richardwu.ca

STAT 331 Course Notes

Applied Linear Models

Peter Balka • Winter 2018 • University of Waterloo

Last Revision: February 5, 2018

Table of Contents

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. 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.

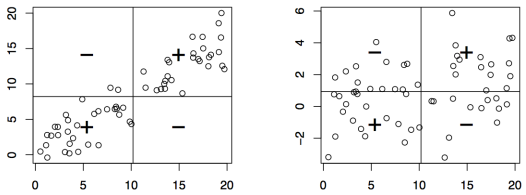
2 January 9, 2018

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 $\hat{\sigma}^2 = \sqrt{\frac{\sum e_i^2}{n-2}}$.

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 varaibles 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

For a given 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)

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

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

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

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.

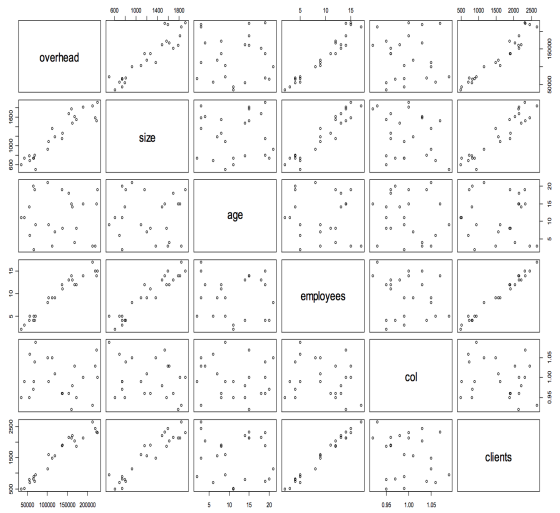


Figure 6.1: Size, employees, and clients are all correlated with overhead. Note however that size, employees, and clients are all correlated with each other therefore it would probably suffice to only include one of these explanatory variates without losing much information in our model.

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) relationshipss 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.

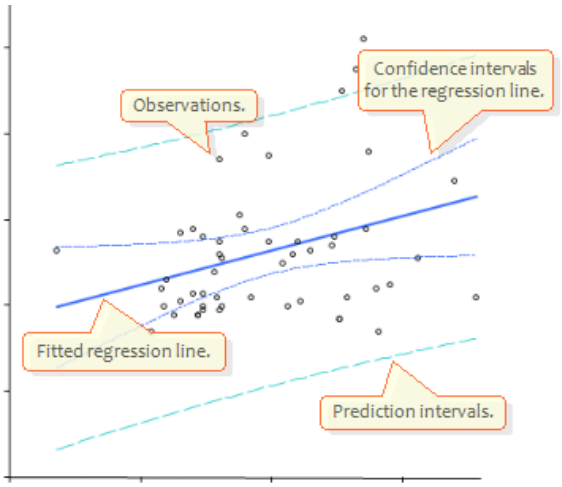


Figure 7.1: The confidence and prediction bands are smaller in closer to the centre of the x's or closer to $\bar{x}$. Furthermore, the prediction bands lie further out from the confidence bands.

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

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

Thus our standard error is

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

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