{y1\cdot 2,\dots,p} = \frac{R(\beta_1|\beta_0, \beta_2, \dots, \beta_p)}{SS[Tot] - R(\beta_2, \beta_3, \dots, \beta_p|\beta_0)}.$$

Bodyfat data, compare models 1,2 and 6 (ignore x_3.)

```
                         bodyfat data

 Obs   x1    x2     y     py_1     ey_1      e2_1      py_2     ey_2      e1_2

   1  19.5  43.1  11.9  15.2190  -3.31903  -2.48145  13.2827  -1.38267   1.34939
   2  24.7  49.8  22.8  19.6764   3.12360  -0.78756  19.0215   3.77847   0.60956
                                  (abbreviated)
  20  25.2  51.0  21.1  20.1050   0.99500  -0.06892  20.0494   1.05061   0.04571
```

The partial correlation coefficient between y and x_1 after accounting for x_2 is $r_{y1\cdot 2} = 0.17$ and the partial for x_2 after accounting for x_1 is $r_{y2\cdot 1} = 0.48$. The partial coefficients of determination are

$$r^2_{y1\cdot 2} = 0.03062 \text{ and } r^2_{y2\cdot 1} = 0.23176.$$

Q: If you had to choose one variable or the other from x_1 and x_2, which would it be?

Q: Anything wrong with throwing both x_1 and x_2 in the final model?

Q: Write coefficients of determination in terms of extra sums of squares. Use $R(\cdot|\cdot)$ notation.

Note: partial correlations obtained in SAS using `PCORR2` option:

```
                                 Squared
                                 Partial
          Variable     DF   Corr Type II

          Intercept     1              .
          x1            1        0.03062
          x2            1        0.23176
```

Partial regression plots

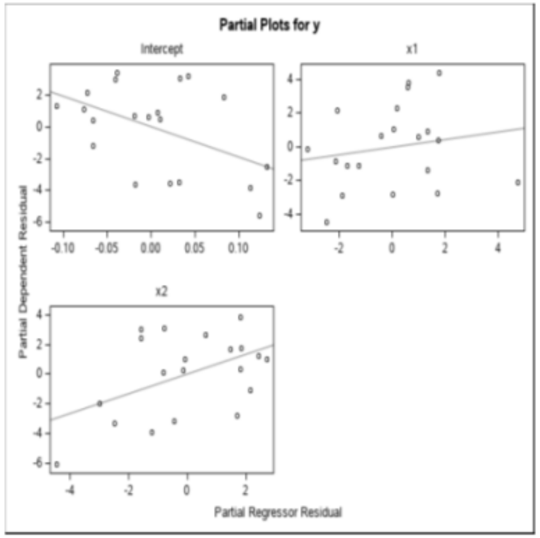
A plot of the residuals from the regression

$$Y = \beta_0 + \beta_2 x_2 + \cdots + \beta_p x_p + E$$

versus the residuals from the regression

$$X_1 = \beta_0 + \beta_2 x_2 + \cdots + \beta_p x_p + E$$

is called a partial regression or leverage plot for x_1 or in the MLR. Can be generated using `ODS GRAPHICS ON` and the `PARTIAL` command in the MODEL statement of PROC REG:



Q: What can these plots tell us?

A1: They convey info. about linear associations between y and candidate variable x_i after accounting for linear dependence of y on other variables $x_1, x_2, \ldots, x_{i-1}, x_{i+1}, \ldots, x_p$

A2: can convey info about nonlinear associations between y and x_i after accounting for other linear associations

A3: They can illuminate possible outliers.

Some exercises (hint: use matrix algebra or SAS).

1. Regarding the `resrun` data as randomly sampled a population of interest. Consider the sub-population of 32 year old males. Fit a quadratic regression function and use it to obtain an estimate of the mean 5k pace in this cohort of all 32 yr-old male runners. Report a standard error and 95% confidence interval.
2. Obtain a 95% prediction interval for one such runner.
3. Explain the difference between the two intervals in questions 1 and 2.
4. At what rate is $\mu(x)$ changing with age? Estimate the appropriate function.
5. Estimate θ, the peak age to run a 5k in the fastest time. Is θ a linear function of regression parameters? Can you obtain an unbiased estimate of the standard error of θ?

Cook's D

Cook's D for an observation i is a measure of influence on predictions:

$$D_i = \frac{\sum_{j=1}^{n} (\widehat{y}_j - \widehat{y}_{j(i)})^2}{pMS(E)}$$

where $\widehat{y}_{j(i)}$ is the fitted value for the j^{th} observation if the i^{th} observation is held out.

```
cdp from ODS output

Obs       pace      age     sexf      CooksD

  1     17.5000      81       0      0.52957
  2     11.9333      76       1      0.45148
  3     17.2667      10       1      0.13515

The MEANS Procedure

          Analysis Variable : diff

        Mean     Corrected SS            USS
--------------------------------------------
   0.0271229        6.6410416      6.7587459
--------------------------------------------
mycooksD computed just for age=81 subject

Obs      _TYPE_     _FREQ_      uss       mycooksd

 1         0         160      6.75875      0.52957
```

```
*resruncooksd.sas;
*Cook's D calculated by PROC REG and from definition;
*inspect code carefully;
data one;  set one;
   race=1*scan(crace,1,':')+1/60*scan(crace,2,':');
   pace=1*scan(cpace,1,':')+1/60*scan(cpace,2,':');
   /* The SCAN command extracts characters from a character string */
   age2=age*age; sexf=(sex="F"); agef=age*sexf; age2f=age2*sexf;
   pace2=pace; if age=81 then pace2=.;
run;
ods graphics on; ods trace on; ods listing close;
proc reg data=one plots=cooksd;
   id name pace age sexf;
   model pace=age age2 sexf/influence;
   ods output cooksdplot=cdp(rename=(id1=name id2=pace id3=age id4=sexf)) ;
   output out=preds1 p=p1;
run;
proc reg data=one; *where age<81;
   model pace2=age age2 sexf/influence;
   output out=preds2 p=p2;
run;
ods listing ;
proc sort data=cdp; by descending cooksd;
proc print data=cdp (obs=3); title "cdp from ODS output";
   var pace age sexf cooksd;
run;
```

Cook's D for every observation may be "delivered" using PROC REG and SAS ODS with the keyword "cooksdplot" discovered using `ods trace on`.

```
cdp from ODS output

Obs       pace      age     sexf      CooksD

  1     17.5000      81       0      0.52957
  2     11.9333      76       1      0.45148
  3     17.2667      10       1      0.13515
```

Calculating Cook's D from the definition . . .

```
proc sort data=preds1; by name; run;
proc sort data=preds2; by name; run;
data both;
   merge preds1 preds2;
   by name;
   diff=p1-p2;
run;
proc sort data=both; by descending age;run;
proc means data=both mean css uss;
   var diff;
   output out=uss uss=uss;
run;
data uss; set uss; mycooksd=uss/(4*3.19068); run;
/* MSE=3.19068 was hard-coded after inspection of output from MODEL1*/
proc print data=uss;
   title "mycooksD computed just for age=81 subject";
run;
```

```
The MEANS Procedure

          Analysis Variable : diff

        Mean     Corrected SS              USS
--------------------------------------------
   0.0271229        6.6410416        6.7587459
--------------------------------------------
mycooksD computed just for age=81 subject
3

Obs     _TYPE_     _FREQ_       uss       mycooksd

 1         0         160      6.75875      0.52957
```

More about model selection: R^2, R_a^2 and Mallow's C_p

In statistical modelling in general, one goal is often to identify a model explains variability in some response (y) of interest through its association with explanatory factors or variables. The principle of model parsimony dictates that it is best to construct a model which explains things, but with as few variables as possible.

Suppose that the true regression function underlying observed data is given by

$$E(Y|x_1,\ldots,x_{q+1}) = \beta_0 + \beta_1 x_1 + \ldots \beta_q x_q \quad (1)$$

but that an analysis leads to the model

$$E(Y|x) = \widehat{\beta}_0 + \widehat{\beta}_1 x_1 + \ldots \widehat{\beta}_{q-2} x_{q-2} \quad (2)$$

Model (2) is said to be *underspecified*. On the other hand, suppose another analysis leads to the model

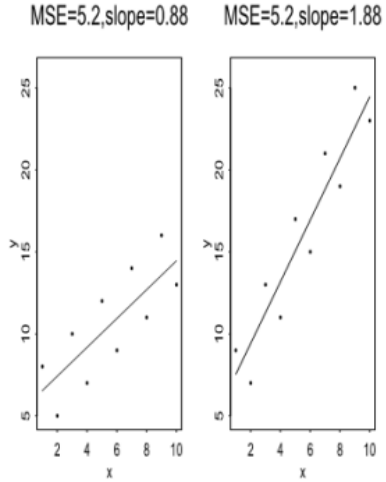
$$E(Y|x) = \widehat{\beta}_0 + \widehat{\beta}_1 x_2 + \ldots \widehat{\beta}_q x_q + \widehat{\beta}_{q+1} x_{q+1} \quad (3)$$

Then model (3) is said to be *overspecified*.

- Underspecified models introduce bias ($E(\hat{\mu}(x) \neq E(Y|x)$.)
- overspecified models inflate the sampling variances of estimators.

Which mistake is worse? (In the sense that underspecification is equivalent to fewer type I errors for tests of the form $H_0 : \beta_i = 0$, it may be preferable, as a rule of thumb.)
The coefficient of multiple determination in MLR, R^2:

- proportion of variability accounted for by a linear model, also the squared correlation between observed $(y_1, y_2, \ldots)$ and predicted $(\hat{y}_1, \hat{y}_2, \ldots,)$ values
- a reasonable criterion for model selection, but not infallible.



For two datasets with "equal" variability unexplained by SLR, the model with larger absolute slope will have higher R^2. To see this, recall that

$$R^2 = \frac{SS[R]}{SS[Tot]} = \frac{SS[Tot] - SS[E]}{SS[Tot]} = 1 - \frac{SS[E]}{SS[Tot]}.$$

bigger spread in $y \Longrightarrow$ bigger R^2

Q: Which line yields a higher r^2? Is this a better fit?

Adjusted R^2

R_a^2, or the *adjusted coefficient of multiple correlation* is given by

$$R_a^2 = 1 - \left(\frac{n-1}{n-p-1}\right)\frac{SS[E]}{SS[Tot]}$$

It imposes a penalty on added independent variables.

Mallow's C_p statistic

Suppose m denotes number of independent variables in full model, $p \leq m$ denotes number of candidates under consideration in reduced model and n denotes sample size.

$$C_p = p + 1 + \frac{(MS[E](p) - MS[E](m)) * (n-p-1)}{MS[E](m)}$$

Subset models for which $C_p \leq p + 1$ are preferred.

In addition to R^2, C_p adjusted R^2, we have AIC,AICc,BIC, ...
Let the likelihood function for a model parameterized by $k-$dimensional θ (including intercept, if any), using a sample of size n be denoted $\mathcal{L}$

$$\mathcal{L}(\theta) = f(y_1, \ldots, y_n; \theta)$$

Let the maximum likelihood estimator of θ be denoted $\widehat{\theta}$. Then

$$AIC = -2\log\mathcal{L}(\widehat{\theta}) + 2k$$

When sample size n is small there is a corrected version of AIC:

$$AICc = AIC + \frac{2k^2 + 2k}{n - k - 1}$$

Schwarz or Bayesian Information Criterion (SIC/BIC)

$$BIC = -2\log\mathcal{L}(\widehat{\theta}) + \log(n)k$$

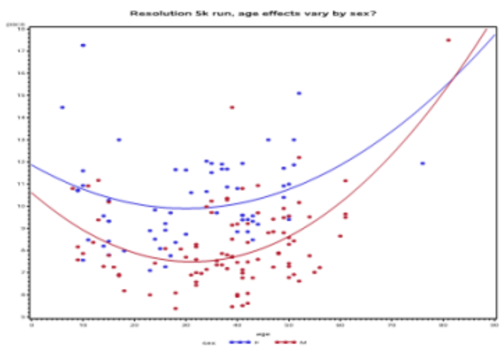
(penalty in BIC larger than in AIC)
Mallow's C_p for reduced model of dimension q.

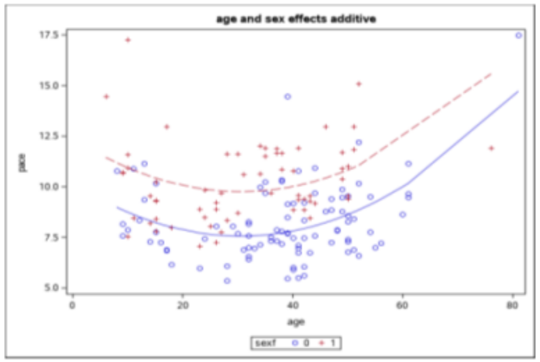
$$\begin{aligned} C_p &= \frac{SS[E]_r}{MS[E]_f} + 2p - n \\ &= p + \frac{MS(E)_r - MS(E)_f}{MS(E)_f}(n - p) \end{aligned}$$

Values small $MS(E)_r$ but also small p.

```
/* models with potentially nonlinear age effects allowed to vary with sex  */
proc reg data=one;
   model pace=age age2 sexf agef age2f/selection=cp aic bic rsquare;
run;
```

```
The SAS System
The REG Procedure
Dependent Variable: pace
C(p) Selection Method
Number of Observations Used         160
Number in                          Adjusted
  Model          C(p)    R-Square  R-Square        AIC          BIC          MSE    Variables in Model

      3        2.9901      0.3684    0.3563   189.5866     191.8431      3.19068    age age2 sexf
      4        4.8893      0.3688    0.3525   191.4825     193.8103      3.20918    age age2 sexf age2f
      4        4.9883      0.3684    0.3521   191.5848     193.9061      3.21123    age age2 sexf agef
      4        5.0408      0.3682    0.3519   191.6390     193.9568      3.21232    age age2 agef age2f
      5        6.0000      0.3725    0.3521   192.5612     195.0257      3.21147    age age2 sexf agef age2f
      3       11.7363      0.3328    0.3199   198.3700     200.1864      3.37073    age age2 agef
                                          (abbreviated)
      1       89.0585      0.0014    -.0049   258.8883     259.2590      4.98100    age
```





For MLR with i.i.d. normal errors, and $\beta((p+1)\times 1)$

$$\begin{aligned}
\mathcal{L}(\beta,\sigma^2) &= \prod_1^n \frac{1}{\sqrt{2\pi\sigma^2}}\exp\{-\frac{1}{2}\sigma^2[(y_i - x_{i\cdot}\beta)/\sigma]^2\} \\
\widehat{\beta} &= (X'X)^{-1}X'Y \\
\widehat{\sigma}^2 &= \frac{n-(p+1)}{n}MS(E) \\
\log\mathcal{L}(\beta,\sigma^2) &= -\frac{n}{2}\log 2\pi - \frac{n}{2}\log\sigma^2 - \frac{1}{2\sigma^2}(Y-X\beta)'(Y-X\beta) \\
\log\mathcal{L}(\widehat{\beta},\widehat{\sigma}^2) &= -\frac{n}{2}\log 2\pi - \frac{n}{2}\log\widehat{\sigma}^2 - \frac{1}{2\widehat{\sigma}^2}(Y-X\widehat{\beta})'(Y-X\widehat{\beta}) \\
&= -\frac{n}{2}\log\widehat{\sigma}^2 + \text{constant}
\end{aligned}$$

`PROC REG` reports $AIC = n\log\left(\frac{SSE}{n}\right) + 2(p+1)$.
link to SAS PROC REG DOC
For the full model, $MS(E) = 3.21147$ and

```
> 160*(log(3.21147*(160-6)/160)) + 2*6
[1] 192.5612
```

So, check your software's computations!

Residual diagnostics

- Residuals can be plotted against independent/predictor variables to check for model inadequacy. (e.g. if relationship is quadratic, but only a linear model was fit, this plot will reveal a pattern between residuals and predictor.)
- Residuals can be plotted against predicted values to look for inhomogeneity of variance (heteroscedasticity). Look for residuals for which variability increases or "fans out" as one looks left-to-right in this plot (or vice-versa).
- The sorted residuals can be plotted against the normal inverse of the empirical CDF of the residuals in a normal plot to assess the normal distributional assumption. A nonlinear association in such a q-q plot indicates nonnormality. If data-rich, a histogram of residuals can also be used.

Normal plots of residuals

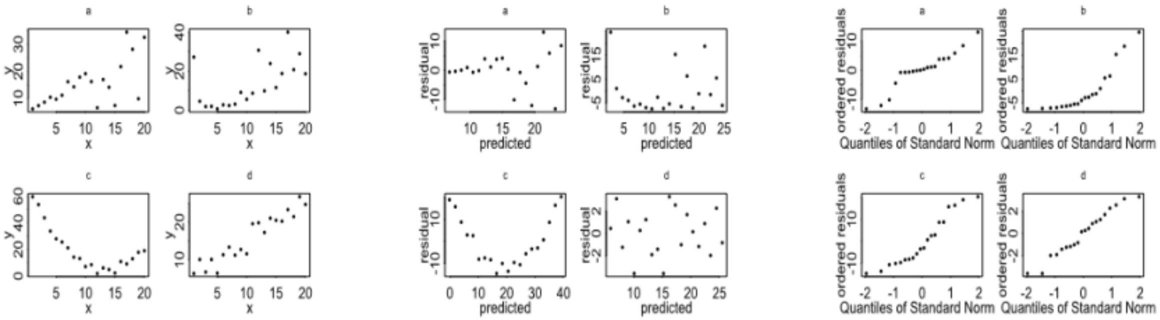
1. Obtain the observed quantiles by ordering the residuals:
$$e_{(1)} \le e_{(2)} \le \cdots \le e_{(n)}.$$
2. For each $i = 1, \ldots, n$ compute the expected quantile from
$$q_{(i)} = z(1 - \frac{i}{n+1}).$$
3. Plot the (ordered) residuals on the vertical axis versus the (ordered) theoretical quantiles on the horizontal axis.

The *empirical cumulative probability* associated with $e_{(i)}$ is
$$p_{(i)} = \frac{\text{Rank of } e_{(i)}}{n+1}.$$
Corresponding theoretical quantiles obtained via
$$q_{(i)} = z(1 - p_{(i)}).$$
e.g. suppose $n = 9$ then for $i = 1$ we look up the 10^{th} percentile of $N(0, 1)$ which is -1.282 $\ldots$ for $i = 9$ we look up $q_{(9)} = +1.282$. Plot the ordered residuals (empirical quantiles) against the theoretical quantiles and expect linearity.

```
ods listing close;
ods graphics on;
proc reg data=running;
   model pace=sexf age age2;   *general linear model.  will discuss soon;
   output out=resids p=yhat r=resid;
run;
proc rank data=resids out=resids2;
   ranks rankresid;
   var resid;
run;
data resids2;
   set resids2;
   ecdf=rankresid/(160+1);    *160 runners;
   q=probit(ecdf);
run;
ods listing ;
proc print data=resids2 ;
   var age pace yhat resid rankresid ecdf q;
run;
proc gplot data=resids;
   plot resid*q;
run;
```

```
                              The SAS System                                  1

 Obs    age      pace        yhat        resid     rankresid       ecdf          q

   1     28     5.3833     7.5837    -2.20040        14.0       0.08696    -1.35974
   2     39     5.4667     7.7671    -2.30046        10.0       0.06211    -1.53728
   3     41     5.5167     7.8735    -2.35681         6.0       0.03727    -1.78332
   4     42     5.6167     7.9351    -2.31841         9.0       0.05590    -1.59015
   5     40     5.9333     7.8175    -1.88416        18.0       0.11180    -1.21700
                         (abbreviated)
 156      6    14.4667    11.4534     3.01324       155.0       0.96273     1.78332
 157     52    15.1000    11.0579     4.04215       157.0       0.97516     1.96263
 158     10    17.2667    10.9473     6.31937       158.5       0.98447     2.15636
 159     10    17.2667    10.9473     6.31937       158.5       0.98447     2.15636
 160     81    17.5000    14.7178     2.78223       152.0       0.94410     1.59015
```

A fun exercise: Match up letters a,b,c,d with the model violation



y v x resid v predicted (y v $\widehat{y}$) normal plots of resids

1. Heteroscedasticity (nonconstant ________)
2. Nonlinearity ($\mu(x)$ not linear in ____)
3. Nonnormality (vertical variation in y about $\mu(x)$ not ____-shaped)
4. Model fits (hurray!)