Introduction to Statistical Learning

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Module 4 The Full Rank Linear Model

Contents

1 Introduction

1.1 Recall linear models matrix formulation - MM3.1

Linear models and Random vectors

In Module 3 we extended the traditional concepts of expectation, variance, etc. to random vectors.

Now let's remind ourselves what a linear model is so that we can apply these concepts:

- We have n subjects, labelled 1 to n;
- Responses (y variable) denoted $y_1, y_2, \ldots, y_n$;
- Explanatory variables $x_1, \ldots, x_k$, with measured values for subject i denoted $x_{i1}, x_{i2}, \ldots, x_{ik}$.

Linear models

The linear model is

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \ldots + \beta_k x_{ik} + \varepsilon_i$$

for all $i = 1, 2, \ldots, n$, or

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & x_{12} & \dots & x_{1k} \\ 1 & x_{21} & x_{22} & \dots & x_{2k} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_{n1} & x_{n2} & \dots & x_{nk} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \vdots \\ \beta_k \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

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

Linear models

Under the terminology we have developed, $\mathbf{y}$ and $\boldsymbol{\varepsilon}$ are random vectors. A common assumption is that $\boldsymbol{\varepsilon}$ is multivariate normal with mean $\mathbf{0}$ and variance $\sigma^2 I$.

X and $\boldsymbol{\beta}$ are NOT random vectors. Although it is common for X to be a measurement, we assume that there is no uncertainty/error in these measurements. In practice, there is often also uncertainty in X, but then our model is conditional on the observed X and we do treat X as constants.

In Bayesian inference, $\boldsymbol{\beta}$ is also a random vector and inference conditions on both $\mathbf{y}$ and X, but this will be deferred to the second half of MAST90104.

1.2 Full rank - MM3.2

Pulling rank

We say the *model* has full rank when the design matrix X has full rank, i.e. $r(X) = k + 1$. This small condition is of crucial importance in the analysis of the model.

For this Module, we assume that X is of full rank.

This means that $X^T X$ is invertible, i.e. $(X^T X)^{-1}$ exists.

1.3 Example house prices - MM3.1

The full rank model

Example. We want to analyse the selling price of a house (y). We think that this depends on two variables, its age (x_1) and the house area (x_2). Our linear model is

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

We sample 5 random houses and obtain the data:

Price ($\times$ \$10k)	Age (years)	Area ($\times 100m^2$)
50	1	1
40	5	1
52	5	2
47	10	2
65	20	3

The full rank model

The model generates the 5 linear equations

$$\begin{aligned} 50 &= \beta_0 + 1\beta_1 + 1\beta_2 + \varepsilon_1 \\ 40 &= \beta_0 + 5\beta_1 + 1\beta_2 + \varepsilon_2 \\ 52 &= \beta_0 + 5\beta_1 + 2\beta_2 + \varepsilon_3 \\ 47 &= \beta_0 + 10\beta_1 + 2\beta_2 + \varepsilon_4 \\ 65 &= \beta_0 + 20\beta_1 + 3\beta_2 + \varepsilon_5 \end{aligned}$$

The full rank model

The matrix form of the model is $\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\varepsilon}$, where

$$\mathbf{y} = \begin{bmatrix} 50 \\ 40 \\ 52 \\ 47 \\ 65 \end{bmatrix}, \quad X = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 5 & 1 \\ 1 & 5 & 2 \\ 1 & 10 & 2 \\ 1 & 20 & 3 \end{bmatrix}, \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}, \quad \boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \end{bmatrix}.$$

Direct calculation will show that X is of full rank (to see this, look at the constant first column, the variable second column and the second and third rows of the X matrix). This is an example of *multiple regression.*

1.4 Example simple linear regression - MM3.1

The full rank model

Example. Simple linear regression can be cast in the framework of a linear model, where the response variable y depends on only one variable x:

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i.$$

For n responses, this gives the linear equations

$$\begin{aligned} y_1 &= \beta_0 + \beta_1 x_1 + \varepsilon_1 \\ y_2 &= \beta_0 + \beta_1 x_2 + \varepsilon_2 \\ &\vdots \\ y_n &= \beta_0 + \beta_1 x_n + \varepsilon_n \end{aligned}$$

The full rank model

In the matrix formulation, we have

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \quad X = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \\ 1 & x_n \end{bmatrix}, \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}, \quad \boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}.$$

X has full rank provided the x_i are not all the same.

We will show later how the linear model framework can be used to derive the well-known regression formulas for the parameters β_0 and β_1.

2 Parameters

2.1 Model assumptions, fitted values and residuals - MM3.2

Model assumptions

The first thing we do with the linear model is to estimate the parameters $\beta_0, \beta_1, \ldots, \beta_k$. We do this using the *method of least squares*.

Firstly, we assume that the error vector $\boldsymbol{\varepsilon}$ has mean $\mathbf{0}$ and variance $\sigma^2 I$; in other words, that the model is unbiased and the errors are uncorrelated with each other.

We do NOT necessarily assume that the errors are *independent* of each other. Nor do we assume they are normal (at first).

Model assumptions

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

The error term is the only random term in the model, so

$$E[\mathbf{y}] = X\boldsymbol{\beta}$$

and

$$\text{Var } \mathbf{y} = \sigma^2 I.$$

The expected value of each response is a linear function of the parameters (hence the term "linear model").

Fitted values and residuals

Suppose that $b_0, b_1, \ldots, b_k$ are estimates of the parameters $\beta_0, \beta_1, \ldots . \beta_k$.

Then we can estimate the expected value of y_i by

$$\widehat{E[y_i]} = b_0 + b_1 x_{i1} + \ldots + b_k x_{ik},$$

called the *fitted* values $\widehat{\mathbf{y}}$.

The ith *residual* is defined to be the difference between the observed value and the estimated value:

$$e_i = y_i - \widehat{E[y_i]}.$$

2.2 Least squares estimates - MM3.2

Parameter estimation using least squares

If our estimates are good, the residuals should be very close to the errors:

$$\begin{aligned} \boldsymbol{\varepsilon}_i &= y_i - E[y_i] \;=\; y_i - \widehat{E[y_i]} + \widehat{E[y_i]} - E[y_i] \\ &= e_i + \widehat{E[y_i]} - E[y_i]. \end{aligned}$$

We choose our estimates to minimise the residuals; specifically, we minimise the sum of the squares of the residuals. This is *least squares estimation* of the parameters.

(We could also try to minimise e.g. the sum of the absolute values of the residuals, but this is much harder because the absolute value is not differentiable.)

Parameter estimation using least squares

Define the vectors of estimated parameters and residuals:

$$\mathbf{b} = \begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ b_k \end{bmatrix}, \quad \mathbf{e} = \begin{bmatrix} e_0 \\ e_1 \\ \vdots \\ e_n \end{bmatrix}.$$

Then we have

$$\mathbf{y} = X\mathbf{b} + \mathbf{e}$$

so

$$\sum_{i=1}^{n} e_i^2 = \mathbf{e}^T\mathbf{e} = (\mathbf{y} - X\mathbf{b})^T(\mathbf{y} - X\mathbf{b}).$$

Parameter estimation using least squares

We choose $\mathbf{b}$ to minimise

$$\begin{aligned} \mathbf{e}^T\mathbf{e} &= (\mathbf{y} - X\mathbf{b})^T(\mathbf{y} - X\mathbf{b}) \\ &= \mathbf{y}^T\mathbf{y} - \mathbf{y}^T X\mathbf{b} - \mathbf{b}^T X^T\mathbf{y} + \mathbf{b}^T X^T X\mathbf{b} \\ &= \mathbf{y}^T\mathbf{y} - 2\mathbf{y}^T X\mathbf{b} + \mathbf{b}^T X^T X\mathbf{b} \\ &= \mathbf{y}^T\mathbf{y} - 2(X^T\mathbf{y})^T\mathbf{b} + \mathbf{b}^T(X^T X)\mathbf{b}, \end{aligned}$$

the third equality is because the scalar $\mathbf{y}^T X\mathbf{b}$ is symmetric and thus $\mathbf{y}^T X\mathbf{b} = (\mathbf{y}^T X\mathbf{b})^T = \mathbf{b}^T X^T\mathbf{y}$.

That is, we need

$$\frac{\partial \mathbf{e}^T\mathbf{e}}{\partial \mathbf{b}} = \mathbf{0}.$$

Parameter estimation using least squares

Since our measurements $\mathbf{y}$ do not depend on our parameter estimates $\mathbf{b}$, we get

$$\begin{aligned} \frac{\partial}{\partial \mathbf{b}}\mathbf{y}^T\mathbf{y} &= \mathbf{0} \\ \frac{\partial}{\partial \mathbf{b}}(-2(X^T\mathbf{y})^T\mathbf{b}) &= -2X^T\mathbf{y} \\ \frac{\partial}{\partial \mathbf{b}}(\mathbf{b}^T(X^T X)\mathbf{b}) &= (X^T X)\mathbf{b} + (X^T X)^T\mathbf{b}. \end{aligned}$$

Thus we need

$$-2X^T\mathbf{y} + 2(X^T X)\mathbf{b} = \mathbf{0}.$$

Parameter estimation using least squares

Rearranging gives the *normal equations*:

$$X^T X\mathbf{b} = X^T\mathbf{y}.$$

Because X is of full rank, $X^T X$ has an inverse. Therefore we can solve for $\mathbf{b}$ to find the least squares estimator

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

Parameter estimation using least squares

Theorem 4.1. *Let $\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\varepsilon}$ where X is a $n \times (k+1)$ matrix of full rank, $\boldsymbol{\beta}$ is a $(k+1) \times 1$ vector of parameters, and $\boldsymbol{\varepsilon}$ is a $n \times 1$ random vector with mean $\mathbf{0}$. Then the least squares estimator for $\boldsymbol{\beta}$ is*

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

2.3 Least squares - house price example - MM3.2

Parameter estimation using least squares

Example. We return to the house price example. Our data are the house prices (response) and the house age and area (design):

$$\mathbf{y} = \begin{bmatrix} 50 \\ 40 \\ 52 \\ 47 \\ 65 \end{bmatrix}, \quad X = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 5 & 1 \\ 1 & 5 & 2 \\ 1 & 10 & 2 \\ 1 & 20 & 3 \end{bmatrix}$$

Parameter estimation using least squares

```
y <- c(50,40,52,47,65)
(X <- matrix(c(rep(1,5),1,5,5,10,20,1,1,2,2,3),5,3))
```

```
##      [,1] [,2] [,3]
## [1,]    1    1    1
## [2,]    1    5    1
## [3,]    1    5    2
## [4,]    1   10    2
## [5,]    1   20    3
```

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

```
##             [,1]
## [1,] 33.0626151
## [2,] -0.1896869
## [3,] 10.7182320
```

Parameter estimation using least squares

Matrix calculations give

$$X^TX = \begin{bmatrix} 5 & 41 & 9 \\ 41 & 551 & 96 \\ 9 & 96 & 19 \end{bmatrix}, \quad X^T\mathbf{y} = \begin{bmatrix} 254 \\ 2280 \\ 483 \end{bmatrix}.$$

Parameter estimation using least squares

We can then find the inverse of X^TX to be

$$(X^TX)^{-1} = \begin{bmatrix} 2.31 & 0.16 & -1.88 \\ 0.16 & 0.03 & -0.2 \\ -1.88 & -0.2 & 1.98 \end{bmatrix}.$$

This gives the least squares estimators as

$$\begin{aligned} \mathbf{b} &= (X^TX)^{-1}X^T\mathbf{y} = \begin{bmatrix} 2.31 & 0.16 & -1.88 \\ 0.16 & 0.03 & -0.2 \\ -1.88 & -0.2 & 1.98 \end{bmatrix} \begin{bmatrix} 254 \\ 2280 \\ 483 \end{bmatrix} \\ &= \begin{bmatrix} 33.06 \\ -0.19 \\ 10.72 \end{bmatrix}. \end{aligned}$$

Parameter estimation using least squares

Therefore our fitted model is

$$y_i = 33.06 - 0.19x_{i1} + 10.72x_{i2} + \varepsilon_i.$$

Note that we often drop the index i when writing down the model:

$$\begin{aligned} y &= 33.06 - 0.19x_1 + 10.72x_2 + \varepsilon \\ \text{price} &= 33.06 - 0.19\,\text{age} + 10.72\,\text{area} + \varepsilon \end{aligned}$$

2.4 Least squares - simple linear regression example - MM3.2

Simple linear regression

Example. Recall that the simple linear regression model can be written as a linear model with two parameters

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i,$$

which gives

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \quad X = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}.$$

Simple linear regression

Then

$$X^TX = \begin{bmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_n \end{bmatrix} \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}$$
$$= \begin{bmatrix} n & \sum_i x_i \\ \sum_i x_i & \sum_i x_i^2 \end{bmatrix} \text{ and}$$

$$X^T\mathbf{y} = \begin{bmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_n \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$
$$= \begin{bmatrix} \sum_i y_i \\ \sum_i x_i y_i \end{bmatrix}.$$

Simple linear regression

We have

$$(X^TX)^{-1} = \frac{1}{n\sum_i x_i^2 - \left(\sum_i x_i\right)^2} \begin{bmatrix} \sum_i x_i^2 & -\sum_i x_i \\ -\sum_i x_i & n \end{bmatrix}.$$

Therefore the least squares estimator for $\boldsymbol{\beta}$ is

$$\begin{aligned} \mathbf{b} &= (X^TX)^{-1}X^T\mathbf{y} \\ &= \frac{1}{n\sum_i x_i^2 - \left(\sum_i x_i\right)^2} \begin{bmatrix} \sum_i x_i^2 & -\sum_i x_i \\ -\sum_i x_i & n \end{bmatrix} \begin{bmatrix} \sum_i y_i \\ \sum_i x_i y_i \end{bmatrix} \\ &= \frac{1}{n\sum_i x_i^2 - \left(\sum_i x_i\right)^2} \begin{bmatrix} \sum_i x_i^2 \sum_i y_i - \sum_i x_i \sum_i x_i y_i \\ n\sum_i x_i y_i - \sum_i x_i \sum_i y_i \end{bmatrix}. \end{aligned}$$

Simple linear regression

The estimator for the slope of the regression line is

$$\begin{aligned} b_1 &= \frac{n\sum_i x_i y_i - \sum_i x_i \sum_i y_i}{n\sum_i x_i^2 - \left(\sum_i x_i\right)^2} \\ &= \frac{\frac{1}{n}\sum_i x_i y_i - \frac{1}{n^2}\sum_i x_i \sum_i y_i}{\frac{1}{n}\sum_i x_i^2 - \frac{1}{n^2}\left(\sum_i x_i\right)^2} \\ &= \frac{\overline{xy} - \bar{x}\bar{y}}{\overline{x^2} - \bar{x}^2}, \end{aligned}$$

which is the standard linear regression formulae that we obtained in MAST90105.

Simple linear regression

The estimator for the intercept of the regression line is

$$b_0 = \frac{\sum_i x_i^2 \sum_i y_i - \sum_i x_i \sum_i x_i y_i}{n\sum_i x_i^2 - \left(\sum_i x_i\right)^2}$$

which may not look so familiar.

Usually the estimator is given as $\bar{y} - b_1\bar{x}$, but it is quite simple to show that they are the same.

2.5 Key orthogonality properties - Not in MM

Residuals orthogonal to the column space of X

The fitted values, $X\mathbf{b}$, are in the column space of X.

The general element of the column space is $X\mathbf{a}$ where $\mathbf{a}$ is a $(k+1) \times 1$ vector. The elements of the column space of X and the residuals $\mathbf{y} - X\mathbf{b}$ are *orthogonal* to each other.

This is because the residuals can be written as $(I-H)\mathbf{y}$ where $H = X(X^TX)^{-1}X^T$ and

$$(X\mathbf{a})^T(I-H)\mathbf{y} = \mathbf{a}^T(X^T(I-H))\mathbf{y}$$

and

$$X^T(I-H) = X^T - X^T(X(X^TX)^{-1}X^T) = 0.$$

Consequences incl. Proof of Theorem 4.1

Since the fitted values are in the column space, the fitted values and residuals are orthogonal and thus *uncorrelated*.

We found the least squares estimators by differentiation but can now show that they minimise the sum of squares of errors between $\mathbf{y}$ and the fitted values with any parameters $\boldsymbol{\beta}$ since then

$$\begin{aligned}
&(\mathbf{y} - X\boldsymbol{\beta})^T(\mathbf{y} - X\boldsymbol{\beta}) = (\mathbf{y} - X\mathbf{b} + X\mathbf{b} - X\boldsymbol{\beta})^T(\mathbf{y} - X\mathbf{b} + X\mathbf{b} - X\boldsymbol{\beta}) \\
&= (\mathbf{y} - X\mathbf{b})^T(\mathbf{y} - X\mathbf{b}) + (X\mathbf{b} - X\boldsymbol{\beta})^T(X\mathbf{b} - X\boldsymbol{\beta}) \\
&\geq (\mathbf{y} - X\mathbf{b})^T(\mathbf{y} - X\mathbf{b}), \qquad (1)
\end{aligned}$$

because orthogonality makes the cross-product terms, $(\mathbf{y}-X\mathbf{b})^T(X\mathbf{b}-X\boldsymbol{\beta})$ & $(X\mathbf{b}-X\boldsymbol{\beta})^T(\mathbf{y}-X\mathbf{b})$, zero and $(X\mathbf{b}-X\boldsymbol{\beta})^T(X\mathbf{b}-X\boldsymbol{\beta})$ is the sum of squares of the vector $X(\mathbf{b} - \boldsymbol{\beta})$.

Geometric Interpretation of Least Squares

The proof of the formula for the least squares estimator is important because it shows the geometry of the fitted values and the residuals. The fitted values are $X\mathbf{b}$, also $\hat{y}$ or $X\hat{\boldsymbol{\beta}}$ or $H\mathbf{y}, H = X(X^TX)^{-1}X^T$, are the orthogonal projection of the response variable $\mathbf{y}$ onto the column space of X. By choosing $\boldsymbol{\beta} = \mathbf{b}$, the squared distance $(\mathbf{y} - X\boldsymbol{\beta})^T(\mathbf{y} - X\boldsymbol{\beta})$ between $\mathbf{y}$ and the vectors in the column space, $X\boldsymbol{\beta}$, is minimised. The residuals, $\mathbf{y} - X\mathbf{b}$, or $\hat{\boldsymbol{\varepsilon}}$ or $\mathbf{y} - X\hat{\boldsymbol{\beta}}$ or $(I - H)\mathbf{y}$, are orthogonal to the column space. Figure 1 shows this graphically for $n = 3$ and X with 2 column vectors X_1, X_2.

2.6 How good is the least squares estimator? - MM 3.2

How good is the least squares estimator?

What makes an estimator "good"?

Two desirable properties for an estimator are that it is unbiased (on target) and of minimal variance.

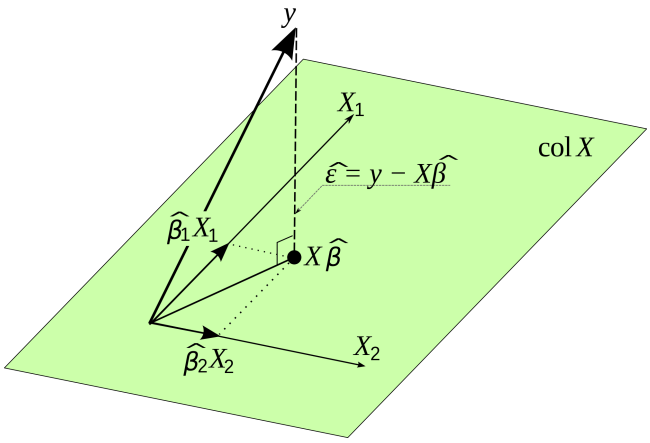


Figure 1: Projecting $\mathbf{y}$ onto the column space of X - source: Wikipedia

Theorem 4.2. *In the general linear model, the least squares estimator* $\mathbf{b} = (X^T X)^{-1} X^T \mathbf{y}$ *is an unbiased estimator for* $\boldsymbol{\beta}$*. In other words,*

$$E[\mathbf{b}] = \boldsymbol{\beta}.$$

Furthermore,

$$Var\ \mathbf{b} = (X^T X)^{-1} \sigma^2.$$

How good is the least squares estimator?

Proof. Our random vector theory is now essential!

$$\begin{aligned} E[\mathbf{b}] &= E[(X^T X)^{-1} X^T \mathbf{y}] \\ &= (X^T X)^{-1} X^T E[\mathbf{y}] \\ &= (X^T X)^{-1} X^T (X\boldsymbol{\beta}) \\ &= \boldsymbol{\beta}. \end{aligned}$$

$$\begin{aligned} \text{Var } \mathbf{b} &= \text{Var } (X^T X)^{-1} X^T \mathbf{y} \\ &= (X^T X)^{-1} X^T \sigma^2 I \left((X^T X)^{-1} X^T\right)^T \\ &= (X^T X)^{-1} X^T X((X^T X)^T)^{-1} \sigma^2 \\ &= (X^T X)^{-1} \sigma^2. \end{aligned}$$

2.7 Gauss-Markov Theorem- MM 3.2

But really, how good is the least squares estimator?

Let's look at *linear* estimators. These are estimators which take the form $L\mathbf{y}$, where L is a matrix of constants. The least squares estimator is a linear estimator with $L = (X^T X)^{-1} X^T$.

Now suppose we have a model with some parameters $\boldsymbol{\beta}$ and linear estimators $\mathbf{b}$ for these parameters.

Definition 4.3. If $E[\mathbf{b}] = \boldsymbol{\beta}$ and the variances of $b_0, b_1, \ldots, b_k$ are minimised over all linear estimators, then $\mathbf{b}$ is called a *best linear unbiased estimator* of $\boldsymbol{\beta}$ (or BLUE).

I'm feeling BLUE

Theorem 4.4 (Gauss-Markov Theorem)**.** *In the full rank general linear model $\mathbf{y} = X\boldsymbol{\beta}+\boldsymbol{\varepsilon}$, the least squares estimator $\mathbf{b} = (X^TX)^{-1}X^T\mathbf{y}$ is the unique BLUE for $\boldsymbol{\beta}$. Let $\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\varepsilon}$ where X is a $n \times (k+1)$ matrix of full rank, $\boldsymbol{\beta}$ is a $(k+1) \times 1$ vector of unknown parameters, and $\boldsymbol{\varepsilon}$ is a $n \times 1$ random vector with mean $\mathbf{0}$ and variance $\sigma^2 I$. Then the least squares estimator $\mathbf{b}$ is the unique best linear unbiased estimator for $\boldsymbol{\beta}$.*

Proof.

Suppose we have another unbiased linear estimator for $\boldsymbol{\beta}$, called $\mathbf{b}^*$. We can write this as

$$\mathbf{b}^* = [(X^TX)^{-1}X^T + B]\mathbf{y}$$

where B is a $(k+1) \times n$ matrix.

I'm feeling BLUE

We then take expectations of both sides:

$$\begin{aligned} E[\mathbf{b}^*] &= [(X^TX)^{-1}X^T + B]E[\mathbf{y}] \\ &= [(X^TX)^{-1}X^T + B]X\boldsymbol{\beta} \\ &= [I + BX]\boldsymbol{\beta}. \end{aligned}$$

Since $\mathbf{b}^*$ is an unbiased estimator for $\boldsymbol{\beta}$, we know that $E[\mathbf{b}^*] = \boldsymbol{\beta}$. Therefore $[I + BX]\boldsymbol{\beta} = \boldsymbol{\beta}$ for all $\boldsymbol{\beta}$. This is the same as $BX\boldsymbol{\beta} = 0$ for all $\boldsymbol{\beta}$. Since $BX\boldsymbol{\beta}$ is a linear combination of the columns of BX, choosing $\boldsymbol{\beta}$ to be each of the standard basis vectors, we see that each column of $BX =$ is 0, giving $BX = 0$.

I'm feeling BLUE

Now look at the variance of $\mathbf{b}^*$:

$$\begin{aligned} \text{Var } \mathbf{b}^* &= \text{Var } [(X^TX)^{-1}X^T + B]\mathbf{y} \\ &= [(X^TX)^{-1}X^T + B]\sigma^2 I[(X^TX)^{-1}X^T + B]^T \\ &= \sigma^2[(X^TX)^{-1}X^T + B][X(X^TX)^{-1} + B^T] \\ &= \sigma^2[(X^TX)^{-1}X^TX(X^TX)^{-1} + (X^TX)^{-1}X^TB^T \\ &\qquad +BX(X^TX)^{-1} + BB^T]. \end{aligned}$$

I'm feeling BLUE

Now $BX = 0$ and $X^TB^T = (BX)^T = 0$, which gives

$$\begin{aligned} \text{Var } \mathbf{b}^* &= \sigma^2[(X^TX)^{-1} + BB^T] \\ &= (X^TX)^{-1}\sigma^2 + BB^T\sigma^2 \\ &= \text{Var } \mathbf{b} + BB^T\sigma^2. \end{aligned}$$

Let's look at the variances of $b_0^*, b_1^*, \ldots, b_k^*$ (ignoring the covariances for now.)

The variances are given by

$$\text{Var } b_i^* = [\text{Var } \mathbf{b}^*]_{ii} = \text{Var } b_i + \sigma^2 \sum_{j=1}^{n} B_{ij}^2.$$

I'm feeling BLUE

Each term in the sum is non-negative, so the variance of b_i^* can never go below Var b_i.

Moreover, the minimum is obtained if and only if $B_{ij} = 0$ for all i, j, in which case $B = 0$ and $\mathbf{b}^* = \mathbf{b}$.

2.8 Example Gauss-Markov and house prices- MM 3.2

Gauss-Markov Theorem

Example. Consider the house price example. The variance of the least squares estimators is given by

$$(X^T X)^{-1}\sigma^2 = \begin{bmatrix} 2.31 & 0.16 & -1.88 \\ 0.16 & 0.03 & -0.2 \\ -1.88 & -0.2 & 1.98 \end{bmatrix} \sigma^2.$$

This means that there is no (unbiased) linear estimator of β_0 which has a smaller variance than $2.31\sigma^2$, and no linear estimator of β_1 which has a smaller variance than $0.03\sigma^2$, etc.

This is true even though we don't know what σ^2 is!

2.9 Estimating linear functions of the parameters- MM 3.2

Estimation of linear functions

What if we want to estimate something other than the parameters?

We are often interested in estimating some linear function of the parameters, $\mathbf{t}^T\boldsymbol{\beta}$, where $\mathbf{t}$ is a $(k+1) \times 1$ vector of constants. How can we estimate these?

It turns out that obvious answer is correct: we simply take the identical linear function of the least squares estimator.

Estimation of linear functions

Theorem 4.5. *Take the full rank general linear model* $\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\varepsilon}$ *and let* $\mathbf{t}$ *be a* $(k+1) \times 1$ *vector of constants. Then the best linear unbiased estimator for* $\mathbf{t}^T\boldsymbol{\beta}$ *is* $\mathbf{t}^T\mathbf{b}$*, where* $\mathbf{b}$ *is the least squares estimator for* $\boldsymbol{\beta}$*.*

The proof of this theorem is very similar to that of the Gauss-Markov theorem.

2.10 Example estimating mean house price- MM 3.2

Estimation of linear functions

The most common use of this theorem is to estimate the (mean) value of the response variable given certain values of the predictor variables.

Example. Consider the house price example. The model is

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \varepsilon,$$

where y is the house price, x_1 is its age, and x_2 is its area.

Suppose we are given a specific house with age x_1^* and area x_2^*, and we wish to estimate what price it will fetch.

Estimation of linear functions

We want to estimate the linear function of the parameters

$$E[y] = \beta_0 + \beta_1 x_1^* + \beta_2 x_2^* = \mathbf{t}^T \boldsymbol{\beta}$$

where $\mathbf{t} = \begin{bmatrix} 1 & x_1^* & x_2^* \end{bmatrix}^T$.

Therefore an unbiased estimator for the house price is

$$\mathbf{t}^T \mathbf{b} = \begin{bmatrix} 1 & x_1^* & x_2^* \end{bmatrix} \mathbf{b} = b_0 + b_1 x_1^* + b_2 x_2^*$$

where $\mathbf{b}$ is the least squares estimator for $\boldsymbol{\beta}$.

Estimation of linear functions

For example, suppose we have a house which is 15 years old and has an area of 250 m^2.

```
b
```

```
##             [,1]
## [1,] 33.0626151
## [2,] -0.1896869
## [3,] 10.7182320
```

```
c(1,15,2.5)%*%b
```

```
##          [,1]
## [1,] 57.01289
```

We expect the house to sell for $570,000 (3 significant figures).

3 Variance estimation

3.1 Variance Estimation- MM 3.3

Variance estimation

Remember that we assume that the errors $\boldsymbol{\varepsilon}$ (and thus $\mathbf{y}$) have covariance matrix $\sigma^2 I$. It is also important to estimate the common variance σ^2.

Everything varies - including our estimates of parameters from different datasets or a response based on parameter estimates. The variance of the responses, σ^2, is a vital component of this variability.

And this variance estimation will be essential for confidence intervals for the true values of the parameters.

Variance estimation

How should we estimate σ^2?

σ^2 can be written as

$$\sigma^2 = E\left[\frac{(\mathbf{y} - X\boldsymbol{\beta})^T(\mathbf{y} - X\boldsymbol{\beta})}{n}\right]$$

and so a reasonable estimator for the variance might be

$$\hat{\sigma^2} = \frac{(\mathbf{y} - X\mathbf{b})^T(\mathbf{y} - X\mathbf{b})}{n}.$$

It turns out that this is slightly biased; we need to make a small adjustment.

Variance estimation

Theorem 4.6. *The* sample variance

$$s^2 = \frac{(\mathbf{y} - X\mathbf{b})^T(\mathbf{y} - X\mathbf{b})}{n - (k+1)}$$

is an unbiased estimator for σ^2.

Define the sum of squares of the residuals

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

and denote the number of parameters by $p = k + 1$. Then we can write

$$s^2 = \frac{SS_{Res}}{n - p}.$$

Variance estimation

Proof. Recall that in Section 2.5, the hat matrix $H = X(X^TX)^{-1}X^T$ was introduced. The matrix H is called the hat matrix because the fitted values $\widehat{E(\mathbf{y})}$ are $H\mathbf{y}$ and the residuals are $(I_n - H)\mathbf{y}$. In the first workshop we showed $I_n - H$ is idempotent and it is symmetric. Hence

$$\begin{aligned}
E[s^2] &= \frac{1}{n-(k+1)}E[(\mathbf{y} - X\mathbf{b})^T(\mathbf{y} - X\mathbf{b})] \\
&= \frac{1}{n-(k+1)}E[(I_n - H)\mathbf{y})^T(I_n - H)\mathbf{y}] \\
&= \frac{1}{n-(k+1)}E[\mathbf{y}^T(I_n - H)(I_n - H)\mathbf{y}] \\
&= \frac{1}{n-(k+1)}E[\mathbf{y}^T(I_n - H)\mathbf{y}].
\end{aligned}$$

Variance estimation

The expectation of this quadratic form is given in Theorem 3.2:

$$E[\mathbf{y}^T A\mathbf{y}] = tr(AV) + \boldsymbol{\mu}^T A\boldsymbol{\mu}.$$

Here

$$\begin{aligned} \boldsymbol{\mu}^T A\boldsymbol{\mu} &= (X\boldsymbol{\beta})^T(I_n - H)(X\boldsymbol{\beta}) \\ &= \boldsymbol{\beta}^T X^T X\boldsymbol{\beta} - \boldsymbol{\beta}^T X^T X(X^T X)^{-1} X^T X\boldsymbol{\beta} \\ &= 0 \end{aligned}$$

Variance estimation

and, using the fact that $tr(AB) = tr(BA)$

$$\begin{aligned} tr(AV) &= tr((I_n - H)\sigma^2 I_n) \\ &= \sigma^2(tr(I_n) - tr(H)) \\ &= \sigma^2(n - tr((X^T X)^{-1} X^T X)) \\ &= \sigma^2(n - tr(I_{k+1})) \\ &= \sigma^2(n - (k+1)) \end{aligned}$$

which gives the result.

3.2 Example - variance estimation for house prices- MM 3.3

Variance estimation

Example. Back to the house price example.

```
b
```

```
##             [,1]
## [1,] 33.0626151
## [2,] -0.1896869
## [3,] 10.7182320
```

```
(e <- y - X%*%b)
```

```
##           [,1]
## [1,]  6.408840
## [2,] -2.832413
## [3,] -1.550645
## [4,] -5.602210
## [5,]  3.576427
```

Variance estimation

```
(SSRes <- sum(e^2))
```

```
## [1] 95.67587
```

```
(s2 <- SSRes/(5-3))
```

```
## [1] 47.83794
```

The sample variance is $s^2 = 47.84$.

3.3 Example - paint cracking- MM 3.3

Variance estimation

Example. A study is designed to predict the extent of the cracking of latex paint in field conditions, based on the extent of the cracking in 'accelerated' tests in the laboratory. We generate the data

Test cracking (x)	Actual cracking (y)
2.0	1.9
3.0	2.7
4.0	4.2
5.0	4.8
6.0	4.8
7.0	5.1

Variance estimation

```
y <- c(1.9,2.7,4.2,4.8,4.8,5.1)
(X <- matrix(c(rep(1,6),2:7),6,2))

##      [,1] [,2]
## [1,]    1    2
## [2,]    1    3
## [3,]    1    4
## [4,]    1    5
## [5,]    1    6
## [6,]    1    7

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

##           [,1]
## [1,] 0.9723810
## [2,] 0.6542857
```

Variance estimation

```
(e <- y - X%*%b)

##             [,1]
## [1,] -0.38095238
## [2,] -0.23523810
## [3,]  0.61047619
## [4,]  0.55619048
## [5,] -0.09809524
## [6,] -0.45238095

(s2 <- sum(e^2)/(6-2))

## [1] 0.2741905
```

Thus we estimate the common variance of the response variables to be ≈ 0.27.

4 0 Intercept

Regression through the origin

So far we have always considered the linear model to include a parameter β_0, which is associated with a column of 1's in the design matrix X. This parameter is called the *intercept*.

Sometimes it is reasonable to assume (from prior knowledge of the data) that no intercept is needed, in which case we can remove it.

Surprisingly little changes. The model becomes

$$y = \beta_1 x_1 + \beta_2 x_2 + \ldots + \beta_k x_k + \varepsilon,$$

but to analyse it, the design matrix loses the first column, the parameter vector loses the first entry, and everything proceeds as before.

Regression through the origin

The least squares estimator is still

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

and the variance estimator is still

$$s^2 = \frac{SS_{Res}}{n-p}.$$

However, we now have $p = k$ instead of $k + 1$.

5 Diagnostics

5.1 Standardised Residuals - Not in MM

Diagnostics: standardised residuals

To assess the fit of our linear models, and to observe possible departures from our model assumptions, we use various diagnostic tools.

Firstly we can look at our residuals. If there is an extremely large residual, or a pattern in the residuals, we might question our assumptions.

However we must be careful. The variance of the errors is (assumed to be) $\sigma^2 I$, but the variance of the *residuals* is not $\sigma^2 I$. In general, the variance of a particular residual depends on how 'far from the centre' the design variables are: the farther away, the lower is the variance of the residual.

Diagnostics: standardised residuals

Recall that $H = X(X^T X)^{-1} X^T$ is the *hat* matrix, because it converts $\mathbf{y}$ (the observed responses) into $\hat{\mathbf{y}}$ (the estimated responses).

To make this precise, we calculate the variance of the residuals

$$\mathbf{e} = \mathbf{y} - X\mathbf{b} = (I - H)\mathbf{y}.$$

$$\begin{aligned} \text{Var } \mathbf{e} &= \text{Var } (I-H)\mathbf{y} \\ &= (I-H)\sigma^2 I(I-H)^T \\ &= \sigma^2(I-H) \end{aligned}$$

since $I-H$ is symmetric and idempotent.

Diagnostics: standardised residuals

To make residuals comparable, we would like to divide them by their standard deviations. However we don't know σ^2, and so use our estimator s^2 instead.

This creates the *standardised residuals*

$$z_i = \frac{e_i}{\sqrt{s^2(1-H_{ii})}}.$$

The standardised residuals have (approximately) equal variance and thus can be compared reasonably.

5.2 Leverage and Cook's Distance - Not in MM

Diagnostics: leverage and Cook's distance

Consider what happens when we calculate the fitted values by $\hat{\mathbf{y}} = X\mathbf{b} = H\mathbf{y}$.

H tends to have its largest values on the diagonal (the best estimate for the mean of y_i is generally close to y_i).

The size of H_{ii} reflects how much $\hat{y}_i$ is based on y_i, as opposed to the other y_j. If H_{ii} is particularly large, then y_i has a large effect on the fit.

We thus define the *leverage* of point i as H_{ii}. For points of high leverage (that is, Hii close to 1), the variance of the residual is close to 0. It is as if there is a magnet on the response variable for a point of high leverage attracting the least squares line to it. There are two exercises in Lab 4 studying this (Workshop question 2 and Lab question 2).

Diagnostics: leverage and Cook's distance

Points with large leverage may have an unusually large effect on the estimated parameters. We must be extra careful with these points to avoid a bad fit.

By itself, a large leverage is not necessarily detrimental. However, if this is combined with a large residual, then the corresponding point may distort the fit.

To check this, we calculate the *Cook's distance* of each point. This measures the change in the estimated parameters $\mathbf{b}$ if we remove the point.

Diagnostics: leverage and Cook's distance

The definition of Cook's distance is

$$D_i = \frac{(\mathbf{b}_{(-i)} - \mathbf{b})^T X^T X(\mathbf{b}_{(-i)} - \mathbf{b})}{(k+1)s^2} = \frac{1}{k+1} z_i^2 \left(\frac{H_{ii}}{1-H_{ii}}\right)$$

where $\mathbf{b}_{(-i)}$ is the estimated parameters if point i is removed. The second equality for Cook's distance makes it easy to compute but its demonstration relies on results on the inverse of the hat matrix when point i is removed.

We can see that this is large if both the standardised residual and the leverage is large — this is where we must be careful.

There is no particular 'must watch' value for Cook's distance, but it is generally considered large if it is greater than 1, and small if it is less than a guideline value of $\frac{4}{n-k-1}$. Those above the value 0.5 are worthy of attention.

5.3 Example: Clover Leaves - Not in MM

R example: clover leaves

We estimate the area of a clover leaf (`area`) based on the midrib length (`midrib`) and estimated area by template (`estim`).

It turns out that (based on knowledge of the geometry and data) it is more appropriate to take the logarithms of the data. The data is available on the LMS.

```
clover <- read.csv("../data/clover.csv")
str(clover,vec.len=2)

## 'data.frame': 145 obs. of  3 variables:
##  $ midrib: num  5.5 6 7 7 7 ...
##  $ estim : num  2 1 1.58 1.58 1.26 ...
##  $ area  : num  1.33 0.75 0.8 1.05 1.47 ...

clover <- log(clover)
```

Command to plot data in pairs

Figure 2 shows plots of the data using the following command.

```
bound <- par("plt")
pairs(clover)
```

Our model is

$$\text{area} = \beta_0 + \beta_1 \text{midrib} + \beta_2 \text{estim} + \varepsilon.$$

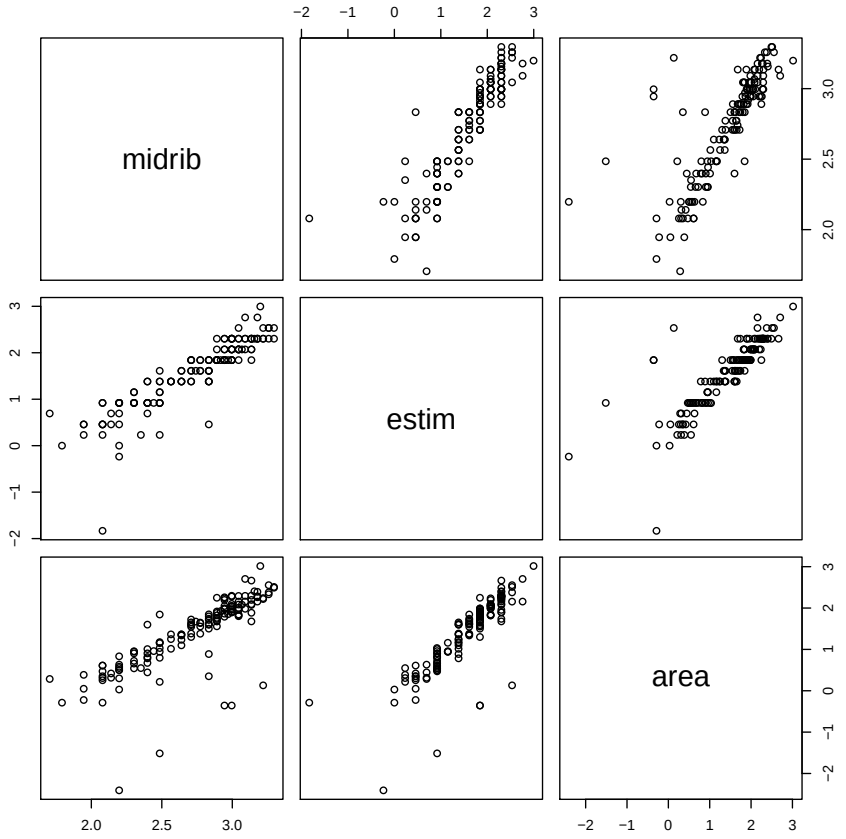
```
y <- clover$area
str(y)

##  num [1:145] 0.2852 -0.2877 -0.2231 0.0488 0.3853 ...

X <- matrix(c(rep(1,145),clover$midrib,clover$estim)
                  ,145,3)
X[1:3,]

##      [,1]     [,2]      [,3]
## [1,]    1 1.704748 0.6931472
## [2,]    1 1.791759 0.0000000
## [3,]    1 1.945910 0.4574248
```

Figure 2: Plots of the variables in pairs



```r
library(Matrix)
n <- dim(X)[1]
p <- dim(X)[2]

rankMatrix(X)[1]

## [1] 3
```

so this is a full rank model.

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

##             [,1]
## [1,] -1.1741275
## [2,]  0.5239692
## [3,]  0.7337812

e <- y - X %*% b
str(e,vec.len=3)

##  num [1:145, 1] 0.0575 -0.0524 -0.4043 -0.1323 ...
```

5.4 The R Command lm - Faraway 2.5

```r
model <- lm(area ~ midrib + estim,data=clover)
summary(model)

##
## Call:
## lm(formula = area ~ midrib + estim, data = clover)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -2.31730 -0.07022  0.08005  0.18787  1.14160
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  -1.1741     0.4604   -2.55   0.0118 *
## midrib        0.5240     0.2248    2.33   0.0212 *
## estim         0.7338     0.1157    6.34 2.87e-09 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.4659 on 142 degrees of freedom
## Multiple R-squared:  0.7078,Adjusted R-squared:  0.7036
## F-statistic:   172 on 2 and 142 DF,  p-value: < 2.2e-16
```

```r
model$coefficients

## (Intercept)      midrib       estim
##  -1.1741275   0.5239692   0.7337812

str(model$residuals, len.vec = 2, digits.d = 2)

##  Named num [1:145] 0.057 -0.052 -0.404 -0.132 0.37 ...
##  - attr(*, "names")= chr [1:145] "1" "2" "3" "4" ...
```

```
str(model$fitted.values, len.vec = 2, digits.d = 2)

##  Named num [1:145] 0.228 -0.235 0.181 0.181 0.015 ...
##  - attr(*, "names")= chr [1:145] "1" "2" "3" "4" ...
```

```
model$rank

## [1] 3

model$df.residual

## [1] 142
```

Point estimate of the log of the area of a leaf with midrib 10 and template area 10:

```
tt <- c(1,log(10),log(10))
tt %*% b

##          [,1]
## [1,] 1.72195
```

```
newclover <- list(midrib=log(10),estim=log(10))
predict(model,newclover)

##       1
## 1.72195
```

Variance estimation

```
(SSRes <- sum(e^2))

## [1] 30.82559

(s2 <- SSRes/(n-p))

## [1] 0.2170816

deviance(model)

## [1] 30.82559

deviance(model)/model$df.residual

## [1] 0.2170816
```

5.5 R Plots - Faraway Chapter 4

Diagnostic plots

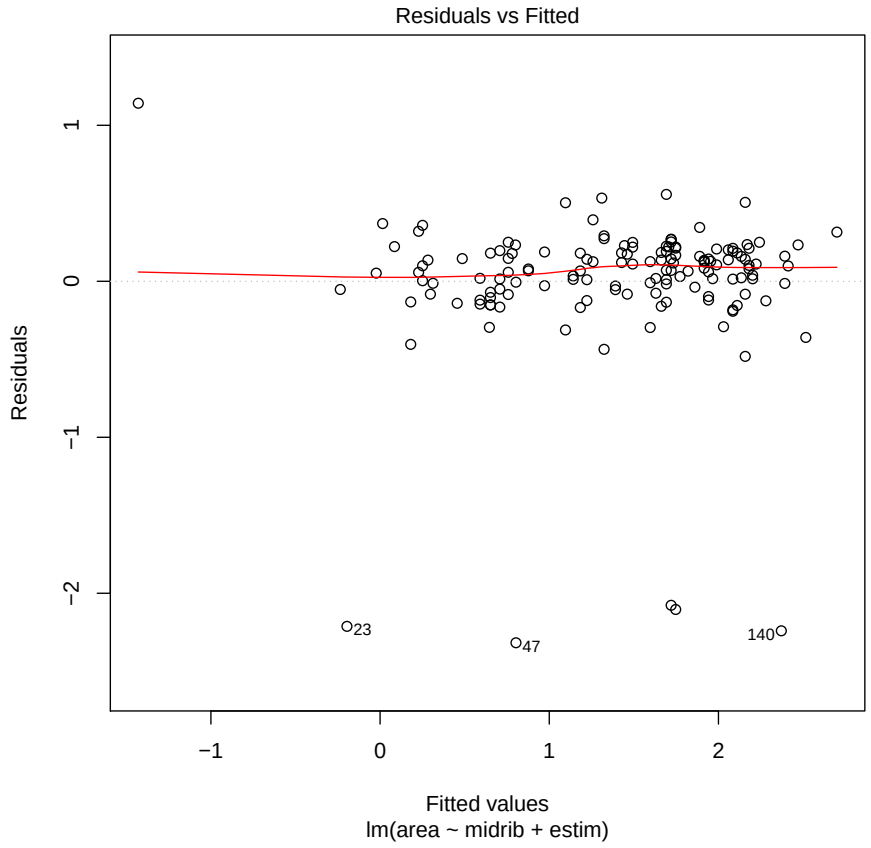


Figure 3: Plot of residuals versus fitted values

R (and in particular the `lm` command) produces many useful plots for checking the fit of the model and deviations from assumptions.

The first plot is residuals vs. fitted values. We look for:

- points with large residual (unequal variances);
- a trend in the residuals (bias);
- a pattern in the residuals (correlation).

The R command is

```
plot(model, which=1)
```

and the output is in Figure 3.

The second plot is a normal quantile-quantile plot of the standardised residuals.

More on this later.

We look for the residuals to be normally distributed. Although the normal distribution has not yet been assumed, assuming it will be central for confidence intervals and hypothesis tests. If the qqplot shows departures from normality, then we look for how the residulas deviate — for example:

- a small number of outliers;
- over- or under-estimation in the tails;
- skewness.

The R command is

```
plot(model, which=2)
```

and the output is in Figure 4.

The third plot is square roots of absolute values of standardised residuals against fitted values. It is quite similar to the first plot. We look for:

- points with high residual (unequal variance);
- a trend in the size of the residuals (heteroskedasticity).
- the nature of the trend if there is one.

The R command is

```
plot(model, which=3)
```

and the output is in Figure 5.

The fourth plot gives standardised residuals vs. leverage. We look for:

- points with high residual (unequal variance);
- points with high leverage (potentially dangerous);
- points with high Cook's distance (poor fit);
- a pattern in the residuals (correlation).

The R command is

```
plot(model, which=5)
```

and the output is in Figure 6.

5.6 What if? - Faraway Ch 4

What if we remove the offending points?

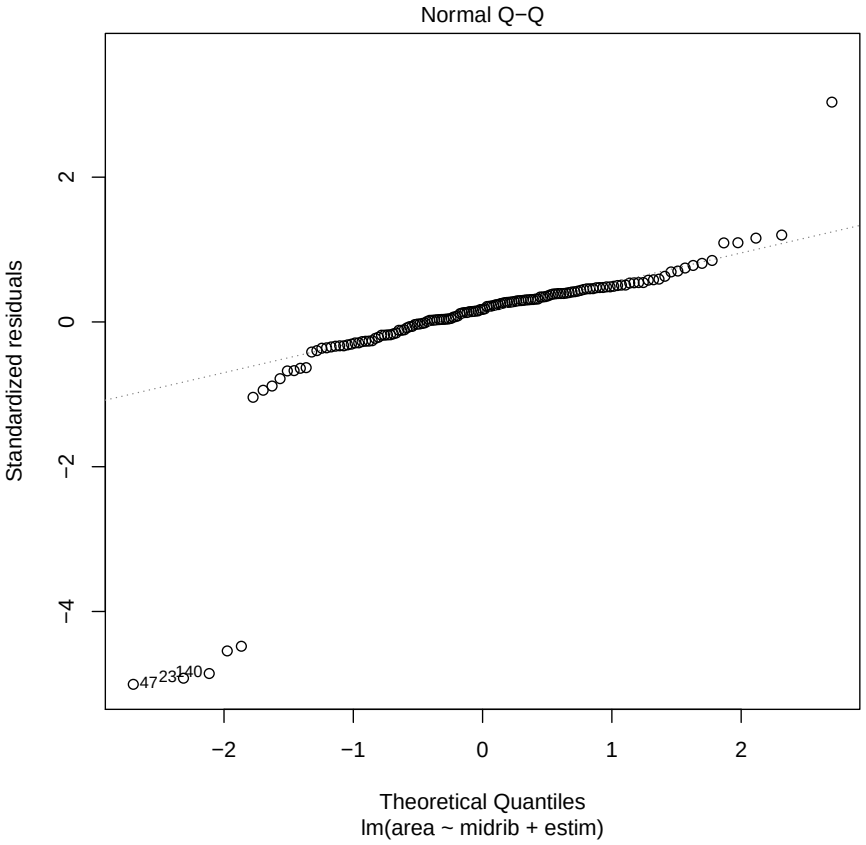


Figure 4: Normal qq plot for residuals

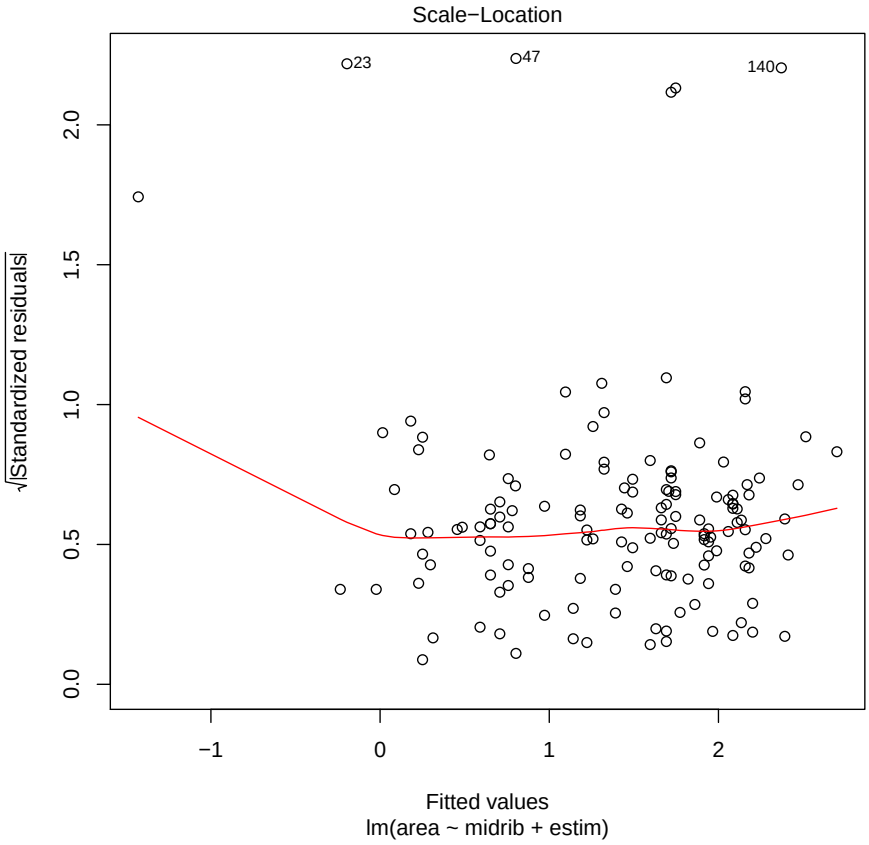


Figure 5: Standardised residuals vs. fitted values

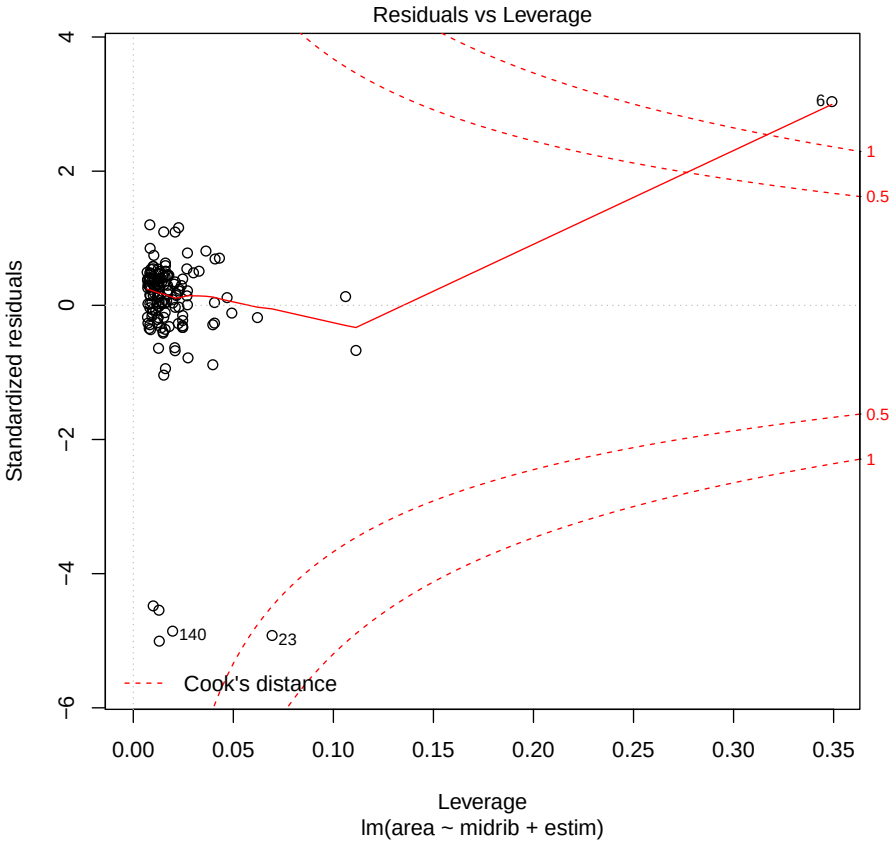


Figure 6: Standardised residuals vs. leverage

```r
goodclover <- clover[-c(6,23,47,97,111,140),]
model2 <- lm(area ~ midrib + estim, data=goodclover)
summary(model2)
```

```
##
## Call:
## lm(formula = area ~ midrib + estim, data = goodclover)
##
## 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
```

What if we didn't take logarithms?

```r
expclover <- exp(clover)
model3 <- lm(area ~ midrib + estim, data=expclover)
summary(model3)
```

```
##
## Call:
## lm(formula = area ~ midrib + estim, data = expclover)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -10.0050  -0.3447   0.1299   0.6378   5.2594
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) -1.06609    0.49919  -2.136   0.0344 *
## midrib       0.15049    0.05265   2.858   0.0049 **
## estim        0.67054    0.08158   8.219 1.16e-13 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.599 on 142 degrees of freedom
## Multiple R-squared:  0.7953,Adjusted R-squared:  0.7924
## F-statistic: 275.8 on 2 and 142 DF,  p-value: < 2.2e-16
```

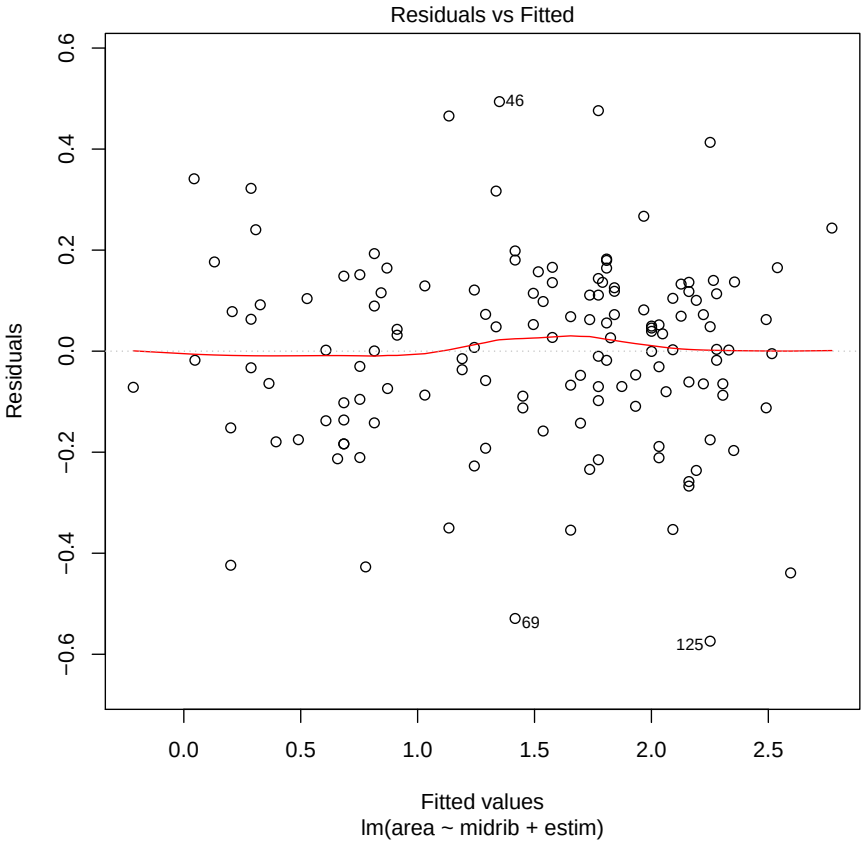


Figure 7: Plot of residuals versus fitted values with points removed

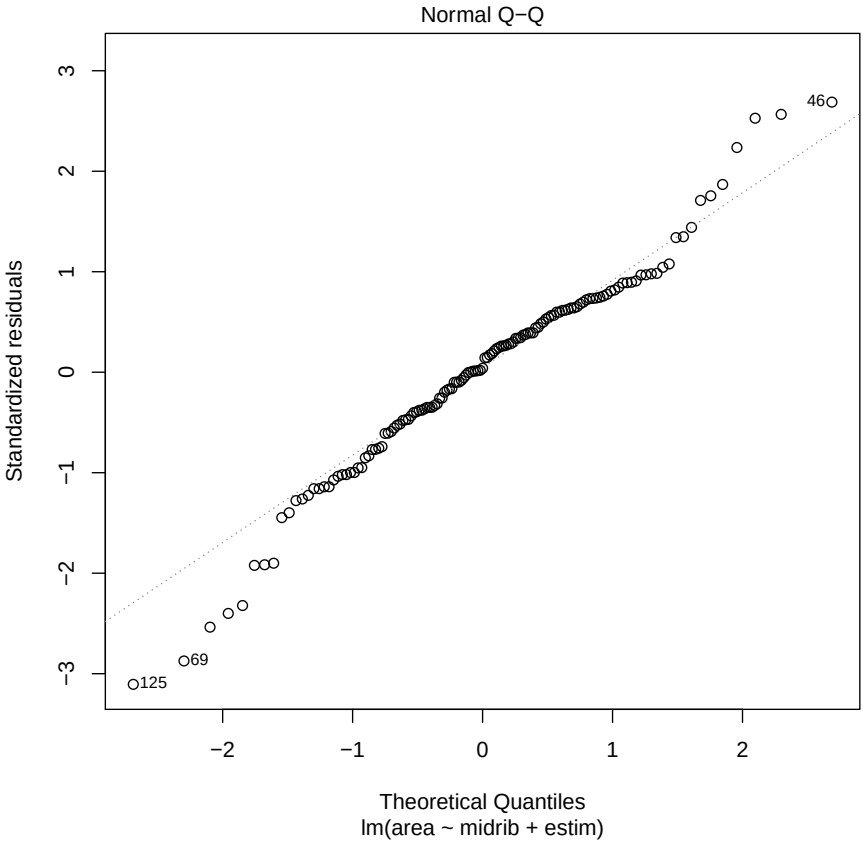


Figure 8: Normal qq plot for residuals with points removed

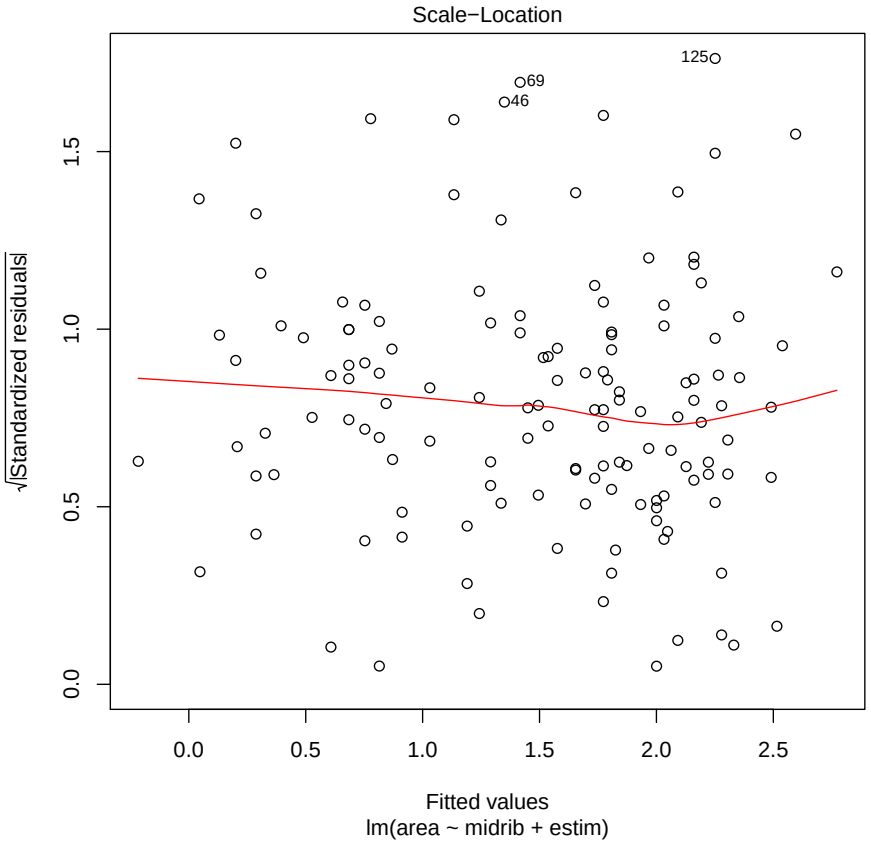


Figure 9: Standardised residuals vs. fitted values with points removed

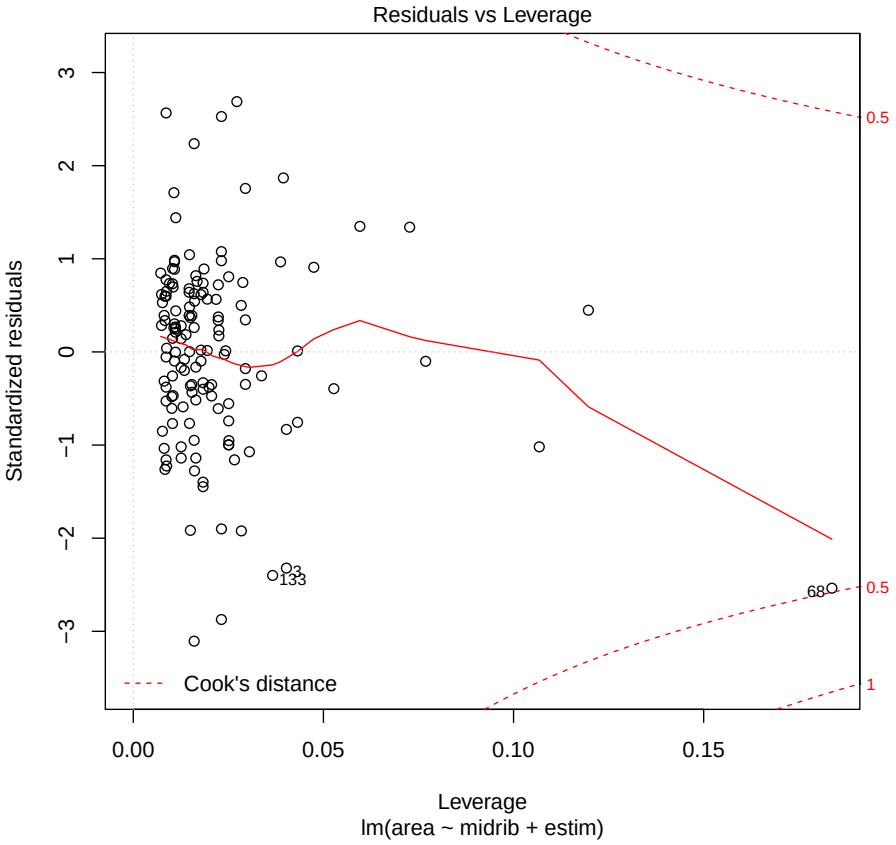


Figure 10: Standardised residuals vs. leverage with points removed

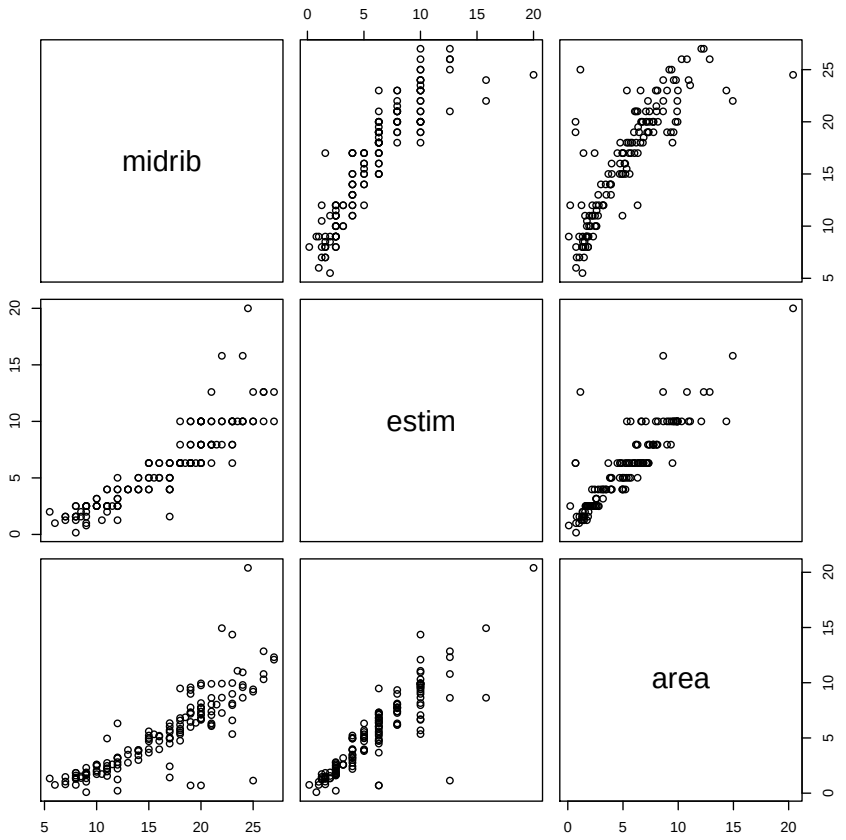


Figure 11: Scatterplots of the pairs of variables in clover with no logs

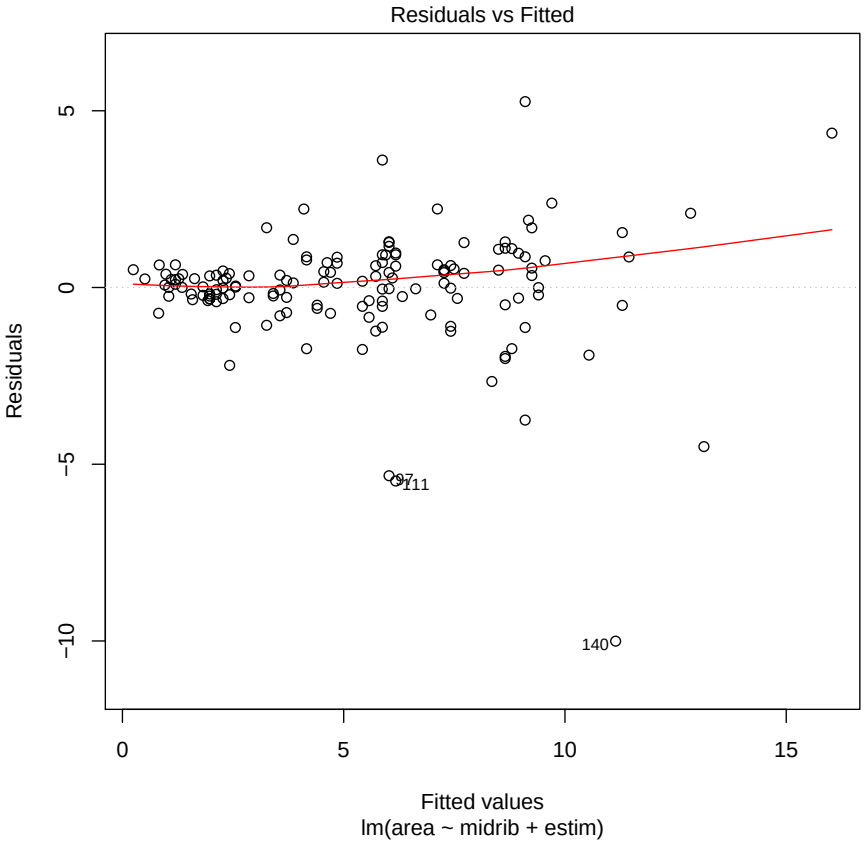


Figure 12: Plot of residuals versus fitted values with no logs

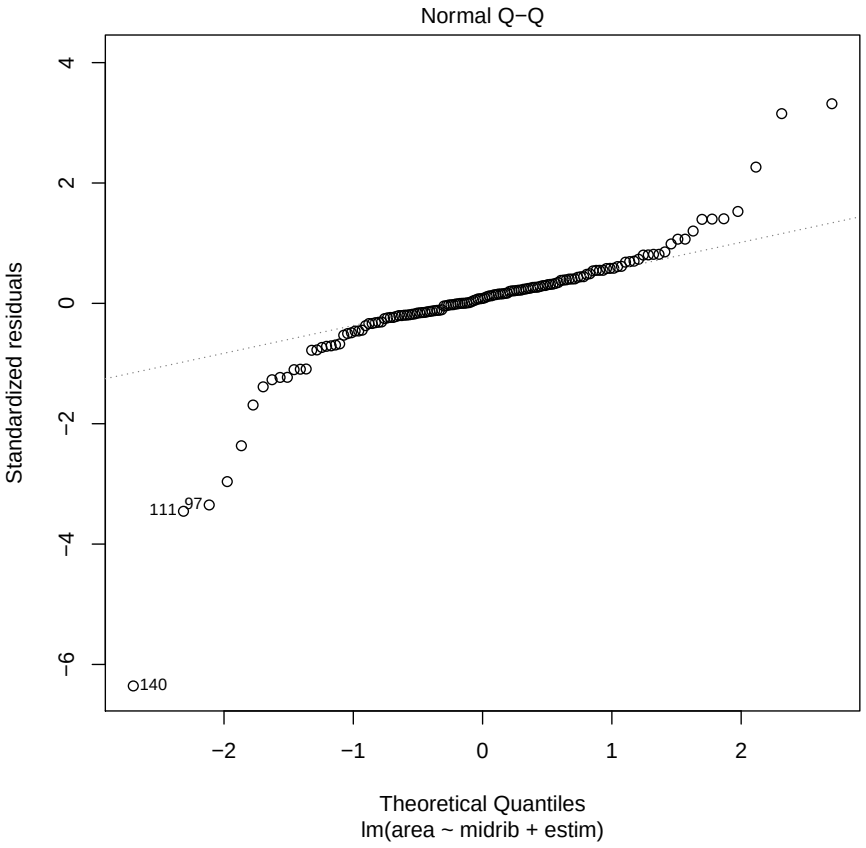


Figure 13: Normal qq plot for residuals with no logs

What if we eliminate the intercept term?

```
X3 <- matrix(c(goodclover$midrib, goodclover$estim),
             ncol=2)
X3[1:3,]

##          [,1]      [,2]
## [1,] 1.704748 0.6931472
## [2,] 1.791759 0.0000000
## [3,] 1.945910 0.4574248
```

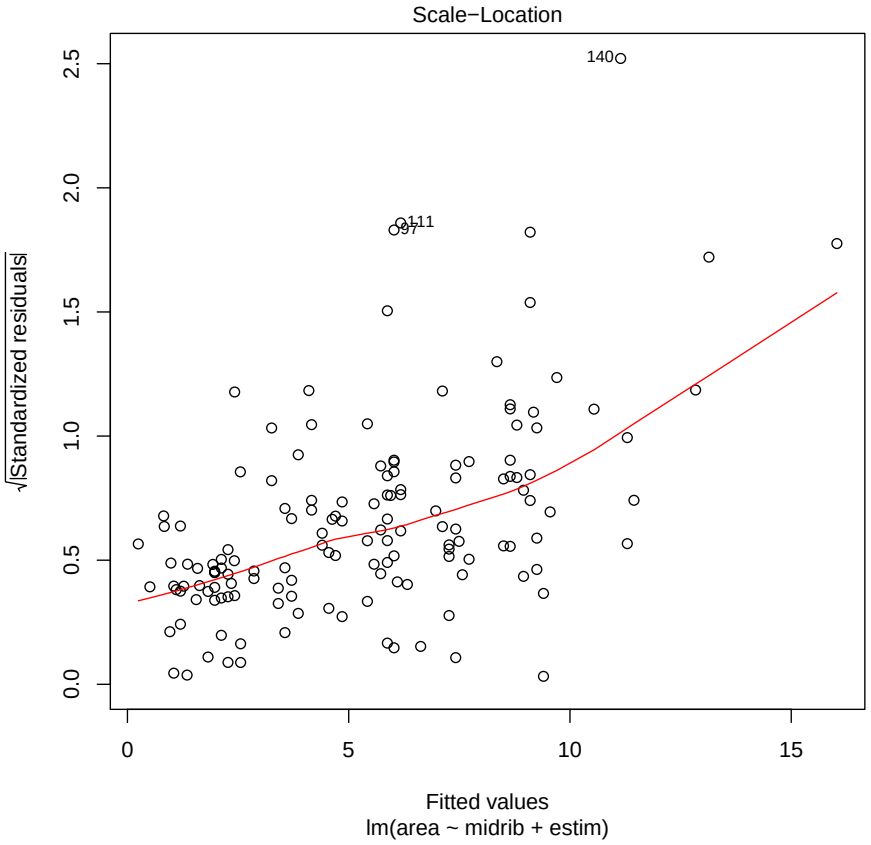


Figure 14: Standardised residuals vs. fitted values with no logs

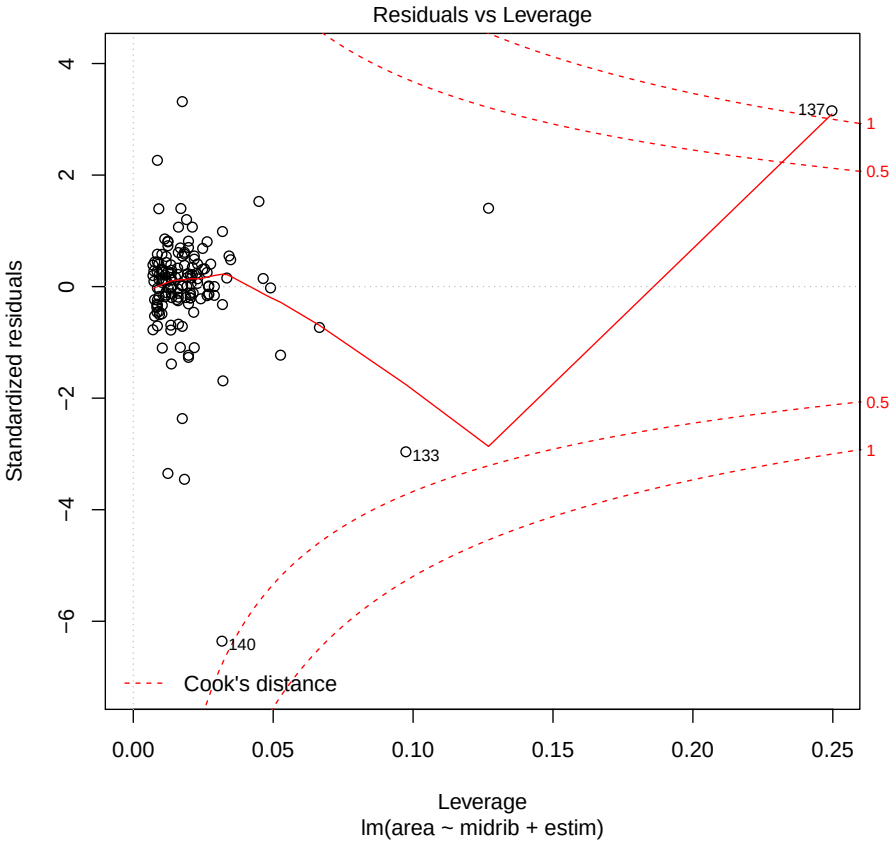


Figure 15: Standardised residuals vs. leverage with no logs

```
y3 <- goodclover$area
(b3 <- solve(t(X3) %*% X3, t(X3) %*% y3))

##              [,1]
## [1,] -0.04673437
## [2,]  1.02242842
```

What if we eliminate the intercept term?

```
model4 <- lm(area ~ 0 + midrib + estim, data = goodclover)
summary(model4)

##
## Call:
## lm(formula = area ~ 0 + midrib + estim, data = goodclover)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.59989 -0.14717  0.03691  0.12036  0.50081
##
## Coefficients:
##        Estimate Std. Error t value Pr(>|t|)
## midrib -0.04673    0.02440  -1.915   0.0576 .
## estim   1.02243    0.03887  26.302   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.2144 on 137 degrees of freedom
## Multiple R-squared:  0.9835,Adjusted R-squared:  0.9832
## F-statistic:  4080 on 2 and 137 DF,  p-value: < 2.2e-16
```

6 Least squares optimal for normal

6.1 MLE for β, σ- MM3.1

MLE assuming Normality

In maximum likelihood estimation (MLE) we choose parameter values to maximise the 'probability' of having observed the given data. We can apply this idea to estimate the parameters of the linear model.

MLEs are popular because they have good *asymptotic* properties: as the sample size goes to ∞ they are unbiased, normally distributed, and have minimum variance under certain conditions.

To find MLEs we need a distribution for the errors. We assume that $\mathbf{y}$ are $MVN(X\boldsymbol{\beta}, \sigma^2 I)$. In particular, this means that the errors are independent (not just uncorrelated).

Maximum likelihood estimation

Since the elements of $\mathbf{y}$ are independent, their joint density is given by

$$f(\mathbf{y}; \boldsymbol{\beta}, \sigma^2) = \frac{1}{(2\pi\sigma^2)}^{n/2} e^{-(\mathbf{y}-X\boldsymbol{\beta})^T(\mathbf{y}-X\boldsymbol{\beta})/(2\sigma^2)}.$$

Considered as a function of the parameters $\boldsymbol{\beta}$ and σ^2, this is called the likelihood, and denoted $L(\boldsymbol{\beta}, \sigma^2)$.

Maximum likelihood estimation

We maximise the likelihood with respect to $\boldsymbol{\beta}$ to generate maximum likelihood estimators for $\boldsymbol{\beta}$. In practice, it is usually easier to maximise the log-likelihood. Because ln is a monotonic function, the maximum is at the same point.

$$\begin{aligned}\ln L(\boldsymbol{\beta}, \sigma^2) = &-\frac{n}{2}\left(\ln(2\pi) + \ln(\sigma^2)\right) \\ &- \frac{1}{2\sigma^2}(\mathbf{y} - X\boldsymbol{\beta})^T(\mathbf{y} - X\boldsymbol{\beta}). \end{aligned} \tag{2}$$

Maximum likelihood estimation

Finding the values of $\boldsymbol{\beta}$ and σ that maximise the log likelihood in equation (2) is the same as removing the constant term and minimising the negative:

$$\begin{aligned}&\frac{n}{2}\ln(\sigma^2) + \frac{1}{2\sigma^2}(\mathbf{y} - X\boldsymbol{\beta})^T(\mathbf{y} - X\boldsymbol{\beta}) \\ &\geq \frac{n}{2}\ln(\sigma^2) + \frac{1}{2\sigma^2}(\mathbf{y} - X\mathbf{b})^T(\mathbf{y} - X\mathbf{b}) \end{aligned} \tag{3}$$

from our derivation of the least squares estimator at inequality (1).

The function $f(x) = a\ln(x) + b/x$ has minimum value at $x = b/a$ (exercise: prove this by differentating twice) and so the minimum value of the loglikelihood is achieved at $\boldsymbol{\beta} = \mathbf{b}$ and $\sigma^2 = (\mathbf{y} - X\mathbf{b})^T(\mathbf{y} - X\mathbf{b})/n$. We have proved:

Maximum likelihood estimation

Theorem 4.7. *In the full rank general linear model $\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\varepsilon}$, assume $\boldsymbol{\varepsilon} \sim MVN(\mathbf{0}, \sigma^2 I)$. Then the maximum likelihood estimator for $\boldsymbol{\beta}$ is also the least squares estimator:*

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

The (joint) maximum likelihood estimator of σ^2 is

$$\widehat{\sigma^2} = (\mathbf{y} - X\mathbf{b})^T(\mathbf{y} - X\mathbf{b})/n$$

Maximum likelihood estimation

The estimate of σ^2 is a biased estimator: the MLE is only asymptotically unbiased.

However, the sample variance

$$s^2 = \frac{SS_{Res}}{n-p} = \frac{n}{n-p}\widehat{\sigma^2}$$

has the same asymptotic properties as $\widehat{\sigma^2}$, but is unbiased for all n, making it the preferred estimator.

Sufficiency

We've seen that the least squares estimator is the best linear unbiased estimator for $\boldsymbol{\beta}$, and that if the errors are normally distributed, it is also the maximum likelihood estimator.

We can in fact go a step further: given the assumption of normality, the least squares estimators are *sufficient*. That is, they use all 'relevant' information about the parameters that is contained in the observed response variables.

The Fisher-Neyman Factorization theorem gives a formal characterisation of sufficient statistics.

Sufficiency

Theorem 4.8 (Fisher-Neyman Factorization Theorem)**.** *Let* $\mathbf{x}$ *be a random variable with parameters* $\boldsymbol{\theta}$*, and let* $\mathbf{x}_1, \ldots, \mathbf{x}_n$ *be a random sample drawn from this distribution, with joint density* $f(\mathbf{x}_1, \ldots, \mathbf{x}_n; \boldsymbol{\theta})$*. Then the statistic* $\mathbf{y} = u(\mathbf{x}_1, \ldots, \mathbf{x}_n)$ *is* sufficient *for* $\boldsymbol{\theta}$ *if and only if* f *can be expressed as*

$$f(\mathbf{x}_1, \ldots, \mathbf{x}_n; \boldsymbol{\theta}) = g(\mathbf{y}; \boldsymbol{\theta}) h(\mathbf{x}_1, \ldots, \mathbf{x}_n).$$

We must be able to factorise the density into one part which depends only on $\mathbf{y}$ and $\boldsymbol{\theta}$, and another part which depends only on the $\mathbf{x}_i$'s.

Example. Suppose we have an i.i.d. sample from a Poisson distribution with parameter λ. The density for a single one of these variables (x_1 say) is

$$f(x_1; \lambda) = \frac{e^{-\lambda} \lambda^{x_1}}{x_1!}$$

Because the samples are independent, the joint density is the product of all the individual densities.

$$\begin{aligned} f(x_1, x_2, \ldots, x_n; \lambda) &= \prod_{i=1}^{n} f(x_i; \lambda) \\ &= \prod_{i=1}^{n} \frac{e^{-\lambda} \lambda^{x_i}}{x_i!} \\ &= e^{-n\lambda} \lambda^{\sum x_i} \left(\prod_{i=1}^{n} x_i! \right)^{-1} \\ &= g\left(\sum x_i; \lambda \right) h(x_1, \ldots, x_n). \end{aligned}$$

It can now be seen that the statistic $\sum_{i=1}^{n} x_i$ is sufficient for λ.

Sufficiency

Theorem 4.9. *In the full rank general linear model* $\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\varepsilon}$*, assume* $\boldsymbol{\varepsilon} \sim MVN(\mathbf{0}, \sigma^2 I)$*. Then the estimators*

$$\mathbf{b} = (X^T X)^{-1} X^T \mathbf{y} \quad \text{and} \quad s^2 = \frac{SS_{Res}}{n - p}$$

are jointly sufficient for $\boldsymbol{\beta}$ *and* σ^2*.*

Optimality

Maximum likelihood theory tells us that asymptotically $\mathbf{b}$ and s^2 have minimum variance. In fact, this is also true for finite samples, as can be show by extending the arguments using the Cramer-Rao inequality used in MAST90105:

Theorem 4.10. *In the full rank general linear model* $\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\varepsilon}$*, assume* $\boldsymbol{\varepsilon} \sim MVN(\mathbf{0}, \sigma^2 I)$*. Then the estimators*

$$\mathbf{b} = (X^T X)^{-1} X^T \mathbf{y} \text{ and } s^2 = \frac{SS_{Res}}{n-p}$$

have the lowest variance among all unbiased estimators of $\boldsymbol{\beta}$ *and* σ^2*.*

This is a stronger condition than BLUE because it includes non-linear estimators. We call this UMVUE (uniformly minimum variance unbiased estimator).

Summary

The least squares estimators $\mathbf{b}$ have the following optimality properties if the error distribution has constant variance:

1. They are BLUE whatever is the error distribution
2. They are maximum likelihood esimators if the error distribution is normal
3. They have minimum variance amongst all unbiased estimators if the error distribution is nornal

If the error distribution is normal, the sample variance s^2 is the minimum variance unbiased estimator of σ^2.

7 Confidence Intervals

7.1 Interval estimation of the coefficients - MM3.6

Interval estimation

The least squares estimators give excellent *point* estimates for the parameters. But this only tells half the story.

To get an idea of how accurate these estimates are, we would like to find *interval* estimates.

We first need to know the distribution of our least squares estimators. This requires an assumption on the distribution of the errors.

We have assumed $\mathbf{y} \sim MVN(X\boldsymbol{\beta}, \sigma^2 I)$ to get optimal estimates, and will need to assume this also for interval estimation.

Interval estimation

Now $\mathbf{b}$ is a linear combinations of $\mathbf{y}$, so it also has a multivariate normal distributions.

Theorem 4.11. *In the full rank general linear model* $\mathbf{y} \sim MVN(X\mathbf{b}, \sigma^2 I)$,

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

has a multivariate normal distribution with mean $\boldsymbol{\beta}$ *and variance* $(X^T X)^{-1}\sigma^2$.

Interval estimation

What about the sample variance?

Theorem 4.12. *In the full rank general linear model* $\mathbf{y} \sim MVN(X\mathbf{b}, \sigma^2 I)$,

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

has a χ^2 *distribution with* $n - p$ *degrees of freedom.*

Interval estimation

Proof. We have shown earlier that the residual sum of squares can be expressed as the quadratic form

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

where $H = X(X^T X)^{-1} X^T$ and $I - H$ is symmetric, idempotent and has rank $n - p$ where p is the number of parameters.

By Corollary 3.7, $\frac{1}{\sigma^2}\mathbf{y}^T[I - X(X^T X)^{-1} X^T]\mathbf{y}$ has a noncentral χ^2 distribution, with $n - p$ d.f. and noncentrality parameter

$$\lambda = \frac{1}{2\sigma^2}\boldsymbol{\mu}^T[I - H]\boldsymbol{\mu}.$$

Interval estimation

But $\boldsymbol{\mu} = X\boldsymbol{\beta}$, so

$$\begin{aligned} \lambda &= \frac{1}{2\sigma^2}(X\boldsymbol{\beta})^T[I - X(X^T X)^{-1} X^T]X\boldsymbol{\beta} \\ &= \frac{1}{2\sigma^2}[\boldsymbol{\beta}^T X^T X\boldsymbol{\beta} - \boldsymbol{\beta}^T X^T X(X^T X)^{-1} X^T X\boldsymbol{\beta}] \\ &= 0. \end{aligned}$$

Thus $\frac{SS_{Res}}{\sigma^2}$ has a (central) χ^2 distribution with $n - p$ degrees of freedom.

Interval estimation

Theorem 4.13. *In the full rank general linear model* $\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\varepsilon}$, *assume* $\boldsymbol{\varepsilon} \sim MVN(\mathbf{0}, \sigma^2 I)$. *Then* $\mathbf{b}$ *and* s^2 *are independent.*

Proof. We use Theorem 3.13. We have

$$\mathbf{b} = (X^T X)^{-1} X^T \mathbf{y}, \quad \frac{SS_{Res}}{\sigma^2} = \mathbf{y}^T \frac{[I - X(X^T X)^{-1} X^T]}{\sigma^2} \mathbf{y}$$

and so

$$\begin{aligned} BVA &= (X^T X)^{-1} X^T \sigma^2 I \frac{[I - X(X^T X)^{-1} X^T]}{\sigma^2} \\ &= (X^T X)^{-1} X^T - (X^T X)^{-1} X^T X (X^T X)^{-1} X^T \\ &= 0. \end{aligned}$$

The t distribution

Recall from MAST90105:

Definition 4.14. Let Z be a standard normal random variable and let X^2_γ be an independent χ^2 random variable with γ degrees of freedom. Then

$$\frac{Z}{\sqrt{X^2_\gamma/\gamma}}$$

has a t distribution with γ degrees of freedom.

The density of the t distribution is

$$f(x) = \frac{\Gamma((\gamma+1)/2)}{\sqrt{\gamma\pi}\Gamma(\gamma/2)} \left(1 + \frac{x^2}{\gamma}\right)^{-(\gamma+1)/2}.$$

Tea distribution

t time

Instructions to use the definition to generate 100 t rv's and plot their histogram against the density. Output in 16.

```
Z <- rnorm(100)
X2 <- rchisq(100,4)
tvals <- Z/sqrt(X2/4)
hist(tvals,freq=FALSE)
```

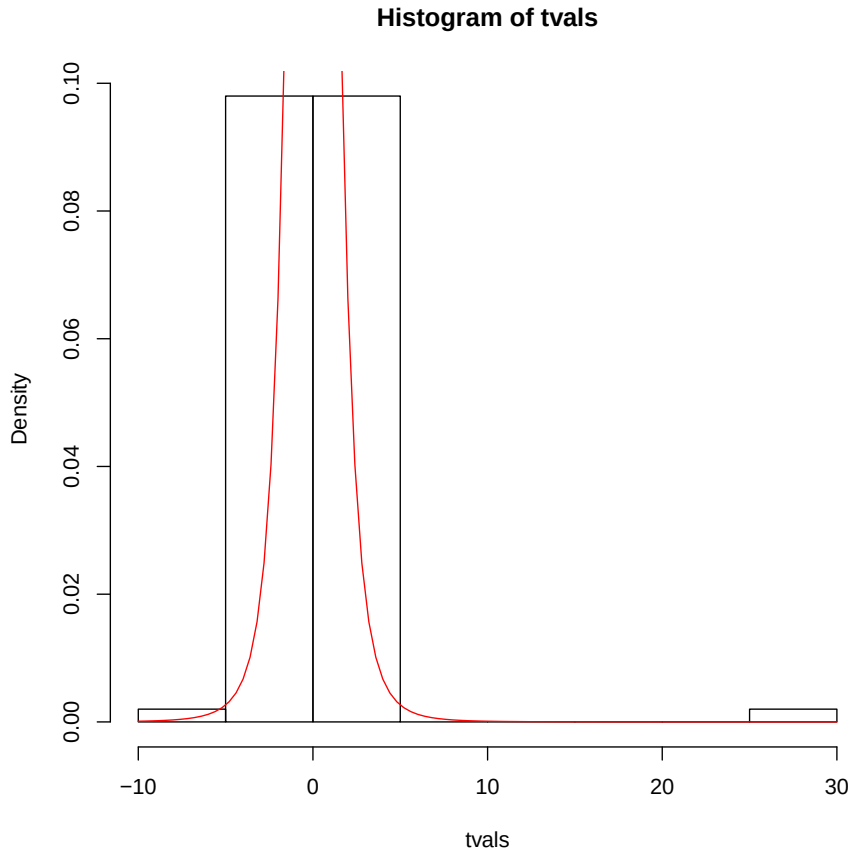


Figure 16: 100 random instances of the t definition with t density shown

```
curve(dt(x,4),add=TRUE,col='red')
```

Interval estimation

We can now create confidence intervals for the parameters. Firstly we will find a confidence interval for a single parameter, β_i.

Consider the covariance matrix of **b**:

$$(X^T X)^{-1}\sigma^2 = \begin{bmatrix} c_{00} & c_{01} & \cdots & c_{0k} \\ c_{10} & c_{11} & \cdots & c_{1k} \\ \vdots & & \ddots & \vdots \\ c_{k0} & c_{k1} & \cdots & c_{kk} \end{bmatrix} \sigma^2.$$

Interval estimation

The least squares estimator of β_i is b_i. The variance of b_i is the ith diagonal element of the covariance matrix, denoted $c_{ii}\sigma^2$.

Since b_i is normal, this means that

$$\frac{b_i - \beta_i}{\sigma\sqrt{c_{ii}}}$$

has a standard normal distribution.

Of course, we do not know what σ is...

Interval estimation

...but from the above theory,

$$\left(\frac{b_i - \beta_i}{\sigma\sqrt{c_{ii}}}\right) / \left(\sqrt{\frac{SS_{Res}/\sigma^2}{n-p}}\right)$$

has a t distribution with $n - p$ degrees of freedom.

Simplifying gives

$$\left(\frac{b_i - \beta_i}{\sigma\sqrt{c_{ii}}}\right) / \left(\sqrt{\frac{s^2}{\sigma^2}}\right) = \frac{b_i - \beta_i}{s\sqrt{c_{ii}}}.$$

Interval estimation

It is now easy to derive a $100(1-\alpha)\%$ confidence interval:

$$\begin{aligned} P[-t_{\alpha/2} \leq (b_i - \beta_i)/(s\sqrt{c_{ii}}) \leq t_{\alpha/2}] &= 1-\alpha \\ P[-t_{\alpha/2}s\sqrt{c_{ii}} \leq b_i - \beta_i \leq t_{\alpha/2}s\sqrt{c_{ii}}] &= 1-\alpha \\ P[b_i - t_{\alpha/2}s\sqrt{c_{ii}} \leq \beta_i \leq b_i + t_{\alpha/2}s\sqrt{c_{ii}}] &= 1-\alpha. \end{aligned}$$

Therefore the confidence interval (using a t distribution with $n-p$ d.f.) is

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

where c_{ii} is the ith diagonal element of $(X^TX)^{-1}$.

7.2 Example - interval estimation of the coefficients - MM3.6

Interval estimation

Example. We model the amount of a chemical that dissolves in a fixed volume of water. This depends (in part) on the water temperature. An experiment is run 6 times and the following data measured:

Temperature (x)	Amount dissolved (y)
0	2.1
10	4.5
20	6.1
30	11.2
40	13.8
50	17.0

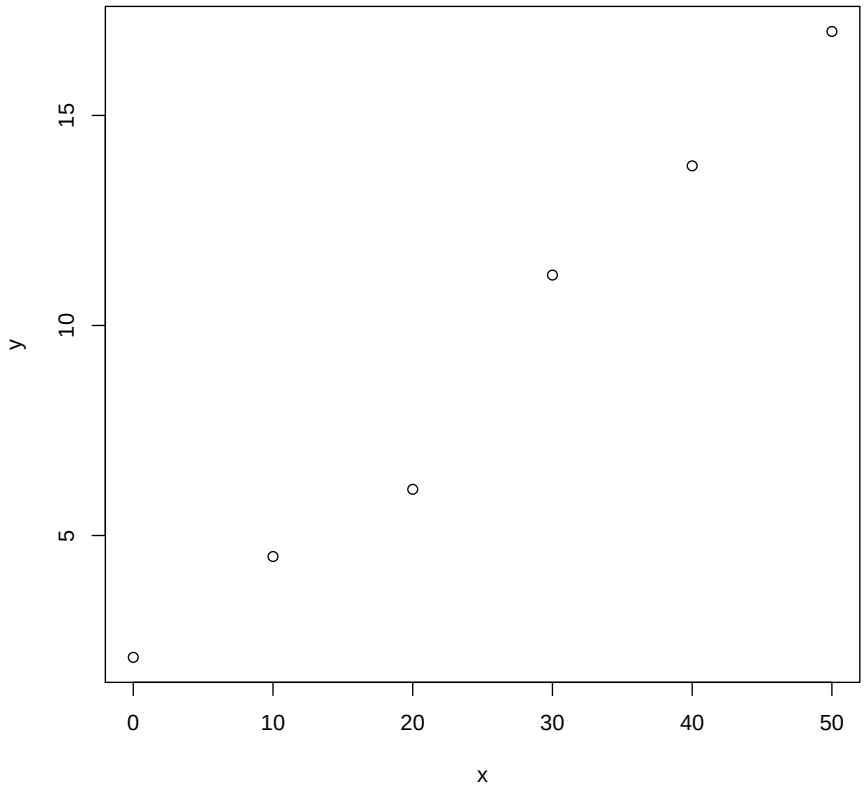


Figure 17: Plot of the amount disolved vs. temperature

Interval estimation

```
y <- c(2.1, 4.5, 6.1, 11.2, 13.8, 17.0)
X <- matrix(c(rep(1,6),seq(0,50,10)),6,2)
(b <- solve(t(X)%*%X, t(X)%*%y))

##           [,1]
## [1,] 1.4380952
## [2,] 0.3071429

(df <- 6-2)

## [1] 4

e <- y - X%*%b
(s <- sqrt(sum(e^2)/df))

## [1] 0.8629959
```

Interval estimation

First we find a confidence interval on β_0, the intercept.

```
c00 <- solve(t(X)%*%X)[1,1]
alpha <- 0.05
ta <- qt(1-alpha/2, df=df)
c(b[1] - ta*s*sqrt(c00), b[1] + ta*s*sqrt(c00))

## [1] -0.2960462  3.1722367
```

We are 95% confident that the true amount of chemical dissolved at 0 temperature lies between -0.30 and 3.17.

Notably, we cannot say with 95% confidence that it is untrue that no chemical dissolves at 0 temperature.

Interval estimation

Next we find a confidence interval on β_1, the slope of the regression.

```
c11 <- solve(t(X)%*%X)[2,2]
c(b[2] - ta*s*sqrt(c11), b[2] + ta*s*sqrt(c11))

## [1] 0.2498661 0.3644197
```

We are 95% confident that for each rise in temperature of 1 degree, the amount of chemical dissolved goes up by an amount between 0.25 and 0.36.

In particular, we are (at least) 95% sure that there is a positive relationship between temperature and chemical dissolved.

7.3 Interval estimation of linear functions - MM3.7

Interval estimation

It is good that we can find confidence intervals for the parameters, but sometimes we want to estimate things other than just the parameters.

In particular, we often want to estimate the mean of the response variable for a given set of inputs.

This is an example of the more general case of linear functions of the parameters.

Interval estimation

Remember that if we want to estimate the function $\mathbf{t}^T\boldsymbol{\beta}$, the best linear unbiased estimator is $\mathbf{t}^T\mathbf{b}$, where $\mathbf{b}$ is the least squares estimator of the parameters. What is its distribution?

Since $\mathbf{b}$ is multivariate normal, any linear combination of b's is normally distributed. We have

$$E[\mathbf{t}^T\mathbf{b}] = \mathbf{t}^T\boldsymbol{\beta}$$

since $\mathbf{b}$ is an unbiased estimator for $\boldsymbol{\beta}$.

Interval estimation

Variance results give us

$$\text{Var } \mathbf{t}^T\mathbf{b} = \mathbf{t}^T(X^TX)^{-1}\sigma^2\mathbf{t} = \mathbf{t}^T(X^TX)^{-1}\mathbf{t}\sigma^2.$$

Therefore

$$\frac{\mathbf{t}^T\mathbf{b} - \mathbf{t}^T\boldsymbol{\beta}}{\sqrt{\mathbf{t}^T(X^TX)^{-1}\mathbf{t}\sigma^2}}$$

has a standard normal distribution.

But again, we do not know what σ is!

Interval estimation

The solution should not be difficult to see: since SS_{Res}/σ^2 is independent of $\mathbf{b}$, it is independent of $\mathbf{t}^T\mathbf{b}$. Therefore

$$\frac{(\mathbf{t}^T\mathbf{b} - \mathbf{t}^T\boldsymbol{\beta})/(\sqrt{\mathbf{t}^T(X^TX)^{-1}\mathbf{t}\sigma^2})}{\sqrt{SS_{Res}/\sigma^2(n-p)}} = \frac{\mathbf{t}^T\mathbf{b} - \mathbf{t}^T\boldsymbol{\beta}}{s\sqrt{\mathbf{t}^T(X^TX)^{-1}\mathbf{t}}}$$

has a t distribution with $n-p$ degrees of freedom.

Using similar steps to before, this gives the $100(1-\alpha)\%$ confidence interval

$$\mathbf{t}^T\mathbf{b} \pm t_{\alpha/2}s\sqrt{\mathbf{t}^T(X^TX)^{-1}\mathbf{t}}.$$

Interval estimation

In particular, if we want to find a confidence interval for the expected response to a particular set of x variables $x_1^*, x_2^*, \ldots, x_k^*$, we wish to estimate

$$E[y] = \beta_0 + \beta_1 x_1^* + \ldots + \beta_k x_k^* = (\mathbf{x}^*)^T\boldsymbol{\beta}$$

where $\mathbf{x}^* = \begin{bmatrix} 1 & x_1^* & x_2^* & \ldots & x_k^* \end{bmatrix}^T$.

This is a linear function of $\boldsymbol{\beta}$, and therefore the $100(1-\alpha)\%$ confidence interval for it is

$$(\mathbf{x}^*)^T\mathbf{b} \pm t_{\alpha/2}s\sqrt{(\mathbf{x}^*)^T(X^TX)^{-1}\mathbf{x}^*}.$$

7.4 Example - interval estimation of linear functions - MM3.7

Interval estimation

Example. In the house price example, we estimated the average selling price of a 15-year-old house with an area of 250 m^2 to be \$570,129. What is the 95% confidence interval for this number?

```
(s <- sqrt(s2))

## [1] 6.916497

xst <- c(1,15,2.5)
xst%*%b

##          [,1]
## [1,] 57.01289
```

```
(ta <- qt(0.975,df=5-3))

## [1] 4.302653

xst%*%b - ta*s*sqrt(t(xst)%*%solve(t(X)%*%X)%*%xst)

##          [,1]
## [1,] 37.83522

xst%*%b + ta*s*sqrt(t(xst)%*%solve(t(X)%*%X)%*%xst)

##          [,1]
## [1,] 76.19056
```

So we are 95% confident that the price will be between \$380,000 and \$760,000 (to the neareast \$10,000) - a wide interval reflecting little data!

8 Prediction intervals

8.1 Prediction intervals theory - MM3.7

Prediction intervals

Given a set of inputs, a 95% confidence interval for the response gives an interval that contains the *expected* response 95% of the time.

In contrast, given a set of inputs, a 95% prediction interval produces an interval in which we are 95% sure that *any new response with those inputs* will lie.

Because a single observation is more variable than the expected response, a prediction interval is wider than the corresponding confidence interval.

Prediction intervals

Suppose we have inputs $\mathbf{x}^* = \begin{bmatrix} 1 & x_1^* & x_2^* & \dots & x_k^* \end{bmatrix}^T$, with corresponding response

$$y^* = (\mathbf{x}^*)^T\boldsymbol{\beta} + \varepsilon^*$$

where Var $\varepsilon^* = \sigma^2$ by assumption.

The mean of $y*$ will be (point) estimated by $(\mathbf{x}^*)^T\mathbf{b}$ but the error is now estimated by $y^* - (\mathbf{x}^*)^T\mathbf{b}$.

Prediction intervals

Since y^* is a new observation, and $\mathbf{b}$ depends only on the current observations $\mathbf{y}$, the two components of error are independent.

This gives

$$\begin{aligned} \text{Var } (y^* - (\mathbf{x}^*)^T\mathbf{b}) &= \text{Var } \varepsilon^* + \text{Var } \left[(\mathbf{x}^*)^T\mathbf{b}\right] \\ &= \sigma^2 + (\mathbf{x}^*)^T(X^TX)^{-1}\sigma^2\mathbf{x}^* \\ &= [1 + (\mathbf{x}^*)^T(X^TX)^{-1}\mathbf{x}^*]\sigma^2 \end{aligned}$$

and since the estimator, $(\mathbf{x}^*)^T\mathbf{b}$, is unbiased, the expectation is $\mathbf{0}$.

Prediction intervals

Following exactly the previous arguments, we derive that

$$\frac{y^* - (\mathbf{x}^*)^T\mathbf{b}}{s\sqrt{1 + (\mathbf{x}^*)^T(X^TX)^{-1}\mathbf{x}^*}}$$

has a t distribution with $n - p$ degrees of freedom.

Thus a prediction interval for y^* is

$$(\mathbf{x}^*)^T\mathbf{b} \pm t_{\alpha/2}s\sqrt{1 + (\mathbf{x}^*)^T(X^TX)^{-1}\mathbf{x}^*}.$$

The only difference with confidence intervals is the presence of the '1', which makes the interval wider (as expected).

8.2 Example - house prediction intervals - MM3.7

Prediction intervals

Example. In the previous example, we estimated the *average* selling price of a 15-year-old house with area 250 m^2 to be in the range [37.84,76.19] ie between \$380,000 and \$760,000.

What is the prediction interval for a *single* such house?

```
xst%*%b - ta*s*sqrt(1+t(xst)%*%solve(t(X)%*%X)%*%xst)

##          [,1]
## [1,] 21.60953

xst%*%b + ta*s*sqrt(1+t(xst)%*%solve(t(X)%*%X)%*%xst)

##          [,1]
## [1,] 92.41626
```

So the prediction interval is $216,100 to $924,200 - a very wide interval! The agent needs more data!

Clover example

Logs were taken of the data and on the log scale, `area` was modelled as a linear function of `estim` and `midrib`. We need i.i.d. normal errors for our confidence intervals to be accurate.

We checked this using a normal quantile-quantile plot in the section on diagnostics. Because of the outlying points, the qqplot in Figure 4 showed distinct departures from normality.

After removing a number of outlying points to produce a smaller data frame called `goodclover`, the qqplot in Figure 8 showed a normal fit if not a close one.

Clover example

The least squares estimates of coefficients can be found from matrix operations.

```
y <- goodclover$area
X <- matrix(c(rep(1,139),goodclover$midrib,
  goodclover$estim),139,3)
n <- dim(X)[1]
p <- dim(X)[2]
b <- solve(t(X) %*% X, t(X) %*% y)
e <- y - X %*% b
SSRes <- sum(e^2)
s2 <- SSRes/(n-p)
```

Clover example

95% confidence interval for β_0, the intercept:

```
C <- solve(t(X) %*% X)
halfwidth <- qt(0.975,df=n-p)*sqrt(s2*C[1,1])
c(b[1] - halfwidth, b[1] + halfwidth)

## [1] -1.7871886 -0.9757665
```

95% confidence interval for β_1, the midrib coefficient:

```
halfwidth <- qt(0.975,df=n-p)*sqrt(s2*C[2,2])
c(b[2] - halfwidth, b[2] + halfwidth)

## [1] 0.4413948 0.8593518
```

Clover example

95% confidence interval for β_2, the estim coefficient:

```
halfwidth <- qt(0.975,df=n-p)*sqrt(s2*C[3,3])
c(b[3] - halfwidth, b[3] + halfwidth)

## [1] 0.5741688 0.8098116
```

Or we can use the command `lm`

```
model2 <- lm(area ~ midrib + estim, data=goodclover)
confint(model2, level=0.95)

##                   2.5 %     97.5 %
## (Intercept) -1.7871886 -0.9757665
## midrib       0.4413948  0.8593518
## estim        0.5741688  0.8098116
```

Clover example

95% confidence interval for the expected area of a leaf with midrib 10 and template area 10:

```
tt <- c(1,log(10),log(10))
halfwidth <- qt(0.975,df=n-p)*sqrt(s2 * t(tt) %*% C %*% tt)
c(tt %*% b - halfwidth, tt %*% b + halfwidth)

## [1] 1.538316 1.880541

newclover <- data.frame(midrib=log(10),estim=log(10))
predict(model2,newclover,interval="confidence",level=0.95)

##        fit      lwr      upr
## 1 1.709429 1.538316 1.880541
```

Clover example

95% *prediction* interval of the area of a leaf with midrib 10 and template area 10:

```
halfwidth <- qt(0.975,df=n-p)*
     sqrt(s2 * (1 + t(tt) %*% C %*% tt))
c(tt %*% b - halfwidth, tt %*% b + halfwidth)

## [1] 1.303147 2.115710

predict(model2,newclover,interval="prediction",level=0.95)

##        fit      lwr     upr
## 1 1.709429 1.303147 2.11571
```

9 Joint confidence intervals

9.1 Joint Cis- MM3.8

Joint confidence intervals

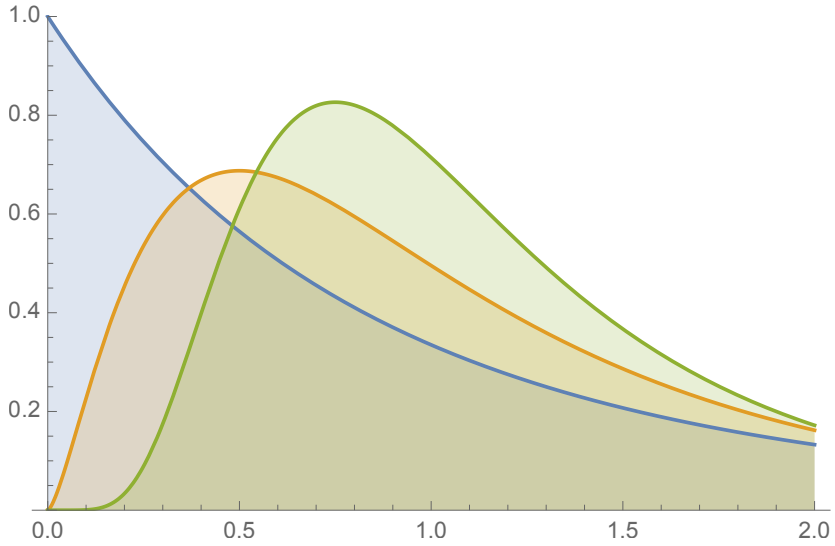


Figure 18: F distributions with 2,5 and 20 df in the numerator and 10 df in the denominator

Sometimes we want confidence intervals for more than one parameter, or linear combination of parameters, at once.

Finding confidence intervals individually for each parameter can be misleading. If we find more than one 95% confidence interval, we do *not* have 95% confidence that all of them will be satisfied at once.

The more confidence intervals we have, the more likely it is that at least one will be wrong!

We need to be able to find a *joint* confidence *region* for a number of parameters at the same time.

9.2 F Distribution - MM3.8

F distribution

Definition 4.15. Let $X^2_{\gamma_1}$ and $X^2_{\gamma_2}$ be independent χ^2 random variables with γ_1 and γ_2 degrees of freedom. Then

$$\frac{X^2_{\gamma_1}/\gamma_1}{X^2_{\gamma_2}/\gamma_2}$$

has an F distribution with γ_1 and γ_2 degrees of freedom.

The F distribution has the density

$$f(x;\gamma_1,\gamma_2) = \frac{1}{\beta(\gamma_1/2,\gamma_2/2)}\left(\frac{\gamma_1}{\gamma_2}\right)^{\gamma_1/2} x^{\gamma_1/2-1}\left(1+\frac{\gamma_1}{\gamma_2}x\right)^{-(\gamma_1+\gamma_2)/2}.$$

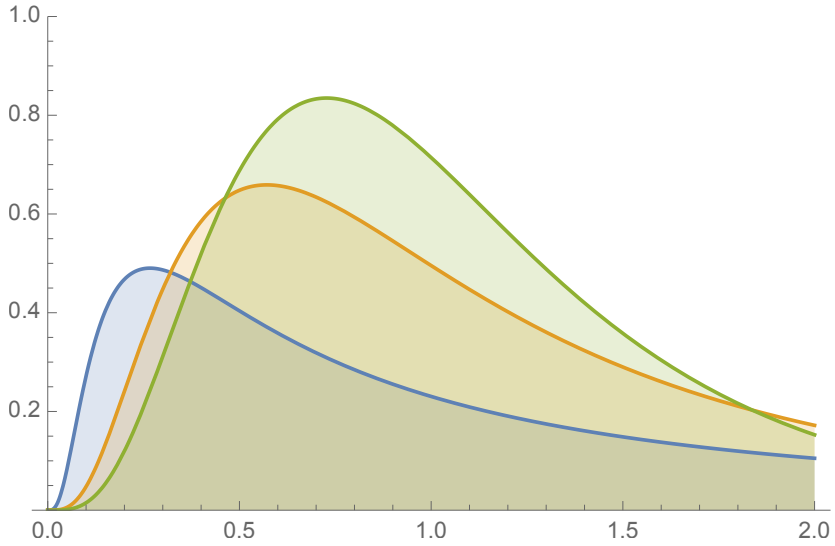


Figure 19: F distributions with 10 df in the numerator and 1,5 and 20 df in the denominator

Simulating the F distribution from its components

```
X1 <- rchisq(100,4)
X2 <- rchisq(100,6)
F <- (X1/4)/(X2/6)
hist(F, freq=FALSE)
curve(df(x,4,6), add=TRUE,col='red')
```

9.3 Derivation of confidence ellipses - MM3.8

Joint confidence intervals

Let's derive a confidence region for $\boldsymbol{\beta}$. The least squares estimator is

$$\mathbf{b} = (X^T X)^{-1} X^T \mathbf{y} \sim MVN(\boldsymbol{\beta}, (X^T X)^{-1}\sigma^2).$$

From Corollary 3.10, the quadratic form

$$\frac{(\mathbf{b}-\boldsymbol{\beta})^T X^T X (\mathbf{b}-\boldsymbol{\beta})}{\sigma^2}$$

has a χ^2 distribution with p degrees of freedom (where p is the number of parameters in the model).

We also know that

$$\frac{(n-p)s^2}{\sigma^2}$$

has a χ^2 distribution with $n-p$ degrees of freedom.

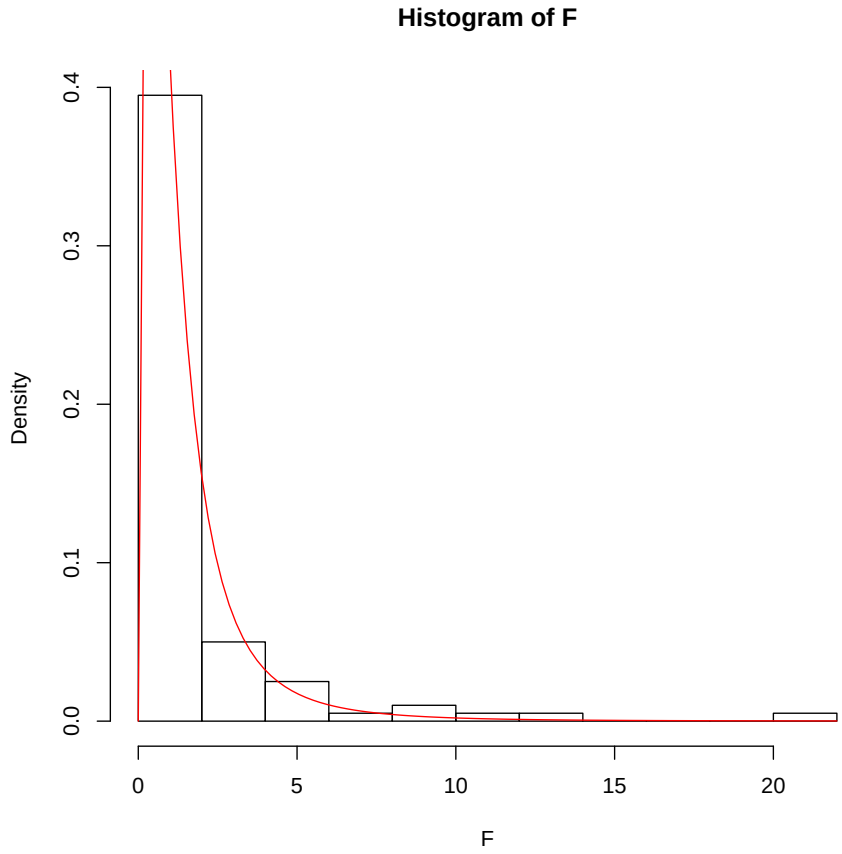


Figure 20: Simulation of 100 ratios of independent χ^2 rv's with df 4 and 6 and corresponding $F_{4,6}$ density

Joint confidence intervals

Since $\mathbf{b}$ and s^2 are independent, the two χ^2 variables above are independent, which means that

$$\left(\frac{(\mathbf{b}-\boldsymbol{\beta})^T X^T X(\mathbf{b}-\boldsymbol{\beta})}{p\sigma^2}\right) / \left(\frac{(n-p)s^2}{(n-p)\sigma^2}\right)$$
$$= \frac{(\mathbf{b}-\boldsymbol{\beta})^T X^T X(\mathbf{b}-\boldsymbol{\beta})}{ps^2}$$

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

Because this statistic is based on $\mathbf{b}-\boldsymbol{\beta}$, which we hope to be small in absolute value, we use the right-hand tail of the F-distribution to create a confidence region.

Joint confidence intervals

Let f_α be the critical value (ie $1-\alpha$ quantile) of the F distribution with p and $n-p$ d.f. and probability α. Then

$$P[(\mathbf{b}-\boldsymbol{\beta})^T X^T X(\mathbf{b}-\boldsymbol{\beta})/ps^2 \leq f_\alpha] = 1-\alpha$$

which gives the confidence region

$$(\mathbf{b}-\boldsymbol{\beta})^T X^T X(\mathbf{b}-\boldsymbol{\beta}) \leq ps^2 f_\alpha.$$

This region is a region bounded by an ellipse (or ellipsoid if $p > 2$) since the left side of the inequality is a quadratic form whose matrix $X^T X$ is positive definite.

9.4 Example - income vs. education - MM3.8

Joint confidence intervals

Example. Modelling income against years of formal education. The data is

Years of education	Income
8	8
12	15
14	16
16	20
16	25
20	40

Joint confidence intervals

```
n <- 6
p <- 2
y <- c(8,15,16,20,25,40)
X <- matrix(c(rep(1,n),8,12,14,16,16,20),n,p)
t(X)%*%X

##      [,1] [,2]
## [1,]    6   86
## [2,]   86 1316
```

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

##          [,1]
## [1,] -15.568
## [2,]   2.528

(s2 <- sum((y-X%*%b)^2)/(n-p))

## [1] 18.692
```

Joint confidence intervals

Calculations give

$$X^T X = \begin{bmatrix} 6 & 86 \\ 86 & 1316 \end{bmatrix}$$

and

$$\mathbf{b} = \begin{bmatrix} -15.57 \\ 2.53 \end{bmatrix}, \quad s^2 = 18.69.$$

So a joint 95% confidence interval is given by

$$\begin{bmatrix} -15.57 - \beta_0 & 2.53 - \beta_1 \end{bmatrix} \begin{bmatrix} 6 & 86 \\ 86 & 1316 \end{bmatrix} \begin{bmatrix} -15.57 - \beta_0 \\ 2.53 - \beta_1 \end{bmatrix} \leq 2 \times 18.69 \times 6.94$$

Joint confidence intervals

```
b1 <- seq(-50, 20, .2)
b2 <- seq(0, 5, .1)
f <- function(beta1, beta2) {
    b <- matrix(c(-15.57, 2.53), 2, 1)
    XTX <- matrix(c(6, 86, 86, 1316), 2, 2)
    f.out <- rep(0, length(beta1))
    for (i in 1:length(beta1)) {
        beta <- matrix(c(beta1[i], beta2[i]), 2, 1)
        f.out[i] <- t(b - beta) %*% XTX %*% (b - beta)
    }
    return(f.out)
}
z <- outer(b1, b2, f)
contour(b1, b2, z, levels=2*18.69*qf(0.95, 2, 4))
```

Notes on the contour plot

The R command `outer` evaluates the function `f` at a matrix of values determined by the values of the vector `b1` and `b2`.

The command `contour` plots the contour for the array of function values corresponding to a 95% confidence interval.

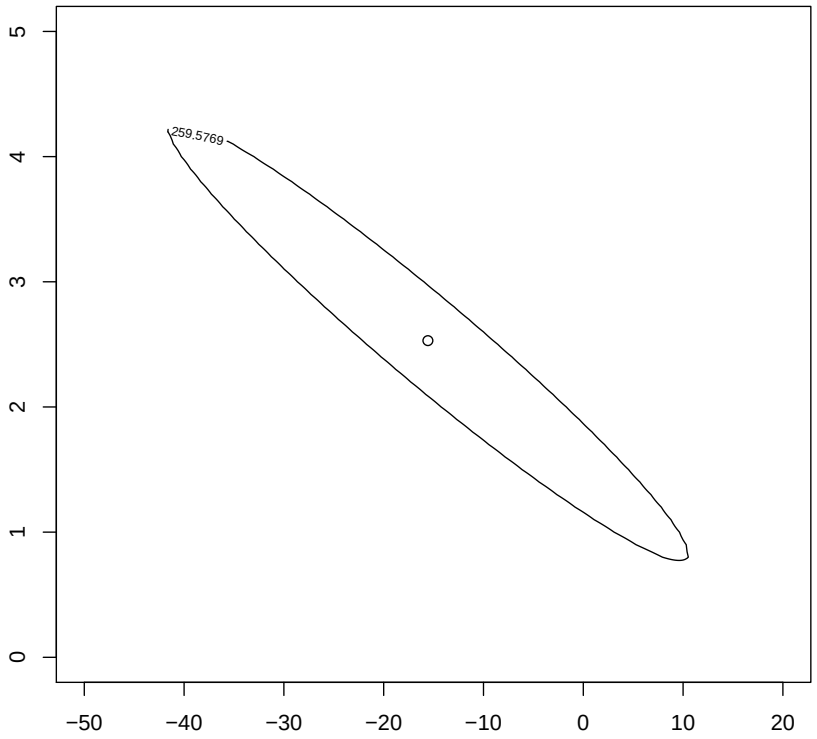


Figure 21: Joint confidence interval of β_0, β_1 with estimates marked

10 Generalised least squares

10.1 General Covariance Matrix - MM3.9

Generalised least squares

So far, we have made the assumption that the errors $\boldsymbol{\varepsilon}$ have mean $\mathbf{0}$ and variance $\sigma^2 I$, and sometimes that they are normally distributed. These assumptions do not always hold.

If the errors do not have $\mathbf{0}$ mean, then we should find another model!

It is not always satisfying to have normal errors, but they occur quite often in practice and the accompanying theory is very appealing.

What if the variance of $\boldsymbol{\varepsilon}$ is not $\sigma^2 I$?

Generalised least squares

Suppose that $\boldsymbol{\varepsilon}$ is multivariate normal but with a positive definite variance V. The maximum likelihood estimator now minimises

$$\mathbf{e}^T V^{-1} \mathbf{e} = (\mathbf{y} - X\mathbf{b})^T V^{-1} (\mathbf{y} - X\mathbf{b})$$

and thus satisfies the (equivalent of) the normal equations

$$X^T V^{-1} X\mathbf{b} = X^T V^{-1} \mathbf{y}.$$

This gives the *generalised least squares estimators*

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

If $V = \sigma^2 I$, this reduces to ordinary least squares.

Generalised least squares

We have

$$\begin{aligned} E[\mathbf{b}] &= \beta, \\ \text{Var } \mathbf{b} &= (X^T V^{-1} X)^{-1}. \end{aligned}$$

Moreover, it can be shown that the Gauss-Markov theorem still holds, i.e. the generalised least squares estimator is still BLUE.

The proof is left as an exercise.

10.2 Weighted Least Squares - MM3.9

Weighted least squares

In this situation, the errors are uncorrelated but do not have a common variance:

$$\text{Var } \boldsymbol{\varepsilon} = diag(\sigma_1^2, \sigma_2^2, \ldots, \sigma_n^2).$$

To estimate the parameters with ML, we minimise

$$(\mathbf{y} - X\mathbf{b})^T V^{-1} (\mathbf{y} - X\mathbf{b}) = \sum_{i=1}^{n} \left(\frac{e_i}{\sigma_i} \right)^2 .$$

That is, we *weight* each residual by the inverse of the corresponding standard deviation. So a point with high variance influences **b** less than a point with low variance.

11 Nonlinearities and transforms

11.1 How to cope with nonlinearities

Nonlinearities

All the models that we study are *linear* models, in the sense that they are linear w.r.t. the parameters. However, this does not mean that they can only model linear relationships. There is still some scope to model nonlinear relationships.

This is particularly true when you know, or have a good idea of what the type of relationship might be.

One way we can handle this is to include extra predictors which are nonlinear functions of the original predictors.

Nonlinearities

For example, suppose lung capacity (y) was predicted by asking participants to blow a single breath into a balloon and measuring the diameter of the balloon (x).

Perhaps we could use a linear model for this, of the form

$$y = \beta_0 + \beta_1 x + \varepsilon.$$

Nonlinearities

However, the diameter of the balloon is not a direct measure of lung capacity, and importantly it is not linearly related to lung capacity.

In fact, lung capacity is more likely to be related linearly to the *volume* of the balloon. The volume is much harder to measure, but is proportional to the cube of the diameter.

Therefore we might instead try a model like

$$y = \beta_0 + \beta_1 x^3 + \varepsilon.$$

Nonlinearities

The analysis actually does not change at all: we have simply changed one design variable for another.

Another alternative might be to model the response on a polynomial that goes up to a cubic:

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \varepsilon.$$

This introduces two extra design variables, but again the analysis is much the same.

Nonlinearities

We can only do this because we understand the source of the data, and thus have a good idea about what kinds of potential relationships might occur.

If we observe an obviously non-linear relationship but have no idea about what the relationship might be, the situation is more difficult.

The best thing to do is to try and deduce the relationship from the data and then fit an appropriate model.

11.2 Transformations?

Transformations

Certain kinds of relationships (in particular multiplicative relationships) also require the transformation of the *response* variable.

We have to be careful with this because a transformation of the response also transforms the error, and the form of the error.

Sometimes this can work in our favour, if the error needs to be transformed in order to fit with the assumptions of a linear model.

Transformations

For example, if the true underlying model is

$$y = \alpha_1 e^{\alpha_2 x} \varepsilon,$$

then we would transform the response variable to $\ln y$:

$$\ln y = \ln \alpha_1 + \alpha_2 x + \ln \varepsilon.$$

We can then fit a linear model to $\ln y$ with design variable x and recover the original coefficients with

$$\alpha_1 = e^{\beta_0}, \quad \alpha_2 = \beta_1.$$

Transformations

On the other hand, if the true underlying model is

$$y = \beta_0 e^{\beta_1 x} + \varepsilon,$$

we can't do this.

We could estimate β_1 in some way (possibly by transforming and fitting as above), but ultimately we would fix it to a value.

Then we would fit a linear model to y with the design variable $e^{\beta_1 x}$ and no intercept. This model will give us β_0.

Transformations

Sometimes we have a good idea at the form of the true underlying model, because we understand the origin of the data.

However, most of the time we do not know the true underlying model and therefore cannot be sure what the correct transformation is.

In this case we usually try out a few reasonable-looking transformations and evaluate them in turn, using diagnostic plots.

Transformations

There are certain signs which may indicate that a transformation is required:

- All the values are positive;
- The distribution of the data is skewed;
- There is an obvious non-linear relationship with another variable;
- The variances show a relationship with one of the variables.

Transformations

Logarithmic transformations are very common because they convert multiplicative effects into additive ones. Useful transformations are:

$\ln y$, x	exponential
$\ln y$, $\ln x$	power law
$\sqrt{y}$	areas, or occurences inside areas
$\sqrt[3]{y}$	volumes
$\frac{1}{y}$	rates
$\ln \frac{y}{1-y}$	proportions

11.3 Example

Clover example

Recall that we first transformed the clover data by taking logarithms. Let us go through that decision process.

Firstly, we 'eyeball' the data.

```
expclover <- read.csv("../data/clover.csv")
pairs(expclover)
```

Clover example

It is clear that there are some non-linearities which necessitate action before fitting a linear model.

Let us look closer at just the `area` to `midrib` relationship using the following commands:

```
plot(area ~ midrib, data=expclover)
m <- lm(area ~ midrib, data=expclover)
curve(m$coeff[1]+m$coeff[2]*x,add=T,col="red")
```

Figure 22: Plots of the clover leaf variables

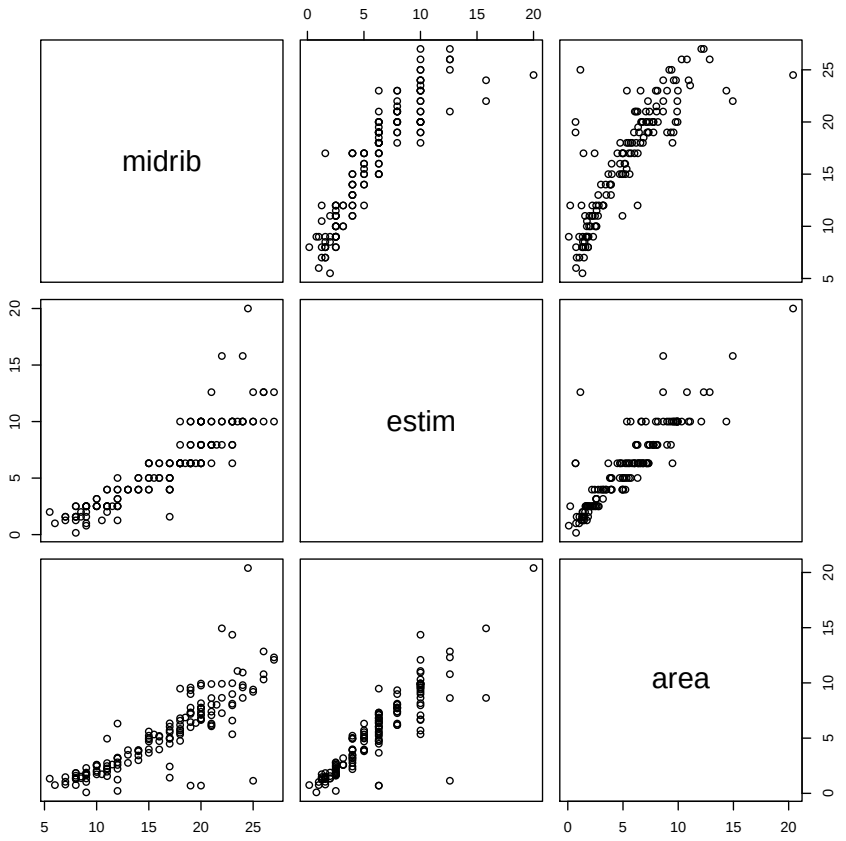
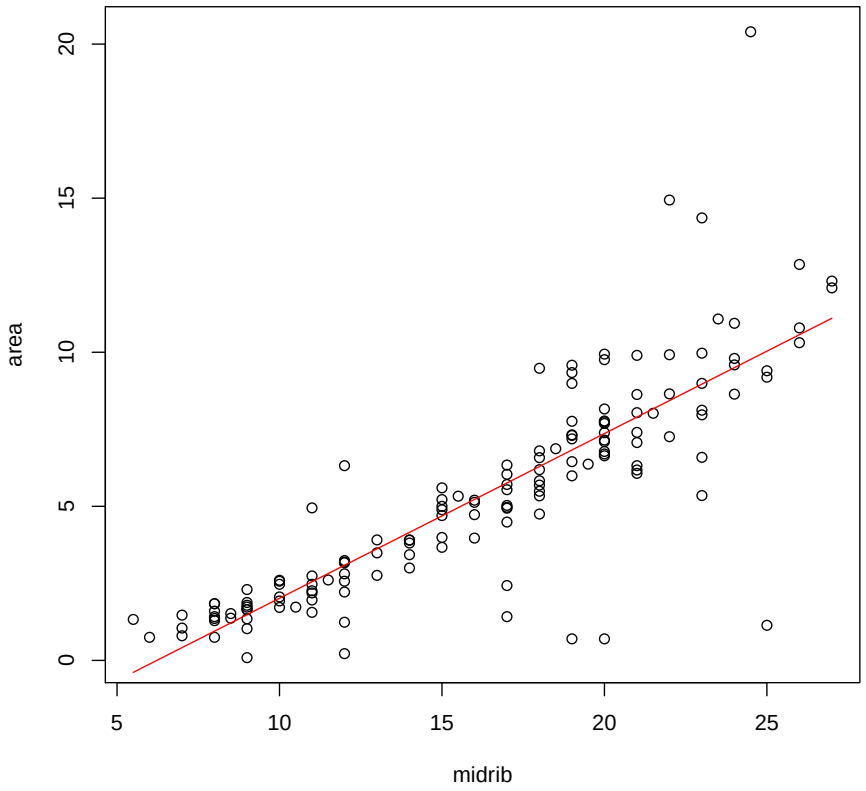


Figure 23: Plot of `area` versus `midrib`



Clover example

One thing which is very noticeable in the plot of `area` versus `midrib` is that the magnitude of the errors increase with both the variables.

This indicates a multiplicative error, which we can check with a diagnostic plot.

```
plot(m, which=3)
```

Clover example

There is some evidence of increase, but not much in the trendline.

It becomes really obvious if we include both `midrib` and `estim`:

Figure 24: Diagnostic plot of square root of abs. residuals vs. fitted values

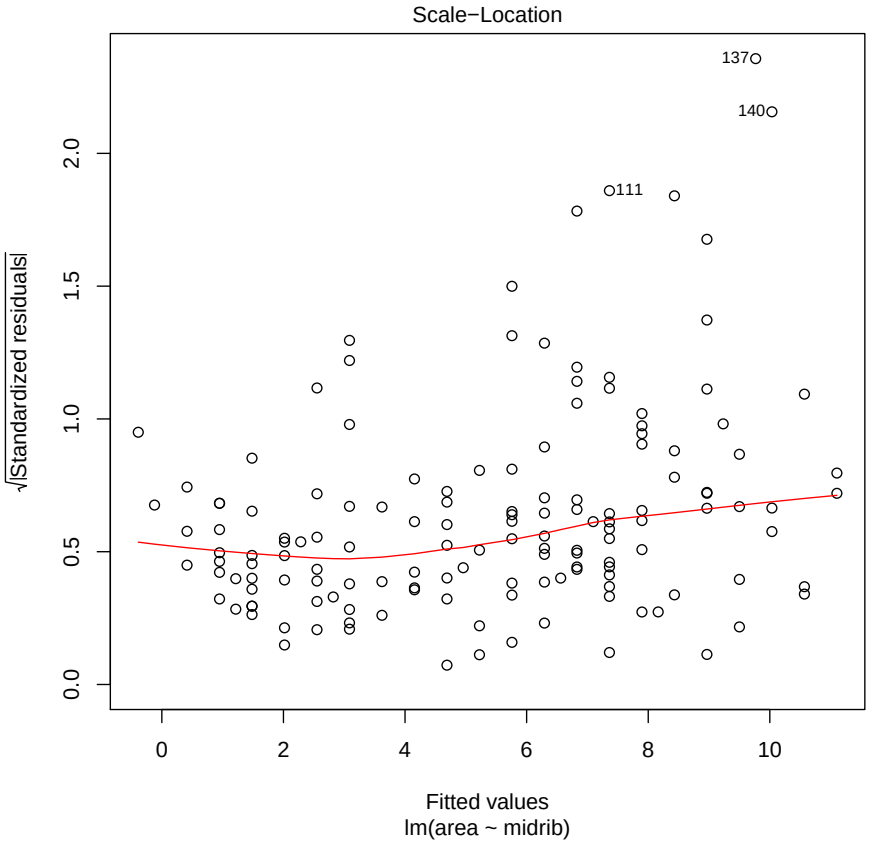
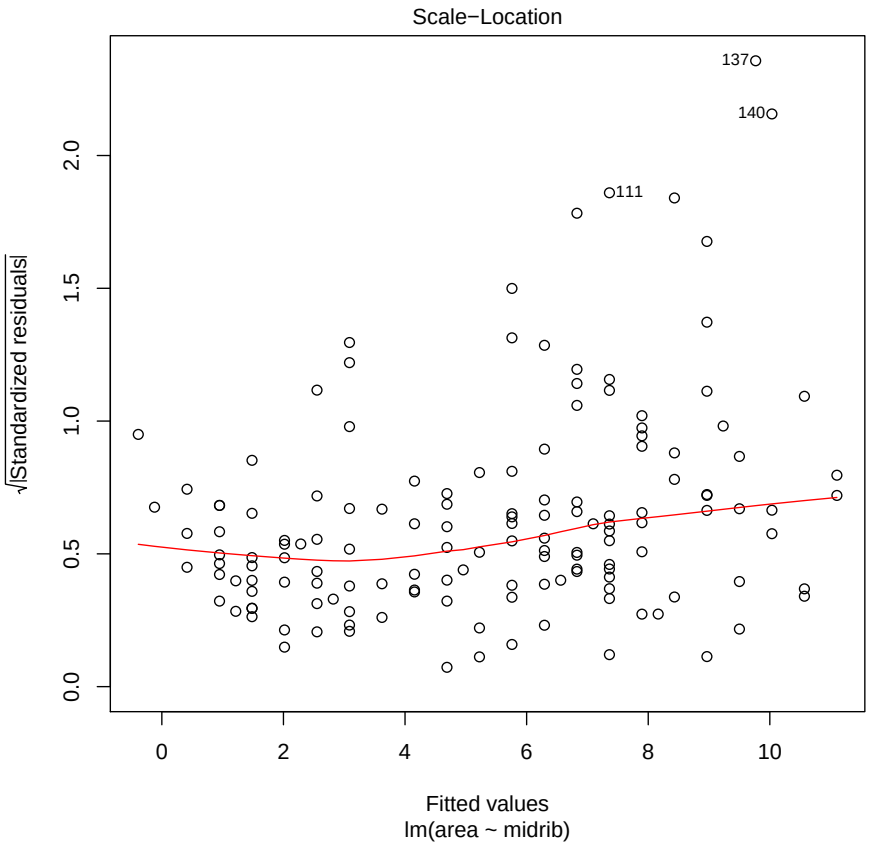


Figure 25: Diagnostic plot, this time including `estim`




```
plot(model3,which=3)
```

Clover example

Now what sort of relationship could happen here?

Looking at the non-linear trend and multiplicative errors in the data, it would seem that the most likely kinds are power law or exponential relationships.

Let us try both types of transformations and see which one fits better.

```
plot(log(area) ~ midrib, data=expclover, ylim=c(-1,3))
m <- lm(log(area) ~ midrib, data=expclover)
curve(m$coeff[1]+m$coeff[2]*x,add=TRUE,col="red")
```

Figure 26: Log `area`

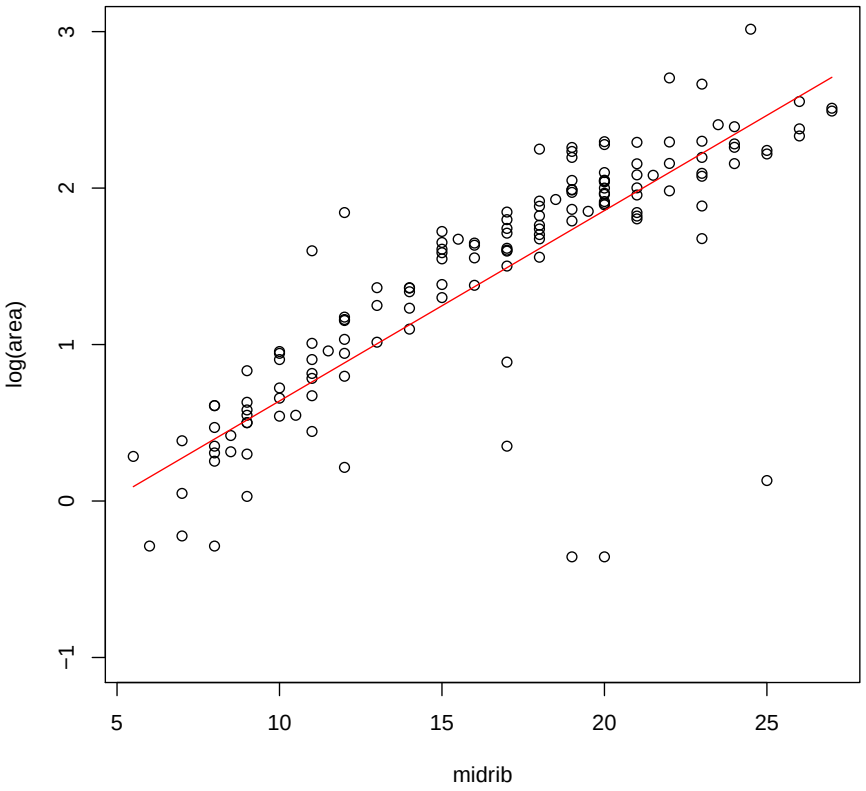
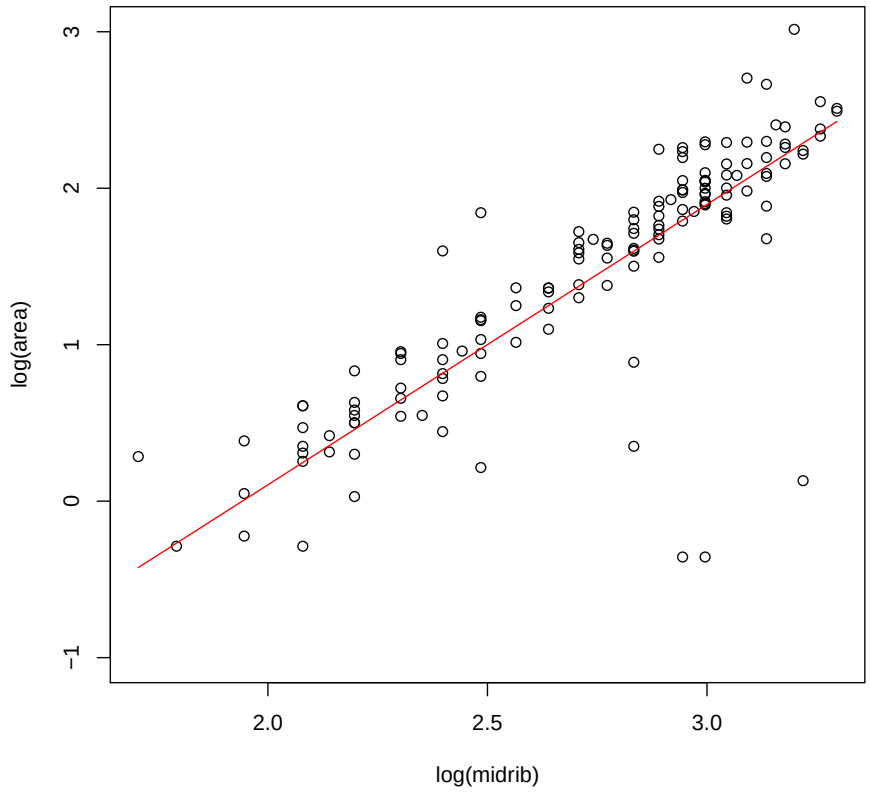


Figure 27: Both logs



Clover example

Now try both with log's

```
plot(log(area) ~ log(midrib), data=expclover, ylim=c(-1,3))
m <- lm(log(area) ~ log(midrib), data=expclover)
curve(m$coeff[1]+m$coeff[2]*x,add=TRUE,col="red")
```

Clover example

Clover example

It is obvious that the model

$$\ln \texttt{area} = \beta_0 + \beta_1 \ln \texttt{midrib} + \varepsilon$$

works the best.

Similar reasoning can also be applied to the relationship between `area` and `estim` to deduce a power law.

It turns out that there are also botanical models which predict a power law, so there are good data-independent reasons to use it too.

Clover example

Using our best fit from before:

```
goodclover <- log(expclover[-c(6, 23, 47, 97, 111, 140), ])
model2 <- lm(area ~ midrib + estim, data = goodclover)
model2$coefficients

## (Intercept)      midrib       estim
##  -1.3814775   0.6503733   0.6919902
```

Our fitted model is

$$\ln \texttt{area} = -1.38 + 0.65 \ln \texttt{midrib} + 0.69 \ln \texttt{estim} + \varepsilon.$$

Converting back into the original measurements, we fit the model

$$\texttt{area} = e^{-1.38} \times \texttt{midrib}^{0.65} \times \texttt{estim}^{0.69} \times \varepsilon'.$$

11.4 Response transformation using residual pattern

A rationale for the transfomations?

In the Clover leaf example, the best model used a ln transformation of the response variable, `area`.

This was done looking at the `plot` of the model with `which = 3`.

If the square root of the absolute standardised residuals had been constant in that plot, $\sqrt{\texttt{area}}$ might be a good response variable, since the assumption is that the variance of the residuals is constant across fitted values.

But this doesn't explain why we chose the `ln` transformation.

A rationale for choosing transfomations

To see a reason, consider a general transformation, $h(y)$, of the response variable y.

The definition of the derivative says that to first order approximation,

$$h(y) - h(E(y)) \approx h'(E(y))(y - E(y))$$

.

Although, in general, $h(E(y)) \neq E(h(y))$, if we square the left side of the approximation and take expectation, we might expect the result to approximate Var (y).

This then gives

$$\text{Var } (h(y)) \approx (h'(E(y)))^2 \text{ Var } (y).$$

For Var $(h(y))$ to be constant (as assumed in our linear model), at least approximately, we need:

$$h'(E(y)) \propto \text{Var } (h(y))^{-1/2} = SD(y)^{-1}.$$

This suggests a rational choice for a transformation $h(y)$ of our response variable might be:

$$h(y) = \int \frac{dy}{SD(y)}.$$

If $SD(y) = SD(\epsilon) \propto \sqrt{E(y)}$, this suggests trying $h(y) = \sqrt{y}$, or for $SD(y) = SD(\epsilon) \propto E(y)$, this suggests trying $h(y) = \ln(y)$.

In practice

Both of these suggestions may be appropriate for non-negative variables.

In practice, if the plot of residuals versus fitted values shows a fanning out with larger fitted values but the `which = 3` plot is approximately constant, then $h(y) = \sqrt{y}$ may be appropriate.

If, as in the clover example, the `which = 3` plot shows some increase in the square root of the absolute values of the residuals with fitted values increasing, then $h(y) = \ln(y)$ may be appropriate.

In all cases, refitting with the chosen transformation and examination of the resulting residual plots is the ultimate test. Even then, if the resulting residual plots look OK, discussion with experts in the variables in the linear model is vital to see if there is a scientific or business reason why the transformation makes sense.