SCIENCE MEETS LIFE

Introduction to Linear Regression

With a continuous or categorical predictor





Aims

- Understand linear regression with one predictor
- Understand how we assess the fit of a regression model
 - ▶ Total sum of squares
 - Model sum of squares
 - Residual sum of squares
 - F
 - R^2
- Know how to do regression using R/SAS
- Interpret a regression model





OLS with continuous predictor





What is Regression?

- A way of predicting the value of one variable from another.
 - It is a hypothetical model of the relationship between two variables.
 - ▶ The model used is a linear one.
 - ▶ Therefore, we describe the relationship using the equation of a straight line.





Describing a Straight Line

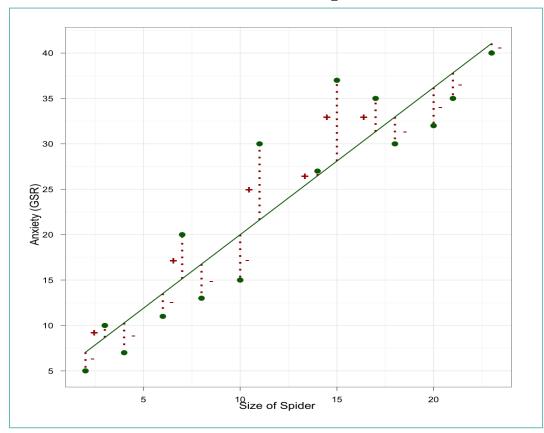
$$Y_i = b_0 + b_1 X_i + \epsilon_i$$

- *b*₁
 - ▶ Regression coefficient for the predictor
 - ▶ Gradient (slope) of the regression line
 - Direction/strength of relationship
- **b**_o
 - Intercept (value of Y when X = 0)
 - ▶ Point at which the regression line crosses the *Y*-axis (ordinate)





The Method of Least Squares



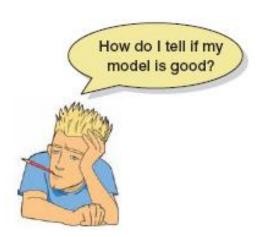
How do I fit a straight line to my data?



This graph shows a scatterplot of some data with a line representing the general trend. The vertical lines (dotted) represent the differences (or residuals) between the line and the actual data

How Good Is the Model?

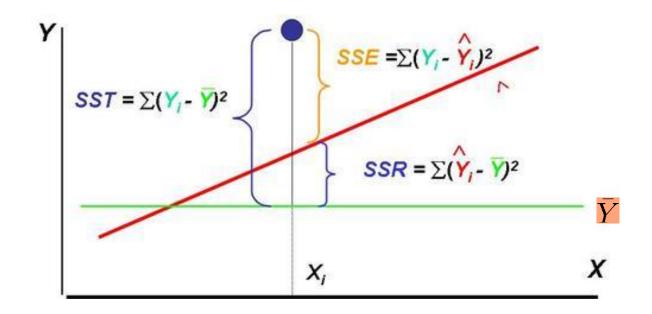
- The regression line is only a model based on the data.
- This model might not reflect reality.
 - ▶ We need some way of testing how well the model fits the observed data.
 - ► How?







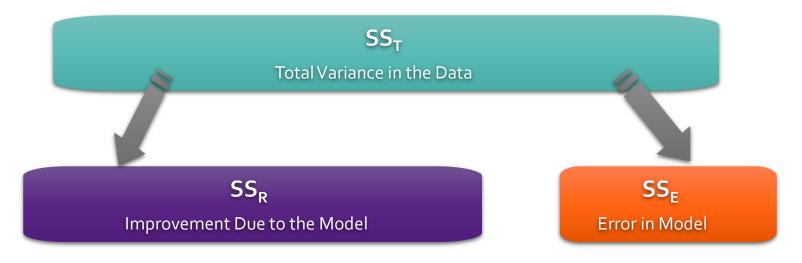
Sums of Squares







Testing the Model



• If the model results in better prediction than using the mean, then we expect SS_R to be much greater than SS_E





Testing the Model: R²

- R²
 - ▶ The proportion of variance accounted for by the regression model.
 - ▶ The Pearson Correlation Coefficient Squared

$$R^2 = SS_R/SS_T$$





Testing the Model

- Mean squared error
 - Sums of squares are total values.
 - ▶ They can be expressed as averages.
 - ▶ These are called mean squares, MS.

F=MS_R/MS_E
with MSR=SSR/1
MSE=SSE/(n-2)





Assessing individual predictors

- Interpretation b₁
 - Change in average predicted outcome resulting from a unit change in the predictor
- Significance of b₁
 - \triangleright H_o: b₁=o, tested with t-test

$$t_{df=N-p-1} = \frac{b_{1observed} - b_{1expected}}{SE_{b1}} = \frac{b_{1observed}}{SE_{b1}}$$

(p is the number of predictors in the model, thus p=1)





Graphics in R with ggplot2

• In **ggplot2** a plot is made up of layers.

Eg:

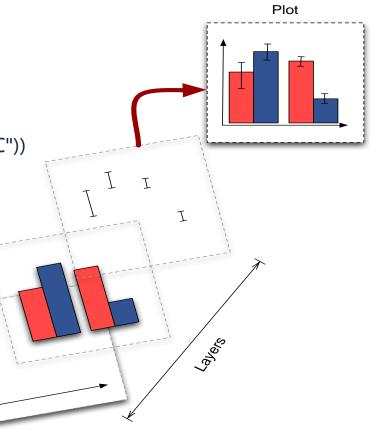
```
bar <- ggplot(chickFlick, aes(x, y, fill = z))
bar + stat_summary(fun.y = mean, ...)
     + stat_summary(fun.data = mean_cl_normal, ...)
     + scale_fill_manual(values=c("#339966", "#6699CC"))
     + labs(...)</pre>
```

More information on:

https://www.r-graph-gallery.com/

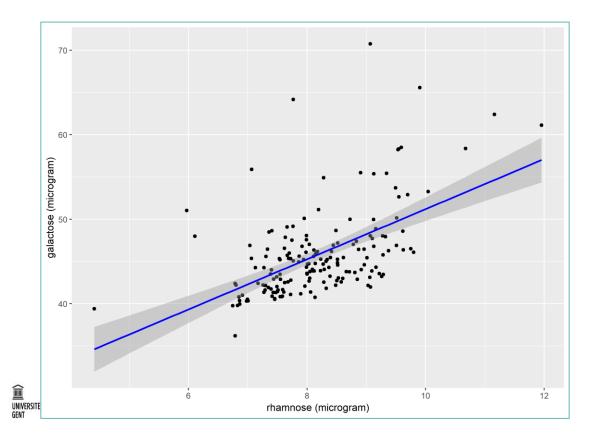






example

• Investigate the relationship between rhamnose and galactose in Arabidopsis lignin mutants





Example (continued)

- Im(outcome ~ predictor, data=dsn)
- Im.fit <- Im(galact_microg ~ rhamn_microg, data = arab)
- > summary(lm.fit)





Output of a Simple Regression

```
##
## Call:
## lm(formula = galact_microg ~ rhamn_microg, data = arab)
##
## Residuals:
             1Q Median
                                 Max
      Min.
## -6.454 -2.382 -1.041 1.432 22.316
##
## Coefficients:
##
               Estimate Std. Error t value Pr(>|t|)
## (Intercept) 21.533
                             2.825 7.623 1.63e-12 ***
## rhamn_microg 2.967
                             0.343 8.650 3.63e-15 ***
## ---
## Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
##
## Residual standard error: 4.342 on 171 degrees of freedom
     (13 observations deleted due to missingness)
## Multiple R-squared: 0.3044, Adjusted R-squared: 0.3003
## F-statistic: 74.83 on 1 and 171 DF, p-value: 3.63e-15
```





Using the Model

$$galactose_i = b_0 + b_1 rhamnose_i$$

= $21.53 + (2.97 * rhamnose_i)$
= $21.53 + (2.97 * 1)$
= 24.5





Checking Assumptions

- Variable type:
 - Pred cont or cat with non-zero variance
 - Outcome var: continuous or interval
- Linearity:
 - Linear in the parameters
- Normally distributed errors
- Homoscedasticity:
 - At each level of the predictor(s), the variance of the residuals should be the same
- Independent errors



Fitted Values and Residuals

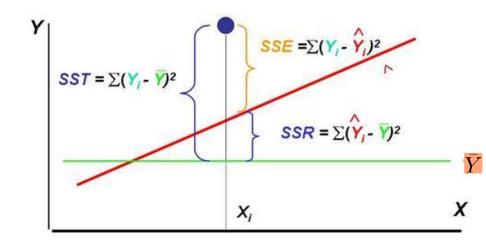
- Fitted values are the estimates of Y as determined by the regression equation.
- Residuals are the differences between each observed value and the corresponding fitted value.

$$y_i = b_0 + b_1 x_i + e_i$$

$$\hat{y}_i = b_0 + b_1 x_i$$

$$y_i = \hat{y}_i + e_i$$

$$y_i - \hat{y}_i = e_i$$



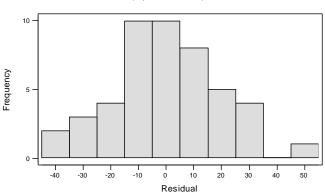




Residual Plots

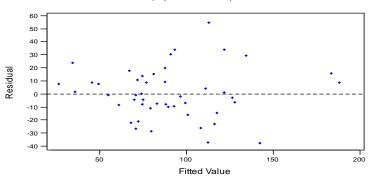
Histogram of the Residuals

(response is Crimrate)



Residuals Versus the Fitted Values

(response is Crimrate)

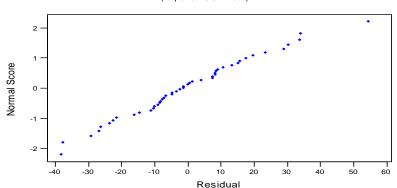


SYSTEMS BIOLOGY



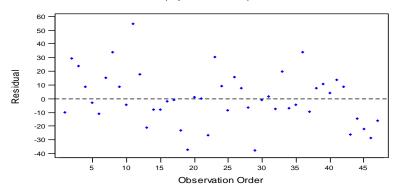
Normal Probability Plot of the Residuals

(response is Crimrate)



Residuals Versus the Order of the Data

(response is Crimrate)



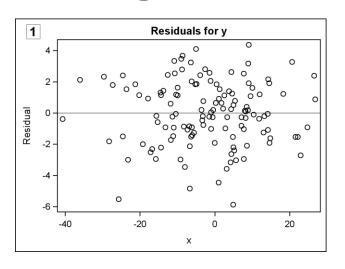
Studentized Residuals

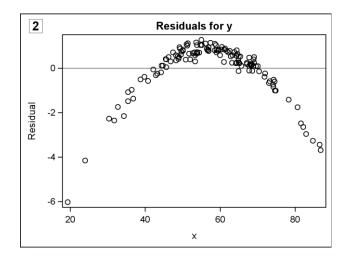
- Disadvantage raw residuals:
 - In same unit as observation (what is small/large?)
- Studentized residual:
 - Residual divided by the estimated standard deviation of the residuals (95% within -2 and +2)
- Suggested cutoffs are as follows:
 - |SR| > 2 for data sets with a relatively small number of observations
 - ▶ |SR| > 3 for data sets with a relatively large number of observations

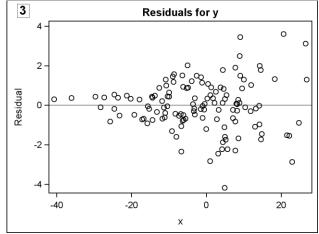


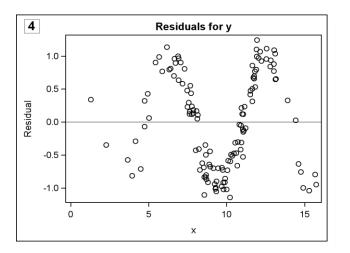


Examining Residual Plots









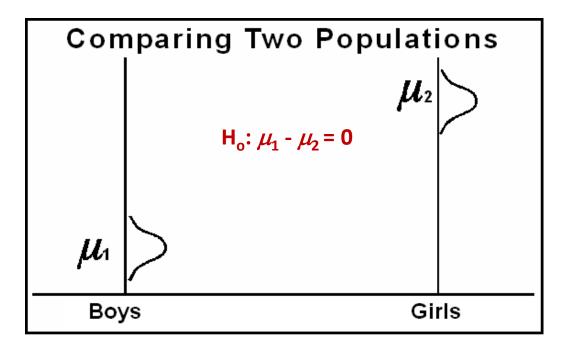


OLS with a binary predictor





Comparing Two Population Means: T-test



Statistical Assumptions:

- independent observations
- normally distributed population means
- equal population variances (Folded F Test)





The T-test as a GLM

$$Y_i = b_0 + b_1 Group_i + \epsilon_i$$





Dummy coding

- Provides a way of using categorical predictors in linear regression
- Uses zeros and ones to convey group membership
- For k groups, we can create k-1 dummies
- For 2 groups, only one dummy variable
 - X=1 when an observation belongs to group 2 and o otherwise





Design matrix

Assume treatment: control and treated

b _o *1 +	b₁*treatmenttreated
---------------------	---------------------

obs	sample	treatment	
1	C1	control	
2	C ₂	control	
3	C ₃	control	
4	T1	treated	
5	T ₂	treated	
6	T ₃	treated	

obs	Intercept	treatmenttreated	
1	1	0	
2	1	0	
3	1	0	
4	1	1	
5	1	1	
6	1	1	



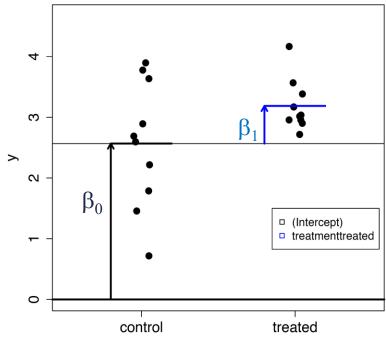


Design matrix

$$E[Y|X = control] = \beta_0$$

$$E[Y|X = treated] = \beta_0 + \beta_1$$

$$H_0: E[Y|X = treated] - E[Y|X = control] = \beta_1 = 0$$







OLS with a categorical predictor





ANOVA as Regression

Consider a control group, a low dose treatment group and a high dose treatment group and some outcome.

The regression model is:

$$outcome_i = b_0 + b_1 X_1 + b_2 X_2 + e_i$$

With $X_1 = 1$ if observation belongs to the Low Dose group and o otw $X_2 = 1$ if observation belongs to the High Dose group and o otw





Example with 3 treatment levels

observation	Intercept	Low Dose	High dose
Control	1	0	0
Control	1	0	0
Control	1	0	0
Low Dose	1	1	0
Low Dose	1	1	0
Low Dose	1	1	0
High Dose	1	0	1
High Dose	1	0	1
High Dose	1	0	1





Conditional models

Control group

$$X_1 = X_2 = 0$$

$$E[outcome|Control] = b_0 = \overline{x_{Control}}$$

Low dose group

$$E[outcome|LowDose] = b_0 + b_1 = \overline{x_{LowDose}}$$

$$b_1 = \overline{x_{LowDose}} - \overline{x_{Control}}$$

High dose group

$$E[outcome|HighDose] = b_0 + b_2 = \overline{x_{HighDose}}$$

$$b_2 = \overline{x_{HighDose}} - \overline{x_{Control}}$$







Performing Simple Linear Regression in R and SAS

R code regression.R and SAS code regression.sas illustrate the concepts discussed previously.



