Introduction to Statistical Learning

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Module 5: Hypothesis Testing for the Full Rank Model

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1 Model Relevance

1.1 Analysis of Variance- MM4.1

The full rank model

In this section, we develop various forms of hypothesis testing on the full rank model. To recap, the full rank model is

$$\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

where X is $n \times p$, $n \geq p$, $r(X) = p$, and the errors $\boldsymbol{\varepsilon}$ have:

- mean $\mathbf{0}$;
- variance $\sigma^2 I$;
- (in this module) are normally distributed (and independent because they are uncorrelated).

The full rank model

The first thing we want to test is *model relevance*: does our model contribute anything at all?

If none of the x variables have any relevance for predicting y, then all the parameters $\boldsymbol{\beta}$ will be $\mathbf{0}$.

We test for this using the null hypothesis

$$H_0 : \boldsymbol{\beta} = \mathbf{0}.$$

The full rank model

Alternatively, if at least some of the x variables are relevant to predicting y, then the corresponding parameters will be nonzero. So our alternative hypothesis is

$$H_1 : \boldsymbol{\beta} \neq \mathbf{0}.$$

To test these hypotheses, we assume throughout this section that the errors $\boldsymbol{\varepsilon}$ are multivariate normal.

ANOVA

The method used to test the hypotheses is analysis of variance (ANOVA).

If $\boldsymbol{\beta} = \mathbf{0}$, then $\mathbf{y} = \boldsymbol{\varepsilon}$ consists entirely of errors. In this case, $\mathbf{y}^T\mathbf{y}$, the sum of squares of the errors, measures the variability of the errors.

However, if $\boldsymbol{\beta} \neq \mathbf{0}$, then $\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\varepsilon}$. In this case, some of $\mathbf{y}^T\mathbf{y}$ will come from errors, but some will come from the model predictions.

By separating $\mathbf{y}^T\mathbf{y}$ into these two parts, we can compare them to see how well the model is doing.

ANOVA

Equation (1) in Module 4 on p.11 (in the proof determining the least squares estimator $\mathbf{b}$) allows us to take $\beta = 0$ and get the Analysis of Variance identity:

$$\mathbf{y}^T\mathbf{y} = (\mathbf{y} - X\mathbf{b})^T(\mathbf{y} - X\mathbf{b}) + (X\mathbf{b})^T(X\mathbf{b}) \tag{1}$$

The first term on the right of equation (1) is the residual sum of squares, SS_{Res}, which can be expressed as

$$SS_{Res} = (\mathbf{y} - X\mathbf{b})^T(y - X\mathbf{b}) = \mathbf{y}^T(I - H)\mathbf{y}$$

where $H = X(X^TX)^{-1}X^T$ is the hat matrix that takes the response variable $\mathbf{y}$ to its fitted value.

ANOVA

The second term on the right of (1) is

$$(X\mathbf{b})^T(X\mathbf{b}) = \hat{\mathbf{y}}^T\hat{\mathbf{y}} = \mathbf{y}^TH\mathbf{y} = y^TX\mathbf{b}, \tag{2}$$

the equalities using the fact that H is idempotent and symmetric.

This second term is called the *regression sum of squares* and denoted SS_{Reg}. It reflects the variation in the response variable that is explained by the model.

We call the total variation in the response variable $SS_{Total} = \mathbf{y}^T\mathbf{y}$. We have divided it into:

$$SS_{Total} = SS_{Reg} + SS_{Res}.$$

ANOVA

Example. Suppose that there is no error, so that $\mathbf{y} = X\boldsymbol{\beta}$. (This situation does not occur in practice except if $n = p$ in which case there are no degrees of freedom in the residuals, so the model is likely to be over-specified.) Then

$$\begin{aligned} SS_{Reg} &= \mathbf{y}^TX(X^TX)^{-1}X^T\mathbf{y} \\ &= \boldsymbol{\beta}^TX^TX(X^TX)^{-1}X^TX\boldsymbol{\beta} \\ &= \boldsymbol{\beta}^TX^TX\boldsymbol{\beta} \\ &= \mathbf{y}^T\mathbf{y} = SS_{Total} \end{aligned}$$

and $SS_{Res} = 0$.

ANOVA

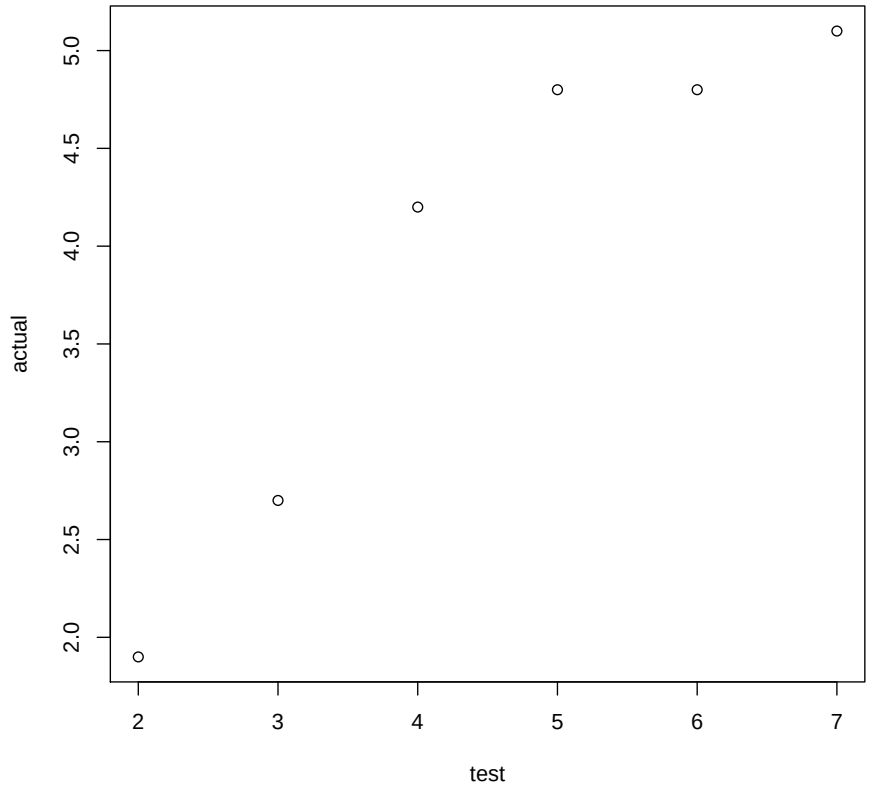
On the other hand, suppose that there is no signal, so that $\boldsymbol{\beta} = \mathbf{0}$ and $\mathbf{y} = \boldsymbol{\varepsilon}$. (Again this does not occur in practice - it is only a limiting case.) If we put $\mathbf{b} = \boldsymbol{\beta} = \mathbf{0}$ then

$$\begin{aligned} SS_{Res} &= (\mathbf{y} - X\mathbf{b})^T(\mathbf{y} - X\mathbf{b}) \\ &= \mathbf{y}^T\mathbf{y} = SS_{Total} \end{aligned}$$

and $SS_{Reg} = 0$.

These are the two extremes of the spectrum.

Figure 1: Actual cracking versus test cracking



1.2 Example - paint cracking - MM4.1

Paint Example - ANOVA

Example. Recall our previous paint cracking example, in which the data had a strong linear relationship.

```
actual <- c(1.9,2.7,4.2,4.8,4.8,5.1)
X <- matrix(c(rep(1,6),2:7),6,2)
b <- solve(t(X)%*%X,t(X)%*%actual)
e <- actual-X%*%b
(SSRes <- sum(e^2))

## [1] 1.096762

(SSTotal <- sum(actual^2))

## [1] 100.63

(SSReg <- SSTotal - SSRes)

## [1] 99.53324
```

Since $99.53 \gg 1.1$, informally we would say that there is a strong linear signal in the data.

1.3 Analysis of Variance Hypothesis Test- MM4.1

ANOVA

To create a formal test of $\boldsymbol{\beta} = \mathbf{0}$, we compare SS_{Reg} against SS_{Res}. If SS_{Reg} is large compared to SS_{Res}, then we have evidence that $\boldsymbol{\beta} \neq \mathbf{0}$.

To know exactly *how* large, we must first derive the distributions of SS_{Reg} and SS_{Res}. Of course, we already know the latter (which we re-state).

ANOVA

Theorem 5.1 (4.13)**.** *In the full rank general linear model* $\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\varepsilon}$*,* SS_{Res}/σ^2 *has a* χ^2 *distribution with* $n - p$ *degrees of freedom.*

Theorem 5.2. *In the full rank general linear model* $\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\varepsilon}$*,* SS_{Reg}/σ^2 *has a noncentral* χ^2 *distribution with* p *degrees of freedom and noncentrality parameter*

$$\lambda = \frac{1}{2\sigma^2}\boldsymbol{\beta}^T X^T X \boldsymbol{\beta}.$$

ANOVA

Proof. From (2)

$$\frac{SS_{Reg}}{\sigma^2} = \frac{1}{\sigma^2}\mathbf{y}^T H \mathbf{y}.$$

By assumption, $\mathbf{y} \sim MVN(X\boldsymbol{\beta}, \sigma^2 I)$. Also H is an idempotent and symmetric matrix. Therefore from Theorem 2.3 its rank is equal to its trace:

$$\begin{aligned} r(H) &= tr(H) \\ &= tr((X^T X)^{-1} X^T X) = tr(I_p) \\ &= p, \end{aligned}$$

using the fact (from p.16 in Module 2) that trace is the same for products in both orders (this argument was also used in Theorem 4.6).

ANOVA

By Theorem 3.5, SS_{Reg}/σ^2 has a noncentral χ^2 distribution with p degrees of freedom and noncentrality parameter

$$\begin{aligned} \lambda &= \frac{1}{2\sigma^2}(X\boldsymbol{\beta})^T H (X\boldsymbol{\beta}) \\ &= \frac{1}{2\sigma^2}\boldsymbol{\beta}^T X^T X \boldsymbol{\beta}. \end{aligned}$$

since $X^T H X = X^T X (X^T X)^{-1} X^T X = X^T X$.

ANOVA

Theorem 5.3. *In the full rank general linear model* $\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\varepsilon}$, SS_{Res} *and* SS_{Reg} *are independent.*

This can be proved by observing that they are both quadratic forms in $\mathbf{y}$ and applying Theorem 3.11.

Alternatively, we can write $SS_{Reg} = \mathbf{b}^T X^T X \mathbf{b}$ and observe that $\mathbf{b}$ and s^2 are independent.

ANOVA

Now how do we test $\boldsymbol{\beta} = \mathbf{0}$?

Observe that if this is true, the noncentrality parameter for SS_{Reg}/σ^2 must be 0.

Thus, under H_0,

$$\frac{SS_{Reg}/p\sigma^2}{SS_{Res}/(n-p)\sigma^2} = \frac{SS_{Reg}/p}{SS_{Res}/(n-p)} = \frac{MS_{Reg}}{MS_{Res}}$$

has an F distribution with p and $n-p$ degrees of freedom.

ANOVA

What happens if H_0 is not true? The expected value of MS_{Reg} is

$$E\left[\frac{SS_{Reg}}{p}\right] = \sigma^2 + \frac{1}{p}\boldsymbol{\beta}^T X^T X \boldsymbol{\beta}.$$

(Recall $SS_{Reg} = \mathbf{y}^T H \mathbf{y}$ and $E[\mathbf{x}^T A \mathbf{x}] = tr(AV) + \boldsymbol{\mu}^T A \boldsymbol{\mu}$.)

The expected value of the denominator MS_{Res} is

$$E\left[\frac{SS_{Res}}{n-p}\right] = E[s^2] = \sigma^2.$$

ANOVA

So if $\boldsymbol{\beta} = \mathbf{0}$, $E[\frac{SS_{Reg}}{p}] = \sigma^2$ and the statistic should be close to 1.

But if $\boldsymbol{\beta} \neq \mathbf{0}$, since $X^T X$ is positive definite (why?), we get $E[\frac{SS_{Reg}}{p}] > \sigma^2$ and the statistic should generally be bigger than 1.

Therefore, we should reject H_0 if the statistic is large and not reject it otherwise, with the critical value determined from the F distribution with p and $n-p$ degrees of freedom.

ANOVA

To lay out all the calculations, we can use an ANOVA table.

Source of variation	Sum of squares	degrees of freedom	Mean square	F ratio
Regression	$\mathbf{y}^T H \mathbf{y}$	p	$\frac{SS_{Reg}}{p}$	$\frac{MS_{Reg}}{MS_{Res}}$
Residual	$\mathbf{y}^T (I-H) \mathbf{y}$	$n-p$	$\frac{SS_{Res}}{n-p}$	
Total	$\mathbf{y}^T \mathbf{y}$	n		

1.4 Example - Analysis of Variance Hypothesis Test- MM4.1

Example: system cost

A data processing system uses three types of structural elements: files, flows and processes. Files are permanent records, flows are data interfaces, and processes are logical manipulations of the data. The cost of developing software for the system is based on the number of these three elements. A study is conducted with the following results:

Cost (y)	Files (x_1)	Flows (x_2)	Processes (x_3)
22.6	4	44	18
15	2	33	15
78.1	20	80	80
28	6	24	21
80.5	6	227	50
24.5	3	20	18
20.5	4	41	13
147.6	16	187	137
4.2	4	19	15
48.2	6	50	21
20.5	5	48	17

Example: system cost

The model we use is

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \varepsilon_i.$$

We want to test the hypothesis of model relevance, i.e.

$$H_0 : \boldsymbol{\beta} = \mathbf{0} \text{ vs. } H_1 : \boldsymbol{\beta} \neq \mathbf{0}.$$

The R output to test this directly from the calculations follows.

```
(b <- solve(t(X)%*%X,t(X)%*%y))
```

```
##             [,1]
## [1,] 1.9617795
## [2,] 0.1177586
## [3,] 0.1767263
## [4,] 0.7964477
```

```
(SSReg <- t(y)%*%X%*%b)
```

```
##          [,1]
## [1,] 38978.38
```

```
(SSTotal <- sum(y^2))
```

```
## [1] 39667.01
```

```
(SSRes <- SSTotal - SSReg)
```

```
##          [,1]
## [1,] 688.6262
```

```
(MSReg <- SSReg/p)
```

```
##          [,1]
## [1,] 9744.596
```

```
(MSRes <- SSRes/(n-p))

##           [,1]
## [1,] 98.37517

(Fstat <- MSReg/MSRes)

##           [,1]
## [1,] 99.05544

qf(0.95,p,n-p)

## [1] 4.120312

pf(Fstat,p,n-p,lower.tail=FALSE)

##               [,1]
## [1,] 3.060186e-06
```

Example: system cost

We can say that $\boldsymbol{\beta} \neq \mathbf{0}$ with a lot of confidence.

Variation	SS	d.f.	MS	F
Regression	38978.38	4	9744.60	99.06
Residual	688.63	7	98.38	
Total	39667.01	11		

Alternatively, we can use the `lm` and `anova` commands in R to do the calculations.

Example: system cost

```
model <- lm(y~X[,-1])
null <- lm(y~0)
anova(null,model)

## Analysis of Variance Table
##
## Model 1: y ~ 0
## Model 2: y ~ X[, -1]
##   Res.Df   RSS Df Sum of Sq      F   Pr(>F)
## 1     11 39667
## 2      7   689  4     38978 99.055 3.06e-06 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

1.5 Clover example - MM4.1

Clover example

Recall the clover example:

```
clover <- read.csv("../data/clover.csv")
clover <- log(clover)
clover <- clover[-c(6,23,47,97,111,140),]
y <- clover$area
X <- cbind(1, clover$midrib, clover$estim)
b <- solve(t(X) %*% X, t(X) %*% y)
n <- length(y)
p <- dim(X)[2]
```

We test for model relevance, $H_0 : \boldsymbol{\beta} = \mathbf{0}$.

```
(SSTotal <- sum(y^2))
```

```
## [1] 381.3093
```

```
(SSRes <- sum((y - X %*% b)^2))
```

```
## [1] 4.722065
```

```
(SSReg <- SSTotal - SSRes)
```

```
## [1] 376.5873
```

```
(Fstat <- (SSReg/p)/(SSRes/(n-p)))
```

```
## [1] 3615.358
```

```
pf(Fstat, p, n-p, lower.tail=FALSE)
```

```
## [1] 1.916608e-129
```

```
basemodel <- lm(area ~ 0, data=clover)
model <- lm(area ~ midrib + estim, data=clover)
anova(basemodel, model)
```

```
## Analysis of Variance Table
##
## Model 1: area ~ 0
## Model 2: area ~ midrib + estim
##   Res.Df    RSS Df Sum of Sq      F    Pr(>F)
## 1    139 381.31
```

```
## 2    136   4.72  3    376.59 3615.4 < 2.2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Again we reject the null hypothesis and conclude that the model is relevant.

2 General linear hypothesis

2.1 Theory - parts of MM4.1 - 4.7

The general linear hypothesis

We can now progress to testing the *general linear hypothesis*:

$$H_0 : C\boldsymbol{\beta} = \boldsymbol{\delta}^* \text{ vs. } H_1 : C\boldsymbol{\beta} \neq \boldsymbol{\delta}^*,$$

where C is an $r \times p$ matrix of rank $r \leq p$ and $\boldsymbol{\delta}^*$ is an $r \times 1$ vector of constants.

This hypothesis makes it possible to test for many things, including relationships among the parameters, or testing the individual parameters against a constant.

The general linear hypothesis

Example. Consider the null hypothesis of model relevance, $H_0 : \boldsymbol{\beta} = \mathbf{0}$.

We can express this in the form of the general linear hypothesis with $C = I_p$ (which has rank p) and $\boldsymbol{\delta}^* = \mathbf{0}$.

2.2 Application to test for equality of slopes - parts of MM4.1 - 4.7

The general linear hypothesis

Example. Consider a regression model with 4 parameters (3 predictors)

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \varepsilon_i.$$

Let

$$C = \begin{bmatrix} 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & -1 \end{bmatrix}, \quad \boldsymbol{\delta}^* = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

If we test $H_0 : C\boldsymbol{\beta} = \boldsymbol{\delta}^*$, this is equivalent to

$$\begin{aligned} \beta_1 - \beta_2 &= 0 \\ \beta_2 - \beta_3 &= 0. \end{aligned}$$

In other words, we are testing the hypothesis $\beta_1 = \beta_2 = \beta_3$.

2.3 Test Statistic - parts of MM4.1 - 4.7

Test statistic

To develop a test statistic, we start with $C\mathbf{b} - \boldsymbol{\delta}^*$, the least squares estimator for $C\boldsymbol{\beta} - \boldsymbol{\delta}^*$.

The vector $C\mathbf{b}-\boldsymbol{\delta}^*$ has elements which are linear combinations of $\mathbf{b}$, a multivariate normal, plus a constant vector. Hence $C\mathbf{b}-\boldsymbol{\delta}^*$
also multivariate normal.

Using expectation and variance properties from Module 3

$$\begin{aligned} E(C\mathbf{b}-\boldsymbol{\delta}^*) &= C\boldsymbol{\beta}-\boldsymbol{\delta}^* \\ \text{Var }(C\mathbf{b}-\boldsymbol{\delta}^*) &= C(X^TX)^{-1}C^T\sigma^2. \end{aligned}$$

Test statistic

From Corollary 3.10, the quadratic form

$$\frac{(C\mathbf{b}-\boldsymbol{\delta}^*)^T[C(X^TX)^{-1}C^T]^{-1}(C\mathbf{b}-\boldsymbol{\delta}^*)}{\sigma^2}$$

has a noncentral χ^2 distribution with r degrees of freedom and noncentrality parameter

$$\lambda = \frac{(C\boldsymbol{\beta}-\boldsymbol{\delta}^*)^T[C(X^TX)^{-1}C^T]^{-1}(C\boldsymbol{\beta}-\boldsymbol{\delta}^*)}{2\sigma^2},$$

since Question 7 in Workshop 5 shows that $C(X^TX)^{-1}C^T$ is invertible.

Test statistic

If the null hypothesis is true, then $C\boldsymbol{\beta}=\boldsymbol{\delta}^*$ and the quadratic form has an ordinary χ^2 distribution.

Since the quadratic form depends (stochastically) only on $\mathbf{b}$, it is independent from s^2.

Therefore under the null hypothesis, the statistic

$$\frac{(C\mathbf{b}-\boldsymbol{\delta}^*)^T[C(X^TX)^{-1}C^T]^{-1}(C\mathbf{b}-\boldsymbol{\delta}^*)/r}{SS_{Res}/(n-p)}$$

has an F distribution with r and $n-p$ degrees of freedom.

We use this statistic to test the general linear hypothesis.

Test statistic

To justify rejecting the null hypothesis for large values of the test statistic, the expected value of the numerator can be calculated to be

$$\begin{aligned} & E\left[\frac{(C\mathbf{b}-\boldsymbol{\delta}^*)^T[C(X^TX)^{-1}C^T]^{-1}(C\mathbf{b}-\boldsymbol{\delta}^*)}{r}\right] \\ &= \sigma^2+\frac{1}{r}(C\boldsymbol{\beta}-\boldsymbol{\delta}^*)^T[C(X^TX)^{-1}C^T]^{-1}(C\boldsymbol{\beta}-\boldsymbol{\delta}^*), \end{aligned}$$

where $[C(X^TX)^{-1}C^T]^{-1}$ is shown in Workshop 5 Question 7 to be positive definite.

If the null hypothesis is true, then the expectation is σ^2. However, if H_0 is false, it will be generally be greater than σ^2.

Therefore we reject H_0 when the statistic is large.

2.4 Example: System Cost - parts of MM4.1 - 4.7

Example: system cost

We revisit the data processing system example. We test the hypothesis $H_0 : \boldsymbol{\beta} = \begin{bmatrix} 2 & 0 & 0 & 1 \end{bmatrix}^T$.

```
bst <- c(2,0,0,1)
C <- diag(4)
r <- 4
num <- t(C%*%b-bst)%*%solve(C%*%solve(t(X)%*%X)%*%t(C))%*%
     (C%*%b-bst)/r
(Fstat <- num/(SSRes/(n-p)))

##          [,1]
## [1,] 2.795888

pf(Fstat, r, n-p, lower=F)

##           [,1]
## [1,] 0.1115939
```

Example: system cost

The critical value of the F distribution with 4 and 7 degrees of freedom at $\alpha = 0.05$ is 4.12, so we cannot reject the null hypothesis, as confirmed also by the p-value of 0.11.

This doesn't mean that it is true, just that it is close!

Workshop 5 Question 8: show that

$$(\mathbf{b} - \boldsymbol{\beta}^*)^T X^T X (\mathbf{b} - \boldsymbol{\beta}^*) = (\mathbf{y} - X\boldsymbol{\beta}^*)^T (\mathbf{y} - X\boldsymbol{\beta}^*) - (\mathbf{y} - X\mathbf{b})^T (\mathbf{y} - X\mathbf{b}).$$

That is, the SS_{Res} for the model under H_0 minus the SS_{Res} for the full model.

Example: system cost

```
library(car)
bst <- c(2,0,0,1)
C <- diag(4)
linearHypothesis(model,C,bst)

## Linear hypothesis test
##
## Hypothesis:
## (Intercept) = 2
## X[, - 1 = 0
## X[, - 2 = 0
## X[, - 3 = 1
##
## Model 1: restricted model
## Model 2: y ~ X[, -1]
##
##   Res.Df     RSS Df Sum of Sq      F Pr(>F)
## 1     11 1788.81
## 2      7  688.63  4    1100.2 2.7959 0.1116
```

Example: system cost

Now we test the hypothesis $H_0 : C\boldsymbol{\beta} = \boldsymbol{\delta}^*$, where

$$C = \begin{bmatrix} 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & -1 \end{bmatrix}, \quad \boldsymbol{\delta}^* = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

This is equivalent to $\beta_1 = \beta_2 = \beta_3$.

```
dst <- c(0,0)
C <- matrix(c(0,0,1,0,-1,1,0,-1),2,4)
r <- 2
num <- t(C%*%b-dst)%*%solve(C%*%solve(t(X)%*%X)%*%t(C))%*%
     (C%*%b-dst)/r
(Fstat <- num/(SSRes/(n-p)))

##          [,1]
## [1,] 5.785777

pf(Fstat, r, n-p, lower=F)

##             [,1]
## [1,] 0.03287564
```

Example: system cost

The calculations can be done by hand here:

$$\begin{aligned} C\mathbf{b} - \boldsymbol{\delta}^* &= \begin{bmatrix} -0.06 \\ -0.62 \end{bmatrix} \\ C(X^TX)^{-1}C^T &= \begin{bmatrix} 0.013 & 0.0024 \\ 0.0024 & 0.00077 \end{bmatrix} \\ (C\mathbf{b} - \boldsymbol{\delta}^*)^T[C(X^TX)^{-1}C^T]^{-1}(C\mathbf{b} - \boldsymbol{\delta}^*) &= 1138.35 \end{aligned}$$

Thus we can reject the null hypothesis at the 5% level, but not at the 1% level.

That is, there is evidence that the parameters β_1, β_2, and β_3 are not identical, but not strong evidence.

The next slide has the output using the package `car` and command `linearHypothesis`.

```
dst <- c(0,0)
C <- matrix(c(0,0,1,0,-1,1,0,-1),2,4)
linearHypothesis(model,C,dst)

## Linear hypothesis test
##
## Hypothesis:
## X[, - 1 - X[, - 2 = 0
```

```
## X[, - 2 - X[, - 3 = 0
##
## Model 1: restricted model
## Model 2: y ~ X[, -1]
##
##   Res.Df     RSS Df Sum of Sq      F  Pr(>F)
## 1      9 1826.98
## 2      7  688.63  2    1138.3 5.7858 0.03288 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

2.5 Example: Clover - parts of MM4.1 - 4.7

Clover example

For the clover data, consider the null hypothesis

$$H_0 : (\beta_0, \beta_1, \beta_2) = (-1, 0.5, 1).$$

```
bst <- as.vector(c(-1, 0.5, 1))
( Fstat <- ((t(b-bst) %*% t(X) %*% X %*% (b-bst))/p)/
  (SSRes/(n-p)) )

##          [,1]
## [1,] 317.6183

pf(Fstat, p, n-p, lower.tail=FALSE)

##              [,1]
## [1,] 3.230366e-61
```

Using anova

```
h0 <- X %*% bst
basemodel <- lm(area ~ 0, data=clover, offset=h0)
model <- lm(area ~ midrib + estim, data=clover)
anova(basemodel, model)

## Analysis of Variance Table
##
## Model 1: area ~ 0
## Model 2: area ~ midrib + estim
##   Res.Df    RSS Df Sum of Sq      F    Pr(>F)
## 1    139 37.806
## 2    136  4.722  3    33.084 317.62 < 2.2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

$H_0 : (\beta_0, \beta_1, \beta_2) = (-1.1, 0.5, 0.7)$

```
bst <- as.vector(c(-1.1, 0.5, 0.7))
Fstat <- ((t(b-bst) %*% t(X) %*% X %*% (b-bst))/p)/(SSRes/(n-p))
Fstat

##          [,1]
## [1,] 21.37493

pf(Fstat, p, n-p, lower.tail=FALSE)

##             [,1]
## [1,] 2.10218e-11
```

$H_0 : (\beta_0, \beta_1, \beta_2) = (-1.1, 0.5, 0.7)$ **using anova**

```
h0 <- X %*% bst
basemodel <- lm(area ~ 0, data=clover, offset=h0)
anova(basemodel, model)

## Analysis of Variance Table
##
## Model 1: area ~ 0
## Model 2: area ~ midrib + estim
##   Res.Df    RSS Df Sum of Sq      F    Pr(>F)
## 1    139 6.9485
## 2    136 4.7221  3    2.2265 21.375 2.102e-11 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

$H_0 : \beta_0 = -1, \beta_1 = \beta_2$

Let's try the null hypothesis $H_0 : \beta_0 = -1, \beta_1 = \beta_2$.

```
( C <- matrix(c(1,0,0,1,0,-1),2,3) )

##      [,1] [,2] [,3]
## [1,]    1    0    0
## [2,]    0    1   -1

library(Matrix)
(r <- rankMatrix(C)[1])

## [1] 2

dst <- c(-1,0)
```

$H_0 : \beta_0 = -1, \beta_1 = \beta_2$

```
( Fstat <- (t(C %*% b - dst) %*%
  solve(C %*% solve(t(X) %*% X) %*% t(C)) %*%
  (C %*% b - dst)/r)/(SSRes/(n-p)) )

##          [,1]
## [1,] 19.54309

pf(Fstat, r, n-p, lower=FALSE)

##              [,1]
## [1,] 3.463526e-08
```

```
linearHypothesis(model, C, dst)

## Linear hypothesis test
##
## Hypothesis:
## (Intercept) = - 1
## midrib - estim = 0
##
## Model 1: restricted model
## Model 2: area ~ midrib + estim
##
##   Res.Df    RSS Df Sum of Sq      F    Pr(>F)
## 1    138 6.0792
## 2    136 4.7221  2    1.3571 19.543 3.464e-08 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

3 Splitting β

3.1 Testing if part of β is 0 - parts of MM4.2

Testing if part of β is 0

If we find that $\boldsymbol{\beta} \neq \mathbf{0}$, we cannot say which β_i are nonzero, only that at least one is not.

If a particular β_i is zero, then it is best to remove it from the model. Otherwise it will only fit noise, and reduce the ability of the model to predict.

Thus, we need to find a way of testing whether *parts* of the parameter vector are $\mathbf{0}$ or not.

Testing if part of β is 0

We split the parameter vector

$$\boldsymbol{\beta} = \left[\begin{array}{c} \beta_0 \\ \vdots \\ \beta_{r-1} \\ \hline \beta_r \\ \vdots \\ \beta_k \end{array}\right] = \left[\begin{array}{c} \boldsymbol{\gamma}_1 \\ \hline \boldsymbol{\gamma}_2 \end{array}\right]$$

and test the hypotheses

$$H_0 : \boldsymbol{\gamma}_1 = \mathbf{0} \text{ vs. } H_1 : \boldsymbol{\gamma}_1 \neq \mathbf{0}.$$

By relabelling the indices, we can test the relevance of any subset of the parameters.

Testing if part of $\boldsymbol{\beta}$ is 0

We can do this in the framework of the general linear hypothesis.

Let $C = [I_r|\mathbf{0}]$ and $\delta^* = \mathbf{0}$. Then $C\beta = \delta^*$ iff $\boldsymbol{\gamma}_1 = \mathbf{0}$.

We define the regression sum of squares for $\boldsymbol{\gamma}_1$ in the presence of $\boldsymbol{\gamma}_2$ as

$$\begin{aligned} R(\boldsymbol{\gamma}_1|\boldsymbol{\gamma}_2) &= (C\mathbf{b} - \delta^*)^T (C(X^T X)^{-1} C^T)^{-1} (C\mathbf{b} - \delta^*) \\ &= \hat{\boldsymbol{\gamma}_1}^T A_{11}^{-1} \hat{\boldsymbol{\gamma}_1}, \end{aligned}$$

where $\hat{\boldsymbol{\gamma}_1}$ is the least squares estimator for $\boldsymbol{\gamma}_1$, and A_{11} is the upper left $r \times r$ matrix of $(X^T X)^{-1}$.

Testing if part of $\boldsymbol{\beta}$ is 0

Our test statistic is

$$\frac{R(\boldsymbol{\gamma}_1|\boldsymbol{\gamma}_2)/r}{SS_{Res}/(n-p)}.$$

From our previous results on the general linear hypothesis, we know that this has an $F_{r,n-p}$ distribution under the null hypothesis $\boldsymbol{\gamma}_1 = \mathbf{0}$. We reject the null when this statistic is too large.

Theorem 5.4. *Let X be a $n \times p$ full rank matrix. Let X and $\boldsymbol{\beta}$ be partitioned as*

$$X = \left[\begin{array}{c|c} X_1 & X_2 \end{array}\right], \boldsymbol{\beta} = \left[\begin{array}{c} \boldsymbol{\gamma}_1 \\ \hline \boldsymbol{\gamma}_2 \end{array}\right],$$

where X_1 is $n \times r$ and $\boldsymbol{\gamma}_1$ is $r \times 1$. Then

$$R(\boldsymbol{\gamma}_1|\boldsymbol{\gamma}_2) = \hat{\boldsymbol{\gamma}_1}^T A_{11}^{-1} \hat{\boldsymbol{\gamma}_1}$$

where $\hat{\boldsymbol{\gamma}_1}$ is the least squares estimator for $\boldsymbol{\gamma}_1$, and A_{11} is the upper left $r \times r$ matrix of $(X^T X)^{-1}$:

$$A_{11}^{-1} = X_1^T X_1 - X_1^T X_2 (X_2^T X_2)^{-1} X_2^T X_1.$$

The key to the proof is:

Lemma 5.5. *Suppose that*

$$A = \left[\begin{array}{c|c} A_{11} & A_{12} \\ \hline A_{21} & A_{22} \end{array}\right], A^{-1} = B = \left[\begin{array}{c|c} B_{11} & B_{12} \\ \hline B_{21} & B_{22} \end{array}\right],$$

and B_{22}^{-1} *exists. Then*

$$A_{11}^{-1} = B_{11} - B_{12}B_{22}^{-1}B_{21}.$$

which is applied with

$$A = (X^T X)^{-1}, \quad B = X^T X = \left[\begin{array}{cc} X_1^T X_1 & X_1^T X_2 \\ X_2^T X_1 & X_2^T X_2 \end{array}\right].$$

Note that this is also the key to the expression of Cook's distance involving the hat matrix and the standardised residuals.

3.2 Analysis of Variance Table - parts of MM4.2

Testing if part of $\boldsymbol{\beta}$ is 0

There is a simpler way to think about the regression sum of squares which follows after a lot of algebra:

Theorem 5.6.

$$R(\boldsymbol{\gamma}_1|\boldsymbol{\gamma}_2) = R(\boldsymbol{\beta}) - R(\boldsymbol{\gamma}_2),$$

where $R(\boldsymbol{\beta})$ *is the regression sum of squares for the full model*

$$\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\varepsilon} = [X_1|X_2]\left[\begin{array}{c} \boldsymbol{\gamma}_1 \\ \boldsymbol{\gamma}_2 \end{array}\right] + \boldsymbol{\varepsilon},$$

and $R(\boldsymbol{\gamma}_2)$ *is the regression sum of squares for the reduced model*

$$\mathbf{y} = X_2\boldsymbol{\gamma}_2 + \boldsymbol{\varepsilon}.$$

Testing if part of $\boldsymbol{\beta}$ is 0

We again express the test calculations in an ANOVA table.

Source of variation	Sum of squares	degrees of freedom	Mean square	F ratio
Regression				
Full model	$R(\boldsymbol{\beta})$	p		
Reduced model	$R(\boldsymbol{\gamma}_2)$	$p-r$		
$\boldsymbol{\gamma}_1$ in presence of $\boldsymbol{\gamma}_2$	$R(\boldsymbol{\gamma}_1\|\boldsymbol{\gamma}_2)$	r	$\frac{R(\boldsymbol{\gamma}_1\|\boldsymbol{\gamma}_2)}{r}$	$\frac{R(\boldsymbol{\gamma}_1\|\boldsymbol{\gamma}_2)/r}{MS_{Res}}$
Residual	$\mathbf{y}^T\mathbf{y} - R(\boldsymbol{\beta})$	$n-p$	$\frac{SS_{Res}}{n-p}$	
Total	$\mathbf{y}^T\mathbf{y}$	n		

Exercise: show that $R(\boldsymbol{\gamma}_2)$, $R(\boldsymbol{\gamma}_1|\boldsymbol{\gamma}_2)$ and SS_{Res} are all independent.

3.3 Example: Testing if part of $\boldsymbol{\beta}$ is 0 - parts of MM4.2

Example: system cost

Example. Consider again the data processing system example. We rejected the hypothesis of model relevance, $\boldsymbol{\beta} = \mathbf{0}$. But that is obvious because the cost of all the systems can't have average 0.

The question we want to test is, does the cost depend on the files, flows or processes? In other words, is one of β_1, β_2, or β_3 nonzero?

To do this, we re-arrange the parameter vector as

$$\boldsymbol{\beta} = \left[\begin{array}{c} \beta_1 \\ \beta_2 \\ \beta_3 \\ \hline \beta_0 \end{array}\right] = \left[\begin{array}{c} \boldsymbol{\gamma}_1 \\ \hline \boldsymbol{\gamma}_2 \end{array}\right].$$

Example: system cost

We must rearrange the columns of X correspondingly:

$$X = \left[\begin{array}{ccc|c} 4 & 44 & 18 & 1 \\ 2 & 33 & 15 & 1 \\ \vdots & \vdots & \vdots & \vdots \\ 5 & 48 & 17 & 1 \end{array}\right] = \left[\begin{array}{c|c} X_1 & X_2 \end{array}\right].$$

We want to test $H_0 : \boldsymbol{\gamma}_1 = \mathbf{0}$ (only the intercept is relevant) against $H_1 : \boldsymbol{\gamma}_1 \neq \mathbf{0}$. The reduced model is

$$\mathbf{y} = X_2\beta_0 + \boldsymbol{\varepsilon}_2,$$

i.e independent normal errors with constant mean.

Example: system cost

```
X2 <- X[,1]
(Rg2 <- t(y)%*%X2%*%solve(t(X2)%*%X2)%*%t(X2)%*%y)

##          [,1]
## [1,] 21800.55

(Rg1g2 <- SSReg - Rg2)

##          [,1]
## [1,] 17177.83

(Fstat <- (Rg1g2/3)/(SSRes/(n-p)))

##          [,1]
## [1,] 58.20517

pf(Fstat,3,n-p,lower=F)

##              [,1]
## [1,] 2.577615e-05
```

Example: system cost

The intercept alone does not explain the variation in the response variable adequately, and we are (reasonably) certain that we need at least one of the terms in the model.

Variation	SS	d.f.	MS	F
Regression				
Full	38978	4		
Reduced	21800	1		
$\boldsymbol{\gamma}_1$ in presence of $\boldsymbol{\gamma}_2$	17178	3	5726	58.2
Residual	689	7	98	
Total	39667	11		

4 Corrected SS

Corrected sum of squares

In general, we have the following ANOVA table for the test $H_0 : \beta_1 = \cdots = \beta_k = 0$ versus the alternative that some $\beta_i \neq 0$, $i \in \{1, \ldots, k\}$.

Source of variation	Sum of squares	degrees of freedom	Mean square	F ratio
Regression				
Full model	$R(\boldsymbol{\beta}) = \mathbf{y}^T H \mathbf{y}$	$k+1$		
Reduced model	$\left(\sum_{i=1}^n y_i\right)^2 / n$	1		
$\boldsymbol{\gamma}_1$ in presence of $\boldsymbol{\gamma}_2$	$R(\boldsymbol{\gamma}_1 \vert \boldsymbol{\gamma}_2)$	k	$\frac{R(\boldsymbol{\gamma}_1 \vert \boldsymbol{\gamma}_2)}{k}$	$\frac{R(\boldsymbol{\gamma}_1 \vert \boldsymbol{\gamma}_2)/k}{MS_{Res}}$
Residual	$\mathbf{y}^T \mathbf{y} - R(\boldsymbol{\beta})$	$n-k-1$	$\frac{SS_{Res}}{n-p}$	
Total	$\mathbf{y}^T \mathbf{y}$	n		

Corrected sum of squares

The SS_{Reg} for the reduced model comes from

$$\mathbf{y}^T \mathbf{1} (\mathbf{1}^T \mathbf{1})^{-1} \mathbf{1}^T \mathbf{y} = \left(\sum_{i=1}^n y_i \right) \frac{1}{n} \left(\sum_{i=1}^n y_i \right).$$

This ANOVA table is sometimes presented differently. Observe that

$$\sum_{i=1}^n (y_i - \bar{y})^2 = \sum_{i=1}^n y_i^2 - \frac{\left(\sum_{i=1}^n y_i\right)^2}{n} = \mathbf{y}^T \mathbf{y} - R(\boldsymbol{\gamma}_2).$$

This is called the *corrected sum of squares*, and $R(\boldsymbol{\gamma}_2)$ the *correction factor*.

Corrected sum of squares

We break down the corrected sum of squares into $R(\boldsymbol{\gamma}_1 | \boldsymbol{\gamma}_2)$ and SS_{Res}, and test using an F statistic ratio. The end result is the same as before, but the table looks slightly different.

Source of variation	Sum of squares	degrees of freedom	Mean square	F ratio
Regression	$SS_{Reg} - \left(\sum_{i=1}^n y_i\right)^2 / n$	k	$\frac{R(\boldsymbol{\gamma}_1 \vert \boldsymbol{\gamma}_2)}{k}$	$\frac{R(\boldsymbol{\gamma}_1 \vert \boldsymbol{\gamma}_2)/k}{MS_{Res}}$
Residual	SS_{Res}	$n-k-1$	$\frac{SS_{Res}}{n-k-1}$	
Total	$\mathbf{y}^T \mathbf{y} - \left(\sum_{i=1}^n y_i\right)^2 / n$	$n-1$		

Some computer software (including R!) will use a corrected sum of squares layout instead of an uncorrected sum, so you should be familiar with both.

Example: system cost

Example. In the data processing example, we rejected the hypothesis that $\begin{bmatrix} \beta_1 & \beta_2 & \beta_3 \end{bmatrix}^T = \mathbf{0}$. The ANOVA table for a corrected sum of squares test is

Variation	SS	d.f.	MS	F
Regression	17178	3	5726	58.2
Residual	689	7	98	
Total	17867	10		

The actual test does not change: the F statistic and degrees of freedom are the same.

Example: system cost

```
model <- lm(y~X[,-1])
null <- lm(y~1)
anova(null,model)

## Analysis of Variance Table
##
## Model 1: y ~ 1
## Model 2: y ~ X[, -1]
##   Res.Df     RSS Df Sum of Sq      F    Pr(>F)
## 1     10 17866.5
## 2      7   688.6  3     17178 58.205 2.578e-05 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

5 Clover example

Clover example — $H_0 : \beta_0 = 0$

We return to the clover example.

```
X2 <- X[,-1]
b2 <- solve(t(X2) %*% X2, t(X2) %*% y)
(SSRes2 <- sum((y - X2 %*% b2)^2))

## [1] 6.296435

(Rg2 <- SSTotal - SSRes2)

## [1] 375.0129

(Rg2 <- t(y) %*% X2 %*% b2)

##          [,1]
## [1,] 375.0129

(Rg1g2 <- SSReg - Rg2)

##         [,1]
## [1,] 1.57437
```

Clover example — $H_0 : \beta_0 = 0$

```
r <- 1
(Fstat <- (Rg1g2/r)/(SSRes/(n-p)))

##          [,1]
## [1,] 45.34336

pf(Fstat, r, n-p, lower.tail=FALSE)

##              [,1]
## [1,] 4.255185e-10
```

Clover example — $H_0 : \beta_0 = 0$

```
null <- lm(area ~ 0 + midrib + estim, data=clover)
anova(null, model)

## Analysis of Variance Table
##
## Model 1: area ~ 0 + midrib + estim
## Model 2: area ~ midrib + estim
##   Res.Df    RSS Df Sum of Sq      F    Pr(>F)
## 1    137 6.2964
## 2    136 4.7221  1    1.5744 45.343 4.255e-10 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Clover example — $H_0 : \beta_1 = 0$

```
X2 <- X[,-2]
(Rg2 <- t(y) %*% X2 %*% solve(t(X2) %*% X2) %*% t(X2) %*% y)

##          [,1]
## [1,] 375.2721

(Rg1g2 <- SSReg - Rg2)

##          [,1]
## [1,] 1.315149

r <- 1
(Fstat <- (Rg1g2/r)/(SSRes/(n-p)))

##          [,1]
## [1,] 37.87756

pf(Fstat, r, n-p, lower.tail=FALSE)

##              [,1]
## [1,] 7.920166e-09
```

Clover example — $H_0 : \beta_1 = 0$

```
null <- lm(area ~ estim, data=clover)
anova(null, model)

## Analysis of Variance Table
##
## Model 1: area ~ estim
## Model 2: area ~ midrib + estim
##   Res.Df    RSS Df Sum of Sq      F   Pr(>F)
## 1    137 6.0372
## 2    136 4.7221  1    1.3152 37.878 7.92e-09 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Clover example — $H_0 : \beta_2 = 0$

```
X2 <- X[,-3]
(Rg2 <- t(y) %*% X2 %*% solve(t(X2) %*% X2) %*% t(X2) %*% y)

##          [,1]
## [1,] 371.9034

(Rg1g2 <- SSReg - Rg2)

##          [,1]
## [1,] 4.683866

r <- 1
(Fstat <- (Rg1g2/r)/(SSRes/(n-p)))

##          [,1]
## [1,] 134.8998

pf(Fstat, r, n-p, lower.tail=FALSE)

##              [,1]
## [1,] 4.288499e-22
```

Clover example — $H_0 : \beta_2 = 0$

```
null <- lm(area ~ midrib, data=clover)
anova(null, model)

## Analysis of Variance Table
##
## Model 1: area ~ midrib
## Model 2: area ~ midrib + estim
##   Res.Df    RSS Df Sum of Sq     F    Pr(>F)
## 1    137 9.4059
## 2    136 4.7221  1    4.6839 134.9 < 2.2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Clover example — $H_0 : \beta_1 = \beta_2 = 0$

```
X2 <- X[,1]
(Rg2 <- t(y) %*% X2 %*% solve(t(X2) %*% X2) %*% t(X2) %*% y)

##          [,1]
## [1,] 310.708

(Rg1g2 <- SSReg - Rg2)

##          [,1]
## [1,] 65.87925

r <- 2
(Fstat <- (Rg1g2/r)/(SSRes/(n-p)))

##          [,1]
## [1,] 948.6927

pf(Fstat, r, n-p, lower.tail=FALSE)

##              [,1]
## [1,] 1.323441e-80
```

Clover example — $H_0 : \beta_1 = \beta_2 = 0$

```
null <- lm(area ~ 1, data=clover)
anova(null, model)

## Analysis of Variance Table
##
## Model 1: area ~ 1
## Model 2: area ~ midrib + estim
##   Res.Df    RSS Df Sum of Sq      F    Pr(>F)
## 1    138 70.601
## 2    136  4.722  2    65.879 948.69 < 2.2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Can you find the p-values?

```
summary(model)

##
## Call:
## lm(formula = area ~ midrib + estim, data = clover)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.57403 -0.10000  0.00737  0.11681  0.49398
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) -1.38148    0.20516  -6.734 4.26e-10 ***
## midrib       0.65037    0.10567   6.154 7.92e-09 ***
## estim        0.69199    0.05958  11.615  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
```

```
## Residual standard error: 0.1863 on 136 degrees of freedom
## Multiple R-squared:  0.9331,Adjusted R-squared:  0.9321
## F-statistic: 948.7 on 2 and 136 DF,  p-value: < 2.2e-16
```

6 Sequential testing

6.1 Sequential testing theory - not in MM

Sequential testing

Suppose that we have a number of explanatory variables in a model, but it's not obvious if all of them are relevant.

We could fit a model using all of them, but this runs the risk of *overfitting*: using irrelevant variables to explain noise by coincidence.

Ideally, we prefer to fit a parsimonious model, i.e. using a minimal number of explanatory variables.

A parsimonious model is less likely to suffer from overfitting.

Sequential testing

In a parsimonious model, if we were to test if the parameter β_i is 0, in the presence of the other model parameters, we should always reject the null.

We can use the tests we have developed to tell if a model is parsimonious or not.

How do we find such a minimal set of parameters?

Sequential testing

Conceivably, with the help of a computer, we could test all the possible parameter sets to find the largest $\boldsymbol{\gamma}_1$ such that the hypothesis $\boldsymbol{\gamma}_1 = \mathbf{0}$ is not rejected.

The problem with this approach (apart from the time required) is that it can give inconsistent results. For example we might reject $\beta_1 = \beta_2 = 0$ given β_3, but not reject $\beta_1 = 0$ given β_2 and β_3, and also not reject $\beta_2 = 0$ given β_1 and β_3.

This can happen when x_1 and x_2 are strongly correlated, so that given one of them the other isn't needed, but you need to have at least one of them.

Partial testing

If we have $p = k + 1$ parameters $\beta_0, \ldots, \beta_k$ we could consider p tests of the form $H_0 : \beta_i = 0$, given all the other parameters are in the model. Such tests are called *partial* tests.

Then we could remove all parameters where we do not reject $\beta_i = 0$.

The discussion above suggests that this could lead us to remove too many variables, *because the partial tests are not independent.*

In a partial test, acceptance or rejection of H_0 does not mean that the parameter is useful or useless in the *best* model, just useful or useless in the *full* model.

Sequential testing

To avoid the problem of dependence between partial tests we can consider a nested sequence of models.

That is, we can start with a simple model and sequentially add parameters until adding parameters does not significantly improve the fit. Then we have a parsimonious model.

Alternatively we can start with a full model and sequentially remove parameters until removing parameters significantly worsens the fit. Then we again have a parsimonious model.

Sequential testing

Consider the series of models (subject to relabelling)

$$\begin{aligned} y &= \beta_0 + \varepsilon^{(0)} \\ y &= \beta_0 + \beta_1 x_1 + \varepsilon^{(1)} \\ &\vdots \\ y &= \beta_0 + \beta_1 x_1 + \ldots + \beta_k x_k + \varepsilon^{(k)}. \end{aligned}$$

We denote the corresponding X matrices by X_j, which are the first $j+1$ columns of X. Let $H_j = H(X_j)$, where for any matrix B of full rank, $H(B) = B(B^TB)^{-1}B^T$ is the hat matrix for B.

The regression sum of squares, R_j, for each of these models is calculated in the usual way:

$$R_j = R(\beta_0, \beta_1, \ldots, \beta_j) = \mathbf{y}^T H_j \mathbf{y},$$

Sequential testing

Note that these are 'full' regression sums of squares, i.e. we are looking at the total variation explained by the model in the presence of *no* other parameters.

Now by taking the difference between the sums of squares, we get the extra variation explained as we add variables to the model one at a time:

$$\begin{aligned} R(\beta_1|\beta_0) &= R_1 - R_0 \\ R(\beta_2|\beta_0, \beta_1) &= R_2 - R_1 \\ &\vdots \\ R(\beta_k|\beta_0, \beta_1, \ldots, \beta_{k-1}) &= R(\boldsymbol{\beta}) - R_{k-1}. \end{aligned}$$

Sequential testing

Theorem 5.7. *In the full rank general linear model* $\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\varepsilon}$*, assume* $\boldsymbol{\varepsilon} \sim N(0, \sigma^2 I)$*:*

$$\begin{aligned} \frac{1}{\sigma^2}\mathbf{y}^T\mathbf{y} &= \frac{1}{\sigma^2}SS_{Res} + \frac{1}{\sigma^2}R(\beta_0) + \frac{1}{\sigma^2}R(\beta_1|\beta_0) + \frac{1}{\sigma^2}R(\beta_2|\beta_0, \beta_1) + \\ &\quad \cdots + \frac{1}{\sigma^2}R(\beta_k|\beta_0, \beta_1, \ldots, \beta_{k-1}), \end{aligned}$$

and the quadratic forms on the right are all independent with noncentral χ^2 *distributions.* SS_{Res} *has* $n - p$ *d.f. and the rest have* 1 *d.f. each.*

Sequential testing

To prove this theorem, we first prove the following lemma.

Lemma 5.8. *Let $A = [A_1|A_2]$ be a matrix of full rank. Then the matrix $H(A) - H(A_1)$ is idempotent.*

Proof.

First we note that

$$\begin{aligned} A^T[I - H(A)] &= A^T - A^T A(A^T A)^{-1} A^T \\ &= 0. \end{aligned}$$

Sequential testing

Partitioning the first factor,

$$\begin{aligned} \left[\frac{A_1^T}{A_2^T}\right][I - H(A)] &= 0 \\ A_1^T[I - H(A)] &= 0 \\ A_1^T &= A_1^T H(A) \\ A_1 &= H(A)A_1. \end{aligned}$$

since $H(A)$ is symmetric.

Sequential testing

So, using the fact that $H(B)$ is idempotent for any matrix B,

$$\begin{aligned} &(H(A) - H(A_1))^2 \\ &= H(A) - H(A)A_1(A_1^T A_1)^{-1} A_1^T \\ &\qquad -A_1(A_1^T A_1)^{-1} A_1^T H(A) + H(A_1) \\ &= H(A) - H(A_1) - H(A_1) + H(A_1) \\ &= H(A) - H(A_1). \end{aligned}$$

Sequential testing

Proof of theorem. The sum follows from the definitions. To prove the rest, we use Theorem 3.14 with the hypothesis that we have idempotent matrices whose sum is idempotent.

The conclusion is that quadratic forms in a multivariate normal random vector, based on the components of the sum, have independent non-central chi-square distributions with degrees of freedom equal to the rank of the matrices. From the lemma, $H_j - H_{j-1}$ is idempotent. Furthermore both H_0 and $I - H_p$ are idempotent.

Thus we have a set of idempotent matrices $H_1, H_2 - H_1, \cdots H_p - H_{p-1}, I - H_p$ whose sum I also idempotent. Theorem 3.14 thus gives that the quadratic forms all have independent noncentral χ^2 distributions.

Sequential testing

To show the degrees of freedom, observe that the sum of the ranks is n and $r(I - H_p) = n - p$.

Each sequential regression sum of squares, $H_j - H_{j-1}$ has 1 degree of freedom because, being idempotent,

$$r(H_j - H_{j-1}) = tr(H_j - H_{j-1}) = tr(H_j) - tr(H_{j-1}) = j - (j-1) = 1,$$

after noting that we already showed that the trace of a hat matrix is the number of columns of the matrix on which it is based.

Sequential testing

Therefore under the hypothesis $\beta_j = 0$, the test statistic

$$F = \frac{R(\beta_j | \beta_0, \beta_1, \ldots, \beta_{j-1})}{SS_{Res}/(n-p)}$$

has an F distribution with 1 and $n - p$ degrees of freedom.

This is still not entirely satisfactory.

Suppose we declare a parameter relevant if the null hypothesis that it is 0 is rejected in a sequence of $F-$tests.

Unfortunately, the order in which the parameters are tested can heavily influence the results. Thus, different orderings can result in different sets of parameters being included in the final model.

6.2 Example: sequential testing squids - not in MM

Squid example

Example. An experiment is conducted to study the size of squid. The response is the weight of the squid, and the predictors are

- x_1: Beak length
- x_2: Wing length
- x_3: Beak to notch length
- x_4: Notch to wing length
- x_5: Width

A total of 22 squid are sampled. Figure 2 shows pairwise plots of the data.

```
squid <- read.csv('../data/squid.csv')
pairs(squid)
```

Squid example

Let's first test if any parameters should be in the model, i.e. if $\boldsymbol{\beta} = \mathbf{0}$.

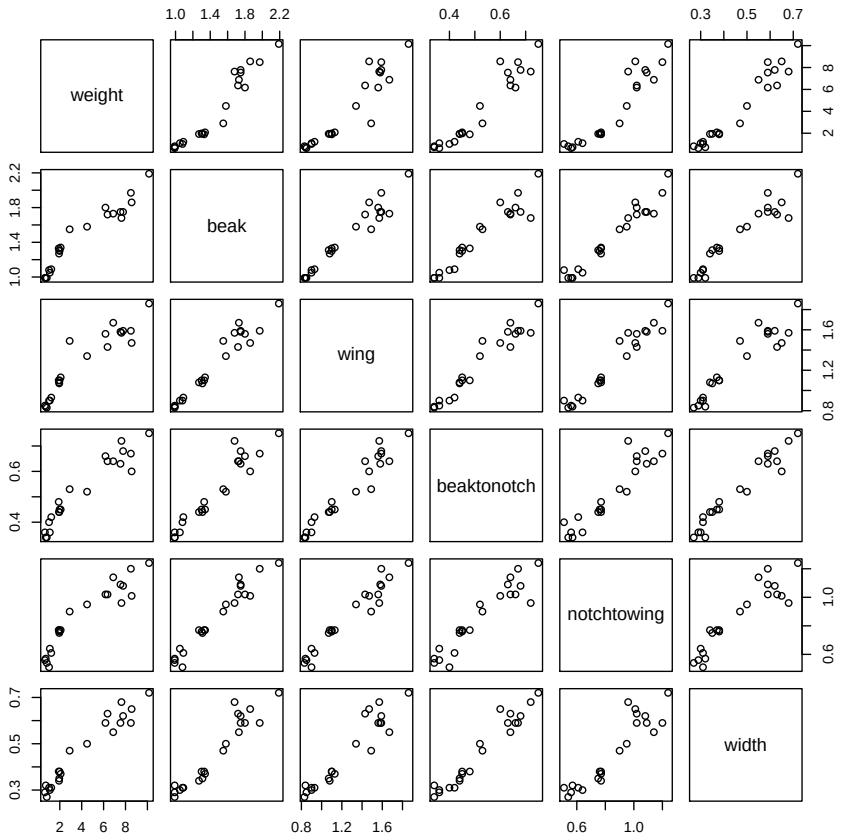


Figure 2: Pairwise plots of the variables in the squid data set

```
n <- dim(squid)[1]
p <- dim(squid)[2]
y <- squid$weight
X <- as.matrix(cbind(rep(1,n),squid[,-1]))
b <- solve(t(X)%*%X,t(X)%*%y)
SSRes <- sum((y-X%*%b)^2)
SSReg <- sum(y^2) - SSRes
(Fstat <- (SSReg/p)/(SSRes/(n-p)))

## [1] 200.4545

pf(Fstat,p,n-p,lower=F)

## [1] 3.879047e-14
```

Squid example

```
sqmodel <- lm(weight~.,data=squid)
sqnull <- lm(weight~0,data=squid)
anova(sqnull, sqmodel)

## Analysis of Variance Table
##
## Model 1: weight ~ 0
## Model 2: weight ~ beak + wing + beaktonotch + notchtowing + width
##   Res.Df    RSS Df Sum of Sq      F    Pr(>F)
## 1     22 603.08
## 2     16   7.92  6    595.16 200.45 3.879e-14 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

The null hypothesis $\boldsymbol{\beta} = \mathbf{0}$ is rejected strongly.

Squid example

Next we test to see which parameters should be included in the model.

```
R <- c()
for (i in 1:p) {
  Xi <- X[,1:i]
  R[i] <- t(y)%*%Xi%*%solve(t(Xi)%*%Xi,t(Xi)%*%y)
}
R

## [1] 387.1566 586.3019 586.4285 590.5481 590.8116 595.1638

R - c(0,R[-length(R)])

## [1] 387.1565500 199.1453356   0.1266641   4.1195388   0.2634957   4.3521933
```

Squid example

Thus the sequential sums of squares are:

$$
\begin{aligned}
R(\beta_0) &= 387.16 \\
R(\beta_1|\beta_0) &= 199.15 \\
R(\beta_2|\beta_0,\beta_1) &= 0.127 \\
R(\beta_3|\beta_0,\beta_1,\beta_2) &= 4.12 \\
R(\beta_4|\beta_0,\beta_1,\beta_2,\beta_3) &= 0.263 \\
R(\beta_5|\beta_0,\beta_1,\beta_2,\beta_3,\beta_4) &= 4.35
\end{aligned}
$$

Squid example

These sum to the regression sum of squares for the full model:

```
sum(R - c(0,R[-length(R)]))
```

```
## [1] 595.1638
```

```
SSReg
```

```
## [1] 595.1638
```

Each of these sums of squares should be compared against the critical F value with 1 and $n-p$ degrees of freedom, multiplied by $SS_{Res}/(n-p)$. With $\alpha = 0.05$, this is:

```
SSRes/(n-p)*qf(0.95,1,n-p)
```

```
## [1] 2.223833
```

Squid example

So starting with a model with no parameters, we should definitely add β_0 and then β_1, but not β_2.

The subsequent tests are harder to interpret. For example, if $\beta_0, \beta_1, \beta_2$, and β_3 are in the model, we should not add β_4. But β_2 is not in the model!

The tests for β_3, β_4 and β_5 need to be repeated, supposing only that β_0 and β_1 are in the model.

Squid example

Note that we use the SS_{Res} (and residual degrees of freedom) of the *full* model in the denominator of our F statistics.

This is because we cannot assume that variables that are not in the model are irrelevant. If there are relevant variables, SS_{Res} of a reduced model may be disproportionately large, and more importantly not conform to our distributional assumptions.

The only way to be safe about this is to use the SS_{Res} of the full model, even if it means losing a few degrees of freedom to truly irrelevant variables.

Squid example

Note: R can not do this unless all the models are presented at once (see the clover example below)! To test for β_i in the presence of $\beta_0, \ldots, \beta_{i-1}$ it uses the residual sum of squares from the model using $\beta_0, \ldots, \beta_i$. This still gives a valid test, though in general not as powerful as the test using SS_{Res} from the full model.

6.3 Example: sequential testing clover example - not in MM

Clover example

We try some sequential tests on the clover example. We test in the order $\beta_0 \to \beta_1 \to \beta_2$.

```
R <- c()
for (i in 1:p) {
  Xi <- X[,1:i]
  R[i] <- t(y)%*%Xi%*%solve(t(Xi)%*%Xi,t(Xi)%*%y)
}
R - c(0,R[-length(R)])

## [1] 310.708028  61.195381   4.683866

(R - c(0,R[-length(R)]))/(SSRes/(n-p))

## [1] 8948.6892 1762.4857  134.8998

qf(0.95, 1, n-p)

## [1] 3.910747
```

Clover example

```
model <- lm(area ~ midrib + estim, data=clover)
nm1 <- lm(area ~ 0, data=clover)
nm2 <- lm(area ~ 1, data=clover)
nm3 <- lm(area ~ midrib, data=clover)
```

Clover example

```
anova(nm1, nm2, nm3, model)

## Analysis of Variance Table
##
## Model 1: area ~ 0
## Model 2: area ~ 1
## Model 3: area ~ midrib
## Model 4: area ~ midrib + estim
##   Res.Df    RSS Df Sum of Sq      F    Pr(>F)
## 1    139 381.31
## 2    138  70.60  1   310.708 8948.7 < 2.2e-16 ***
## 3    137   9.41  1    61.195 1762.5 < 2.2e-16 ***
```

```
## 4    136   4.72  1     4.684  134.9 < 2.2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

7 Selection

7.1 Forward selection - not in MM

Forward selection

To resolve the difficulties of different final models depending on parameter ordering, there are strategies to find a parsimonious model using sequential tests.

Forward selection starts off with an empty model, and adds the variable which is found to be most significant.

Significance is measured in relation to the current model, so all tests are conducted in the presence of already included parameters, but not the other parameters.

When no variables are significant enough to add, we stop and take the current model as the final model.

Forward selection

1. Start with an empty model.
2. Calculate the F-values for the tests $H_0 : \beta_i = 0$, for all parameters not in the model, in the presence of parameters already in the model.
3. If none of the tests are significant (we do not reject any null hypotheses), then stop.
4. Otherwise add the most significant parameter (i.e. parameter with the largest F-value).
5. Return to step 2.

7.2 Example: forward selection - not in MM

Cement example: forward selection

We model the heat expended y (in calories) in cement during 180 days hardening, depending on percentages of 4 different chemicals in the mixture. Note that 1 to 5 percent of the cement is not in these chemicals. Figure 109 shows the pairwise scatter plots.

```
heat <- read.csv("../data/heat.csv")
str(heat)
```

```
## 'data.frame': 13 obs. of  5 variables:
##  $ x1: int  7 1 11 11 7 11 3 1 2 21 ...
##  $ x2: int  26 29 56 31 52 55 71 31 54 47 ...
##  $ x3: int  6 15 8 8 6 9 17 22 18 4 ...
```

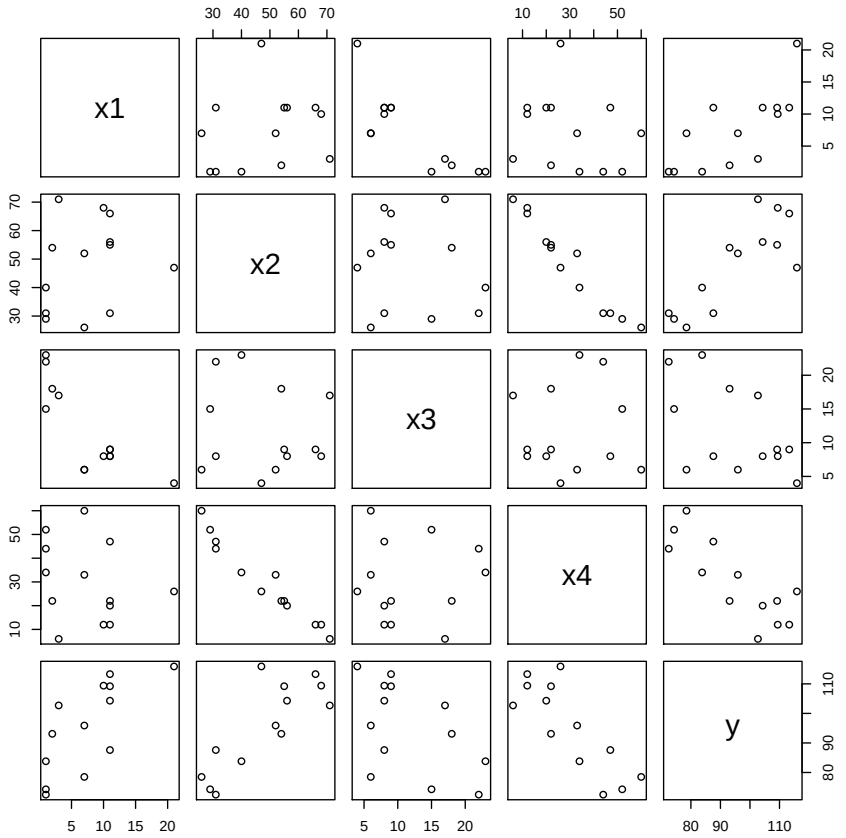


Figure 3: Pairwise plots of cement data

```
##  $ x4: int  60 52 20 47 33 22 6 44 22 26 ...
##  $ y : num  78.5 74.3 104.3 87.6 95.9 ...

basemodel <- lm(y ~ 1, data=heat)
```

Cement example: forward selection

```
add1(basemodel, scope= ~ . + x1 + x2 + x3 + x4, test="F")

## Single term additions
##
## Model:
## y ~ 1
##        Df Sum of Sq     RSS    AIC F value    Pr(>F)
```

```
## <none>              2715.76 71.444
## x1      1   1450.08 1265.69 63.519 12.6025 0.0045520 **
## x2      1   1809.43  906.34 59.178 21.9606 0.0006648 ***
## x3      1    776.36 1939.40 69.067  4.4034 0.0597623 .
## x4      1   1831.90  883.87 58.852 22.7985 0.0005762 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

model2 <- lm(y ~ x4, data=heat)
```

Cement example: forward selection

```
add1(model2, scope= ~ . + x1 + x2 + x3, test="F")

## Single term additions
##
## Model:
## y ~ x4
##        Df Sum of Sq    RSS    AIC  F value    Pr(>F)
## <none>              883.87 58.852
## x1      1    809.10  74.76 28.742 108.2239 1.105e-06 ***
## x2      1     14.99 868.88 60.629   0.1725    0.6867
## x3      1    708.13 175.74 39.853  40.2946 8.375e-05 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

model3 <- lm(y ~ x1 + x4, data=heat)
```

Cement example: forward selection

```
add1(model3, scope= ~ . + x2 + x3, test="F")

## Single term additions
##
## Model:
## y ~ x1 + x4
##        Df Sum of Sq    RSS    AIC F value  Pr(>F)
## <none>              74.762 28.742
## x2      1    26.789 47.973 24.974  5.0259 0.05169 .
## x3      1    23.926 50.836 25.728  4.2358 0.06969 .
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

We use variables x_1 and x_4 in our final model.

7.3 Backward elimination - not in MM

Backward elimination

A conceptually similar method is *backward elimination*:

1. Start with the full model.

2. Calculate the F-values for the tests $H_0 : \beta_i = 0$, for all parameters in the model, in the presence of the other parameters in the model.

3. If all of the tests are significant (we reject all null hypotheses), then stop.

4. Otherwise, remove the least significant parameter (i.e. parameter with smallest F-value).

5. Return to step 2.

Backward elimination

Backward elimination is complementary to forward selection, i.e. starts from the full model and removes the least important variable until all variables are important.

Forward selection and backward elimination are easy to understand and to apply, but do not always produce the optimal results.

One reason this is so is the inability to remove an already added variable (or add an already removed variable). This inflexibilty is often limiting.

7.4 Example: backward elimination cement - not in MM

Cement example: backward elimination

```
fullmodel <- lm(y ~ .,data=heat)
drop1(fullmodel, scope= ~ ., test="F")

## Single term deletions
##
## Model:
## y ~ x1 + x2 + x3 + x4
##        Df Sum of Sq    RSS    AIC F value  Pr(>F)
## <none>              47.864 26.944
## x1      1   25.9509 73.815 30.576  4.3375 0.07082 .
## x2      1    2.9725 50.836 25.728  0.4968 0.50090
## x3      1    0.1091 47.973 24.974  0.0182 0.89592
## x4      1    0.2470 48.111 25.011  0.0413 0.84407
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

model2 <- lm(y~x1+x2+x4,data=heat)
```

Cement example: backward elimination

```
drop1(model2, scope= ~., test="F")

## Single term deletions
##
## Model:
## y ~ x1 + x2 + x4
##        Df Sum of Sq    RSS    AIC  F value    Pr(>F)
## <none>               47.97 24.974
## x1      1    820.91 868.88 60.629 154.0076 5.781e-07 ***
```

```
## x2      1     26.79  74.76 28.742   5.0259   0.05169 .
## x4      1      9.93  57.90 25.420   1.8633   0.20540
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

model3 <- lm(y ~ x1 + x2, data=heat)
```

Cement example: backward elimination

```
drop1(model3, scope = ~ ., test="F")

## Single term deletions
##
## Model:
## y ~ x1 + x2
##        Df Sum of Sq     RSS    AIC F value    Pr(>F)
## <none>               57.90 25.420
## x1      1    848.43  906.34 59.178  146.52 2.692e-07 ***
## x2      1   1207.78 1265.69 63.519  208.58 5.029e-08 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

We use variables x_1 and x_2 in our final model.

7.5 Stepwise selection - not in MM

Stepwise selection

Stepwise selection functions similarly to forward or backward selection, but with the possibility of either adding or eliminating a variable at each step.

In order to assess the appropriateness of a model, we use a *goodness-of-fit* measure.

We give a procedure using a goodness-of-fit measure called Akaike's information criterion (AIC), but it is easy to adjust the procedure for any other goodness-of-fit statistic. The smaller is the AIC, the better is the model - details follow after describing stepwise selection.

Stepwise selection

1. Start with any model.
2. Compute the AIC of all models which either have one extra variable or one less variable than the current model.
3. If the AIC of all such models is more than the AIC of the current model, stop.
4. Otherwise, change to the model with the lowest AIC.
5. Return to step 2.

Stepwise selection

Stepwise selection is generally better than forward or backward selection, because it avoids the problem that an already added variable can never be removed (or the opposite).

However the final model depends on the starting model, so it does not necessarily find a global optimum for the goodness-of-fit statistic. Instead it finds a local optimum.

It is possible for small numbers of variables to find a global minimum through an exhaustive search of all possible combinations. However, as the number of variables increases, this will take too long.

7.6 Goodness of fit measures - not in MM

Goodness-of-fit measures

The F test is used to compare *nested* models, that is, it requires the variable set of one model to be fully contained in the variable set of the other model.

We cannot use an F test to compare models which, for example, have replaced one variable with another variable.

Also, use of the F test requires the somewhat arbitrary choice of a significance level.

To overcome these problems many authors have proposed *goodness-of-fit* measures, which try to give a measure of how good a model is, independently of other models.

Residual sum of squares

The residual sum of squares, SS_{Res}, measures how well the model fits the (training) data. However, it is not a good goodness-of-fit measure, as it does not take into account model complexity, and thus can not prevent overfitting.

We can overcome this by using s^2 as a goodness-of-fit statistic. When we add a variable to the model, SS_{Res} always decreases. However, the degrees of freedom $n - p$ also decreases, so s^2 will decrease only if the variable is "good".

Unfortunately, in practice using s^2 for goodness-of-fit does not discourage overfitting enough.

R^2

A commonly reported goodness-of-fit statistic is the proportion of corrected total sums of squares that is explained by the model:

$$R^2 = 1 - \frac{SS_{Res}}{SS_{Total} - \left(\sum_i y_i\right)^2 / n}.$$

R^2 lies between 0 and 1, and the larger it is, the more variation in y is explained by the model. It is also equal to the square of the correlation between y and $\hat{y}$.

However R^2 can never decrease when we add a variable to a model, as even an irrelevant variable will 'explain' a small extra amount of variation. We would like to remove irrelevant variables, so, like SS_{Res}, R^2 is not appropriate for model selection.

Adjusted R^2

The adjusted R^2 tries to account for model complexity by introducing a penalty based on the number of parameters in the model:

$$\text{adj } R^2 = 1 - \frac{n-1}{n-1-k}(1-R^2).$$

Here we assume that β_0 is in the model, and k is the number of other parameters in the model.

The adjusted R^2 is better for model selection than s^2, but there are other more sophisticated goodness-of-fit measures that we can use, such as the AIC, BIC or Mallows' C_p statistic.

AIC

A very popular goodness-of-fit statistic is *Akaike's information criterion*, or AIC. This is based on the likelihood of the observed values of the response.

$$\begin{aligned} AIC &= -2\ln(\text{likelihood}) + 2p \\ &= n\ln\left(\frac{SS_{Res}}{n}\right) + 2p + \text{const.} \end{aligned}$$

(Here the likelihood is the maximised likelihood.) A smaller value of AIC indicates a better model.

The form of the AIC can be justified using information theory.

Mallows' C_p

Another goodness-of-fit statistic is *Mallows' C_p statistic*. This statistic compares the residual sum of squares of an intermediate model against the the residual sum of squares for a full model:

$$C_p = \frac{SS_{Res}(\text{model})}{s^2(\text{full model})} + 2p - n,$$

where p is the number of parameters in the (intermediate) model. The smaller C_p is, the better the model.

Goodness-of-fit measures

Note that any goodness-of-fit statistic should only to be used to compare various models for the same data. For none of them is there an absolute measure of how good a model is.

7.7 Example: stepwise selection cement - not in MM

Cement example: stepwise selection

```
model2 <- step(basemodel, scope=~.+x1+x2+x3+x4,steps=1)

## Start:  AIC=71.44
## y ~ 1
##
```

```
##        Df Sum of Sq     RSS    AIC
## + x4    1   1831.90  883.87 58.852
## + x2    1   1809.43  906.34 59.178
## + x1    1   1450.08 1265.69 63.519
## + x3    1    776.36 1939.40 69.067
## <none>              2715.76 71.444
##
## Step:  AIC=58.85
## y ~ x4
```

Cement example: stepwise selection

```
model3 <- step(model2, scope=~.+x1+x2+x3,steps=1)

## Start:  AIC=58.85
## y ~ x4
##
##        Df Sum of Sq     RSS    AIC
## + x1    1    809.10   74.76 28.742
## + x3    1    708.13  175.74 39.853
## <none>               883.87 58.852
## + x2    1     14.99  868.88 60.629
## - x4    1   1831.90 2715.76 71.444
##
## Step:  AIC=28.74
## y ~ x4 + x1
```

Cement example: stepwise selection

```
model4 <- step(model3, scope=~.+x2+x3,steps=1)

## Start:  AIC=28.74
## y ~ x4 + x1
##
##        Df Sum of Sq     RSS    AIC
## + x2    1     26.79   47.97 24.974
## + x3    1     23.93   50.84 25.728
## <none>                74.76 28.742
## - x1    1    809.10  883.87 58.852
## - x4    1   1190.92 1265.69 63.519
##
## Step:  AIC=24.97
## y ~ x4 + x1 + x2
```

Cement example: stepwise selection

```
step(model4, scope=~.+x3)

## Start:  AIC=24.97
## y ~ x4 + x1 + x2
##
```

```
##        Df Sum of Sq    RSS    AIC
## <none>               47.97 24.974
## - x4    1      9.93  57.90 25.420
## + x3    1      0.11  47.86 26.944
## - x2    1     26.79  74.76 28.742
## - x1    1    820.91 868.88 60.629
##
## Call:
## lm(formula = y ~ x4 + x1 + x2, data = heat)
##
## Coefficients:
## (Intercept)           x4           x1           x2
##     71.6483      -0.2365       1.4519       0.4161
```

Cement example: stepwise selection

```
model2 <- step(fullmodel, scope=~., steps=1)

## Start:  AIC=26.94
## y ~ x1 + x2 + x3 + x4
##
##        Df Sum of Sq    RSS    AIC
## - x3    1    0.1091 47.973 24.974
## - x4    1    0.2470 48.111 25.011
## - x2    1    2.9725 50.836 25.728
## <none>               47.864 26.944
## - x1    1   25.9509 73.815 30.576
##
## Step:  AIC=24.97
## y ~ x1 + x2 + x4
```

Cement example: stepwise selection

```
step(model2, scope=~.+x3)

## Start:  AIC=24.97
## y ~ x1 + x2 + x4
##
##        Df Sum of Sq    RSS    AIC
## <none>               47.97 24.974
## - x4    1      9.93  57.90 25.420
## + x3    1      0.11  47.86 26.944
## - x2    1     26.79  74.76 28.742
## - x1    1    820.91 868.88 60.629
##
## Call:
## lm(formula = y ~ x1 + x2 + x4, data = heat)
##
## Coefficients:
## (Intercept)           x1           x2           x4
##     71.6483       1.4519       0.4161      -0.2365
```

7.8 t-tests - not in MM

t tests

We can also use a t test for a partial test of one parameter. That is, to test $H_0 : \beta_i = 0$ against $H_1 : \beta_i \neq 0$ in the presence of all the other parameters.

Recall our confidence interval for β_i:

$$b_i \pm t_{\alpha/2} s \sqrt{c_{ii}},$$

where c_{ii} is the (i,i)th entry of $(X^T X)^{-1}$, and we use a t distribution with $n-p$ degrees of freedom.

If this confidence interval includes 0, we do not reject H_0; otherwise, we can reject it.

t tests

In other words, we use the t statistic (with $n-p$ degrees of freedom)

$$\frac{b_i}{s\sqrt{c_{ii}}}.$$

Let us compare this with our partial F test. The statistic we use for this is

$$\frac{R(\beta_i|\beta_0, \beta_1, \ldots, \beta_{i-1}, \beta_{i+1}, \ldots, \beta_k)}{SS_{Res}/(n-p)}.$$

The denominator is of course s^2.

t tests

We saw previously that the numerator is

$$R(\beta_i|\beta_0, \beta_1, \ldots, \beta_{i-1}, \beta_{i+1}, \ldots, \beta_k) = \hat{\boldsymbol{\gamma}}_1{}^T A_{11}^{-1} \hat{\boldsymbol{\gamma}}_1$$

where $\hat{\boldsymbol{\gamma}}_1 = b_i$, and A_{11} is the top left element of $(X^T X)^{-1}$ after the columns have been re-arranged so that the ith column comes first.

In other words, $A_{11} = c_{ii}$ and

$$\begin{aligned} R(\beta_i|\beta_0, \beta_1, \ldots, \beta_{i-1}, \beta_{i+1}, \ldots, \beta_k) &= b_i (c_{ii})^{-1} b_i = \frac{b_i^2}{c_{ii}} \\ \frac{R(\beta_i|\beta_0, \beta_1, \ldots, \beta_{i-1}, \beta_{i+1}, \ldots, \beta_k)}{s^2} &= \frac{b_i^2}{c_{ii} s^2}. \end{aligned}$$

This is exactly the square of the t statistic!

t tests

This is actually not too surprising. The t distribution can be expressed as a normal variable divided by the square root of a χ^2 variable.

Therefore when we square it, we get the square of a normal variable divided by a χ^2 variable. But the square of a normal variable is a χ^2 variable with 1 d.f.

Therefore the square of a t variable with n d.f. is an F variable with 1 and n d.f.

This means that the t test and the F test are (nearly) identical; the t test is actually slightly more useful, because it also gives an indication of the sign of the parameter.

7.9 Example: t-tests chemicals - not in MM

t tests

Example. In the previous section, we modelled the amount of a chemical which dissolves in water, when held at a certain temperature. We found that the 95% confidence interval for β_1 was

$$0.31 \pm 2.78 \times 0.86\sqrt{0.00057} = [0.25, 0.36].$$

A t test would use the statistic

$$\frac{b_1}{s\sqrt{c_{11}}} = \frac{0.31}{0.86\sqrt{0.00057}} = 14.89$$

using a t distribution with $n - p = 6 - 2 = 4$ degrees of freedom.

This rejects the hypothesis $\beta_1 = 0$ at the 0.05 level (critical value 2.78). We can also say that β_1 is almost certainly positive.

t tests

On the other hand, if we use an F test:

```
(Rb <- t(y)%*%X%*%b)

##         [,1]
## [1,] 663.771

(Rb0 <- t(y)%*%X[,1]%*%solve(t(X[,1])%*%X[,1],t(X[,1])%*%y))

##          [,1]
## [1,] 498.6817

(Rb1_b0 <- Rb - Rb0)

##          [,1]
## [1,] 165.0893

(Fstat <- Rb1_b0/s^2)

##          [,1]
## [1,] 221.6672
```

t tests

```
pf(Fstat,1,df,lower=F)

##                [,1]
## [1,] 0.0001185219

sqrt(Fstat)

##           [,1]
## [1,] 14.88849

pt(sqrt(Fstat),df,lower=F)*2

##                [,1]
## [1,] 0.0001185219
```

t tests

The critical value of the F distribution with 1 and 4 degrees of freedom is $7.71 = 2.77^2$. So we can again reject the null hypothesis of $\beta_1 = 0$.

Variation	SS	d.f.	MS	F
Regression				
Full	663.77	2		
Reduced	498.68	1		
β_1 in presence of β_0	165.09	1	165.09	221.7
Residual	2.98	4	0.74	
Total	666.75	6		

7.10 Shrinkage - Not in MM

Shrinkage

Not all selection procedures employ sequential addition and/or deletion of variables. Some go for a more holistic approach.

A common approach is to try and 'shrink' all fitted parameters toward 0, so that irrelevant variables have little or no effect on the model.

Some of the fitted parameters might actually become 0, and the associated variables can then be removed.

Shrinkage

For example, *ridge regression* uses a penalized least squares approach. Here we minimise the residual sum of squares, but include a term which penalises the size of the parameters. We choose $\mathbf{b}$ to minimise

$$\sum_{i=1}^{n} e_i^2 + \lambda \sum_{j=0}^{k} b_j^2.$$

The λ term controls the amount of 'shrinkage' of the parameters. The penalized least squares estimators can be calculated to be

$$\mathbf{b} = (X^T X + \lambda I)^{-1} X^T \mathbf{y}.$$

This approach will never shrink parameters to 0.

Shrinkage

Another approach is the LASSO (Least Absolute Shrinkage and Selection Operator), which minimises

$$\sum_{i=1}^{n} e_i^2 + \lambda \sum_{j=0}^{k} |\mathbf{b}_j|.$$

The LASSO actually shrinks small parameters to 0, and can be used for variable selection by removing those variables.

Choosing an appropriate shrinking parameter λ is quite involved. A common method is *cross-validation*, which estimates the predictive power of the model by removing parts of the dataset and using them as test sets.