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STAT 331 Course Notes

Applied Linear Models

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Abstract

These notes are intended as a resource for myself; past, present, or future students of this course, and anyone interested in the material. The goal is to provide an end-to-end resource that covers all material discussed in the course displayed in an organized manner. These notes are my interpretation and transcription of the content covered in lectures. The instructor has not verified or confirmed the accuracy of these notes, and any discrepancies, misunderstandings, typos, etc. as these notes relate to course's content is not the responsibility of the instructor. If you spot any errors or would like to contribute, please contact me directly.

1 January 4, 2018

1.1 Simple linear regression review

In SLRM, there is a single explanatory variate and a response variate.
A good graphical summary for SLRM are **scatterplots**.
A good numerical summary for SLRM is the **correlation coefficient** defined as

$$r = \frac{\sum(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum(x_i - \bar{x})^2 \sum(y_i - \bar{y})^2}}$$

where $-1 \leq r \leq 1$. If $|r| \approx 1$ then the explanatory/response variates have a strong linear relationship.

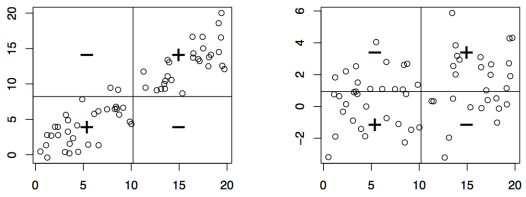
2 January 9, 2018

2.1 Correlation coefficient and covariance

Note: the measure r is also the covariance divided by the standard deviations or

$$r = \frac{cov(X, Y)}{\sigma_X \sigma_Y}$$

Note that the covariance $E[(X - E[X])(Y - E[Y])]$ can be graphically separated by the means $\bar{X}$ and $\bar{Y}$.



One can see that the covariance signage is determined by the sum of the magnitudes in the positive and negative quadrants.

2.2 Simple linear regression (SLR) model

An SLR model can be thought of as a line with covariates x and y where

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i \quad i = 1, \ldots, n$$

where ϵ_i is some error term for each i.

Example 2.1. From the dataset

Overhead	Office Size
218955	1589
224513	1912
⋮	⋮

Thus we have the SLR model

$$218955 = \beta_0 + \beta_1(1589) + \epsilon_1$$
$$224513 = \beta_0 + \beta_1(1912) + \epsilon_2$$

2.3 Methods of least squares

Find (estimate) the value of β_0, β_1 (denoted by $\hat{\beta}_0, \hat{\beta}_1$, respectively) that minimizes the sum of squares of the errors $\sum_{i=1}^n \epsilon_i^2$. That is: we find values of β_0, β_1 that minimizes the function

$$S(\beta_0, \beta_1) = \sum_{i=1}^n \epsilon_i^2 = \sum_{i=1}^n [y_i - (\beta_0 + \beta_1 x_i)]^2$$

We take the partial derivatives and set to 0 to find the minimum (assuming convexity)

$$\frac{\partial S}{\partial \beta_0} = -2 \sum_{i=1}^n y_i - (\beta_0 + \beta_1 x_i) = 0$$
$$\frac{\partial S}{\partial \beta_1} = -2 \sum_{i=1}^n x_i [y_i - (\beta_0 + \beta_1 x_i)] = 0$$

which yields (the notation changes to estimates of β assuming we can calculate those)

$$\sum_{n=1}^n y_i = n\hat{\beta}_0 + \sum_{n=1}^n x_i \hat{\beta}_1$$
$$\sum_{n=1}^n x_i y_i = \sum_{i=1}^n x_i \hat{\beta}_0 + \sum_{n=1}^n x_i^2 \hat{\beta}_1$$

which gives us the estimates

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$
$$\hat{\beta}_1 = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sum (x_i - \bar{x})^2} = \frac{S_{xy}}{S_{xx}}$$

where the second equation follows from substituting in the first and re-deriving for $\frac{\partial S}{\partial \beta_1}$.
The corresponding fitted line is

$$\hat{\mu}_{y|X=x} = \hat{\mu} + \hat{\beta}_0 + \hat{\beta}_1 x$$

For the example with overhead above, we'd have

$$\hat{\mu} = -27877.06 + 126.33x$$

2.4 Fitted residuals

These are the difference between the actual values and our fitted value (distinct from the error terms previously)

$$e_i = (y_i - \hat{\mu_i}) = y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_i)$$

Some **key points** regarding this model

- By estimating two parameters (β_0, β_1), we have imposed two constraints on our residuals (from our partial derivatives)

$$\sum e_i = 0$$
$$\sum x_i e_i = 0$$

  These reduces our number of n independent measures by 2 since we can compute the remaining two residuals from $n-2$ observations. Thus we have $n-2$ **degrees of freedom** (or in general, $n-k$ dfs where k is the number of estimated parameters>).

2.5 Interpretation of estimated parameters $\hat{\beta}_i$

β_1

$$\begin{aligned} \hat{\mu} &= \hat{\beta}_0 + \hat{\beta}_1 x \\ \hat{\mu_{x+1}} &= \hat{\beta}_0 + \hat{\beta}_1 (x+1) \\ &= \hat{\beta}_0 + \hat{\beta}_1 x + \hat{\beta}_1 \\ &= \hat{\mu} + \hat{\beta}_1 \end{aligned}$$

thus $\hat{\beta}_1$ can be interpreted as the estimated mean change in the response (y) associated with one unit change of x.

β_0 For $x = 0$, $\hat{\mu} = \hat{\beta}_0$.

However, in the example with overhead, it's evident that when $x = 0$ overhead is negative (-27877.06) which is nonsensical.

Never extrapolate results outside the range of the values of the explanatory variate(s).

3 January 16, 2018

3.1 Invariants for normal SLR models

Recall for the normal SLR model we have

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i \quad i = 1, \ldots, n$$

where $\epsilon_i \sim N(0, \sigma^2)$ is some error term for each i.

- $\beta_0 + \beta_1 x_i$ is the **deterministic** and ϵ_i is the **random** components of the model.
- $Var(\epsilon_i) = \sigma^2$ for all i (constant variance)
- ϵ_i, ϵ_j for $i \neq j$ are independent (otherwise we'd need time series)

3.2 Estimate of variance in SLR

Each of our error terms follow a $N(0, \sigma^2)$ distribution. The **unbiased** estimate of σ^2 is

$$\hat{\sigma}^2 = \frac{\sum_{i=1}^{n} e_i^2}{n-2}$$

The **residual standard error** is $\hat{\sigma} = \sqrt{\frac{\sum e_i^2}{n-2}}$.

3.3 Unbiased estimator of $\hat{\beta}_1$

The **estimator** of $\hat{\beta}_1$ is a random variable $\hat{\beta}_1$ (usually denoted with a big B) that is similar to the estimate but with r.v. Y_i and $\bar{Y}$

$$\hat{\beta}_1 = \frac{\sum(x_i - \bar{x})(Y_i - \bar{Y})}{\sum(x_i - \bar{x})^2}$$

Note: $\hat{\beta}_1$ can be expressed as a linear combination of response variables Y_i, $i = 1, 2, \ldots, n$.

$$\begin{aligned}
\hat{\beta}_1 &= \frac{\sum(x_i - \bar{x})Y_i - \bar{Y}\sum(x_i - \bar{x})}{S_{xx}} \\
&= \frac{\sum(x_i - \bar{x})Y_i}{S_{xx}} && \sum(x_i - \bar{x}) = 0 \\
&= \sum_{i=1}^{n} c_i Y_i && c_i = \frac{(x_i - \bar{x})}{S_{xx}}
\end{aligned}$$

Remember that

$$\begin{aligned}
&\epsilon_i \sim N(0, \sigma^2) \text{ independent } \Rightarrow Y_i \sim N(\beta_0 + \beta_1 x, \sigma^2) \text{ independent} \\
\Rightarrow &\hat{\beta}_1 \sim \text{ Normal (sum of independent normal r.v.'s)}
\end{aligned}$$

Thus we have

$$\begin{aligned}
E(\hat{\beta}_1) = E(\sum c_i Y_i) &= \sum c_i E(Y_i) \\
&= \sum(\frac{(x_i - \bar{x})}{S_{xx}})(\beta_0 + \beta_1 x_i) \\
&= \frac{\beta_0 \sum(x_i - \bar{x}) + \beta_1 \sum x_i(x_i - \bar{x})}{S_{xx}} \\
&= \frac{\beta_1 \sum x_i(x_i - \bar{x}) - \beta_1 \bar{x} \sum(x_i - \bar{x})}{S_{xx}} && \text{eliminate and introduce 0 term} \\
&= \frac{\beta_1 \sum(x_i - \bar{x})(x_i - \bar{x})}{\sum(x_i - \bar{x})^2} \\
&= \beta_1
\end{aligned}$$

Since $E(\hat{\beta}_1) = \beta_1$, then $\hat{\beta}_1$ is an unbiased estimator of β_1.

The variance of our estimator $\hat{\beta}_1$ is

$$\begin{aligned} Var(\hat{\beta}_1) &= Var(\sum c_i Y_i) \\ &= \sum c_i^2 Var(Y_i) && Y_i \text{ independent} \\ &= \sum \frac{\sigma^2 (x_i - \bar{x})^2}{S_{xx}^2} \\ &= \frac{\sigma^2}{S_{xx}} \\ &= \frac{\sigma^2}{\sum (x_i - \bar{x})^2} \end{aligned}$$

Since our estimator $\hat{\beta}_1$ follows (from above)

$$\hat{\beta}_1 \sim N(\beta_1, \frac{\sigma^2}{S_{xx}})$$

we have

$$\frac{\hat{\beta}_1 - \beta_1}{\frac{\sigma}{\sqrt{S_{xx}}}} \sim N(0,1)$$

in terms of the sample variance (or estimate $\hat{\sigma}$ we have the **T-distribution**)

$$\frac{\hat{\beta}_1 - \beta_1}{\frac{\hat{\sigma}}{\sqrt{S_{xx}}}} \sim t_{n-2}$$

3.4 Identities of distributions

Recall that the distribution of the sample means follows a normal distribution

$$\bar{X} \sim N(\mu, \frac{\sigma^2}{n})$$

so we have

$$\frac{\bar{X} - \mu}{\frac{\sigma}{\sqrt{n}}} \sim N(0,1)$$

$$\frac{\bar{X} - \mu}{\frac{\hat{\sigma}}{\sqrt{n}}} \sim t_{n-1}$$

This follows from

$$\begin{aligned}
SD(X) &= \sigma \\
SE(X) &= \hat{\sigma} \\
SD(\bar{X}) &= \frac{\sigma}{\sqrt{n}} \\
SE(\bar{X}) &= \frac{\hat{\sigma}}{\sqrt{n}} \\
\frac{\bar{X} - \mu}{SE(\bar{X})} &\sim t_{n-1} \\
\frac{\hat{\beta}_1 - \beta_1}{SE(\hat{\beta}_1)} &\sim t_{n-2}
\end{aligned}$$

4 January 18, 2018

4.1 Inference for β_1 in SLR

"Is there a relationship between overhead and office size (for the population of offices)?"
There is no (linear) relationship $\iff \beta_1 = 0$.
We can statistically check this using two methods

1. Confidence interval for β_1
2. Hypothesis test for β_1 ($H_0 : \beta_1 = 0$)

4.2 Confidence interval for SLR

General example, not necessarily SLR: For a distribution with one parameter μ, we can calculate the $(1-\alpha)100\%$ confidence interval for μ (note: we need only one t value since the T-distribution is symmetric)

$$\begin{aligned}
&\hat{\mu} \pm t_{n-1,1-\frac{\alpha}{2}} \cdot SE(\hat{\mu}) \\
\Rightarrow &\bar{x} \pm t_{n-1,1-\frac{\alpha}{2}} \left(\frac{\hat{\sigma}}{\sqrt{n}} \right)
\end{aligned}$$

where $\bar{x}$ is the sample mean of the distribution.
By a similar line of logic, we can produce confidence intervals for our parameters. The $(1-\alpha)100\%$ confidence interval for β_1 (where the we have $n-2$ degrees of freedom)

$$\hat{\beta}_1 \pm t_{n-2,1-\frac{\alpha}{2}} \cdot SE(\hat{\beta}_1)$$

Example 4.1. The 95% C.I. for β_1 for overhead data is

$$\begin{aligned}
&\hat{\beta}_1 \pm t_{22,0.975} SE(\hat{\beta}_1) \\
=&126.33 \pm 2.074(10.88) \\
=&126.33 \pm 22.57 = (103, 76, 148.90)
\end{aligned}$$

where ± 22.57 is the **margin of error**.

Since $\beta_1 = 0$ is not in the interval, we can conclude that there is a *significant* positive relationship between overhead and office size.

Remark 4.1. An X% confidence interval can be interpreted as: X% of X% confidence intervals established from repeated samples contain the true value.
In other words: they are intervals constructed from a procedure that will contain the population mean for a specified proportion of the time (X% of the time).

4.3 Hypothesis testing for SLR

We form a **null hypthoesis** H_0 and an alternative hypothesis H_1, where we assume H_0 unless there is statistical significance rejecting H_0.
For simple linear regression, we suppose

$$H_0 : \beta_1 = 0 \qquad \text{no relationship}$$
$$H_1 : \beta_1 \neq 0 \qquad \text{two-sided alternative}$$

Our **test statistic** t is the distribution

$$t = \frac{\hat{\beta}_1 - \beta_1}{SE(\hat{\beta}_1)} \sim t_{n-2}$$

Example 4.2. Under H_0 we have for our example

$$t = \frac{126.33 - 0}{10.88} = 11.61$$

If we look at our t_{22} distribution, we find the total probability of the pdf at $P(t \leq 11.61)$ and $P(t \geq 11.61)$ (the **p-value**).
We see that $P(t_{22} > 2.819) = 0.0005 \Rightarrow P(t_{22} > 11.61) << 0.005$.
Thus the p-value is $2P(t_{22} > 11.61) << 0.01$ (in fact, it is 7.47×10^{-11}), which is lower than **0.05 (the significance level)**, so we reject the null hypothesis.

Remark 4.2. The p-value of a hypothesis test can be interpreted as: the probability that our sample holds (the observed, or more extreme, results) under the null hypothesis. If it is extremely low (past a certain threshold), then we may reject the null hypothesis as not possible.

4.4 Two-sided vs one sided tests

The reason why we took both CDF ends of the T-distribution in the example above is to account for a $\hat{\beta}_1$ equally as extreme but on the negative side. Since we assume all this happens to chance, $\hat{\beta}_1$ could equally be the same magnitude but with a negative sign.

4.5 Confidence interval vs hypothesis testing

Deciding which method to use is problem dependent: usually, hypothesis testing is simpler to interpret for many variates and a confidence interval is only relevant for single variates.
A 95% confidence interval corresponds with a hypothesis test with a 0.05 significance level i.e. we will derive an equivalent conclusion.

4.6 Multiple linear regression (MLR) model

We want to model the following relationship

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \ldots + \beta_p x_{ip} + \epsilon_i$$

where $\epsilon_i = N(0, \sigma^2)$ and independent.
Note we have p variates and $p+1$ parameters (the bias term) thus we have $n-(p+1)$ degrees of freedom.
In matrix form, this is represented as

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & x_{12} & \dots & x_{1p} \\ 1 & x_{21} & x_{22} & \dots & x_{2p} \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 1 & x_{n1} & x_{n2} & \dots & x_{np} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

which can be written succinctly as

$$Y = X\beta + \epsilon$$

where $\epsilon = N(\vec{0}, \sigma^2 I)$ or $Var(\epsilon) = \sigma^2 I$ (the **covariance matrix**; note that the covariance between ϵ_i, ϵ_j $i \neq j$ is 0 since they are independent).

5 January 23, 2018

5.1 Least squares estimation of β in MLR

Our residual expression is now, for n observations and p explanatory covariates

$$S(\beta_0, \beta_1, \dots, \beta_p) = \sum [y_i - (\beta_0 + \beta_1 x_{i1} + \dots + \beta_p x_{ip})]^2$$

Taking the partial derivatives with respect to each β_j and finding the minimum

$$\begin{aligned} \frac{\partial S}{\partial \beta_0} &= -2 \sum [y_i - (\beta_0 + \beta_1 x_{i1} + \dots + \beta_p x_{ip})] = 0 \\ \frac{\partial S}{\partial \beta_1} &= -2 \sum x_{i1} [y_i - (\beta_0 + \beta_1 x_{i1} + \dots + \beta_p x_{ip})] = 0 \\ &\vdots \\ \frac{\partial S}{\partial \beta_p} &= -2 \sum x_{ip} [y_i - (\beta_0 + \beta_1 x_{i1} + \dots + \beta_p x_{ip})] = 0 \end{aligned}$$

which can also be expressed as

$$\begin{aligned} &n(\beta_0) + (\sum x_{i1})\beta_1 + \dots + (\sum x_{ip})\beta_p = \sum y_i \\ &(\sum x_{i1})\beta_0 + (\sum x_{i1}^2)\beta_1 + \dots + (\sum x_{i1}x_{ip})\beta_p = \sum x_{i1} y_i \\ &\vdots \\ &(\sum x_{ip})\beta_0 + (\sum x_{i1}x_{ip})\beta_1 + \dots + (\sum x_{ip}^2)\beta_p = \sum x_{ip} y_i \end{aligned}$$

In matrix form, this is written as

$$(X^T X)\hat{\beta} = X^T y$$

yields the best square estimate

$$\hat{\beta} = (X^T X)^{-1} X^T y$$

assuming X is of full rank (i.e. $p+1$ linearly independent columns).

5.2 Estimate of variance in MLR

We can estimate the variance for the error terms (or the variance of the random component in our model) by taking the sum of squared residuals and dividing by the degrees of freedom

$$\hat{\sigma}^2 = \frac{\sum e_i^2}{n-(p+1)} = \frac{\sum[y_i - (\beta_0 + \beta_1 x_{i1} + \ldots + \beta_p x_{ip})]^2}{n-(p+1)}$$

The **residual standard error** is the square root of this or

$$\hat{\sigma} = \sqrt{\frac{\sum e_i^2}{n-(p+1)}}$$

5.3 Hat matrix

The **hat matrix** (also known as the *influence matrix*) maps our responses to predicted values.
Given our predicted mean responses

$$\hat{\mu} = X\hat{\beta} = X(X^TX)^{-1}X^Ty = Hy$$

The matrix H is the hat matrix

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

Some properties of H are:

H is symmetric ($H = H^T$) Note that

$$\begin{aligned} H^T = [X(X^TX)^{-1}X^T]^T &= X[(X^TX)^{-1}]^TX^T \\ &= X[(X^TX)^T]^{-1}X^T \\ &= X(X^TX)^{-1}X^T \\ &= H \end{aligned}$$

$(AB)^T = B^TA^T$

$(A^{-1})^T = (A^T)^{-1}$

H is idempotent ($H = HH$)

$$\begin{aligned} HH &= (X(X^TX)^{-1}X^T)(X(X^TX)^{-1}X^T) \\ &= X[(X^TX)^{-1}(X^TX)](X^TX)^{-1}X^T \\ &= X(X^TX)^{-1}X^T \\ &= H \end{aligned}$$

Note that

$$\hat{\mu} = Hy$$

where our residual is

$$\begin{aligned} e &= y - \hat{\mu} \\ &= y - Hy \\ &= (I - H)y \end{aligned}$$

The residuals are a linear combination of our responses.

So we have

$$\begin{aligned} y &= \hat{\mu} + e \\ &= Hy + (I - H)y \end{aligned}$$

where Hy is orthogonal to $(I-H)y$ (that is: $(Hy)^T(I-H)y = 0$ - follows by expansion and the fact that $H^TH = H$). This implies that $\hat{\mu}_i$ and e_i are independent and thus

$$Cov(\hat{\mu}_i, e_i) = 0$$

5.4 Inference for β in MLR

To infer the meaning of the model parameters $(\beta_0, \beta_1, \ldots, \beta_p)$, we note that

$$\epsilon \sim (0, \sigma^2 I) \Rightarrow Y \sim N(XB, \sigma^2 I)$$

since $Y = X\beta + \epsilon$.
The **distribution of** $\hat{\beta}$ is thus

$$\hat{\beta} = (X^TX)^{-1}X^TY$$

so $\hat{\beta} \sim Normal$.
Its model parameters are

$$\begin{aligned} E[\hat{\beta}] &= E[(X^TX)^{-1}X^TY) \\ &= (X^TX)^{-1}X^TE[Y] \\ &= (X^TX)^{-1}X^T(X\beta) \\ &= \beta \end{aligned}$$

and for the variance

$$\begin{aligned} Var(\hat{\beta}) &= Var((X^TX)^{-1}X^TY) \\ &= [(X^TX)^{-1}X^T]Var(Y)[(X^TX)^{-1}X^T]^T \qquad\qquad Var(AY) = AVar(Y)A^T \\ &= \sigma^2(X^TX)^{-1}X^TX[(X^TX)^{-1}]^T \\ &= \sigma^2(X^TX)^{-1} \end{aligned}$$

thus $\hat{\beta} \sim N(\beta, \sigma^2(X^TX)^{-1})$. Note that for a specific β_j, its marginal distribution is

$$\hat{\beta}_j \sim N(\beta_j, \sigma^2(X^TX)^{-1}_{jj}) \quad j = 0, 1, 2, \ldots, p$$

where $SE(\hat{\beta}_j) = \hat{\sigma}\sqrt{(X^TX)^{-1}_{jj}}$.
One can see that the variance is not constant (some parameters will be estimated with a larger confidence interval) since

$$Var(\hat{\beta}_j) = \sigma^2(X^TX)^{-1}_{jj}$$

where the diagonal entries are not the same.
It is often common for β_j to change as more covariates are added to a multiple linear model. This implies each

explanatory covariate are correlated and thus

$$Cov(\hat{\beta}_j, \hat{\beta}_k) = \sigma^2 (X^T X)^{-1}_{jk} \neq 0$$

The covariance of β_j, β_k $j \neq k$ can all be 0 if all explanatory variates are independent.

Remark 5.1. Covariate x_j, x_k are independent *iff* $Cov(\hat{\beta}_j, \hat{\beta}_k) = 0$.

The β_js can be interpreted as: keeping all other covariates in the model constant, what is the mean response of my covariate x_j? In effect, multiple linear regression corrects for other covariates.

5.5 Confidence interval in MLR

Note: this is a confidence interval for the parameter β_j, not the estimate $\hat{\beta}_j$.
For a $(1-\alpha)100\%$ confidence interval we have

$$\hat{\beta}_j \pm t_{n-(p+1),1-\frac{\alpha}{2}} SE(\hat{\beta}_j)$$

Example 5.1. For example, the 95% CI for β_1 (size) in the overhead example is

$$\begin{aligned} &\hat{\beta}_1 \pm t_{18,0.975} SE(\hat{\beta}_1) \\ =&31.26 \pm 2.101(21.47) \\ =&31.26 \pm 45.11 \Rightarrow (-13.85, 76.37) \end{aligned}$$

since the CI encompasses 0, we conclude there is no significant relationship of size with respect to overhead *after accounting for other covariates.*

5.6 Hypothesis testing in MLR

The null hypothesis for testing if a covariate is related to the response is

$$H_0 : \beta_j = 0$$

where we have the test statistic

$$t = \frac{\hat{\beta}_j - 0}{SE(\hat{\beta}_j)} \sim t_{n-(p+1)}$$

under H_0.

Example 5.2. For β_1 (size), we have

$$t = \frac{31.26}{21.47} = 1.46$$

From the t-distribution table for $n = 18$, we see that this corresponds to a p-value between 0.1 and 0.2 (0.1625 to be exact).
We therefore do not reject H_0 (p-value > 0.05) i.e. there is no significant relationship between overhead nad size, after accounting for the other variates.

6 January 25, 2018

6.1 Scater plot matrix

For a given set of explanatory variates and a response variate, we can plot a matrix of 2D scatter plots of each variate against all the other variates.

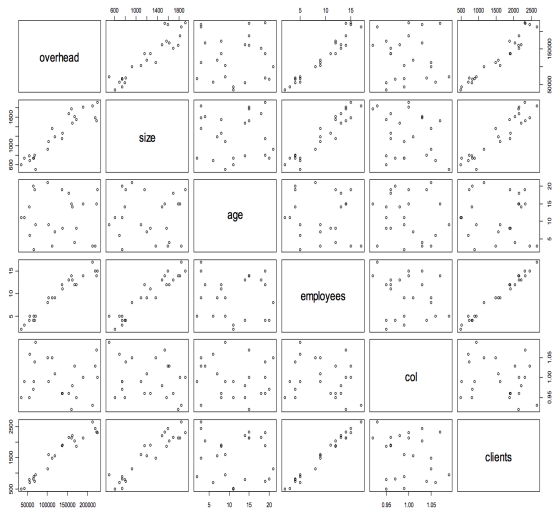


Figure 6.1: Size, employees, and clients are all correlated with overhead. Note however that size, employees, and clients are all correlated with each other therefore it would probably suffice to only include one of these explanatory variates without losing much information in our model.

From this matrix, we can visually see which explanatory variates are correlated to the explanatory variate but also which explanatory variates are correlated with each other.

6.2 Multicollinearity

When strong (linear) relationships are present among two or more explanatory variates, we say the variates exhibit **multicollinearity**.
Intuitively, multicollinearity means some explanatory variates are dependent and it would not be required to have all the extraneous dependent variates in model since they do not introduce much additional explained variance/information.
In fact, multicollinear is **detrimental**: it leads to inflated variances of the associated parameter estimates ($(X^TX)^{-1}$ has inflated diagonal entries, thus $SE(\hat{\beta}_j) = \hat{\sigma}\sqrt{(X^TX)^{-1}_{jj}}$ is inflated), resulting in inaccurate conclusions from hypothesis tests and confidence intervals (which depend on $SE(\hat{\beta}_j)$) (intuitively, our estimate of the impact of one unit change of x_j, $\hat{\beta}_j$, while controlling for the others tend to be less precise since there is some dependency happening when "changing" x_j with another correlated x_k).

6.3 Variance inflation factor (VIF)

To assess whether a variate x_j is a problem in terms of multicollinearity, we can regress x_j onto all other explanatory variates. We can then caclulate the **variance inflation factor** for x_j

$$\text{VIF}_j = \frac{1}{1 - R_j^2}$$

The VIF_j can be interpreted as the factor by which the variance of $\hat{\beta}_j$ is increased relative to the ideal case in which all explanatory variates are uncorrelated (i.e. columns of X are orthogonal).

Example 6.1. Suppose we do this for $x_j = x_3$: we regress the number of employees on all other explanatory variates (see scatter plot matrix above).
We have $R_3^2 = 0.9855$, thus we have a VIF of $\frac{1}{1-R_3^2} = 68.97$. So the variance is inflated $\approx 69x$ because of multicollinearity (compared to the case where we just have x_3).

As a general rule of thumb: multicollinearity is a serious problem if VIF > 10 (or thereabouts), which corresponds to an $R_j^2 > 0.9$.

7 January 30, 2018

7.1 Maximum likelihood estimation (MLE)

A remark on least squares estimation of β: for a model with *normal errors*, *maximum likelihood estimation (MLE)* and *least squares estimation (LSE)* are equivalent.
The **maximum likelihood estimation** is defined as

$$\begin{aligned} L(\beta_0, \beta_1, \ldots, \beta_p \mid y_1, \ldots, y_n) &= \prod_{i=1}^{n} P(y_i) \\ &= \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} e^{\frac{-(y_i-\mu_i)^2}{2\sigma^2}} \\ &= (2\pi\sigma^2)^{\frac{-n}{2}} e^{\frac{-\sum(y_i-\mu_i)^2}{2\sigma^2}} \qquad \mu_i = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} \end{aligned}$$

Taking the log likelihood function

$$l = \log(L) = c - \frac{\sum[y_i - (\beta_0 + \beta_1 x_{i1} + \ldots + \beta_p x_{ip}]^2}{2\sigma^2} \qquad = S(\beta_0, \beta_1, \ldots, \beta_p) = \sum \epsilon_i^2 \quad \text{from LSE}$$

7.2 Gauss-Markov theorem

Consider the model given by $Y = X\beta + \epsilon$ where $E(\epsilon) = 0, Var(\epsilon) = \sigma^2 I$. The G-M theorem states that among all unbiased linear estimators $\hat{\beta}^* = M^* Y$, the LSE given by $\hat{\beta} = MY$ (where $M = (X^T X)^{-1} X^T$ in LSE) has the smallest variance.
That is

$$Var(\hat{\beta}^*) = Var(\hat{\beta}) + \sigma^2 (M^* - M)(M^* - M)^T$$

where $(M^* - M)(M^* - M)^T$ is a positive semidefinite matrix (a matrix A is positive semidefinite if $a^T A a \geq 0$ for any vector a).

7.3 Confidence interval for μ_{new}

Example 7.1. Provide an interval in which the mean overhead of a 1000 sq ft office that is 12 years old, has a $col = 1.02$ and 1300 clients lies.

Note we can find the **confidence interval for** μ_{new} or a new mean response.

$$\hat{\mu}_{new} = \hat{\beta}_0 + \hat{\beta}_1 x_{new,1} + \ldots + \hat{\beta}_p x_{new,p}$$

which is in vector form: $x_{new}^T\hat{\beta}$ where $x_{new}^T = (1, x_{new,1}, \ldots, x_{new,p})$.
The distribution of $\hat{\mu}_{new}$ can be derived. Recall that

$$\hat{\beta} \sim N(\beta, \sigma^2(X^TX)^{-1})$$

so we know that $\hat{\mu}_{new} \sim Normal$. Furthermore

$$\begin{aligned} E[\hat{\mu}_{new}] &= \mu_{new} = x_{new}^T\beta \\ Var(\hat{\mu}_{new}) &= Var(x_{new}^T\hat{\beta}) \\ &= x_{new}^T Var(\hat{\beta}) x_{new} \\ &= \sigma^2 x_{new}^T (X^TX)^{-1} x_{new} \end{aligned}$$

Thus we have

$$\hat{\mu}_{new} \sim N(\mu_{new}, \sigma^2 x_{new}^T (X^TX)^{-1} x_{new})$$

which has the corresponding pivotal distribution

$$\frac{\hat{\mu}_{new} - \mu_{new}}{\hat{\sigma}\sqrt{x_{new}^T(X^TX)^{-1}x_{new}}} \sim t_{n-(p+1)}$$

Thus the $(1-\alpha)100\%$ CI for μ_{new} is

$$\hat{\mu}_{new} \pm t_{n-(p+1),1-\frac{\alpha}{2}}\hat{\sigma}\sqrt{x_{new}^T(X^TX)^{-1}x_{new}}$$

Example 7.2. In the overhead model, we have $x_{new}^T = (1, 1000, 12, 1.02, 1300)$.
So the 95% CI for μ_{new} is

$$(97460.07, 112202.30)$$

where $\hat{\mu}_{new} = 104831.2$ and the margin of error is 7371.1.

Remark 7.1. A confidence interval only establishes an estimate interval *for a population parameter*, but not a particular random variable. We would need to use a **prediction interval** to establish an estimate for Y_{new}.

7.4 Prediction interval for Y_{new}

Example 7.3. An office is 1000 sq ft, 12 years old, with 1300 clients and a $col = 1.02$. Provide an interval for the overhead of **this (particular) office**.

Remark 7.2. This question is different than the previous one since it asks for an interval for a particular office *rather than the mean overhead* of an office of this characteristic in the population.

Consider the prediction error given by $Y_{new} - \hat{\mu}_{new}$. Thus we have

$$\begin{aligned} Var(Y_{new} - \hat{\mu}_{new}) &= Var(Y_{new}) + Var(\hat{\mu}_{new}) && \text{independence} \\ &= \sigma^2 + \sigma^2 x_{new}^T(X^TX)^{-1}x_{new} \\ &= \sigma^2(1 + x_{new}^T(X^TX)^{-1}x_{new}) \end{aligned}$$

where $Y_{new}, \hat{\mu}_{new}$ are independent since any new observations do not depend on our estimate.

Thus the $(1-\alpha)100\%$ prediction interval for Y_{new} is

$$\hat{\mu}_{new} \pm t_{n-(p+1),1-\frac{\alpha}{2}} \hat{\sigma} \sqrt{1 + x_{new}^T (X^T X)^{-1} x_{new}}$$

Example 7.4. In the overhead model, we still have the same x_{new}^T so we get for the 95% prediction interval

$$(73946.20, 135715.70)$$

where $\hat{\mu}_{new} = 104831.2$ (same as CI) and the margin of the error is 30884.5 (much larger than the MoE in the CI).

Note that for the SLR model, the confidence interval and the prediction interval standard errors reduce to

$$\hat{\sigma} \sqrt{\frac{1}{n} + \frac{(x_{new} - \bar{x})^2}{S_{xx}}}$$

and

$$\hat{\sigma} \sqrt{1 + \frac{1}{n} + \frac{(x_{new} - \bar{x})^2}{S_{xx}}}$$

respectively. Note that the errors are smaller as x_{new} is closer to the mean/centre $\bar{x}$ as we can see in the prediction and confidence bands.

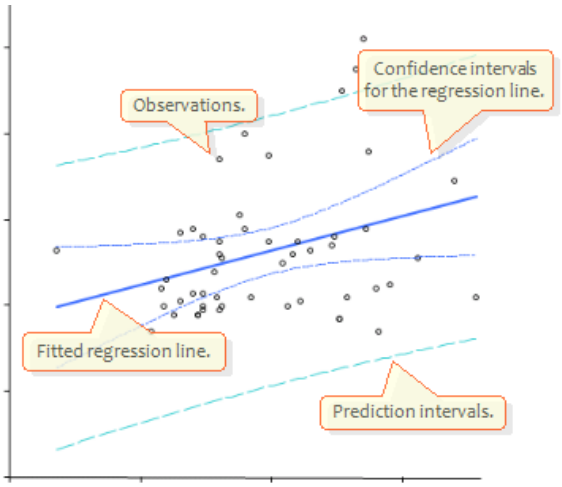


Figure 7.1: The confidence and prediction bands are smaller in closer to the centre of the x's or closer to $\bar{x}$. Furthermore, the prediction bands lie further out from the confidence bands.

8 February 1, 2018

8.1 Modelling categorical variates

Example 8.1. Promotion study: does a wing promotion have any effect on sales? Do different types of promotion affect sales differently?
The sampling protocol is as follows:

- 30 stores randomly selected from population
- 10 stores are randomly assigned to one of three promotion types: promo1, promo2, no promotion (control)

- response variate: change (%) in sales over two-week period of study

One **inappropriate approach may be**:

$$Y_i = \beta_0 + \beta_1 x_i + \epsilon_i \quad \epsilon_i \sim N(0, \sigma^2) \text{ ind.}$$

where

$$x_i = \begin{cases} 1 & \text{if ith store uses promo1} \\ 2 & \text{if ith store uses promo2} \\ 3 & \text{if ith store has no promo} \end{cases}$$

There may be no linear relationship depending on the way we assign x_i (e.g. promo 1 has a higher mean response, promo 2 has a lower mean response, no promo has a higher mean response). This model is too **restrictive**.
A more *flexible model*:

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \epsilon_i \quad \epsilon_i \sim N(0, \sigma^2)$$

where $x_{i1} = 1$ if ith store uses promo1 (0 otherwise) and $x_{i2} = 1$ if ith store uses promo2.
This is similar to *one-hot encoding* and these are called **indicator or dummy variates**.
Our data might look like

store(i)	x_{i1}	x_{i2}
1	0	0
2	0	0
⋮	⋮	⋮
10	1	0
11	1	0
⋮	⋮	⋮
21	0	1
22	0	1
⋮	⋮	⋮
30	0	1

Suppose we consider adding $x_{i3} = 1$ when the ith store has no promo and 0 otherwise. Then we have our X matrix as

$$\begin{bmatrix} 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 0 & 1 & 0 \end{bmatrix} \tag{8.1}$$

note that $x_{i3} = 1 - (x_{i1} + x_{i2})$ so we have a linear dependent column.
This implies $\text{rank}(X) = 3$ which is not of full rank, thus $X^T X$ is not invertible.

To interpret/inference our parameters, note that the estimate response or estimated change of sales (in %) is given by

$$\hat{\mu} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2$$

So for a store that does not have any promos

$$\hat{\mu} = \hat{\beta}_0 + \hat{\beta}_1(0) + \hat{\beta}_2(0) = \hat{\beta}_0$$

Similarly for promo 1 stores

$$\hat{\mu} = \hat{\beta}_0 + \hat{\beta}_1$$

and for the promo 2 stores

$$\hat{\mu} = \hat{\beta}_0 + \hat{\beta}_2$$

From our data, we may get the regression summary

```
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept)   -0.870      1.665  -0.523  0.60552
x1             8.350      2.354   3.547  0.00145 **
x2             2.970      2.354   1.261  0.21792
```

We can't conclude anything about the control case (no promo) and the promo 2 group, but we can conclude that the estimated increase in sales (relative to the control) using promo1 is 8.35% (p-value < 0.05).
More formally, is there a **difference in mean increase in sales** between no promo and promo1 stores? We can assume the null hypothesis $H_0 : \beta_1 = 0$ (no change in promo1 sales) and alternative hypothesis $H_a : \beta_1 \neq 0$.
Thus we have the test statistic

$$\begin{aligned} t &= \frac{\hat{\beta}_1 - \beta_1}{SE\hat{\beta}_1} \\ &= \frac{\hat{\beta}_1 - 0}{SE\hat{\beta}_1} \\ &= 3.547 \end{aligned}$$

We can look up the T-distribution with $30 - 3 = 27$ degrees of freedom to figure out that the p-value is 0.00145. We *reject* H_0: so using promo1 is associated with a significantly higher mean sales than no wing promotion.
A more nuanced question: is there a difference in mean sales between promo1 and promo2? This is not quite clear from our regression summary. Thus we use hypothesis testing with null hypothesis $H_0 : \beta_1 - \beta_2 = 0$. What about our test statistic?
One approach is

$$t = \frac{(\hat{\beta}_1 - \hat{\beta}_2) - 0}{SE(\hat{\beta}_1 - \hat{\beta}_2)} \sim t_{27}$$

under H_0. But what is the standard error? We need to take the variance of $\hat{\beta}_1 - \hat{\beta}_2$. Recall that the variances of $\hat{\beta}$ are

$$\begin{aligned} &\hat{\beta} \sim N(\beta, \sigma^2(X^T X)^{-1}) \\ &\hat{\beta}_j \sim N(\beta_j, \sigma^2(X^T X)^{-1}_{jj}) \\ &\Rightarrow Cov(\hat{\beta}_j, \hat{\beta}_k) = \sigma^2(X^T X)^{-1}_{jk} \end{aligned}$$

so we have

$$\begin{aligned} Var(\hat{\beta}_1 - \hat{\beta}_2) &= Var(\hat{\beta}_1) + Var(\hat{\beta}_2) - 2Cov(\hat{\beta}_1, \hat{\beta}_2) \\ &= \sigma^2(X^TX)^{-1}_{11} + \sigma^2(X^TX)^{-1}_{22} - 2\sigma^2(X^TX)^{-1}_{12} \\ &= \sigma^2[(X^TX)^{-1}_{11} + (X^TX)^{-1}_{22} - 2(X^TX)^{-1}_{12}] \end{aligned}$$

Thus our standard error is

$$SE(\hat{\beta}_1 - \hat{\beta}_2) = \hat{\sigma}\sqrt{(X^TX)^{-1}_{11} + (X^TX)^{-1}_{22} - 2(X^TX)^{-1}_{12}}$$

Another more general approach is the **F-test (ANOVA)**.

9 February 6, 2018

9.1 X matrices with orthogonal columns

$Y = X\beta + \epsilon$. Suppose we are designing an experiment where the response is the shrinkage of a part (%) during molding process. There are 3 factors: Temp(L,H), Pressure(L,H), Speed(L,H). We thus have 2^3 unique experimental runs

run	T	P	S
1	L	L	L
2	L	L	H
3	L	H	L
4	L	H	H
5	H	L	L
6	H	L	H
7	H	H	L
8	H	H	H

Therefore we have as our model

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \epsilon$$

where

$$x_{i1} = \begin{cases} 1 & \text{if ith run uses H temp} \\ 0 & \text{otherwise (L temp)} \end{cases}$$

$$x_{i2} = \begin{cases} 1 & \text{if ith run uses H pressure} \\ 0 & \text{otherwise (L pressure)} \end{cases}$$

$$x_{i3} = \begin{cases} 1 & \text{if ith run uses H speed} \\ 0 & \text{otherwise (L speed)} \end{cases}$$

There is an **alternative coding** scheme where we use -1 instead of 0

$$x_{i1} = \begin{cases} 1 & \text{if ith run uses H temp} \\ -1 & \text{otherwise (L temp)} \end{cases}$$
$$x_{i2} = \begin{cases} 1 & \text{if ith run uses H pressure} \\ -1 & \text{otherwise (L pressure)} \end{cases}$$
$$x_{i3} = \begin{cases} 1 & \text{if ith run uses H speed} \\ -1 & \text{otherwise (L speed)} \end{cases}$$

So our X matrix becomes

$$X = \begin{bmatrix} 1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

Remark 9.1. All the columns in X are orthogonal.

By noting columns i, j where $i \neq j$ are orthogonal, we can easily see that

$$X^T X = \begin{bmatrix} 8 & 0 & 0 & 0 \\ 0 & 8 & 0 & 0 \\ 0 & 0 & 8 & 0 \\ 0 & 0 & 0 & 8 \end{bmatrix}$$

Taking the inverse, we get

$$(X^T X)^{-1} = \begin{bmatrix} \frac{1}{8} & 0 & 0 & 0 \\ 0 & \frac{1}{8} & 0 & 0 \\ 0 & 0 & \frac{1}{8} & 0 \\ 0 & 0 & 0 & \frac{1}{8} \end{bmatrix}$$

10 February 8, 2018

10.1 Interpretation of parameters for categorical $-1, 1$ variates

Previously we chose $-1, 1$ as values for our indicator variates as opposed to $0, 1$. How do we interpret the parameter estimates now that $x_{ik} \in \{1, -1\}$ (how do we interpret 1 unit of change which is now halved on this scale)? Taking a look at the previous example we have for two different trials where Tep is toggled between L and H

$$\begin{aligned} \{L, L, L\} : \hat{\mu} &= \hat{\beta}_0 - \hat{\beta}_1 - \hat{\beta}_2 - \hat{\beta}_3 \\ \{H, L, L\} : \hat{\mu} &= \hat{\beta}_0 + \hat{\beta}_1 - \hat{\beta}_2 - \hat{\beta}_3 \\ &= (\hat{\beta}_0 - \hat{\beta}_1 - \hat{\beta}_2 - \hat{\beta}_3) + 2\hat{\beta}_1 \end{aligned}$$

So we have $\hat{\mu}_{HLL} = \hat{\mu}_{LLL} + 2\hat{\beta}_1$.

Suppose we get $\hat{\beta}_1 = -0.2875$ in the MLR. Then we have

$$2\hat{\beta}_1 = -0.5750$$

So holding all other factors constant running temperature at a high level is associated with an estimated decrease of 0.5750% in shrinkage compared to running at low temp (since the p-value is ≥ 0.05, there is no statistical significant relationship).

10.2 Independence of indicator variates

Note from our X^TX matrix, we see that $Cov(\hat{\beta}_j, \hat{\beta}_k) = \sigma^2(X^TX)^{-1}_{jk} = 0$ for $j \neq k$.
So if we were to take out an explanatory variate, the parameter estimates will not change (no linear dependency between them). **However, it's possible for the p-value to change**.
For example, in a sample dataset we see that the p-value for pressure was 0.0978 (not significant) after correcting for temperature and speed, but was 0.0421 (significant) with just an SLR (just pressure regressed onto shrinkage). Why is this the case? Well when we removed some variates, we **increased our degrees of freedom**. Algebraically we had

$$\hat{\sigma} = \sqrt{\frac{\sum e_i^2}{df}}$$

and for our standard errors for our parameter we had

$$SE(\hat{\beta}_j) = \hat{\sigma} \cdot \sqrt{(X^TX)^{-1}_{jj}}$$

thus in our reduced model, as the degrees of freedom increases as we take away parameters, our residual standard error decreases hence $SE(\hat{\beta}_j)$ decreases. This is especially true for small samples with low degrees of freedom.

Example 10.1. In our shrinkage vs temperature, pressure and speed we originally had in the "full" model

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \epsilon \quad \epsilon \sim N(0, \sigma^2) \text{ independent}$$

This corresponds to

$$\hat{\sigma} = \sqrt{\frac{\sum e_i^2}{4}} = 3.271 \Rightarrow SE(\hat{\beta}_j) = \hat{\sigma}\sqrt{(X^TX)^{-1}_{jj}} = 1.1563$$

By reducing our model down to only one explanatory variate pressure, we have

$$Y = \beta_0 + \beta_2 x_2 + \epsilon \quad \epsilon \sim N(0, \sigma^2) \text{ independent}$$

$$\hat{\sigma} = \sqrt{\frac{\sum e_i^2}{6}} = 2.733 \Rightarrow SE(\hat{\beta}_j) = 0.9662$$

Note however the p-value does not decrease in general when removing variates. This only happens when the explained variance/variation (see **ANOVA**) of the removed variates is relatively small compared to the increase in the degrees of freedom when those variates are removed. If we had repeated the above experiment many times (to have a larger *df*) then the p-value will differ less.

10.3 Analysis of Variance (ANOVA) and additional sum of squares

Recall that the **sample variance** is given by

$$s^2 = \frac{\sum(y_i - \bar{y})^2}{n-1}$$

We want to decompose the sum of squares into two parts: one for the variance we can explain with our model and one for the variance we cannot explain. Doing this algebraically

$$\begin{aligned}\sum_{i=1}^{n}(y_i-\bar{y})^2 &= \sum(y_i-\hat{\mu}_i+\hat{\mu}_i-\bar{y})^2 \\ &= \sum(y_i-\hat{\mu}_i)^2+\sum(\hat{\mu}_i-\bar{y})^2+2\sum(y_i-\hat{\mu}_i)(\hat{\mu}_i-\bar{y})\end{aligned}$$

For the last term we have

$$\begin{aligned}\sum(y_i-\hat{\mu}_i)(\hat{\mu}_i-\bar{y}) &= \sum\hat{\mu}_i(y_i-\hat{\mu}_i)-\bar{y}\sum(y_i-\hat{\mu}_i) \\ &= \sum\hat{\mu}_i e_i-\bar{y}\sum e_i \\ &= \hat{\mu}^T e && \textstyle\sum e_i=0 \\ &= 0 && \hat{\mu}, e \text{ is orthogonal}\end{aligned}$$

Remark 10.1. e and $\hat{\mu}$ are orthogonal because we have

$$\begin{aligned}\hat{\mu}^T e &= \sum\hat{\mu}_i e_i \\ &= \sum(\hat{\beta}_0+\hat{\beta}_1 x_i)e_i \\ &= \hat{\beta}_0\sum e_i+\hat{\beta}_1\sum x_i e_i \\ &= 0 && \textstyle\sum e_i=0 \text{ and } \sum x_i e_i=0 \text{ from derivation of } \hat{\beta}_i \text{ (see Fitted residuals)}\end{aligned}$$

Thus we have

$$\begin{aligned}\sum_{i=1}^{n}(y_i-\bar{y})^2 &= \sum(y_i-\hat{\mu}_i)^2+\sum(\hat{\mu}_i-\bar{y})^2 \\ SS(Tot) &= SS(Res)+SS(Reg)\end{aligned}$$

where $SS(Reg)$ is the variation our regression model accounts for (or **explained sum of squares**), and $SS(Res)$ is the **residual sum of squares**.

10.4 Coefficient of determination R^2

For the SLR case, R^2 is exactly the square of the coefficient of correlation r.
For the MLR case (and in general), it is equivalent to

$$R^2=\frac{SS(Reg)}{SS(Tot)}$$

or the **proportion of variation explained by our model**. Rewriting in terms of $SS(Res)$ or the sum of squares not explained by our model

$$R^2=\frac{SS(Tot)-SS(Res)}{SS(Tot)}=1-\frac{SS(Res)}{SS(Tot)}$$

10.5 Testing if any variates are related to response

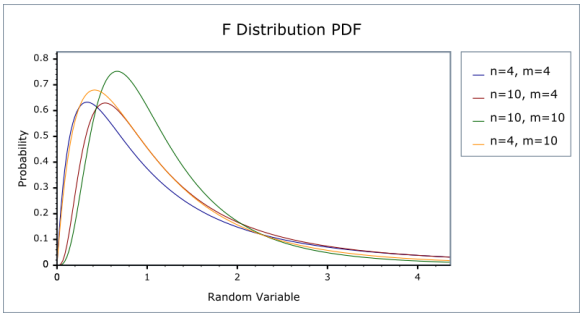
The F-test will check if there is, for example, a relationship between overhead (response variate) and **at least one** of size, age, col, or clients (explanatory variates). That is: its null hypothesis is (note that β_0 is not included)

$$H_0 : \beta_1 = \beta_2 = \beta_3 = \beta_4 = 0$$
$$H_a : \text{ at least one of } \beta_j \neq 0 \quad j = 1, 2, 3, 4$$

What would be the test statistic we use for this? Obviously we cannot use a T distribution and T-statistic like before. We want our statistic to be large when our model explains a lot of variation relative to the variation we cannot explain. We would also like to correct for the degrees of freedom, thus we have

$$F = \frac{MS(Reg)}{MS(Res)} = \frac{\frac{SS(Reg)}{p}}{\frac{SS(Res)}{(n-(p+1))}}$$

where $MS(\cdot)$ is the mean squared error (we will later see that this is a special case of the more general F-statistic). Under $H_0 : F \sim F_{p,n-(p+1)}$. Under H_0, we expect $F = 1$.
Note that $F \geq 0$, so the F-distribution looks something like



Example 10.2. For our overhead study, our $H_0 : \beta_1 = \beta_2 = \beta_3 = \beta_4 = 0$. We got from our regression summary in R

$$F = \frac{MS(Reg)}{MS(Res)} = 100.5$$

Note that the p-value $= P(F > 100.5) = 1.661 \times 10^{-12}$ (one-tailed!). So we reject H_0 so at least one of size, age, col or clients is significantly related to overhead.

11 February 13, 2018

11.1 ANOVA table in R

A sample output from R for the ANOVA table

```
1 Response: y
2 Df Sum Sq  Mean Sq F value Pr(>F)
3 x          1 0.0049 0.004897  0.0574 0.8112
4 Residuals 98 8.3654 0.085361
```

The fields correspond to

Source	df	SS	MS	F	p-value
Reg	p	$SS(Reg)$	$\frac{SS(Reg)}{p}$	$\frac{MS(Reg)}{MS(Res)}$	$P(F > F_{p,n-(p+1)})$
Res	$n-(p+1)$	$SS(Res)$	$\frac{SS(Res)}{n-(p+1)}$		
Tot	$n-1$	$SS(Tot)$	$n-1$		

11.2 F-test and ANOVA

After accounting for col index and # of clients, does either size or age account for significant variation in overhead? So in our "full model" we have

$$Y = \beta_0 + (\beta_1 x_1 + \beta_2 x_2) + \beta_3 x_3 + \beta_4 x_4 + \epsilon \quad \epsilon \sim N(0, \sigma^2)$$

in our "reduced" model with just col index and # of clients we have

$$Y = \beta_0 + \beta_3 x_3 + \beta_4 x_4 + \epsilon \quad \epsilon \sim N(0, \sigma^2)$$

(where we take away size and age β_1, β_2). For the reduced model we have $H_0 : \beta_1 = \beta_2 = 0$ and H_a is at least one of $\beta_1, \beta_2 \neq 0$.
We want to see how much more variation our full model explains vs our reduced model.
We can use the **F-statistic**

$$F = \frac{\frac{SS(Res)_{red} - SS(Res)_{full}}{df_{red} - df_{full}}}{\frac{SS(Res)_{full}}{df_{full}}}$$

where under $H_0 : F \sim F_{df_{red}-df_{full}, df_{full}}$, where $df_{full} = n - (p+1)$ and p is the total number of parameters in the *full model*.
Note that $SS(Res)_{red} - SS(Res)_{full}$ is called the **additional sum of squares** (additional variance explained by full model). Also remark the denominator is simply $MS(Res)_{full} = \hat{\sigma}^2$.

Example 11.1. Recall that

$$\hat{\sigma} = \sqrt{\frac{\sum e_i^2}{n-(p+1)}}$$

So we can calculate it as

$$SS(Res)_{full} = \sum e_i^2 = \hat{\sigma}^2(n-(p+1))$$

so we have

$$SS(Res)_{full} = 14330^2(19)$$

and similarly

$$SS(Res)_{red} = 15360^2(21)$$

So our F-statistic value is

$$F = \frac{(15360^2(21) - 14330^2(19))/2}{14330^2} = 2.564$$

So the p-value is the value of $P(F_{2,19} > 2.564)$. From the F-table we see that $P(F_{2,19} > 3.52) = 0.05$ which implies our p-value is > 0.05. So we do not reject H_0. The reduced model is thus preferred: that is age and size together do not account for significant variation in overhead after acconting for col and clients.

In R, we can accomplish this via

```
1 > anova(audit.red.lm, audit.full.lm)
```

where `audit.red.lm` and `audit.full.lm` are the reduced and full models, respectively. This gives us a p-value of 0.1033 in R for the example.

11.3 F-test special case: testing significance of all parameters of a model

Consider again the case where we wanted to test $H_0 : \beta_1 = \beta_2 = \ldots = \beta_p = 0$ and H_a at least one of $\beta_j \neq 0$ for $j = 1, 2, \ldots, p$. This is simply the F-test but with a 0 parameter reduced model.
Note that if we are testing for the significance of a single model, our "full" model is our model

$$Y = \beta_0 + \beta_1 x_1 + \ldots \beta_p x_p + \epsilon \quad \epsilon \sim N(0, \sigma^2)$$

and the "reduced" model is

$$Y = \beta_0 + \epsilon \quad \epsilon \sim N(0, \sigma^2)$$

First note that the LSE (least square estimate) of β_0 for the reduced model is

$$\begin{aligned}
&\sum (y_i - \hat{\beta}_0)^2 \\
\Rightarrow &-2\sum (y_i - \hat{\beta}_0) = 0 && \text{first-order condition} \\
\Rightarrow &-n\hat{\beta}_0 + \sum y_i = 0 \\
\Rightarrow &\hat{\beta}_0 = \frac{\sum y_i}{n} = \bar{y} = \hat{\mu}
\end{aligned}$$

So we end up with

$$\begin{aligned}
SS(Res)_{red} = \sum e_i^2 &= \sum (y_i - \hat{\mu}_i)^2 \\
&= \sum (y_i - \hat{\beta}_0)^2 && Y = \beta_0 + \epsilon \Rightarrow \hat{\mu} = \hat{\beta}_0 \\
&= \sum (y_i - \bar{y})^2 \\
&= SS(Tot)
\end{aligned}$$

Thus we have

$$\begin{aligned}
F &= \frac{(SS(Tot) - SS(Res)_{full})/p}{MS(Res)_{full}} \\
&= \frac{SS(Reg)_{full}/p}{MS(Res)_{full}} \\
&= \frac{MS(Reg)}{MS(Res)}
\end{aligned}$$

as we had previously used.

11.4 F-test special case: testing significance of one additional parameter

Remember we previously tested for the significance of a parameter using the T-test where $H_0 : \beta_j = 0$ for some $j = 1, \ldots, p$.

Example 11.2. After accounting for size, col, and clients, is age significant related to overhead?
Our full model is thus

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \epsilon$$

and our reduced model (with age removed)

$$Y = \beta_0 + \beta_1 x_1 + \beta_3 x_3 + \beta_4 x_4 + \epsilon$$

We thus want to test for $H_0 : \beta_2 = 0$ and $H_0 : \beta_2 \neq 0$. Instead of using the T-statistic

$$t = \frac{\hat{\beta}_2}{SE(\hat{\beta}_2)}$$

we can instead use the F-statistic

$$F = \frac{(SS(Res)_{red} - SS(Res)_{full})/1}{MS(Res)_{full}}$$

or concretely with our example

$$\begin{aligned} F &= \frac{14210^2(20) - 14330^2(19)}{14330^2} \\ &= 0.666 \end{aligned}$$

Which gives us a p-value > 0.05. We do not reject H_0, so after accounting for size, col, and clients, age is not significantly related to overhead (reduced model is preferred).

Remark 11.1. For the p-values, note that

$$P(F_{1,df} > C) = P(|t_{df}| > C^2) \quad C > 0$$

(our F-statistic value is the square of the t-statistic value). That is: for comparing two models with a difference of one df we have $F = t^2$ (The F-test statistic and t-statistic will yield **identical p-values**).

12 February 15, 2018

12.1 Difference in response from reduced model

In the promo example, we had

$$x_1 = \begin{cases} 1 & \text{if promo1 used} \\ 0 & \text{otherwise} \end{cases}$$

$$x_2 = \begin{cases} 1 & \text{if promo2 used} \\ 0 & \text{otherwise} \end{cases}$$

where our model is $Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon$, $\epsilon \sim N(0, \sigma^2 I)$.
Is there a difference in sales between promo1 and promo2 stores?
One way is to do the following hypothesis test

$$\begin{aligned} H_0 &: \beta_1 - \beta_2 = 0 \\ H_a &: \beta_1 - \beta_2 \neq 0 \end{aligned}$$

thus we have the T-statistic

$$t = \frac{(\hat{\beta}_1 - \hat{\beta}_2) - 0}{SE(\hat{\beta}_1 - \hat{\beta}_2)}$$

Another approach: additional sum of squares. We have the full model

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon$$

and reduced model

$$\begin{aligned} Y &= \beta_0 + \beta^* x_1 + \beta^* x_2 + \epsilon && \beta^* = \beta_1 = \beta_2 \\ &= \beta_0 + \beta^*(x_1 + x_2) + \epsilon \\ &= \beta_0 + \beta^* x_3 + \epsilon && x_3 = x_1 + x_2 \end{aligned}$$

where we can interpret x_3 as

$$x_3 = \begin{cases} 1 & \text{if either promotion 1 or 2 used} \\ 0 & \text{otherwise} \end{cases}$$

So we have the F-statistic

$$F = \frac{(SS(Res)_{red} - SS(Res)_{full})/1}{MS(Res)_{full}}$$

where we get $F = 5.2218$ and p-value 0.03038 in our example for a $F_{1,27}$ distribution.
We therefore reject H_0, therefore mean sales is significantly greater for promo1 than for promo2.

12.2 General linear hypothesis

Consider the hypotheses tested so far using additional sum of squares (p is the number of total parameters in our full model)

1. $H_0 : \beta_1 = \beta_2 = \ldots = \beta_p = 0$
2. $H_0 : \beta_1 = \beta_2 = 0 \quad (p = 4)$
3. $H_0 : \beta_1 = 0 \quad (p = 3)$
4. $H_0 : \beta_1 - \beta_2 = 0$

The additional sum of squares test can be used to test any set of linear constraints that can be expressed in the form

$$H_0 = A\beta = 0$$

where A is an $l \times (p+1)$ matrix of l linear constraints.
For the hypothesis (1) we have

$$H_0 : \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & \ldots & 0 \\ 0 & 0 & 1 & 0 & 0 & \ldots & 0 \\ 0 & 0 & 0 & 1 & 0 & \ldots & 0 \\ \vdots & & & & & & \\ 0 & 0 & 0 & \ldots & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \vdots \\ \beta_p \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

where the left matrix is A and the right matrix is β. Similarly for (2)

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{bmatrix}$$

And for (3)

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 \end{bmatrix}$$

and for (4)

$$A = \begin{bmatrix} 0 & 1 & -1 \end{bmatrix}$$

12.3 Residual analysis and model assumptions

Residual analysis lets us **assess our model assumptions**. Recall our model assumptions of $Y = X\beta + \epsilon$ where $\epsilon \sim N(0, \sigma^2 I)$:

- The "function form" of the relationship is correctly specified (i.e. $\mu = X\beta$)

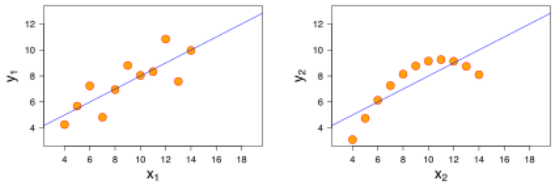


Figure 12.1: The linear function form is correctly specified for the left plot but not for the right plot where although the line fits well, it is not really linear (but rather quadratic).

  We want to make sure we're not fitting a linear regression model to data that is actually quadratic or some other nonlinear fit (the significance of our parameters in the regression summary in say R tells us nothing about this: we can get really significant parameter estimates but the data may not actually be linear).

- Errors are normal (specified as $\epsilon \sim N(\cdot)$).

  Remark 12.1. Normality of errors is not too important: although we assumed Y is normal (which depends on ϵ being normal) to derive β and $\hat{\beta}$, since β is the linear combination of Y normal variables it approaches a normal distribution regardless of Y's distribution for large sample sizes by the Central Limit theorem.

- Errors have constant variance i.e. **homoskedastic** (specified as $\sigma_i^2 = c$ some constant c for all β_i).

  It is possible for data to not have non-constant variance that is a function of X

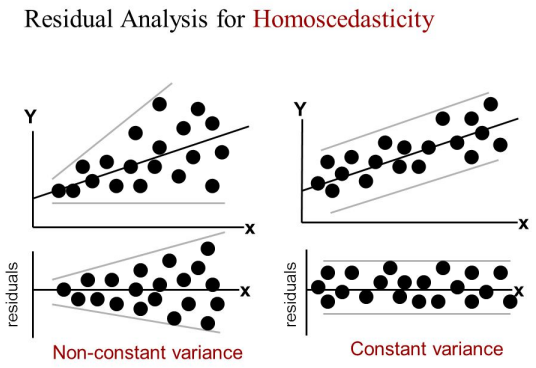


Figure 12.2: Non-constant variance would imply that we have variance as a function of X. For example, if the variance increases linearly as X increases, then we need to transform our data (e.g. square root it or log it) or fit another function to it (e.g. log in GLMs?).

- Errors are independent (specified as variance is $\sigma^2 I$, where the identity matrix has 0 off-diagonal entries).

  This is typically violated for time-series data.

13 February 27, 2018

13.1 Residual plots

One way we can assess our model assumptions is with **residual plots** (where e_i is always on the y-axis):

e_i **vs** $\hat{\mu}_i$ Recall under the model $Y = X\beta + \epsilon$, we have $e^T\hat{\mu} = 0$ (orthogonal vectors) so $Cov(e_i, \hat{\mu}_i) = 0$. Thus they are independent.

A plot of e_i vs $\hat{\mu}_i$ should always reveal no observable pattern or relationship between the residuals and the fitted values. No pattern implies that our **function form** is specified correctly and our **variance is constant**.

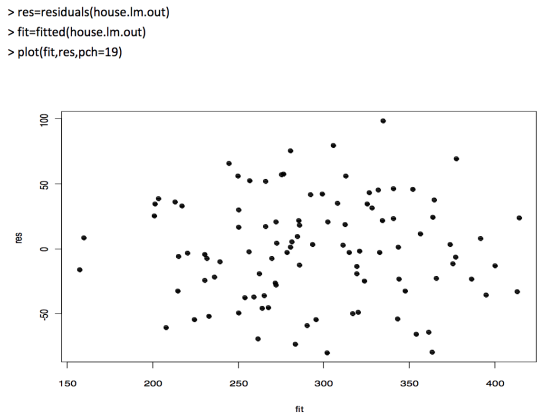


Figure 13.1: Residual plot of e_i vs $\hat{\mu}_i$.

QQ plots These are used to assess assumption of normal errors. It plots ordered (standardized) residuals vs expected quantiles from $N(0, 1)$.

A straight line relationship is an indication that the assumption of normal errors has been reasonably met.

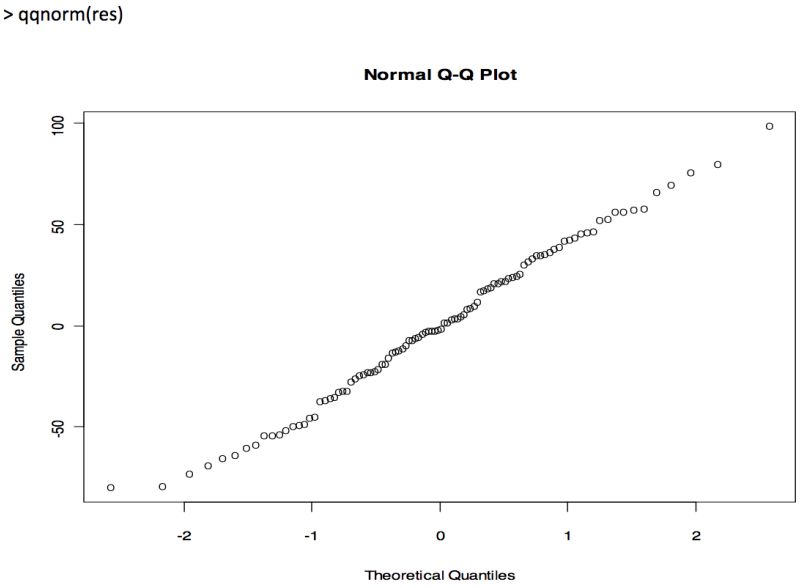


Figure 13.2: The non-standardized residuals (i.e. the residual values are plotted as) are ordered based on their corresponding quantile in the standard normal distribution (e.g. a residual of ≈ -80 corresponds to the theoretical standard normal quantile of -1.96).

We do not currently have a plot to check if the errors are independent (this will be discussed more during time-series).

13.2 Methods to address violated model assumptions

To address perceived violations of model assumptions:

- Transformation of response (and/or one or more explanatory variates). For example, there are **variance-stabilizing transformations** we can use:
  - $\log y$
  - $\sqrt{y}$
  - $\frac{1}{y}$

  (these may also be used for explanatory variates). These can be used if either the errors (variance) is not normal or if the function form is not linear. We can apply each of these transformations and see if it produces a better fit *and produces a "better" fit of our model assumptions.*

  Remark 13.1. After transforming our data, the residual standard error may seemingly decrease (or even increase) dramatically. Note that the RSE is relative to our response values: since the scale of those change based on the transformation we must take care when interpreting the change in the RSE.

  Remark 13.2. We will need to modify our intepretation of our parameter estimates since they are now estimated with respect to the transformed response values, not the original values.

- Inclusion of **higher order terms** (e.g. quadratic (x^2), cubic (x^3) of our explanatory variates (x)). This is sometimes called **polynomial regression**.

This does not violate multicollinearity since these terms are not *linearly* dependent.

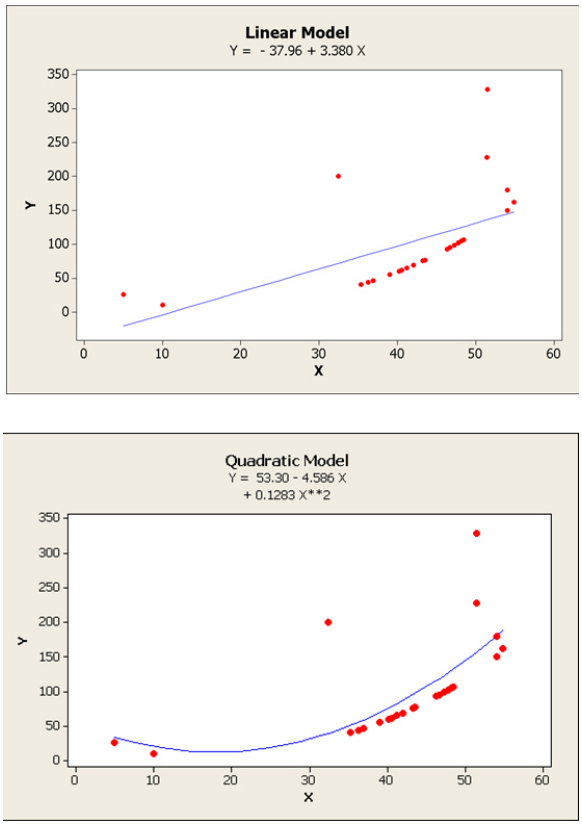


Figure 13.3: We initially have a linear model with a linear explanatory x and response y. We see the relationship between x and y is more quadratic. We then add x^2 as a term to our model which can allow us to fit a quadratic using linear regression with variates x and x^2 (our parameters are then the coefficients A, B, C in the quadratic $y = A + Bx + Cx^2$).

- Inclusion of **interaction terms**.

  When the relationship between an explanatory variate, x_k, and the response depends on the value of another explanatory variate, x_m, we say there is an **interaction** between x_k and x_m (i.e. when other variates have a magnifying/diminishing effect on the relationship between another variate and the response).

  For example, the effect of size on overhead of an office may be magnified if the age of the office is larger (and vice versa).

  May require the inclusion of an interaction term $x_k * x_m$ (where the explicit asterisk $*$ denotes interaction). It is coincidentally often the pairwise product of the variates.

  Remark 13.3. One must be careful introducing too many interaction terms since that will decrease our **degrees of freedom**.

  Example 13.1. In our overhead model, we had

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \epsilon$$

if we want an interaction term between age (x_1) and size (x_2) then we use the model

$$\begin{aligned} Y &= \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_5 (x_1 * x_2) + \epsilon \\ &= \beta_0 + (\beta_1 + \beta_5 x_2) x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \epsilon \end{aligned}$$

We can then interpret β_5 as the magnifying effect of x_2 on x_1.

14 March 1, 2018

14.1 Fitted residuals e vs errors ϵ

We can derive an expression that relates our fitted residuals (e, a distribution) and our assumed random errors (ϵ) Recall that (below are vectors)

$$\begin{aligned} e &= Y - \hat{\mu} \\ &= Y - X\hat{\beta} \\ &= Y - X(X^T X)^{-1} X^T y \\ &= Y - HY \\ &= (I - H)Y \\ &= (I - H)(X\beta + \epsilon) \\ &= X\beta - X(X^T X)^{-1} X^T X\beta + \epsilon - H\epsilon \\ &= X\beta - X\beta + \epsilon - H\epsilon \\ &= (I - H)\epsilon \end{aligned}$$

So we end up with

$$\begin{aligned} e &= (I - H)Y \\ &= (I - H)\epsilon \end{aligned}$$

One might assume $Y = \epsilon$ since

$$\begin{aligned} &(I - H)^{-1}(I - H)Y = (I - H)^{-1}(I - H)\epsilon \\ \Rightarrow &Y = \epsilon \end{aligned}$$

but this is not necessarily true since $I - H$ need not be invertible (it is invertible iff its rank is n)! Note that

$$rank(I - H) = n - rank(H) = n - tr(H) = n - rank(X) = n - (p + 1)$$

(TODO: revisit this) where the rank of a symmetric matrix is its trace. Since $n - (p + 1) < n$, $I - H$ is not of full rank so it is not invertible!

14.2 Distribution of fitted residuals e

Since $e = (I - H)\epsilon$ and $\epsilon \sim N$ then $e \sim N$, and we can derive the normal distribution of e

$$\begin{aligned} E[e] &= (I - H)E(\epsilon) = 0 \\ Var(e) &= (I - H)Var(\epsilon)(I - H)^T \\ &= \sigma^2(I - H)(I - H)^T \\ &= \sigma^2(I - H) \end{aligned}$$

So we have

$$e \sim N(0, \sigma^2(I - H))$$

Assuming our variates are all mutually independent (i.e. $\sigma^2_{jk} = 0$ for $j \neq k$) then we get

$$Cov(e_j, e_k) = -h_{jk} \quad j \neq k$$

where all entries of H are strictly positive (recall H is idempotent so this immediately follows). This makes sense intuitively: since all residuals must sum to 0 in LSE, some positive residual should coerce other residuals to be negative hence the negative covariance.
Another way to express this

$$e_i = N(0, \sigma^2(I - h_{ii}))$$

14.3 Studentized residuals

Analogous to standardizing with respect to the normal distribution, we can do the same with the T-distribution. As before (remember $\bar{e_i} = 0$), the studentized residuals d_i is defined as

$$d_i = \frac{e_i}{\hat{\sigma}\sqrt{1 - h_{ii}}}$$

where we subtract the mean and divide by the standard error.
This looks very similar to, when $\hat{\beta}_i = N(\beta_i, \sigma^2(X^TX)^{-1}_{ii})$

$$\frac{\hat{\beta}_i - \beta_i}{\sigma^2\sqrt{(X^TX)^{-1}_{ii}}} \sim t_{n-(p+1)}$$

d_i does not exactly follow a T-distribution since e_i and $\hat{\sigma}$ are not independent. Thus it follows a distribution *roughly that of the T-distribution.*

Remark 14.1. There are two types of studentized residuals: **internalized** and **externalized**. They differ in $\hat{\sigma}$ where the internalized uses the biased estimate of σ^2 (whereby sum of squared residuals divided by $n - p$) and externalized removes the ith residual suspected of being improbably large since it may skew the distribution (takes sum of residuals square except ith residual and divide by $n - (p + 1)$).
See the Wikipedia page for more details.

14.4 Outliers

These can be:

extreme values of the response variate How do we define one formally?

An observation is considered an "outlier" if its studentized residual d_i satisfies

$$|d_i| > 2.5$$

or thereabouts.

Why might an observation be an outlier?

1. Typo or human error
2. Missing interacting variate (e.g. type of company may be important to consider overhead of the company: not including such may result in outliers)

extreme values in the explanatory variate space These are extreme values of $(x_1, x_2, \ldots, x_p)$. Suppose we have one such outlier.

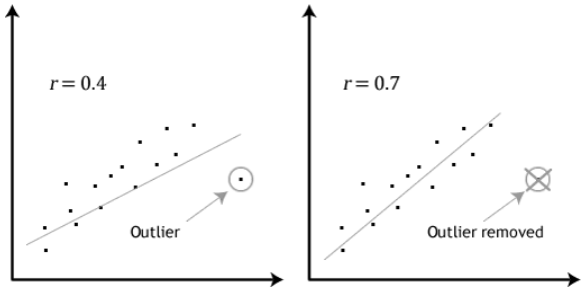


Figure 14.1: An outlier can have a huge effect on the fit and goodness of fit.

Think about the effect of fitting a LSE with and without the outlier. If the outlier lands roughly in the fit without the outlier, then there will be little difference between the two fits (the fit without the outlier will "move away" from where the outlier was before).

If the outlier lands far away from the fit without the outlier, then including it in the fit will skew it dramatically.

We can identify these outliers based on the residual i's h_{ii} (as we derived for its variance in its distribution). h_{ii} is also **called leverage**.

15 March 6, 2018

15.1 Additional variation required for more precise parameter estimates in ANOVA

Quick note about ANOVA:
Recall that a (full) model with additional variates will account for more variation than its reduced model.
The additional variation explained is given as

$$SS(Res)_{red} - SS(Res)_{full}$$

However, it's possible that in the full model our parameter estimates become *less precise*. This is defined as the

residual standard error **possibly increasing**. Note that

$$\hat{\sigma}_{red} = \sqrt{\frac{SS(Res)_{red}}{df_{red}}}$$
$$\hat{\sigma}_{full} = \sqrt{\frac{SS(Res)_{full}}{df_{full}}}$$

In the full model as we introduce more variates to the reduced model, while $SS(Res)_{full}$ decreases, df_{full} also decreases. Therefore if the ratio of df_{full} decreases more dramatically than $SS(Res)_{full}$, then $\hat{\sigma}_{full}$ will increase relative to $\hat{\sigma}_{red}$. This implies *less precise parameter estimates.*
To figure out the additional variation we required, we solve

$$\hat{\sigma}_{full} < \hat{\sigma}_{red}$$
$$\iff \sqrt{\frac{SS(Res)_{full}}{df_{full}}} < \sqrt{\frac{SS(Res)_{red}}{df_{red}}}$$

for the additional variation.

15.2 Leverage

As discussed previously, outliers can be problematic (they can skew our regression). In a multiple variate regression (at least with two explanatory variate), we can identify them visually

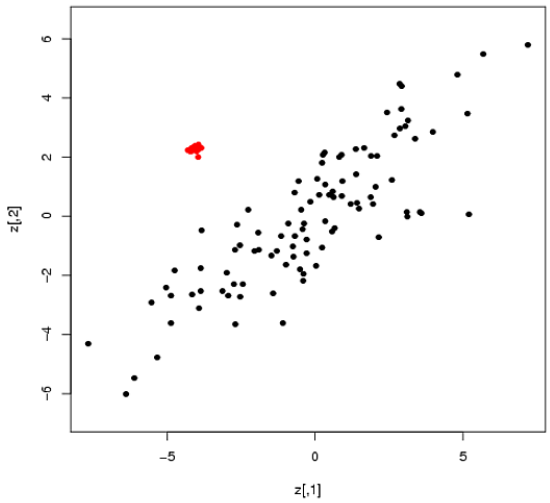


Figure 15.1: For a model with two explanatory variate, outliers show up as points that are not clustered around the cloud where most other points in the 2D plot of the two variates are. These outliers have **high leverage** since they deviate greatly in terms of their *explanatory variates.*

This can extend arbitrarily to some p-dimensional cloud.
Recall that $\hat{\mu} = Hy$. So we get

$$\hat{\mu}_i = h_{ii}y_i + \sum_{j \neq i} h_{ij}y_j$$

The **leverage of the ith observation** is defined as h_{ii}, the ith diagonal element of H. Intuitively h_{ij}'s may skew our $\hat{\mu}_i$ based on its magnitude, however:

Remark 15.1. When we say an observation has **high leverage**, we refer to it deviating from the mean of the **explanatory variate space** and *not* (most of the time) the response variate (see Influential observations).

Note that:

- $\frac{1}{n} \leq h_{ii} \leq 1$
- the *greater the distance* between $(x_{i1}, x_{i2}, \ldots, x_{ip})$ and $(\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_p)$, the *larger the leverage.*

  For example in SLR, we have
  $$h_{ii} = \frac{1}{n} + \frac{(x_i - \bar{x})^2}{SS_x}$$
  (where $SS_x = SS_{xx} = \sum(x_i - \bar{x})^2$).

  This is why leverage is such a good measure for identifying these outliers (i.e. observations that deviate greatly in their explanatory variates).

- $$tr(H) = rank(H) = rank(X) = p + 1$$
- Recall that we have $e \sim N(0, \sigma^2(I - H))$. Thus
  $$e_i \sim N(0, \sigma^2(1 - h_{ii}))$$

  Note that as $h_{ii} \to 1$ (i.e. leverage goes up), the variance of the distribution of the fitted residuals of that ith observation goes towards 0 (thus the fitted residuals are distributed around 0 more closely).

  So in theory the residuals of outliers are small.

  Remark 15.2. We cannot therefore tell if an observation is an outlier just by the residual plot since small residual values do not mean it's an outlier.

So a case (observation) i is considered to have **high leverage** if

$$h_{ii} > 2\bar{h} = \frac{2(p+1)}{n}$$

or thereabouts.

Example 15.1. In the overhead example, we have

$$2\bar{h} = \frac{2(5)}{24} = \frac{10}{24} \approx 0.4$$

If we plot our h_{ii}'s we can see none of our observations have high leverage.

15.3 Influential observations

An observation is considered **influential** if omission of this point has a *considerable effect* (not *significant*, since that implies some statistical/hypothesis testing) on the fitted line (i.e. changes the parameter estimates considerably). Only **high leverage cases** have the *potential* to be influential.

How do we identify these influential observations? One measure: **Cook's distance.**

$$D_i = \frac{h_{ii}}{1-h_{ii}} \cdot \frac{d_i^2}{p+1} \quad \text{where } d_i = \frac{e_i}{\hat{\sigma}\sqrt{1-h_{ii}}}$$

D_i anywhere near 1 (or greater) suggests a strongly influential case.

Remark 15.3. Cook's distance and influential observations combine both outliers in the response values (factored in by d_i) and in their explanatory variate values (factored in by $\frac{h_{ii}}{1-h_{ii}}$).

16 March 8, 2018

16.1 Model selection

We cannot simply use R^2 (multiple R-squared) to compare models (this will always increase (or stay the same) as you introduce parameters). Remember we previously saw that introducing additional variates may actually make our model produce *less precise paramter estimates.*
We saw residual standard error (RSE) would be a better metric since it highlights how precise our estimates are by also taking into account degrees of freedom. There is also the adjusted R-squared value (see below) that we can use, which is equivalent to selection based on RSE.

Sequential methods

Backward elimination

- Fit all p variates
- Remove the variate with the largest p-value if p-value $> \alpha$ (where $\alpha = 0.10$ or higher, typically e.g. R uses something closer to 0.15).
- Fit $p-1$ variate model with removed variate excluded
- Continue removing one variate at a time until no variates can be removed (all p-values $< \alpha$)

Forward selection

- Fit p SLR models (a model for each variate)
- Select the variate associated with smallest p-value, if p-value $< \alpha$ (α typically the same as above)
- Fit $p-1$ two-variate models that all include the variate selected
- Continue adding one variate at a time to your set of models until no models can be added (all p-values $> \alpha$)

Stepwise selection Begin with forward selection, and alternate between forward and backward at each step to determine whether any variates added in previous steps can be removed.

Selection from all possible subsets

- With p potential variates, there are $2^p - 1$ possible models. That is, for models with $k \leq p$ variates

k	# of possible models
1	$\binom{p}{1}$
2	$\binom{p}{2}$
$\vdots$	$\vdots$
p	$\binom{p}{p}$

So the total number of model subsets is

$$\sum_{k=1}^{p}\binom{p}{k} = \sum_{k=0}^{p}\binom{p}{k} - 1 = 2^p - 1$$

which follows from the Binomial theorem

$$\sum_{x=0}^{n}\binom{n}{x}a^n b^{n-x} = (a+b)^n$$

(plug in $a = b = 1$).
For example if $p = 8$, we have 255 possible model subsets.

- Select a suitable model based on a reasonable measure of fit. Two such measures are the R^2_{adj} **(adjusted R-squared)** or **Mallows's** C_p (see below).
- One can use the `leaps` package and command in R to do this.

16.2 Adjusted R-squared R^2_{adj}

Recall that

$$R^2 = 1 - \frac{SS(Res)}{SS(Tot)}$$

which *always goes up* as we introduce more variates and $SS(Res)$ decreases.
The adjusted R-squared R^2_{adj} uses the *mean squared* instead of the sum of squares

$$R^2_{adj} = 1 - \frac{\frac{SS(Res)}{n-(p+1)}}{\frac{SS(Tot)}{n-1}}$$

so we correct for the degrees of freedom as we introduce/remove variates in our models. Note that $R^2_{adj} < R^2$ since $\frac{n-1}{n-(p+1)} > 1$ for all $p \geq 1$.
Note that we can also write

$$R^2_{adj} = 1 - \frac{\hat{\sigma}^2}{\frac{SS(Tot)}{n-1}}$$

so the selection based on R^2_{adj} is equivalent to selection based on *residual standard error* $\hat{\sigma}$.

16.3 Mallows's C_p

For a k variate model ($k = 1, 2, \ldots, p$) then **Mallows's** C_p is defined as

$$C_p = \frac{SS(Res)_k}{MS(Res)_p} + 2(k+1) - n$$

Intuitively, we want our k variate model to have a lower $SS(Res)_k$ and we want to use as few k variates as possible. Thus we want *lower* Mallows's C_p values.
A model is considered suitable if $C_p \leq k + 1$.

Caution: in the full model ($k = p$) we have

$$\begin{aligned} C_p &= \frac{SS(Res)_p}{\frac{SS(Res)_p}{n-(p+1)}} + 2(p+1) - n \\ &= p + 1 \end{aligned}$$

so Mallows's C_p doesn't tell us anything about the full model.

17 March 13, 2018

17.1 `leaps` in R for model selection

We can use the `leaps` package/command to quickly find the best models for each # of variates used in the model. We specify the `nbest` number of models to show in the output for each k in the k variate models.
For example

```
> leaps(house[,-9],value, nbest=2, names=names(house[,-9]))
$which
   size stories baths rooms   age lotsize basement garage
1  TRUE   FALSE FALSE FALSE FALSE   FALSE    FALSE  FALSE
1 FALSE   FALSE  TRUE FALSE FALSE   FALSE    FALSE  FALSE
2  TRUE   FALSE FALSE FALSE  TRUE   FALSE    FALSE  FALSE
2  TRUE    TRUE FALSE FALSE FALSE   FALSE    FALSE  FALSE
3  TRUE   FALSE FALSE FALSE  TRUE    TRUE    FALSE  FALSE
3  TRUE   FALSE FALSE FALSE  TRUE   FALSE    FALSE   TRUE
4  TRUE   FALSE FALSE FALSE  TRUE    TRUE    FALSE   TRUE
4  TRUE    TRUE FALSE FALSE  TRUE    TRUE    FALSE  FALSE
5  TRUE    TRUE FALSE FALSE  TRUE    TRUE    FALSE   TRUE
5  TRUE   FALSE FALSE  TRUE  TRUE    TRUE    FALSE   TRUE
6  TRUE    TRUE  TRUE FALSE  TRUE    TRUE    FALSE   TRUE
6  TRUE    TRUE FALSE  TRUE  TRUE    TRUE    FALSE   TRUE
7  TRUE    TRUE  TRUE  TRUE  TRUE    TRUE    FALSE   TRUE
7  TRUE    TRUE  TRUE FALSE  TRUE    TRUE     TRUE   TRUE
8  TRUE    TRUE  TRUE  TRUE  TRUE    TRUE     TRUE   TRUE

$label
[1] "(Intercept)" "size"        "stories"     "baths"       "rooms"
[6] "age"         "lotsize"     "basement"    "garage"

$size
 [1] 2 2 3 3 4 4 5 5 6 6 7 7 8 8 9

$Cp
 [1] 27.150656 90.632218 21.556807 25.009540 10.144146 16.866082  4.137270
 [8]  9.322945  3.327332  6.091166  5.096306  5.216045  7.027277  7.067730
[15]  9.000000
```

The two best models for each k are show in the list of `TRUE/FALSE` (which specifies which variates were included in the model). The correspond Mallows's C_p values are shown below. Remember we'd like $C_p \leq k + 1$ for a reasonable model.

17.2 Interacting terms

Previously we talked about interacting terms to address model violations. For example, in the overhead example the effect of size on the house value may depend on the age of the house (e.g. size may have a stronger/lesser effect on house value for older/younger houses).
We denote two interacting terms by $x_i * x_j$. For example we might have the model

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_5 (x_2 * x_4) + \epsilon$$

where x_2 represents age and x_4 represents whether the house has a garage.
The interaction term $x_2 * x_4$ poses: does the effect of age on value depend on whether the house has a garage?
We can rewrite our model as

$$Y = \beta_0 + \beta_1 x_1 + (\beta_2 + \beta_5 x_4) x_2 + \beta_3 x_3 + \beta_4 x_4 + \epsilon$$

The interpretation of β_2 **changes**: β_2 is the effect of size if the house has no garage (i.e. when $x_4 = 0$). $\beta_2 + \beta_5$ (i.e. $x_4 = 1$) is the effect of size if the house has a garage.
This supports the claim that we can simply take the pairwise product to introduce an interacting term.

17.3 Forecasting time series data using linear regression models

Consider a dataset of wine sales. Previously we regressed on a response variate (total sales) on some explanatory variates (e.g. store, location, etc.).
What if we had data on just the total sales across time? We generally denote time series with one response variate as

$$\{y_t\} = \{y_1, y_2, \ldots, y_n\} = 1954, 2302, \ldots, 4365, 4290\}$$

where y_t represents the monthly wine sales (1000L) in month t where $t = 1, 2, \ldots, 187$.

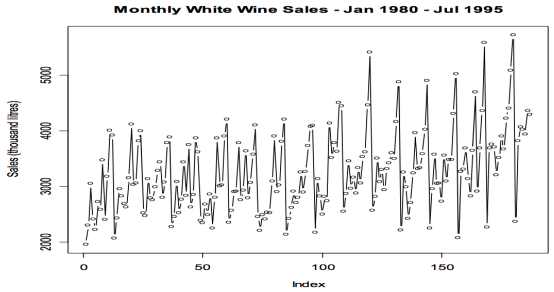


Figure 17.1: Monthly wine sales plotted against time (hence this is a time series).

What is $\hat{y}_{188}$ or the predicted sales for August 1995 (the 188th month since epoch)? (Note that we use $\hat{y}$ instead of $\hat{\mu}$: it does not make sense to think of a time series as a mean response anymore since there could be seasonal variations. Denoting it as $\hat{y}_t$ is more semantically correct).
We notice that there are spikes in the total sales that correspond to every 12 months. There is a strong correlation between sales every 12 months.
Can we assess the strength of lag k **auto-correlation** by calculating the **auto-correlation function (acf)**?

Remark 17.1. This is called **auto-correlation** since it's like correlation but there are no other variates we are considering: rather, it is the correlation of the response variate to itself.

17.4 Auto-correlation function

Definition 17.1. The **auto-correlation funtion (acf)** for some lag k is defined as

$$r_k = \frac{\sum_{t=k+1}^{n}(y_t - \bar{y})(y_{t-k} - \bar{y})}{\sum_{t=1}^{n}(y_t - \bar{y})^2}$$

This tells us how correlated the response values are to response values k time units behind.
For example, when $k = 12$

y_{t-12}	y_t
y_1 (Jan)	y_{13} (Jan)
y_2 (Feb)	y_{14} (Feb)
$\vdots$	$\vdots$

We can produce an **auto-correlation plot** or **correlogram** (e.g. in R) that maps the acf (r_k) against lag k's (e.g. from 0 to 25). Note that for $k = 1$, $r_k = 1$ always (obviously). We look for spikes (positive or negative) in the plot to find reasonable lag k for our models.

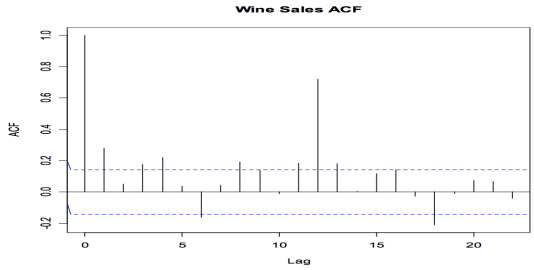


Figure 17.2: ACF against lag k i.e. a correlogram of the wine sales dataset. There is a significant spike in ACF at lag 12. Note there are significance lines drawn to distinguish significant acfs at some lag k (more below in section 18.2).

18 March 15, 2018

18.1 Fitting linear regression to account for seasonality in time series

In our example with wine sales above, we noticed that there was a significant $r_{12} \approx 0.7$ acf value that corresponds to a high auto-correlation between every twelve months. Months like December see spikes in wine sales and January see dips in sales.
How do we fit a linear regression model to account for this correlation between months?

Very restrict and bad approach Consider the model

$$y_t = \beta_0 + \beta_1 x_t + \epsilon_t \quad \epsilon_t \sim N(0, \sigma^2) \text{ independent}$$

where $x_t = 1, 2, \ldots, 12$ for each corresponding month January,February, ..., December.

This however restricts up to have a linear relationship between months (e.g. the difference in wine sale between January and February is restricted to that between February and March, etc.).

A more appropriate model Consider the model

$$y_t = \beta_0 + \beta_1 x_{t1} + \beta_2 x_{t2} + \ldots + \beta_{11} x_{t11} + \epsilon_t \quad \epsilon_t \sim N(0, \sigma^2) \text{ indepdendent}$$

where $x_{t1} = 1$ if the t-th month is January, $x_{t2} = 1$ if February, etc. (indicator variables for each month up to November since December is known if we know all others are 0).

In our regression summary, each β_i, $i = 1, \ldots, 11$ are estimates of how wine sales differ with respect to December (since β_0 or intercept is the estimate for December sales when all x_{ti} are 0).

Note for all $\hat{y}_{\text{Dec}} = \hat{\beta}_0 = 4536.1$ litres. Similarly $\hat{y}_{Jan} = \hat{\beta}_0 + \hat{\beta}_1 = 2288.5$. We also see that

$$\hat{y}_{Jan} = \hat{\beta}_0 + \hat{\beta}_1 \Rightarrow \hat{\beta}_1 = \hat{y}_{Jan} - \hat{y}_{Dec}$$

which supports our earlier claim that the β_i is the estimated difference between a given month's wine sale and December's.

Using this model, we can create a **seasonally-adjusted** wine sales dataset. If we plot the residuals from our model against time, it will show the variation caused by other factors that are not due to seasonality.

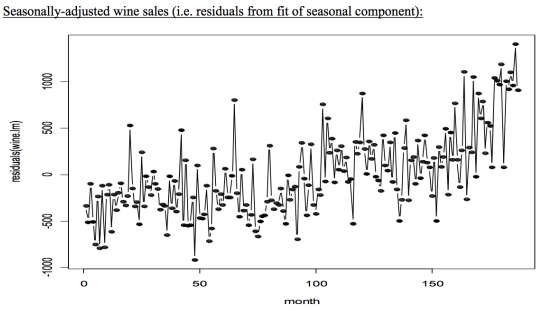


Figure 18.1: Residuals plotted against time (residual plot) from our regression model with indicator variables for each month.

As we see in the residual plot, there is an upward trend in the residuals hence our linear regression model with the assumption constant variance for the given model is violated (there is some trend we have not accounted for).

The residual plot also forms a different time series $\{e_t\}$ with $\bar{e_t} = 0$. Consider its acf

$$r_k = \frac{\sum_{t=k+1}^{n} e_t e_{t-k}}{\sum_{t=1}^{n} e_t^2}$$

And consider r_1 (where we have $e_t e_{t-1}$ as terms in the numerator). Since there is an overall positive trend, the sum of $e_t e_{t-1}$ will be overall positive and thus $r_1 > 0$. Similarly, $r_2 > 0$, etc. We can assess assumption of independent errors **by a plot of the acf** of the residuals

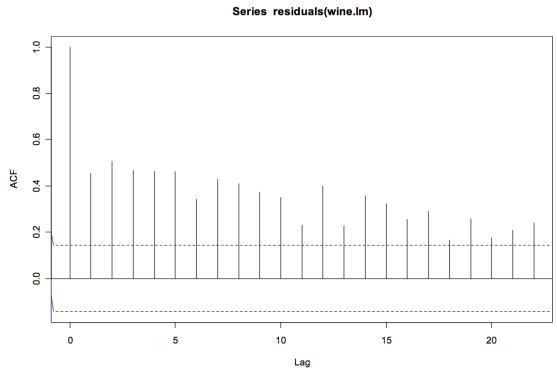


Figure 18.2: ACF plot for the time series data of the residuals from our above model.

Upshot: We clearly have dependent error/residual terms.

18.2 (Sample) acf r_k vs process auto-correlation ρ_k

The (sample) acf r_k is an estimate of the process auto-correlation ρ_k, that is

$$r_k = \hat{\rho}_k$$

This distinction comes from the fact that we are only taking a snapshot/sample/window of the overall time series of our process $\{Y_t\}$. We then use this sample to produce r_k which is an estimate of ρ_k.
The **significance lines** on the acf plot in R allows a crude assessment of the significance of r_k at lag k (i.e. assesses whether $\rho_k = 0$ at lag k).
It can be shown that for large n (under the null hypothesis $\rho_k = 0$), $E[r_k] = 0$ and $Var(r_k) = \frac{1}{n}$, thus

$$0 \pm \frac{2}{\sqrt{n}}$$

yields approximately the 95% confidence limits for ρ_k, assuming $\rho_k = 0$.
E.g. in the wine example, we have $n = 187$ thus the significance lines are at ± 0.146 acf in the correlogram.

18.3 Durbin-Watson test statistic

We can test for lag 1 auto-correlation in errors using the **Durbin-Watson** test statistic

$$D = \frac{\sum_{t=2}^{n}(e_t - e_{t-1})^2}{\sum_{t=1}^{n} e_t^2}$$

where e_t is the residual at time t. We can rewrite this for large n's

$$\begin{aligned} D &\approx \frac{\sum e_t^2 + \sum e_{t-1}^2 - 2\sum e_t e_{t-1}}{\sum e_t^2} \\ &\approx 2 - 2r_1 \\ &= 2(1 - r_1) \end{aligned}$$

(this is r_1 for $\{e_t\}$, not $\{y_t\}$). Since $-1 < r_1 < 1$, then $0 < D < 4$. We can thus relate the value of D to r_1

$D < 2$ **(close to 0)** Suggests $\rho_1 > 0$ (positive lag 1 auto-correlation)

$D > 2$ **(close to 4)** Suggests $\rho_1 < 0$ (negative lag 1 auto-correlation)

$D \approx 2$ Suggests no auto-correlation ($\rho_1 = 0$)

So to test for **positive auto-correlation** at lag 1 using the Durbin-Watson test statistic, we have $H_0 : \rho_1 = 0$ and $H_a : \rho_1 > 0$ and our test statistic D.
We then compare D to critical values D_L and D_U from Durbin-Watson (DW) tables (or use a computer):

$D < D_L$ Reject H_0 (conclude $\rho_1 > 0$)

$D > D_U$ Do not reject H_0 (conclude $\rho_1 = 0$)

$D_L < D < D_U$ inconclusive

Similarly to test for **negative auto-correlation** at lag 1 we have $H_0 : \rho = 0$ and $H_a : \rho_1 < 0$, we use $4 - D$ instead:

$4 - D < D_L$ Reject H_0 (conclude $\rho_1 < 0$)

$4 - D > D_U$ Do not reject H_0 (conclude $\rho_1 = 0$)

$D_L < 4 - D < D_U$ inconclusive

19 March 20, 2018

19.1 Trend component in time series

As noted in Fitting linear regression to account for seasonality in time series we see that there is still some trend component we have not accounted for (though we have indeed accounted for seasonality components with the indicator variables for the months).
We thus include additional terms to our model to account for trend

$$y_t = \beta_0 + \beta_1 x_{t1} + \ldots + \beta_{11} x_{t11} + \beta_{12} t + \beta_{13} t^2 + \epsilon_t$$

where $\epsilon_t \sim N(0, \sigma^2)$ independent. Note that our $\beta_1, \ldots, \beta_{11}$ remain the same (our seasonality component) and we've introduced a **trend component** with $\beta_{12} t + \beta_{13} t^2$ (we have a quadratic trend component since the time series appears to have a quadratic trend).
Including this trend component we see that our R^2 (proportion of variance) increased from 0.6155 to 0.7963! If we *naively plot* our residuals against the fitted values $\hat{\mu}$, we get the plot

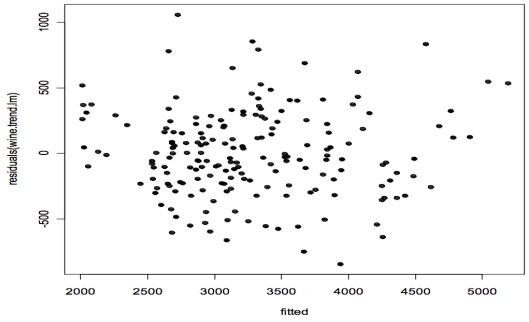


Figure 19.1: Residuals e_i plotted against fitted values $\hat{\mu}_i$ after accounting for the trend in a linear regresion model of time series wine sales data.

However, this doesn't really tell us how our residuals *varies over time* (we may notice that January has lower values so it might be the group of residuals to the left, but in general this is difficult to do for all months).
We thus instead plot residuals against time (i.e. month)

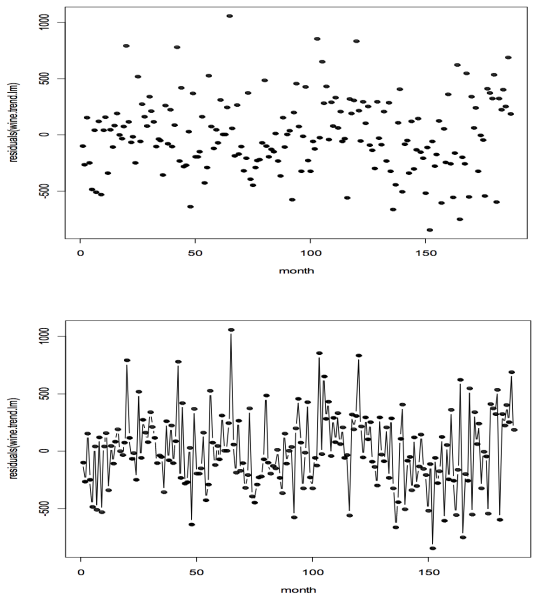


Figure 19.2: Residuals e_i plotted against time t after accounting for the trend in a linear regresion model of time series wine sales data.

We see that the residuals look much better than before after accounting for trend (they look much more randomly distributed about 0 than before). If we plot the acf for $\{e_t\}$ we get

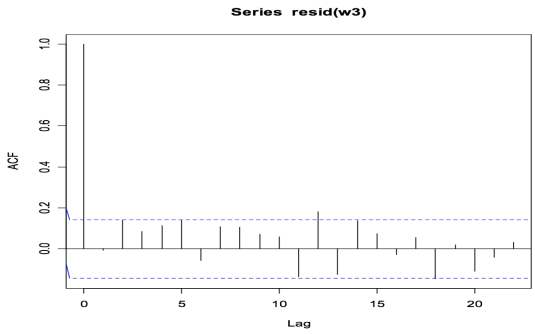


Figure 19.3: ACF plot for residuals $\{e_t\}$ from our linear model that includes seasonality and trend components.

It appears that there is no statistically significant $\rho_k \neq 0$ in our residuals. Therefore, our model assumptions (for residuals) appear to be satisfied.
If we calculated the Durbin-Watson statistic for the above residuals $\{e_t\}$, we get $D = 2.0093$ (p-value of 0.4923) so we do no reject H_0 so we conclude there is no significant **lag-1** autocorrelation ($\rho_1 = 0$).

19.2 Predictions with time series

Suppose we wanted to predict the next month's wine sales for the example wine sales dataset. From our model we have

$$\begin{aligned}\hat{y}_{Aug1998} &= \hat{y}_{188} \\ &= \hat{\beta}_0 + \hat{\beta}_8 + \hat{\beta}_{12}(188) + \hat{\beta}_{13}(188^2) \\ &= 4,369,053 \text{ litres}\end{aligned}$$

20 March 22, 2018

20.1 Faculty salary study: regression model example

The working group used regression modelling to identify anomalies in salary and correct these anomalies.
The response variate to test for is the **salary of full-time Faculty ($)**.
The regression model and questions asked along the way may look something like this:

1. Suppose the model was fitted to identify anomalies in pay in **gender**. A regression model was fitted and it was identified that males were being paid more than females by about $2100. Someone hypothesizes that this is due to male Faculty tending to have more experience than female.

2. We need to account for **experience** in our model by introducing it into our regression model. There is still a statistical difference between gender groups. Someone notices that different Faculties have different pay grades.

3. We introduce the **academic unit variate** (i.e. Department/Faculty). We may also want to introduce the **degree** of the Faculty member.

4. This process continues until we account for as many variates as we can. We can then make a stronger argument for any statistical differences in pay between gender groups.

The sequence of models used in the study is as follows:

First model Fit without gender variate to detect anomalies that were non-gender based.

One notable higher order term introduced is "years since hire squared". This makes sense since salary increases are compounding so a linear term would not be fully adequate (they could have even fit an exponential term or log transformed years).

Interaction terms were introduced between academic group (department/faculty) and rank (professor, associate processor, lecturer, etc.): rank differences may differ among faculties (one term per combination).

Similarly interaction terms were introduced between lag (time between highest degree and year of hire) and rank.

One key point: the group did not employ model selection to remove insignificant variates. Since the target audience is the public, they want to avoid the audience questioning why they did not include certain variates (and making the argument that the hypothetical removed variates could affect salary).

In the report, the mean salary of a hypothetical Faculty member was predicted using the model by calculated $\hat{\mu}$ with the hypothetical set of attributes.

To identify anamolies, we can look at obserations with **large residuals** (specifically those with **extreme negative residuals** since the group would not want to fix people being paid more: they could be paid substantially more because of some other unaccounted variate such as prestigious publications).

How do they define an "anomaly"? They used both the **absolute difference** (between actual and fitted) and **proportional difference** ($\frac{\text{actual} - \text{fitted}}{\text{fitted}}$). Why proportional? A \$20,000 difference is much more substantial for someone who has an actual salary of \$180,000 than someone who has an actual salary of \$1,000,000.

The actual crtierion for anomalies they used was

- actual $< 90\%$ fitted ($\frac{|e_i|}{\hat{\mu}_i} > 0.1$ for $e_i < 0$) AND actual \$> 5000 below fitted ($e_i < -5000$).

They found 88 initial anomalies. After further investigation, they concluded that 59 were indeed anomalies and 12 required even further investigation (some anomalies were explained by other factors like sabbaticals or incorrect rank and year of hire). They also broken down the anomaly proportion by gender and faculty (female Faculty had higher proportion of anomalies).

Revised model The group then included the gender variate and found that the parameter estimate revealed that males were being paid more on average by \$2904.69 ($\hat{\beta}_{gender} = 2904.69$) where $x_{gender} = 1$ if male and 0 otherwise. The p-value was significant.

A summary of some techniques the group used:

1. identified response and explanatory variates
2. fit regression model
3. interpreted parmaeter estimates
4. included higher order terms
5. included interaction terms
6. discussed log transformation of response
7. compared models (additional sum of squares or R^2_{adj}, C_p)
8. residual plot
9. identified outliers
10. prediction
11. addressed model assumptions

21 March 27, 2018

21.1 Logistic regression

So far we have considered on the **normal** linear model where we have

$$Y_i = \beta_0 + \beta_1 x_{i1} + \ldots + \beta_p x_{ip} + \epsilon_i$$

where $\epsilon_i \sim N(0, \sigma^2)$ independent, $Y_i \sim N(\mu_i, \sigma^2$ independent, and

$$\mu_i = \beta_0 + \beta_1 x_{i1} + \ldots + \beta_p x_{ip} = x_i^T \beta$$

where $x_i^T = (1, x_{i1}, \ldots, x_{ip})$. $x_i^T \beta$ is our **linear predictor**.

Now consider a **binary response variate** where

$$Y_i = \begin{cases} 1 & \text{if ith case is a success} \\ 0 & \text{otherwise} \end{cases}$$

Also we have $P(Y_i = 1) = \pi_i$ and $P(Y_i = 0) = 1 - \pi_i$ where π_i is the probability that the ith case is a success. Then we can model Y_i as a **Bernoulli random variable** with probability function

$$f(y_i) = \pi_i^{y_i}(1 - \pi_i)^{1-y_i} \qquad y_i = 0, 1$$

Note that

$$\begin{aligned} E[Y_i] = \mu_i &= \sum_{y_i=0}^{1} y_i f(y_i) \\ &= 1(\pi_i) + 0(1 - \pi_i) \\ &= \pi_i \end{aligned}$$

Also

$$\begin{aligned} Var(Y_i) &= \sum y_i^2 f(y_i) - \left(\sum y_i f(y_i)\right) \\ &= \pi_i - \pi_i^2 \\ &= \pi_i(1 - \pi_i) \end{aligned}$$

So $Var(Y_i)$ is a function of $\mu_i = \pi_i$. Note also that

$$\epsilon_i = y_i - \pi_i = \begin{cases} -\pi_i & y_i = 0 \\ 1 - \pi_i & y_i = 1 \end{cases}$$

In **logistic regression**, we model the mean of the ith response, π_i, as a *nonlinear function* of the parameters $\beta_0, \beta_1, \ldots, \beta_p$. The most common function we use is the sigmoid function

$$\pi_i = \frac{e^{x_i^T \beta}}{1 + e^{x_i^T \beta}}$$

(note that this contains our linear predictor $x_i^T \beta$).
If we solve for our linear equation we get

$$x_i^T \beta = \log\left(\frac{\pi_i}{1 - \pi_i}\right)$$

(natural log). This is called the **logit link** or **log odds**. Recall that odds for an event measure

$$\frac{P(A)}{P(A^c)} = \frac{P(A)}{1 - P(A)}$$

It's called a **link function** because it links our mean μ_i to our linear predictor (the link function for a normal linear model is just the identity function).

21.2 Parameter estimation in logistic regression

Based on the method of **maximum likelihood**. Requires iterative procedure (e.g. Newton's/Newton-Rhapson method or gradient descent).

21.3 Binomial count data and logistic regression

The logistic model can also be fit to binomial count data where Y_i is the nubmer of successes in n_i independent trials, i.e.

$$Y_i \sim BIN(n_i, \pi_i)$$

Example 21.1. For example, consider a study done on the death penalty vs. race of *victim* (not defendant). Data was collected on 362 dealth peanlty cases where the response was $Y_i = 1$ if the ith case resulted in the dealth penalty and 0 otherwise.
The explanatory variates are

1. x_1 - aggravation level (crime severity) where $x_1 = 1, 2, \ldots, 6$ (1 is low, 6 is high)
2. x_2 - race of *victim* (1 if white, 0 otherwise (e.g. black)).

Note that there are a total of 12 distinct **constellations** (number of different groupings with identical sets of explanatory variates i.e. combinations of explanatory variate values).
Let m be the number of constellations. Then we define a new response variate Y_j the number of successes of the jth constellation, which can be modelled by the binomial distribution $Y_j \sim BIN(n_j, \pi_j)$ where $j = 1, \ldots, m$.

21.4 Interpretation of logistic regression parameter estimates $\hat{\beta}_j$

Consider the parameter estimates from our logistic regression fit

$$\log\left(\frac{\pi_i}{1-\pi_i}\right) = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$

and consider β_1. What if we increased it by 1? i.e. we have x_1th and $x_1 + 1$th observations where $x_1 + 1$th has its x_1 increased by 1. Then we have

$$\log\left(\frac{\pi_{x_1}}{1-\pi_{x_1}}\right) = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$
$$\log\left(\frac{\pi_{x_1+1}}{1-\pi_{x_1+1}}\right) = \beta_0 + \beta_1 (x_1 + 1) + \beta_2 x_2$$

So we have

$$\begin{aligned}\beta_1 &= \log\left(\frac{\pi_{x_1+1}}{1-\pi_{x_1+1}}\right) - \log\left(\frac{\pi_{x_1}}{1-\pi_{x_1}}\right) \\ &= \log\left(\frac{\frac{\pi_{x_1+1}}{1-\pi_{x_1+1}}}{\frac{\pi_{x_1}}{1-\pi_{x_1}}}\right)\end{aligned}$$

called the **log odds ratio**. We can also write

$$e^{\beta_1} = \frac{\frac{\pi_{x_1+1}}{1-\pi_{x_1+1}}}{\frac{\pi_{x_1}}{1-\pi_{x_1}}}$$

call the **odds ratio**.
Thus for every 1 unit increase in a given variate x_i, we observe a e^{β_i} multiplicative increase in the odds of the response variate being 1 (e.g if $e^{\beta_i} = 2$, then 1 unit increase sees a *two-fold increase* (two times) the odds of the response variate being 1).

Example 21.2. In the death penalty study above, we end up with $\hat{\beta}_2 = 1.8106$ or $e^{\hat{\beta}_2} = 6.11$ (parameter estimate for the race variate).
So after accounting for aggravation level or severity of crime, the odds of a death penalty sentence is **6.11 times higher** if the victim is White compared to a Black victim (i.e. odds increased by a factor of 6.11 i.e. odds increase by 511%).

22 March 29, 2018

22.1 Inference for β_j logistic regression parameters and Wald statistic

For sufficient large sample sizes, note that

$$\left(\frac{\hat{\beta}_j - \beta_j}{SE(\hat{\beta}_j)}\right)^2 \sim X^2_{n-(p+1)}$$

i.e. the above has the distribution of the chi-squared distribution on $n-(p+1)$ degrees of freedom.
To test $H_0 : \beta_j = 0$, we have the **Wald statistic**

$$z = \left(\frac{\hat{\beta}_j}{SE(\hat{\beta}_j)}\right) \sim N(0,1) \text{ under } H_0$$

22.2 Model deviance (aka residual deviance in R)

The **deviance** is the difference between the likelihood of our fitted model and the likelihood of a perfectly fitted model (the saturated model i.e. model with parameters such that the data are fitted exactly). It is used for assessing goodness of fit for models that use maximum likelihood estimation (MLE) for its parameters. It is defined as

$$D = 2\left(l(\text{saturated}) - l(\text{fitted})\right)$$

where $l(\pi \mid y) = \log(L(\pi \mid y))$ is the log-likelihood function. Recall that the likelihood function is defined as

$$L(\pi \mid y) = \prod_{i=1}^{m} f(y_i)$$

For $Y_i \sim Bin(n_i, \pi_i)$ for $i = 1, \ldots, m$ (m different categories) we have

$$\begin{aligned} L(\pi \mid y) &= \prod_{i=1}^{m} \binom{n_i}{y_i} \pi_i^{y_i} (1-\pi_i)^{n_i - y_i} \\ l(\pi \mid y) &= \sum_{i=1}^{m} \log \binom{n_i}{y_i} + y_i \log(\pi_i) + (n_i - y_i)\log(1-\pi_i) \\ &= \sum_{i=1}^{m} y_i \log(\pi_i) + (n_i - y_i)\log(1-\pi_i) + C \end{aligned}$$

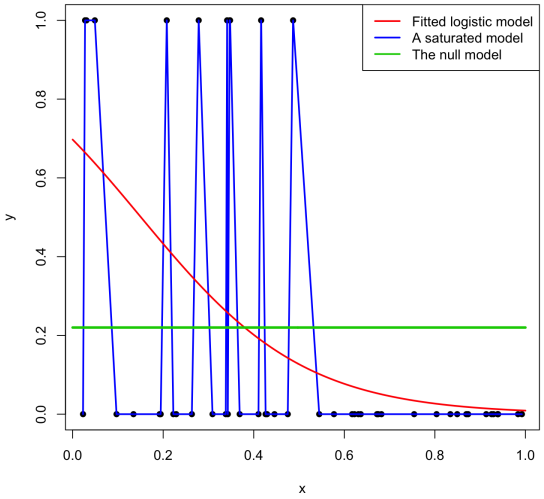


Figure 22.1: Examples of saturated and non-saturated fitted models for a dataset.

For the saturated/perfect model, MLE gives us

$$\hat{\pi}_i = \frac{y_i}{n_i}$$

i.e. when we fit with $p + 1 = n$ parameters so we get a perfect fit.
For the fitted model, $\hat{\pi}_i$ is the MLE (found iteratively) where $pi_i = \frac{e^{x_i^T \hat{\beta}}}{1+e^{x_i^T \hat{\beta}}}$.

22.3 Assessing model adequacy using model deviance

If the model provides an adequate fit, then $D \sim X^2_{n-(p+1)}$ for sufficient large $n - (p+1)$.
We assume that model is adequate if $\frac{D}{n-(p+1)} \approx 1$ *or less.*

Example 22.1. For the death penalty vs race of the victim model, we have

$$\frac{D}{n-(p+1)} = \frac{3.8816}{9} < 1$$

so our model is adequate.

22.4 Comparison of models (reduced vs. full) using model deviance

Under the assumption that the reduced model provides a better fit

$$D_{red} - D_{full} \sim X^2_{df_{red} - df_{full}}$$

for sufficiently large sample sizes.
Note that

$$\begin{aligned} D_{red} - D_{full} &= 2\left(l(\text{fitted})_{full} - l(\text{fitted})_{red}\right) \\ &= 2\log\left(\frac{L(\text{fitted})_{full}}{L(\text{fitted})_{red}}\right) \end{aligned}$$

this is exactly the **likelihood ratio test statistic**.

Example 22.2. Suppose we wanted to see if the reduced model with just the race of the victim (aggravation level removed) is a better model.
We thus have for our full model

$$x_i^T\beta = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2}$$

and the reduced model

$$x_i^T\beta = \beta_0 + \beta_2 x_{i2}$$

We will be testing $H_0 : \beta_1 = 0$ (i.e. reduced model is preferred) and $H_a : \beta_1 \neq 0$.
Note that from R, we get $D_{red} - D_{full} = 163.87 - 3.8816 \approx 160$.
Our test statistics distribution is X_1^2, so our p-value is $P(X_1^2 > 160) << 0.05$ so we reject H_0 so the full model is better.
We can also test for our fitted model as the **null model** i.e. reduced model is $x_i^T\beta = \beta_0$, so we test for $H_0 : \beta_1 = \ldots = \beta_p = 0$.
From the R output, D_{red} is the "null deviance" so $D_{red} - D_{full} = 212.28238 - 3.8816 \approx 203$ so we reject H_0 so the full model is preferred.

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23.1 Akaike information criterion (AIC)

Another way to compare models derived from MLE is using the **Akiake information criterion (AIC)**. It is given as

$$AIC = 2(p+1) - 2l(\text{fitted})$$

we prefer models with the *smallest* AIC.

23.2 Interaction terms in logistic regression

Similary to linear regression, we can also introduce interaction terms in our logistic regression model.

Example 23.1. For example, we had $x_{i1} = 1, \ldots, 6$ denote the crime severity and $x_{i2} = 1$ iff the victim was White. Suppose we introduce the interaction term $x_{i1} * x_{i2}$ i.e. our linear predictor becomes

$$\begin{aligned} x_i^T\beta = \beta_0 &= \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3(x_{i1} * x_{i2}) \\ &= \beta_0 = \beta_1 x_{i1} + (\beta_2 + \beta_3 x_{i1}) x_{i2} \end{aligned}$$

where if $\beta_3 > 0$, then the more severe the crime is the more likely it is for the death penalty if the victim is White. We see in our R output that β_3 is indeed positive, but it is not significant and has even made β_2 (parameter with race variate) not significant.
To test for no interaction using deviance test, we have $H_0 : \beta_3 = 0$ and $H_a : \beta_3 \neq 0$. Thus we use

$$D_{red} - D_{full} = 3.8816 - 3.3438 = 0.5378$$

Remember that this statistic is distributed as X_1^2. Clearly $P(X_1^2 > 0.5378) > 0.05$ so the interaction is not significant.

23.3 Contingency tables vs logistic regression

A contingency table lists the number of occurrences of each variate group in a table. Logistic regression can introduce and take into account other variates such as aggravation levels without much difficulty compared to contigency tables.

Example 23.2. Recall that we had categorical variables with race (White or Black) and the death penalty (Yes or No). The 2-by-2 contingency table for the example is

$$\begin{array}{c} \\ \text{White} \\ \text{Black} \end{array} \begin{array}{c} \begin{array}{ccc} \text{Yes} & \text{No} & \end{array} \\ \begin{bmatrix} 45 & 85 & 130 \\ 14 & 218 & 232 \\ 59 & 303 & 362 \end{bmatrix} \end{array}$$

We can calculate our odds and odds ratios from contigency tables easily

$$\hat{\pi}_W = \frac{45}{130}$$
$$\hat{\pi}_B = \frac{14}{232}$$

So the odds of death penalty for White victims is

$$\frac{\hat{\pi}_W}{1 - \hat{\pi}_W} = \frac{45/130}{85/130} = \frac{45}{85}$$

Similarly the odds of death penalty for Black victims is

$$\frac{\hat{\pi}_B}{1 - \hat{\pi}_B} = \frac{14/232}{218/232} = \frac{14}{218}$$

Thus the odds ratio is

$$\frac{\hat{\pi}_W/(1 - \hat{\pi}_W)}{\hat{\pi}_B/(1 - \hat{\pi}_B)} = \frac{45/85}{14/218} = 8.24$$

Note that when we fit the corresponding logistic regression model, we end up with $e^{\hat{\beta}_1} = e^{2.1094} = 8.24$. So both methods give us the same results.