

Regression Modelling

Maxwell Munford
PhD Biomechanics, Mechanical Engineering

Objectives

- ▶ Correlation
- ▶ Linear Regression
- ▶ Multi-Variable Regression
- ▶ Interpretation and Application
- ▶ NOT focussing on theory

What Is Regression?

... and why do we use it?

What Is Regression?

What Is Regression?

- ▶ A statistical analysis that attempts to predict the effects of one or more variables on another variable
- ▶ Correlation is a mutual relationship between 2 or more variables

The Process

- ▶ Scatter plots
- ▶ Measure the degree of linearity between two variables
- ▶ Quantify this relationship

What do we assume?

- ▶ Assume a causal relationship
- ▶ Equation of line of best fit
- ▶ Test the significance
- ▶ Analyse residuals
- ▶ Predication

} Analyse model

10

54.26

X Mean

47.83

Y Mean

16.76

X Standard Deviation

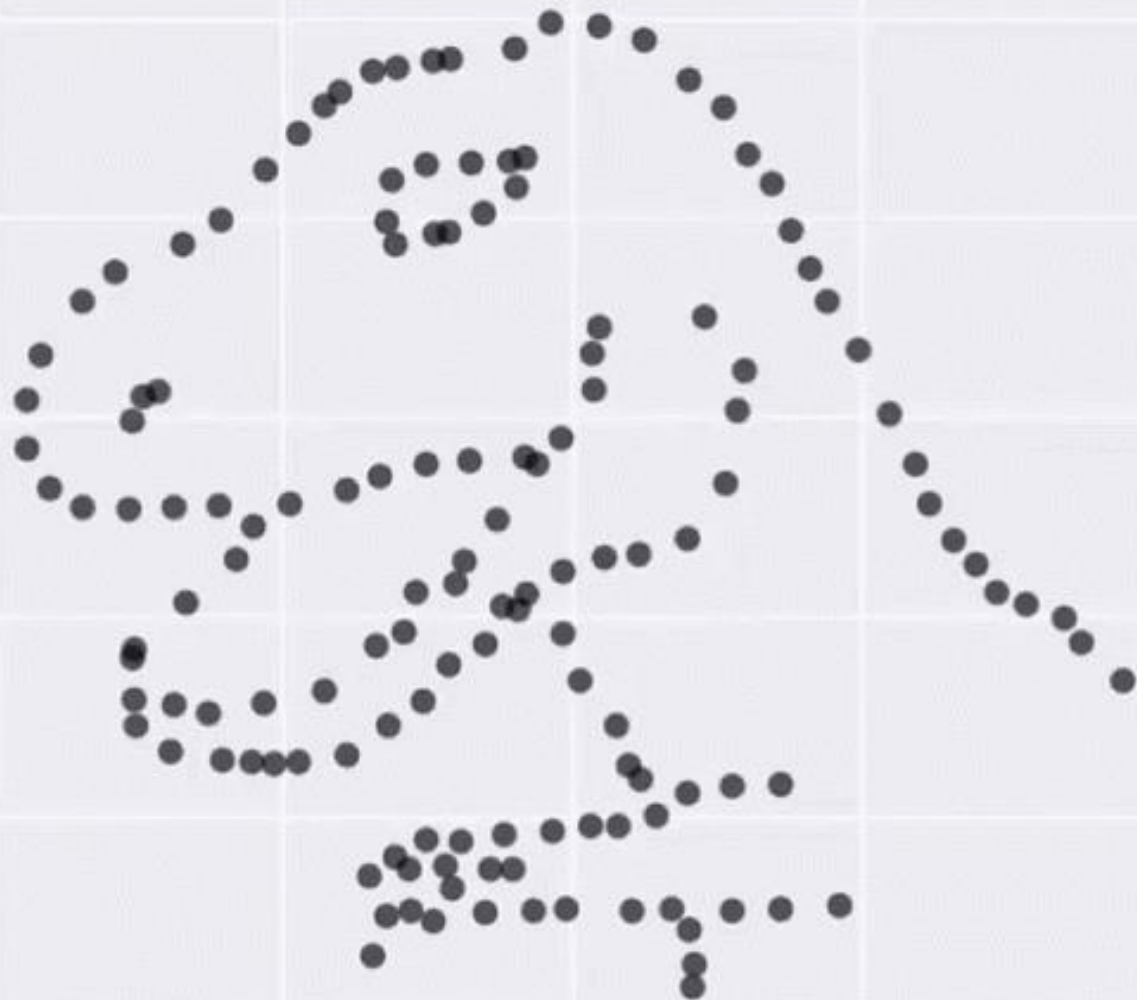
26.93

Y Standard Deviation

-0.06

Correlation Coefficient

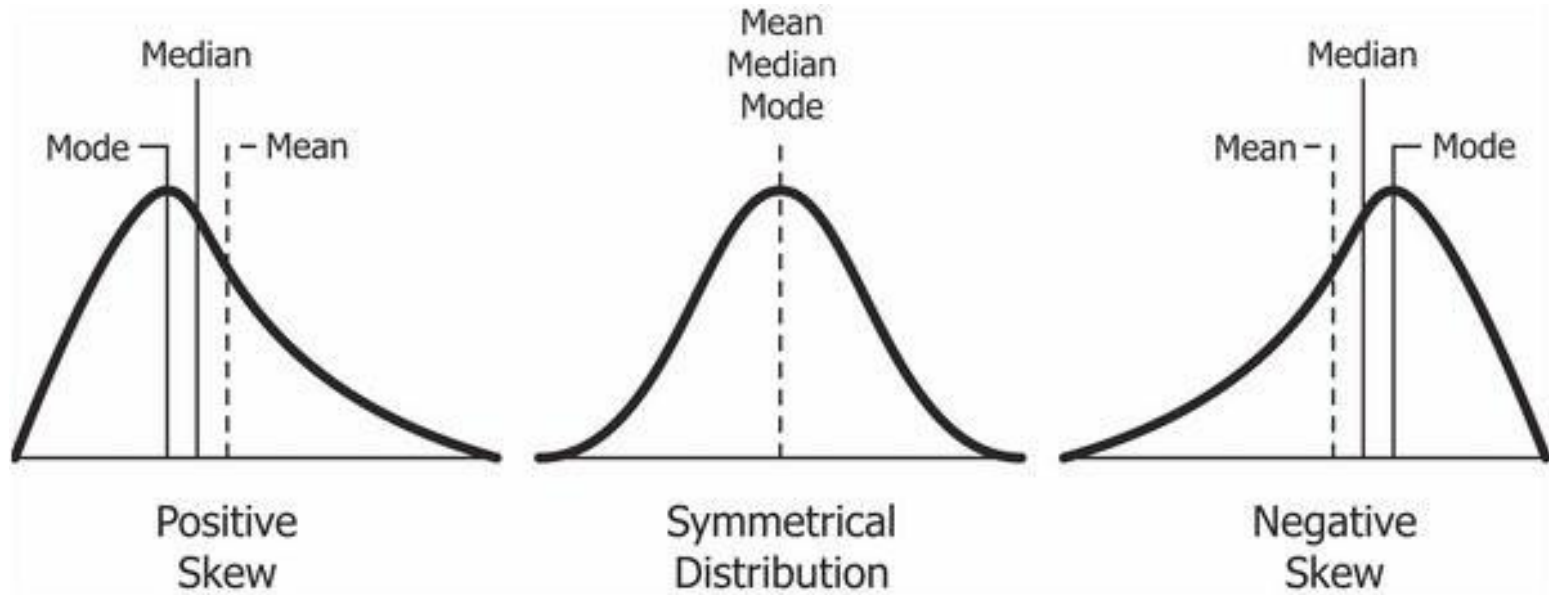
10



Scatter Plots

- ▶ Plot a scatter diagram and look for evidence of linear trend

- ▶ Skewness, in statistics, is the degree of distortion from the symmetrical bell curve in a probability distribution.
- ▶ Can be positive, negative or zero, to a varying degree.
- ▶ Helps to consider the extremes of data, not just the averages, by standardising data.



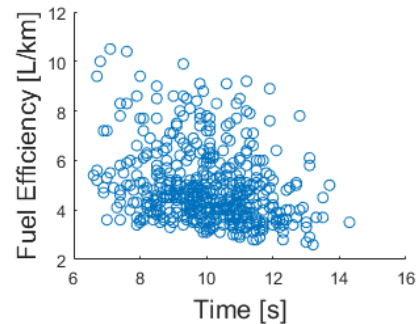
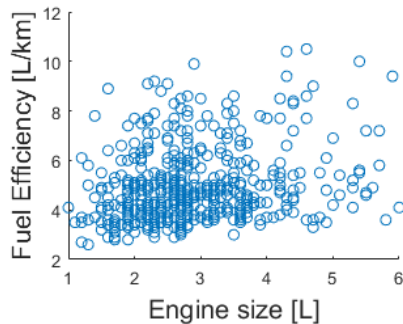
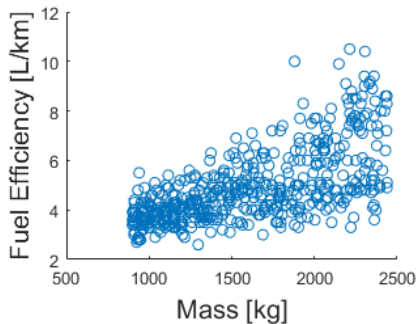
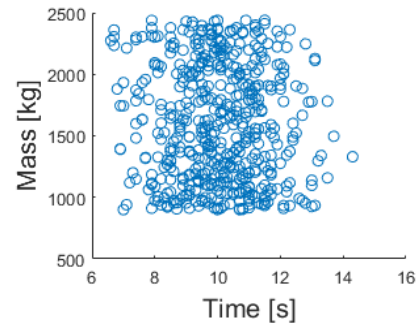
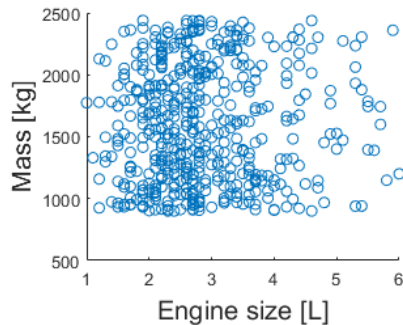
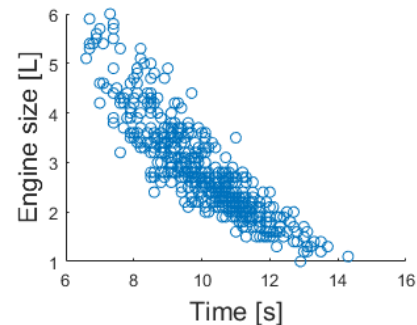
Car Emissions Data Task

Regression Analysis

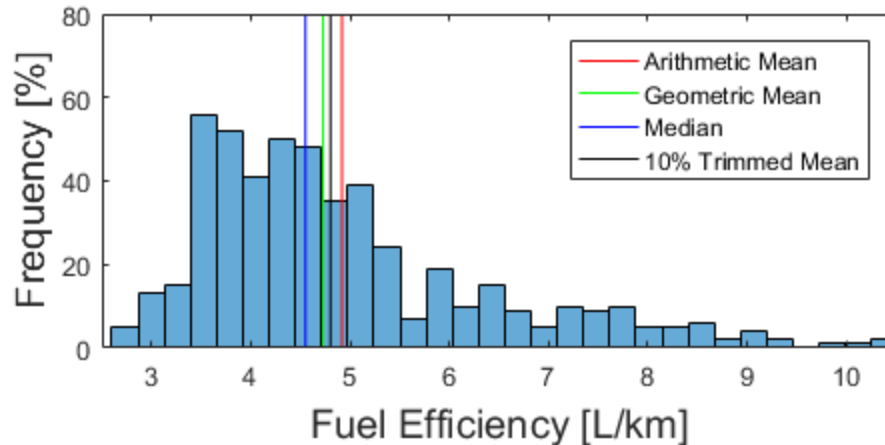
Generate and evaluate a model for fuel efficiency in terms of time, vehicle mass, engine size, fuel type and colour

Scatter Plots

- ▶ Looking for possible correlation



- ▶ Looking for skew in the response variable
- ▶ Positive skew \Rightarrow mode < median < mean

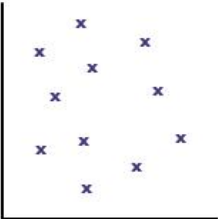
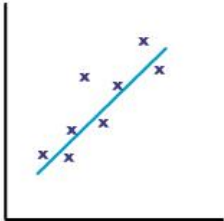
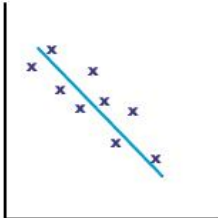


Initial Thoughts...

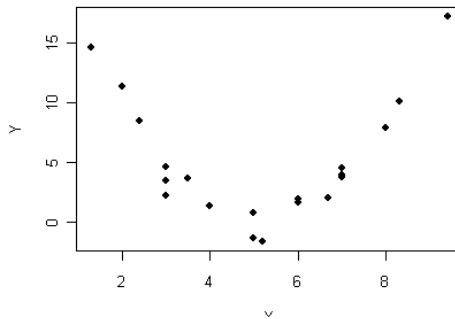
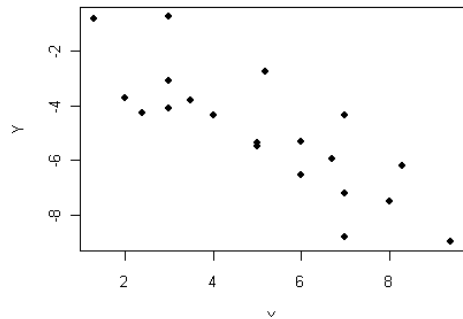
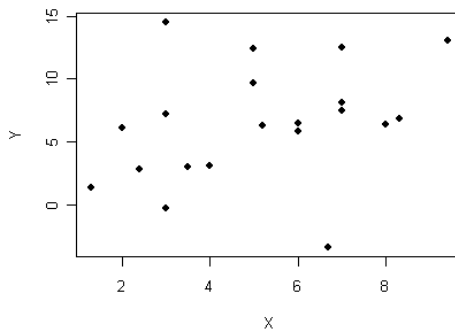
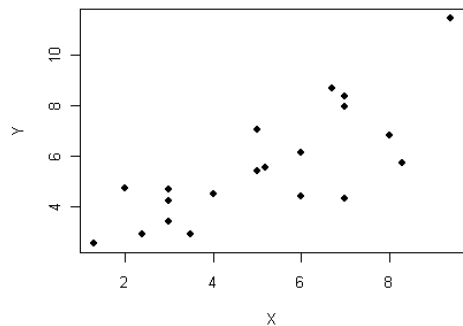
- ▶ Correlation exists between fuel efficiency, vehicle mass, acceleration time and engine size and engine size and acceleration time.
- ▶ Weaker correlation between fuel efficiency and engine size
- ▶ Positive skew, so we should standardise by the geometric mean, $x' = \frac{x - \bar{x}_{Geometric}}{\sigma_{Geometric}}$

- ▶ Having decided that x_i and y_i are paired
- ▶ We want to study the relationship between them
- ▶ The Correlation coefficient measures the degree of linear relation between x and y

Correlation

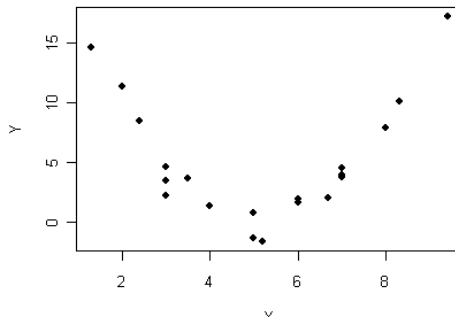
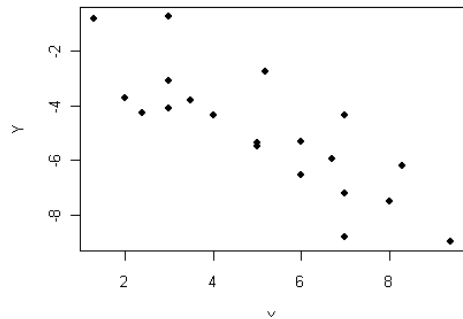
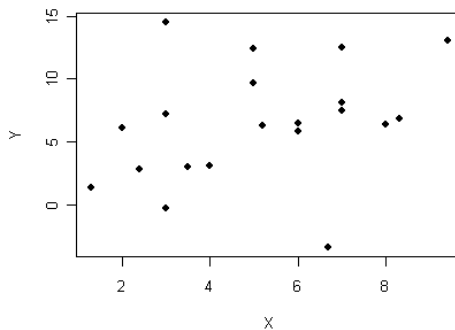
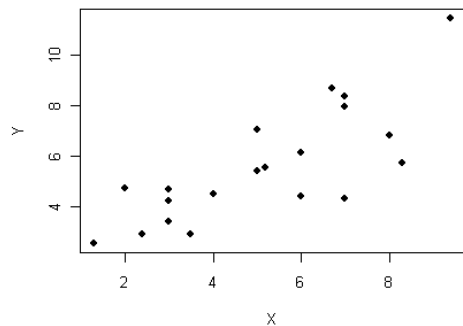
R	Results	Correlation	Example
0	Uncorrelated	No correlation	 A scatter plot with approximately 12 data points (marked with 'x') distributed randomly across the plot area, showing no discernible linear trend.
>0	Positively correlated	$y = \beta x + \alpha$	 A scatter plot with approximately 10 data points (marked with 'x') showing a clear upward linear trend. A solid blue line is drawn through the points, representing a positive linear regression.
<0	Negatively correlated	$y = -\beta x + \alpha$	 A scatter plot with approximately 10 data points (marked with 'x') showing a clear downward linear trend. A solid blue line is drawn through the points, representing a negative linear regression.

Correlation



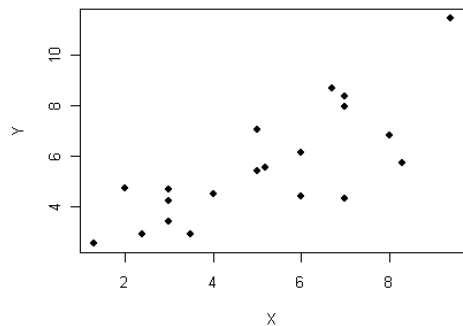
Correlation

correlation = 0.78

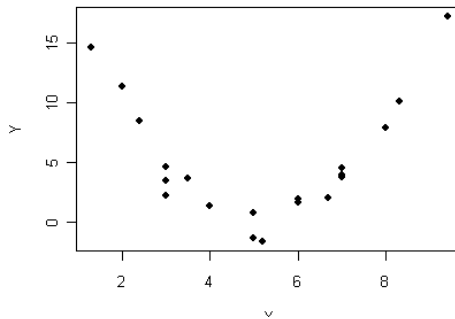
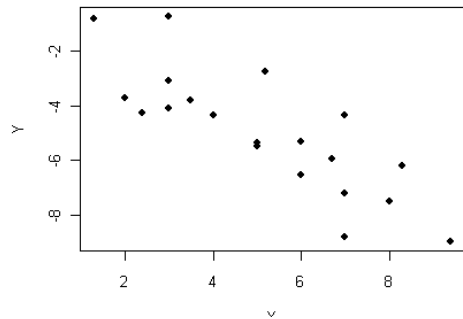
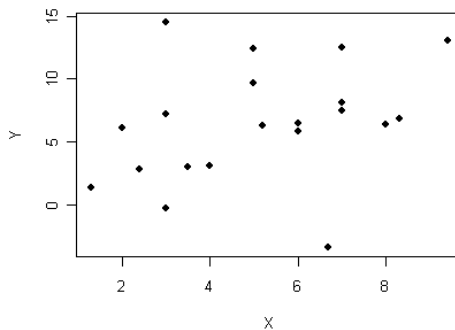


Correlation

correlation = 0.78

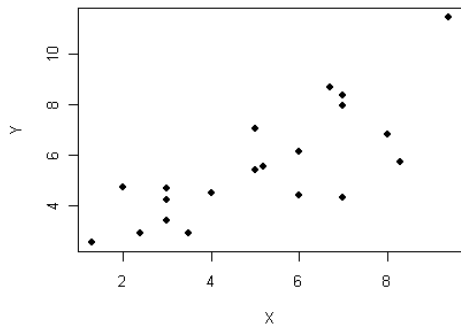


correlation = 0.32

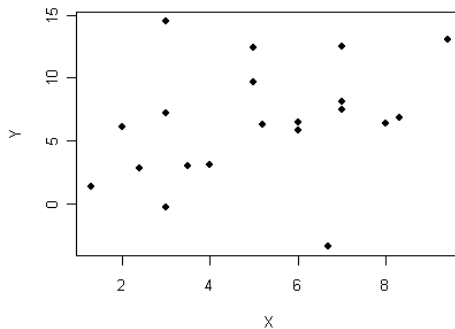


Correlation

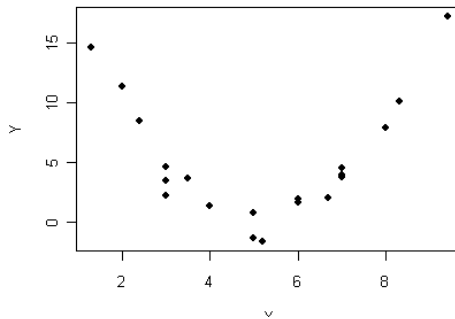
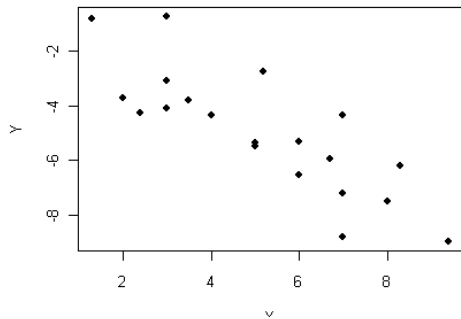
correlation = 0.78



correlation = 0.32

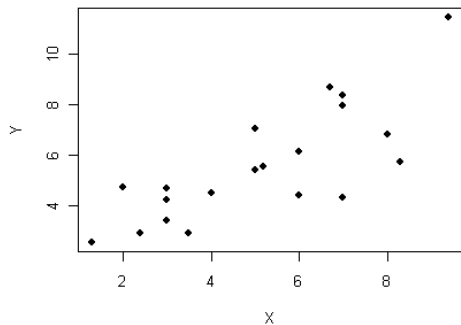


correlation = -0.82

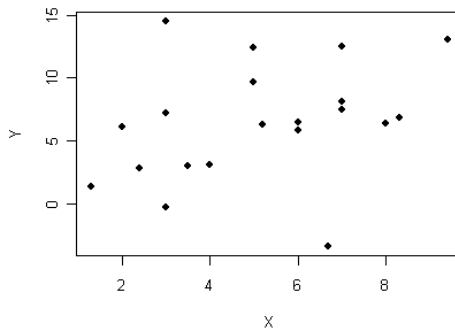


Correlation

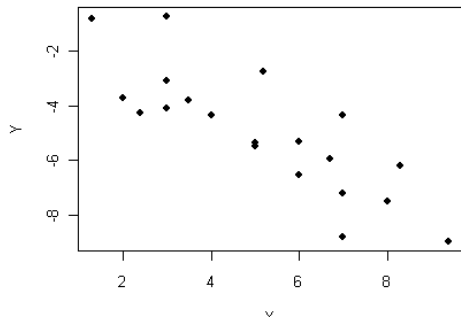
correlation = 0.78



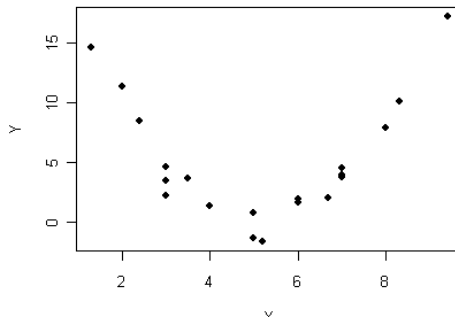
correlation = 0.32

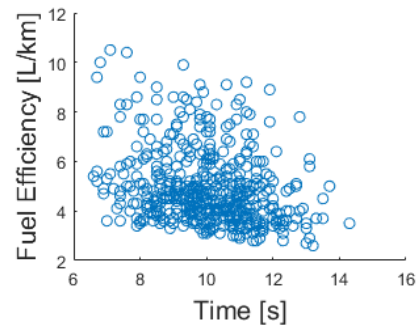
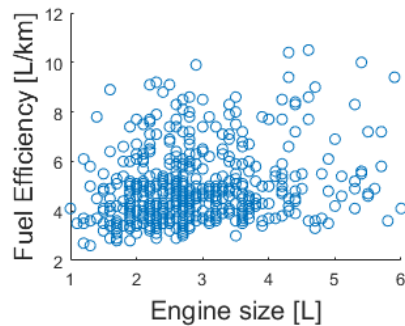
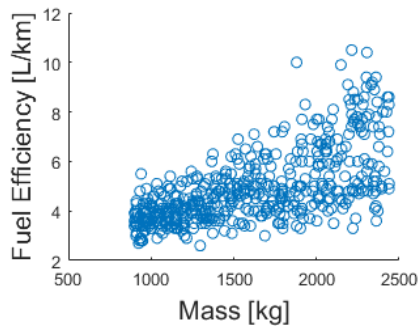
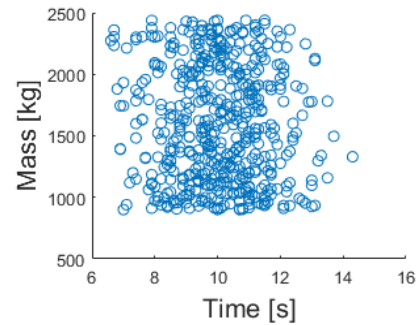
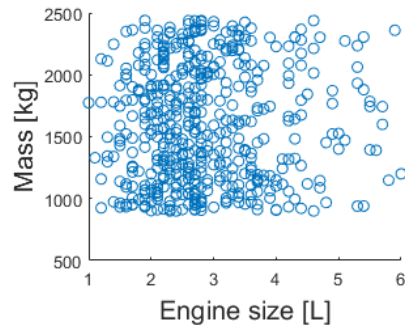
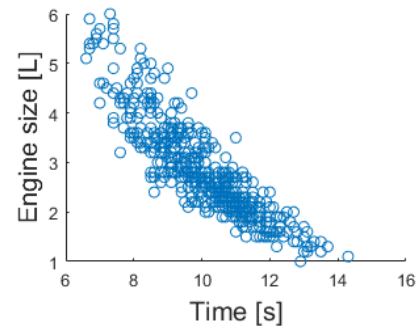


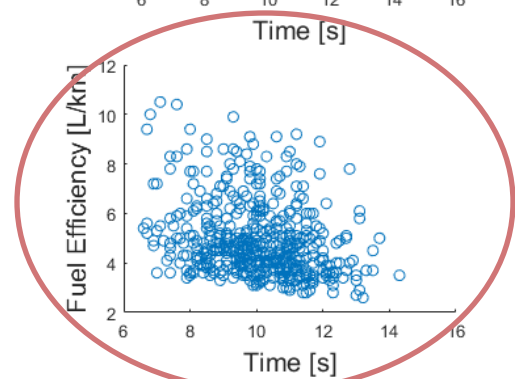
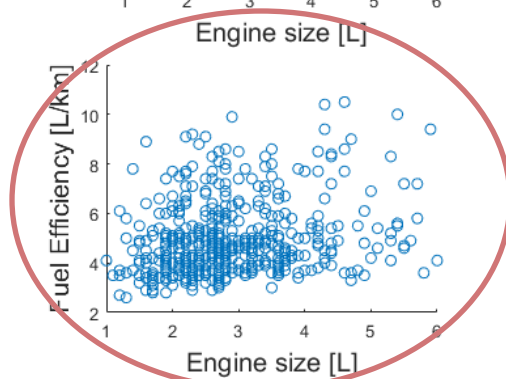
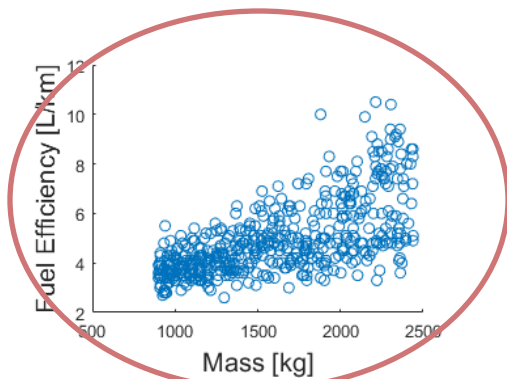
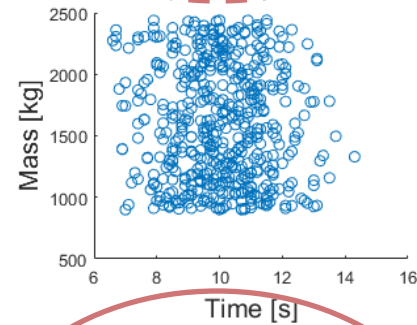
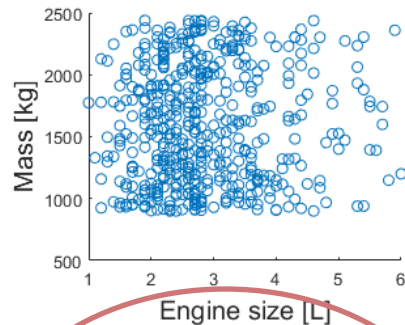
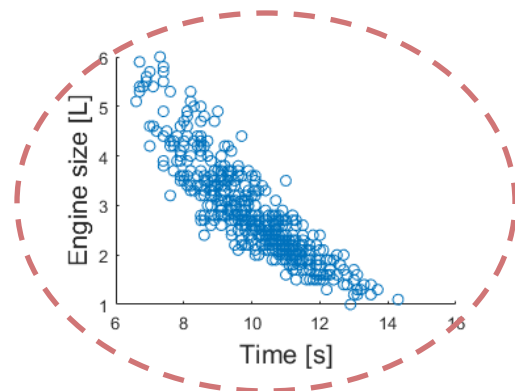
correlation = -0.82



correlation = 0.02



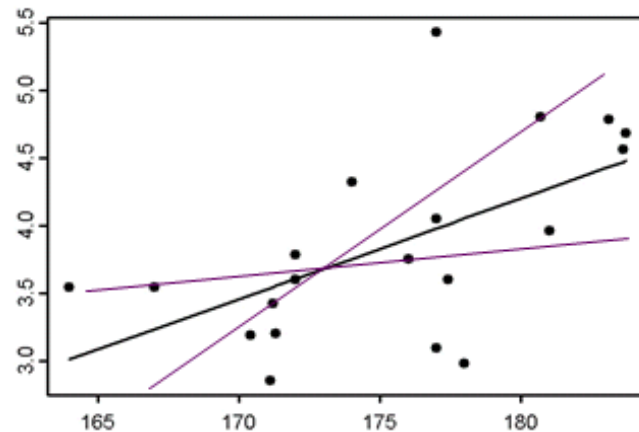




- ▶ Not necessarily interested in the correlation coefficient
- ▶ Where does weaker correlation exist
- ▶ Interaction term may be needed between engine size and time

Regression

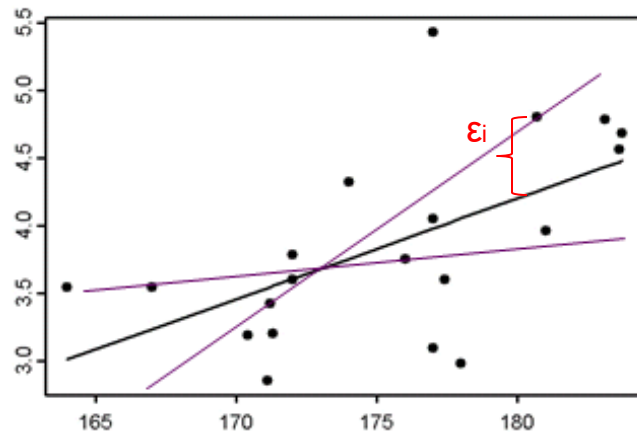
- ▶ $y_i = \alpha + \beta x_i$
- ▶ Let a = estimated α
 b = estimated β



- ▶ a = average fuel consumption at height = 0
- ▶ b = increase in fuel consumption for 1cm increase in height

Regression: Residuals

- ▶ Our model is not perfect
- ▶ $y_i = \alpha + \beta x_i + \epsilon_i$



- ▶ Residuals are the error between our model predictions and the actual data
- ▶ We assume these are normally distributed

Regression: Least Squares

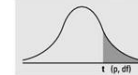
- ▶ Find the line of best fit (estimate α and β) to minimise this error
- ▶
$$\sum_{i=1}^n \epsilon_i^2 = \sum_{i=1}^n (y_i - \alpha - \beta x_i)^2$$
- ▶ MATLAB, Python and excel all have libraries to solve this

Regression: Least Squares

- ▶ $\sum_{i=1}^n \epsilon_i^2 = \sum_{i=1}^n (y_i - \alpha - \beta x_i)^2$
- ▶ This is an optimisation in terms of α and β
- ▶ The resulting model predicts y values given x
- ▶ $y = a + bx$

Regression: Confidence Interval

- ▶ How accurate are our estimated values of a and b ?
- ▶ Confidence intervals based on the standard error
- ▶ 95% CI in b calculated from t scores
- ▶ $(b - t SE(b), b + t SE(b))$



df/p	0.40	0.25	0.10	0.05	0.025	0.01	0.005	0.0005
1	0.324920	1.000000	3.077684	6.313752	12.70620	31.82052	63.65674	636.6192
2	0.288675	0.816497	1.885618	2.919986	4.30265	6.96456	9.92484	31.5991
3	0.276671	0.764892	1.637744	2.353363	3.18245	4.54070	5.84091	12.9240
4	0.270722	0.740697	1.533206	2.131847	2.77645	3.74695	4.60409	8.6103
5	0.267181	0.726687	1.475884	2.015048	2.57058	3.36493	4.03214	6.8688
6	0.264835	0.717558	1.439756	1.943180	2.44891	3.14267	3.70743	5.9588
7	0.263167	0.711142	1.414924	1.894579	2.36462	2.99795	3.49948	5.4079
8	0.261921	0.706387	1.396815	1.859548	2.30600	2.89646	3.35539	5.0413
9	0.260955	0.702722	1.383029	1.833113	2.26216	2.82144	3.24984	4.7809
10	0.260185	0.699812	1.372194	1.812461	2.22814	2.76377	3.16927	4.5869
11	0.259556	0.697445	1.363430	1.795885	2.20099	2.71808	3.10581	4.4370
12	0.259033	0.695483	1.356217	1.782288	2.17881	2.68100	3.05454	4.3178
13	0.258591	0.693829	1.350171	1.770933	2.16037	2.65031	3.01228	4.2208
14	0.258213	0.692417	1.345030	1.761310	2.14479	2.62449	2.97684	4.1405
15	0.257885	0.691197	1.340606	1.753050	2.13145	2.60248	2.94671	4.0728
16	0.257599	0.690132	1.336757	1.745884	2.11991	2.58349	2.92078	4.0150
17	0.257347	0.689195	1.333379	1.739607	2.10982	2.56693	2.89823	3.9651
18	0.257123	0.688364	1.330391	1.734064	2.10092	2.55238	2.87844	3.9216
19	0.256923	0.687621	1.327728	1.729133	2.09302	2.53948	2.86093	3.8834
20	0.256743	0.686954	1.325341	1.724718	2.08596	2.52798	2.84534	3.8495
21	0.256580	0.686352	1.323188	1.720743	2.07961	2.51765	2.83136	3.8193
22	0.256432	0.685805	1.321237	1.717144	2.07387	2.50832	2.81876	3.7921
23	0.256297	0.685306	1.319460	1.713872	2.06866	2.49987	2.80734	3.7676
24	0.256173	0.684850	1.317836	1.710882	2.06390	2.49216	2.79694	3.7454
25	0.256060	0.684430	1.316345	1.708141	2.05954	2.48511	2.78744	3.7251
26	0.255955	0.684043	1.314972	1.705618	2.05553	2.47863	2.77871	3.7066
27	0.255858	0.683685	1.313703	1.703288	2.05183	2.47266	2.77068	3.6896
28	0.255768	0.683353	1.312527	1.701131	2.04841	2.46714	2.76326	3.6739
29	0.255684	0.683044	1.311434	1.699127	2.04523	2.46202	2.75639	3.6594
30	0.255605	0.682756	1.310415	1.697261	2.04227	2.45726	2.75000	3.6460
z	0.253347	0.674490	1.281552	1.644854	1.95996	2.32635	2.57583	3.2905
CI	———	———	80%	90%	95%	98%	99%	99.9%


Warning

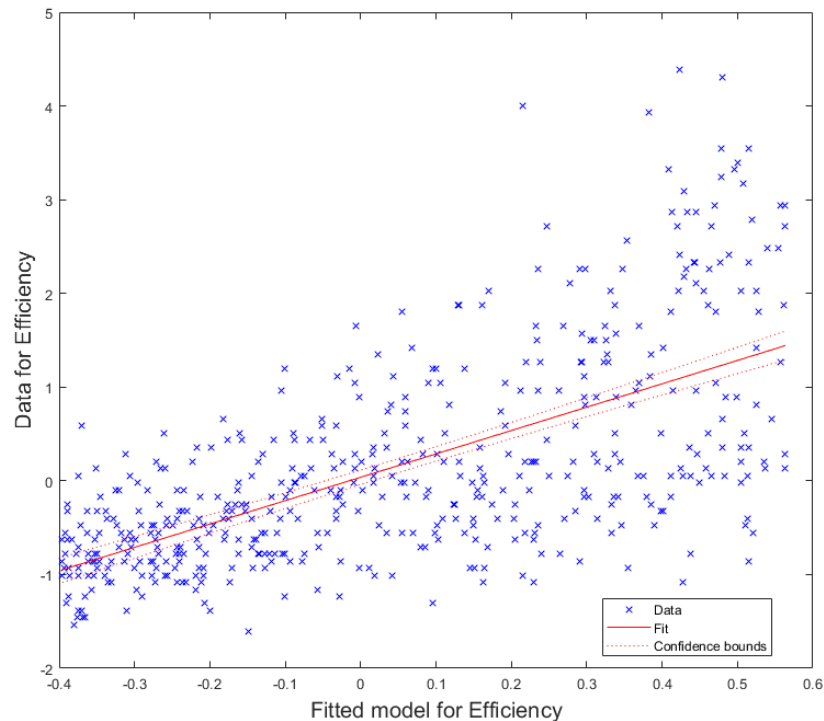
- ▶ Do not use your model to predict data outside the range of values in the **domain** of x
- ▶ Be cautious of overfitting

Regression with a Single Predictor Variable

- ▶ Model with one predictor:
- ▶ $Efficiency = \alpha + \beta Mass$

Regression with a Single Predictor Variable

- ▶ Model with one predictor:
- ▶ $Efficiency = \alpha + \beta Mass$
- ▶ $R^2 = 0.4157$ 
- ▶ $MSE = 0.7402$
- ▶ $AIC = 12705$



What do we think of this model?

- ▷ $R^2 = 0.4157$
- ▷ $MSE = 0.7402$
- ▷ $AIC = 1271$

Multiple Variable Linear Regression?

Multiple Explanatory Variables

- ▶ Multiple variables which simultaneously affect output variable
- ▶ Interpretation can become increasingly difficult with more variables
- ▶ Prevent confounding and reduce residual variation



Multiple Explanatory Variables


- ▶ $y_i = \alpha + \beta_1 x_{1,i} + \beta_2 x_{2,i} + \beta_2 x_{2,i} + \dots + \epsilon_i$
- ▶ i = number of observations
- ▶ $x_{1,i} = i^{th}$ observation of the 1st variable
- ▶ $x_{2,i} = i^{th}$ observation of the 2nd variable
- ▶ β_1 = the increase in y for a unit increase in x_1

Categorical Variables

- ▶ Takes one of a limited number of values
- ▶ Binary variables take values 0 or 1

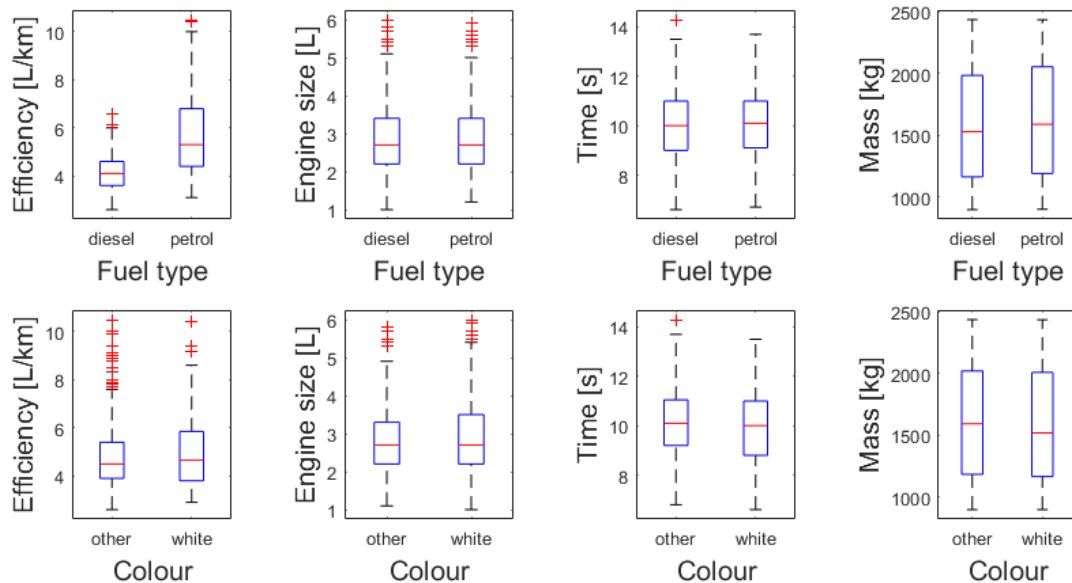
BloodType
State
Gender
Ethnicity
HairColour
ModeOfTransport
LanguageType
EyeColour
CarType
Brand
PoliticalParty

Binary Variables

- ▶ $y_i = \alpha + \beta_1 x_i + \epsilon_i$ 
- ▶ This model fits the mean of y for each category of x
- ▶ α = mean y_i in 1st group
- ▶ $\alpha + \beta$ = mean y_i in 2nd group
- ▶ β = difference in y_i between groups

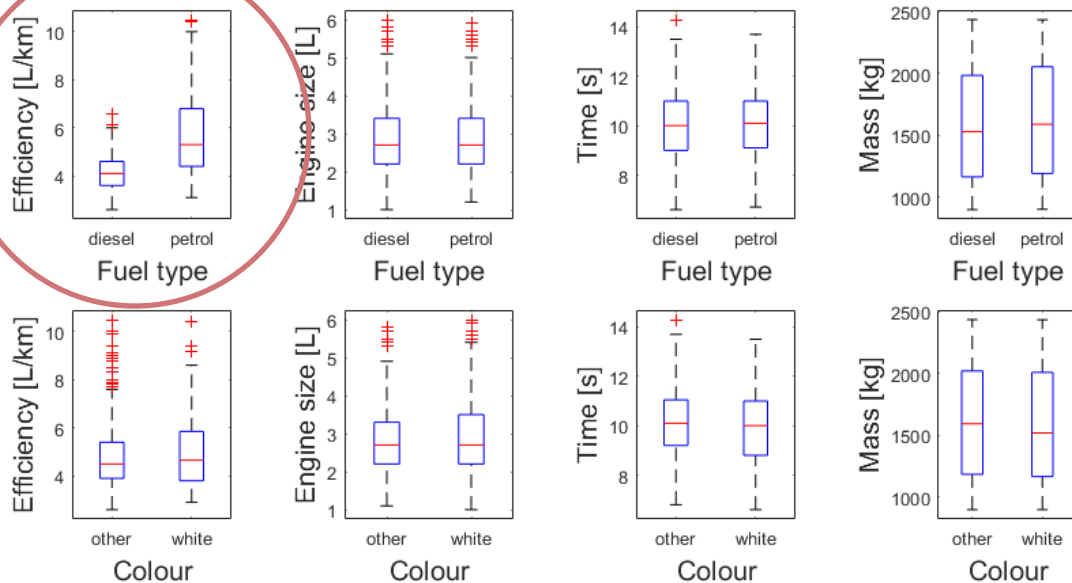
Categorical Variables

- ▶ Box plots of our data against known categorical variables



Categorical Variables

- ▶ Box plots of our data against known categorical variables



Categorical Variables

- ▶ Fuel efficiency looks likely to depend on Fuel type to some degree
- ▶ Fuel type could be a suitable predictor variable in the model

Regression: Least Squares with Multiple Variables

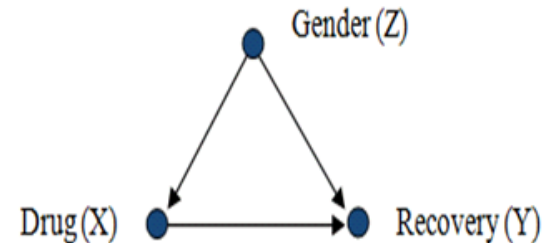
- ▶ $\sum_{i=1}^n \epsilon_i^2 = \sum_{i=1}^n (y_i - \alpha - \beta_1 x_{1,i} - \beta_2 x_{2,i} - \beta_2 x_{2,i})^2$
- ▶ This is an optimisation in terms of α and $\beta_{1,2,3} \dots$
- ▶ The resulting model predicts y values given x

Regression with Multiple Variables

- ▶ Regression coefficients (b) report the effect of each variable while holding all others at their average values

Confounding

- ▶ Consider a researcher attempting to assess the effectiveness of drug X, from population data in which drug usage was a patient's choice.
- ▶ Data show that gender differences influence a patient's choice of drug as well as their chances of recovery (Y).
- ▶ In this scenario, **gender z confounds the relationship between X and Y since Z is a cause of both X and Y.**



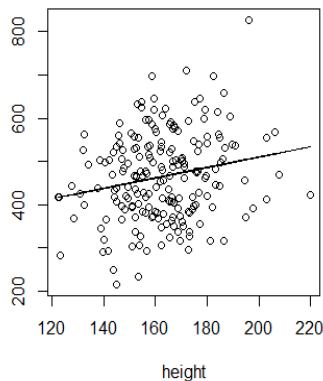
- ▶ $y_i = \alpha + \beta_1 x_{1,i} + \beta_2 x_{2,i} + \beta_3 x_{3,i} + \beta_4 (x_{2,i} x_{3,i}) + \dots + \epsilon_i$
- ▶ $x_{3,i}$ is a categorical variable
- ▶ β_2 = increase in y_i for unit increase in x_2
- ▶ $\beta_3 + \beta_4$ = increase in y_i for unit increase in x_2 for an observation in the categorical variable x_3

- ▶ $ArmLength_i = \alpha + \beta_1 Age_i + \beta_2 Height_i + \beta_3 Gender_i + \beta_4 (Height_i Gender_i) + \epsilon_i$
- ▶ Gender is the categorical variable
- ▶ β_2 = increase in *ArmLength* for unit increase in *Height*
- ▶ $\beta_2 + \beta_3$ = increase in *ArmLength* for unit increase in *Height* for a *Female*

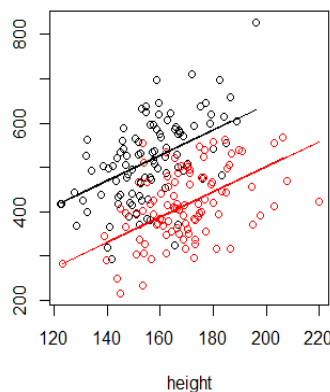
- ▶ If the interaction term is significant then we should include both the interaction and individual terms
- ▶ The effect of gender is the different between males and females in this model on the value of height
- ▶ This must be found considering the interaction term

Model Interactions

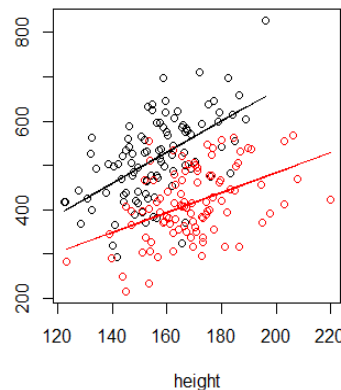
- Assuming the effect of height is significant we can have three models depending on whether gender and the interaction are significant.



$$\text{ArmLength}_i = \alpha + \beta_1 \text{Age}_i + \beta_2 \text{Height}_i$$



$$\text{ArmLength}_i = \alpha + \beta_1 \text{Age}_i + \beta_2 \text{Height}_i + \beta_3 \text{Gender}_i$$



$$\text{ArmLength}_i = \alpha + \beta_1 \text{Age}_i + \beta_2 \text{Height}_i + \beta_3 \text{Gender}_i + \beta_4 (\text{Height}_i \text{Gender}_i)$$

Improve on the Previous Model by Including more Terms

- ▶ Model with one predictor:
- ▶ $Efficiency = \alpha + \beta_1 Mass + \beta_2 FuelType$
- ▶ $R^2 = 0.6540$
- ▶ $MSE = 0.4383$
- ▶ $AIC = 1010$

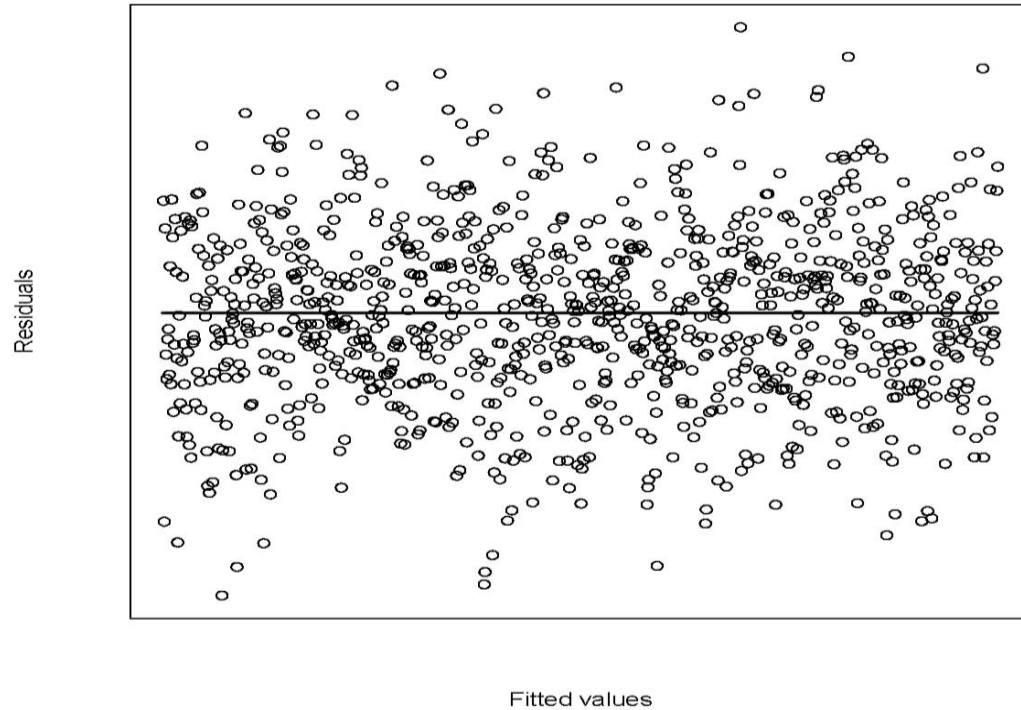
Model Checking

Model checking should be performed to avoid erroneous extrapolation of data trends

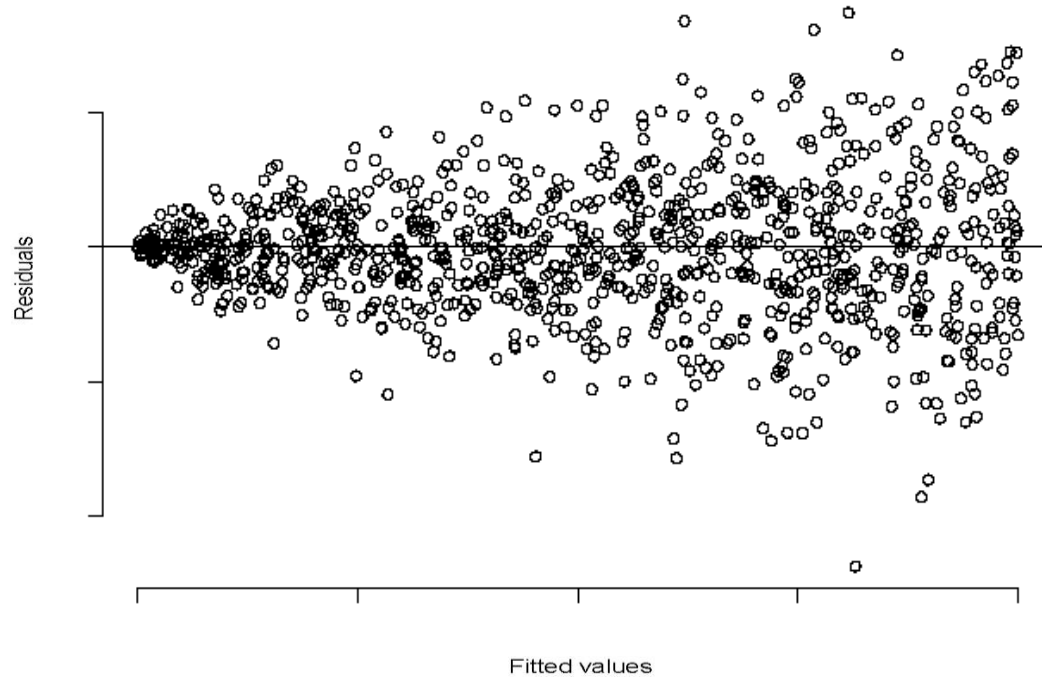
- ▶ Residuals are the error between the observed and predicted data
- ▶ Look for trends or patterns in the residuals which indicate an assumption is not valid

- ▶ Scatter plots of residuals against fitted values help identify:
 - ▶ Non-constant variance
 - ▶ Violation of the linearity assumption
 - ▶ Potential outliers
- ▶ If these assumptions are valid then you will see no trend

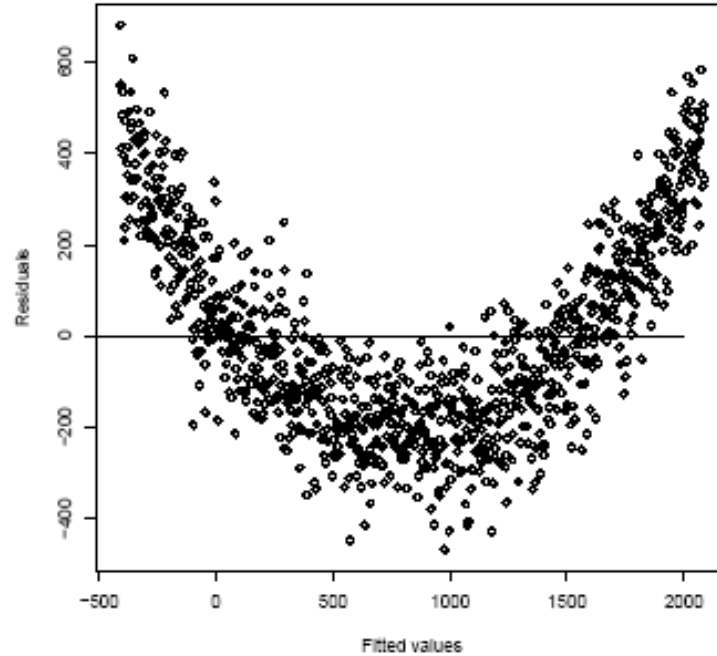
Residual Scatter Plot: Satisfactory



Residual Scatter Plot: Non-constant Variance



Residual Scatter Plot: Non-Linear Relationship

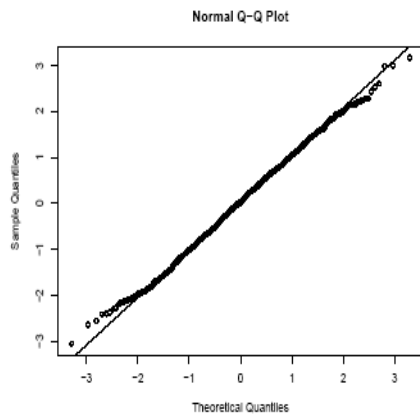


Residual Analysis

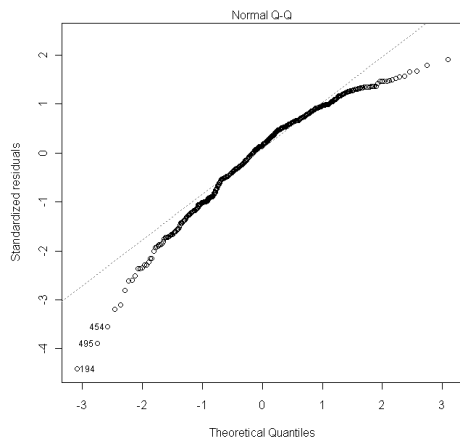
- ▶ Standardise residuals by dividing by their standard deviation
- ▶ They should now be Normal with mean = 0 and variance = 1
- ▶ Box plots – symmetric?
- ▶ Proportion of standardised residuals inside percentiles
- ▶ Q-Q plot – $x = y$ graph should form

Q-Q Plots and Skew

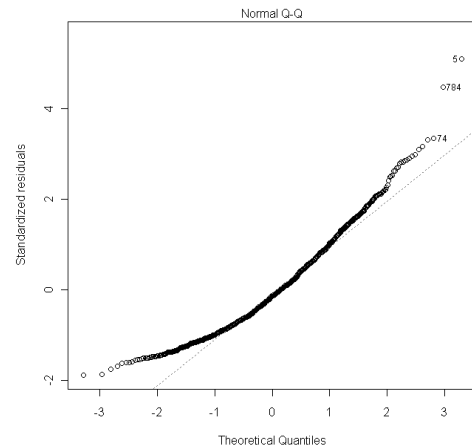
► Satisfactory



► Negative Skew



► Positive Skew



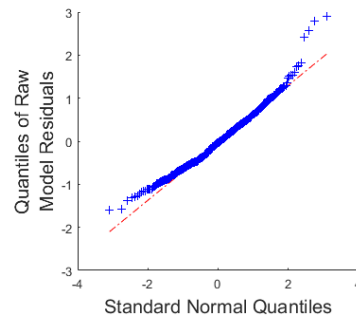
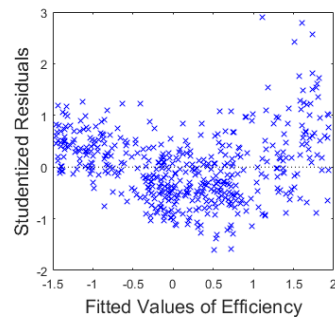
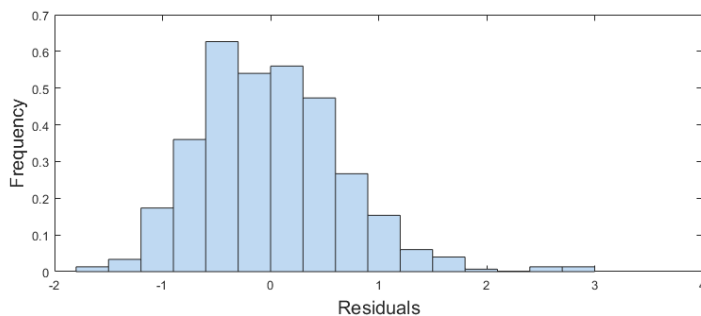
- ▶ Median < Geometric Mean < Arithmetic Mean
- ▶ Positive skew => Standardise by the geometric mean
- ▶ Negative skew=> Standardise

Identifying Outliers

- ▶ Any points which stand out as having larger residuals than other values should be checked
- ▶ Cook's Distance is given by most software and measures the influence of each individual point on the model

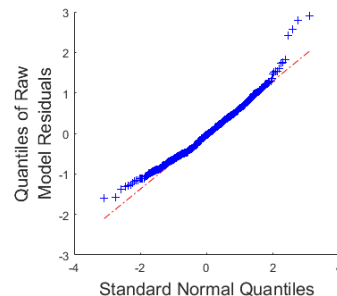
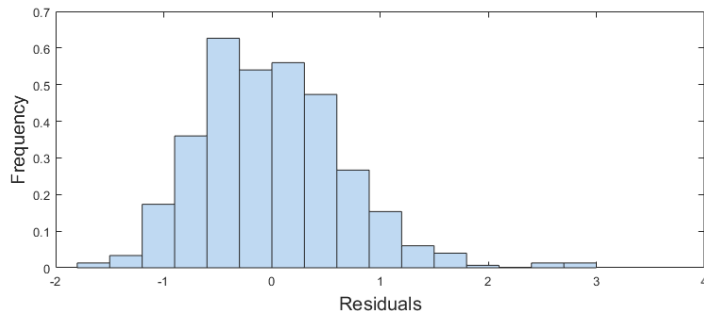
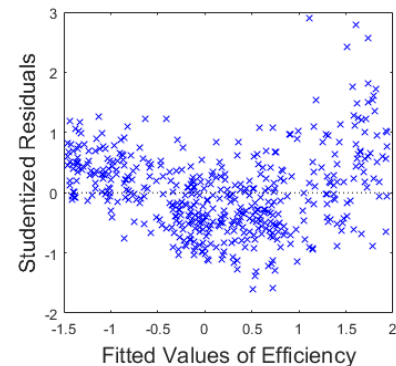
Residual Analysis

▸ $Efficiency = \alpha + \beta_1 Mass + \beta_2 FuelType$



Residual Analysis

- ▶ Possibly a non-linear relationship?
- ▶ Maybe very slightly positively skewed?



Model Fitting

Model checking should be performed to avoid erroneous extrapolation of data trends

Scatter Plots, Box Plots & Histograms

Look for linearly related variables, skewness

Interaction Terms

These may improve the model of your data

Adjust Model

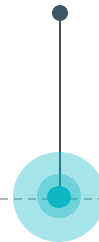
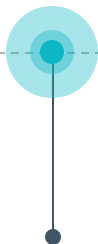
You may transform variables before fitting a model or include additional terms

Fit Model

Based on which variables you suspect are linearly related from scatter diagrams.

Residual Analysis

Look for non-constant variance, non-linearity and potential outliers



MATLAB Script


- ▶ Given data on car emissions in terms of vehicle mass, acceleration time, engine size, fuel type and colour.
- ▶ Fit models seeking to optimise for:
 - ▶ Error
 - ▶ AIC – relative loss of information

Search for Best Models

- ▶ Open file: Regression_Analysis_Car_Emissions
- ▶ Use the scatter and box plots to pick a starting model

How to Use the Script


- ▶ Standardise by the arithmetic or geometric mean



```

94
95
96 % 'G' for geometric standardisation or 'A' for arithmetic standardisation
97 - standard = Standardise(cont,FieldNames,ArMean,ArStd,GeoMean,GeoStd,'A');
98
99
  
```

- ▶ Edit line 115 with your trial model



```

113
114 % Insert Model Here
115 - model = ['Efficiency ~ Mass + FuelType'];
116
117 % Other Examples for models
118 % model = ['Efficiency ~ Mass + EngineSize^2'];
119 % AccelTime
120 % EngineSize
121 % Mass
122 % FuelType
123 % Mass:FuelType % Example of an interaction term
124
  
```

Search for Best Models

- ▶ Keep note of the MSE, Rsquared and AIC
- ▶ Seek to increase Rsquared
- ▶ Seek to reduce MSE and AIC

Things to Try

- ▶ Increasing the number of terms
- ▶ Including categorical variables
- ▶ Using interaction terms (FuelType:AccelerationTime)
- ▶ Standardising Method
- ▶ Raising terms to a power

How did you do?

Prizes for the 'best' model

An Optimum Model?

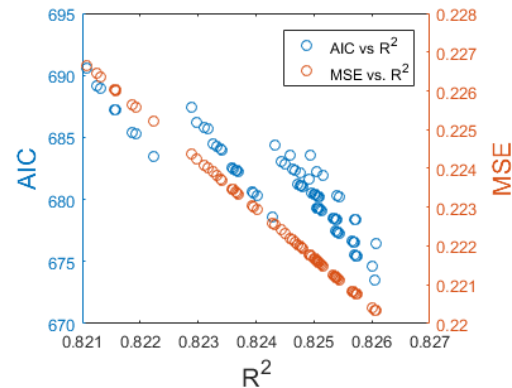
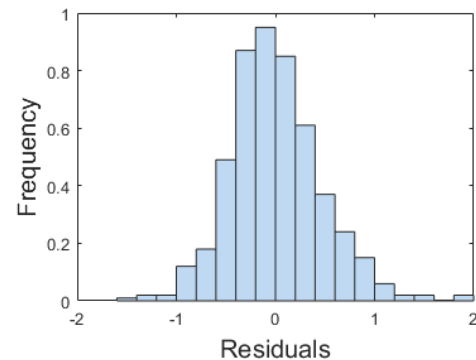
▶ Running the script:

```

125
126 % Make Model:
127 % [Rmax,mdl,Criteria] = MakeModel(tbl,model);
128 - [CountOpt,Rmax,mdl,Criteria] = MakeOptimumModel(tbl,3)
129

```

- ▶ Normally distributed residuals
- ▶ AIC and MSE clearly decrease with Rsquared



Model Simplicity

► Model 1

- Rsquared = 0.8261
- MSE = 0.220
- AIC = 673

$$\begin{aligned} \text{Efficiency} = & \\ & \alpha + \beta_1 \text{Mass} \\ & + \beta_2 \text{EngineSize} \\ & + \beta_3 \text{AccelerationTime} \\ & + \beta_4 \text{MassFuelType}^2 \end{aligned}$$

► Model 2

- Rsquared = 0.8261
- MSE = 0.220
- AIC = 676

$$\begin{aligned} \text{Efficiency} = & \\ & \alpha + \beta_1 \text{Mass}^3 \\ & + \beta_2 \text{EngineSize} \\ & + \beta_3 \text{AccelerationTime}^2 \\ & + \beta_4 \text{MassFuelType}^2 \\ & + \beta_4 \text{EngineSize FuelType} \end{aligned}$$

Further Reading

What are next steps

- ▶ K-means cluster classification
- ▶ Bootstrapping (Confidence Intervals)
- ▶ Introductory courses to Machine Learning (Stanford, coursera)

How did we do?

- ▶ Please let us know what you thought of this course and how we can improve it
- ▶ <https://forms.gle/HAdcNGkFK5fkCimk6>