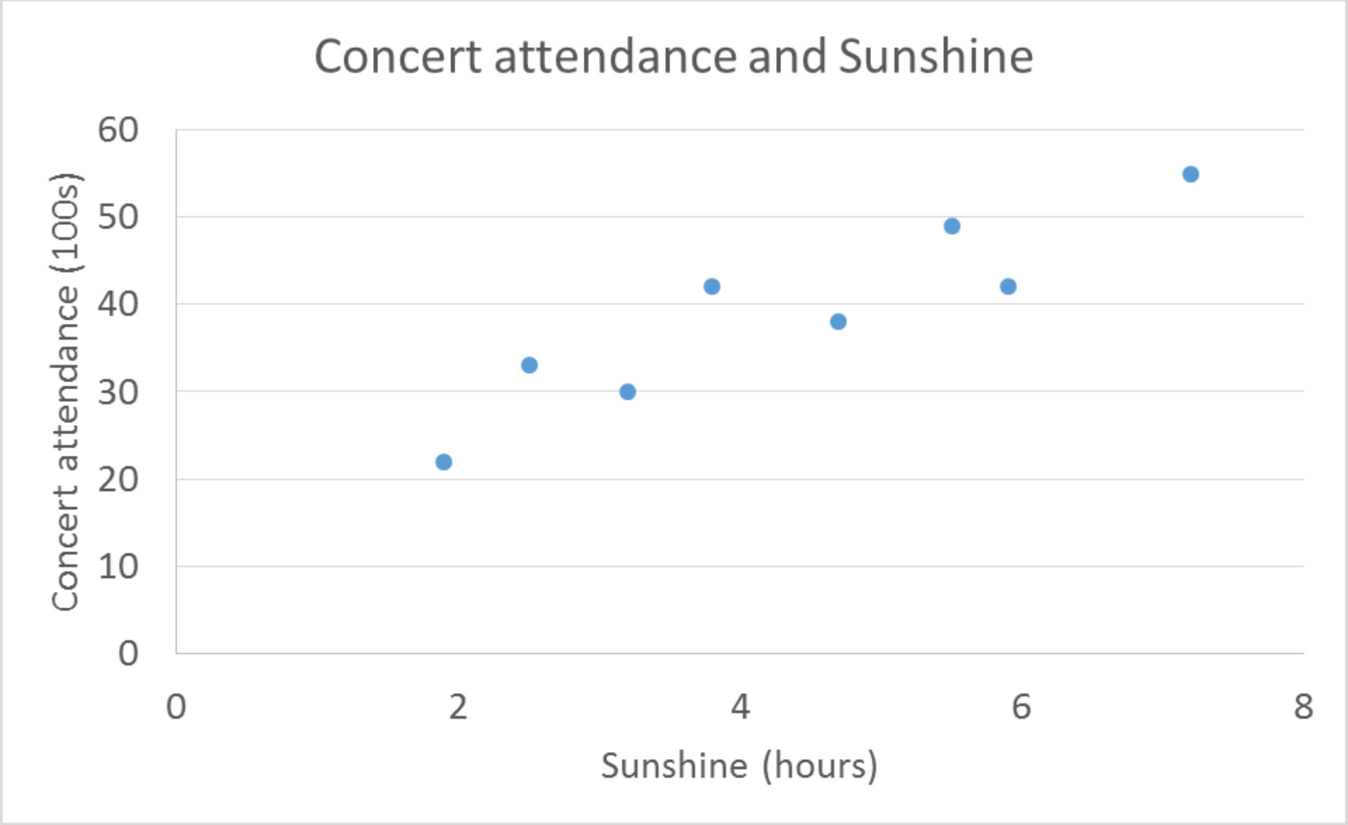
Linear Regression

Simple Linear Regression

Example

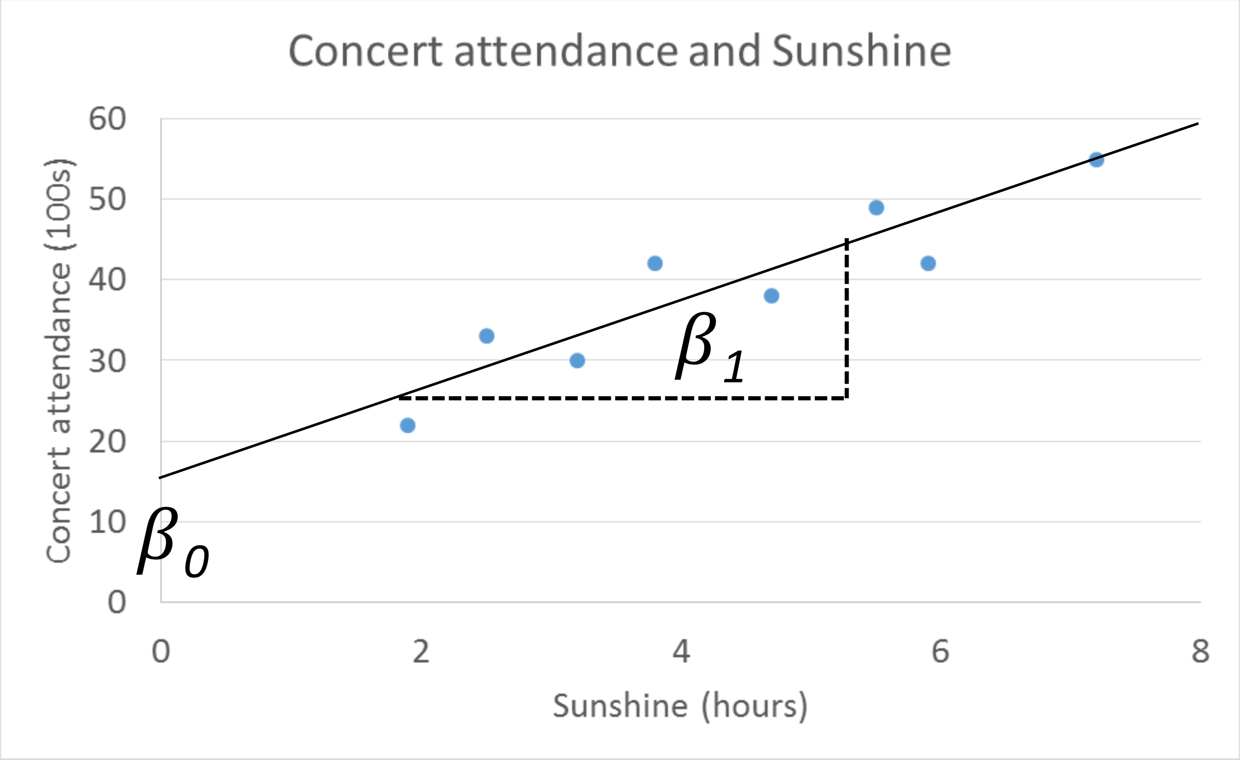
- Impact of weather on event attendance
- Correlated? Predictable?

Sunshine (hours)	1.9	2.5	3.2	3.8	4.7	5.5	5.9	7.2
Concert attendance (100s)	22	33	30	42	38	49	42	55

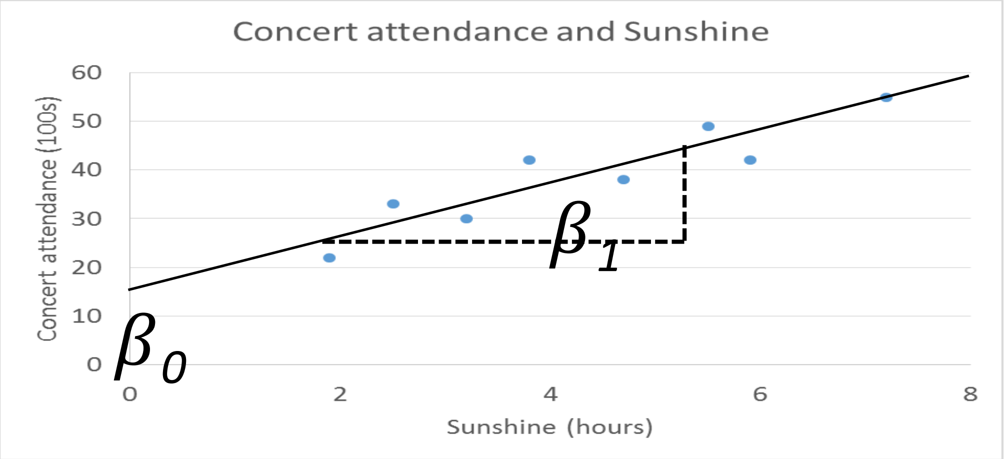


Simple Linear Regression

- Regression
  - Dependent variable is numeric
- Linear
  - Fit a line
  - Line : Coefficients
- Optimization
  - Many possible lines
  - Criteria : Minimize error
- Error
  - Sum of squared residuals



Linear Regression : Math



- Linear Regression
  - Dependent variable is numeric
  - Fit a line
- Line Fitting
  - More than 2 data points ➔ Over-specified problem
  - Criteria : Minimize error (sum of squared residuals)

$$y \approx \beta_0 + \beta_1 x$$

$$y = \beta_0 + \beta_1 x + \epsilon$$

$$\epsilon \sim N(0, \sigma^2)$$

$$RSS = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2$$

- Optimization problem
  - Solve (using calculus)
  - Find coefficients (line) which minimizes the Residual Sum of Squares

$$\min_{\beta} RSS$$

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2}$$

$$\bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$$

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

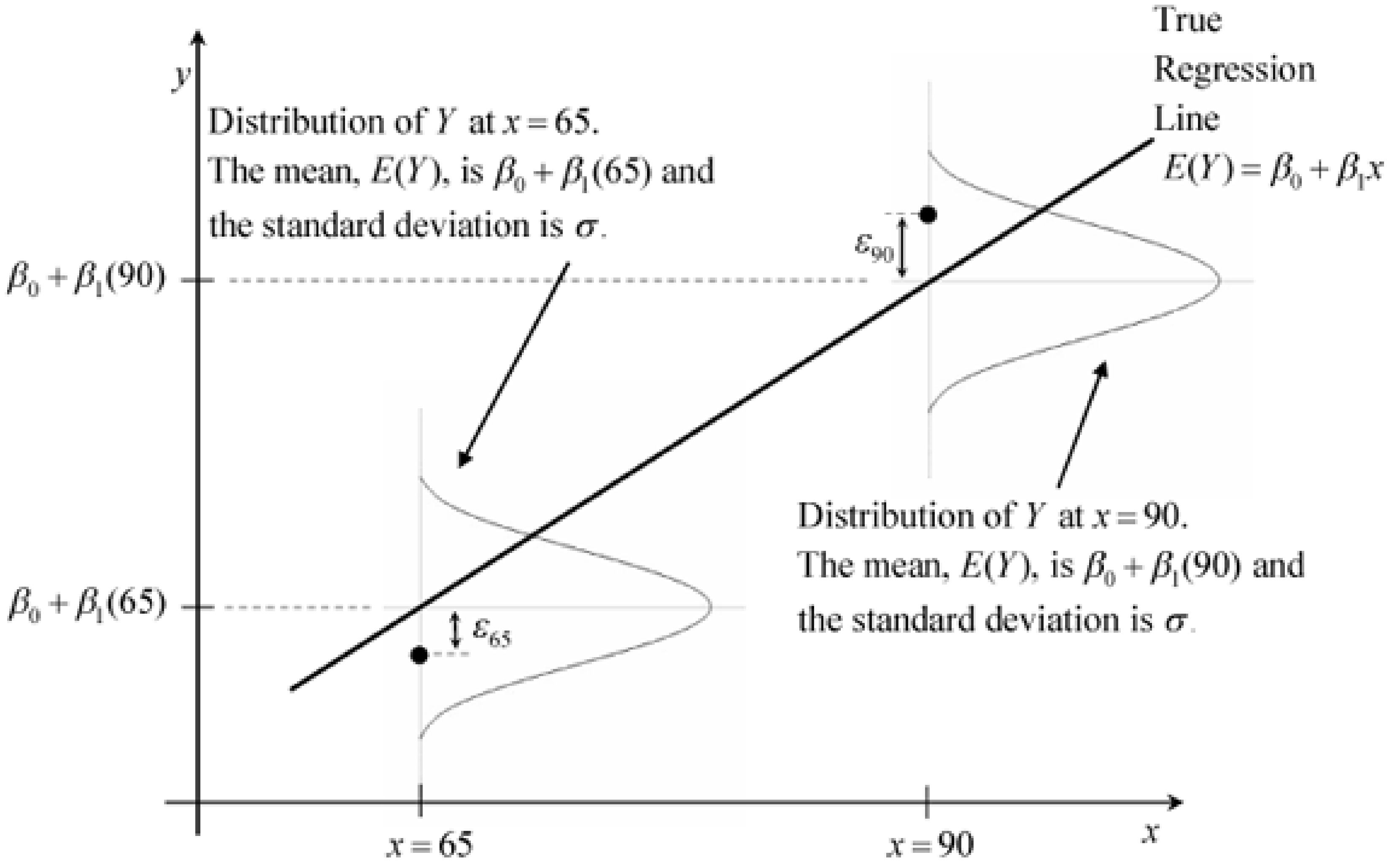
- Use estimated coefficients ("model") to make predictions

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x$$

Linear Regression : Intuition

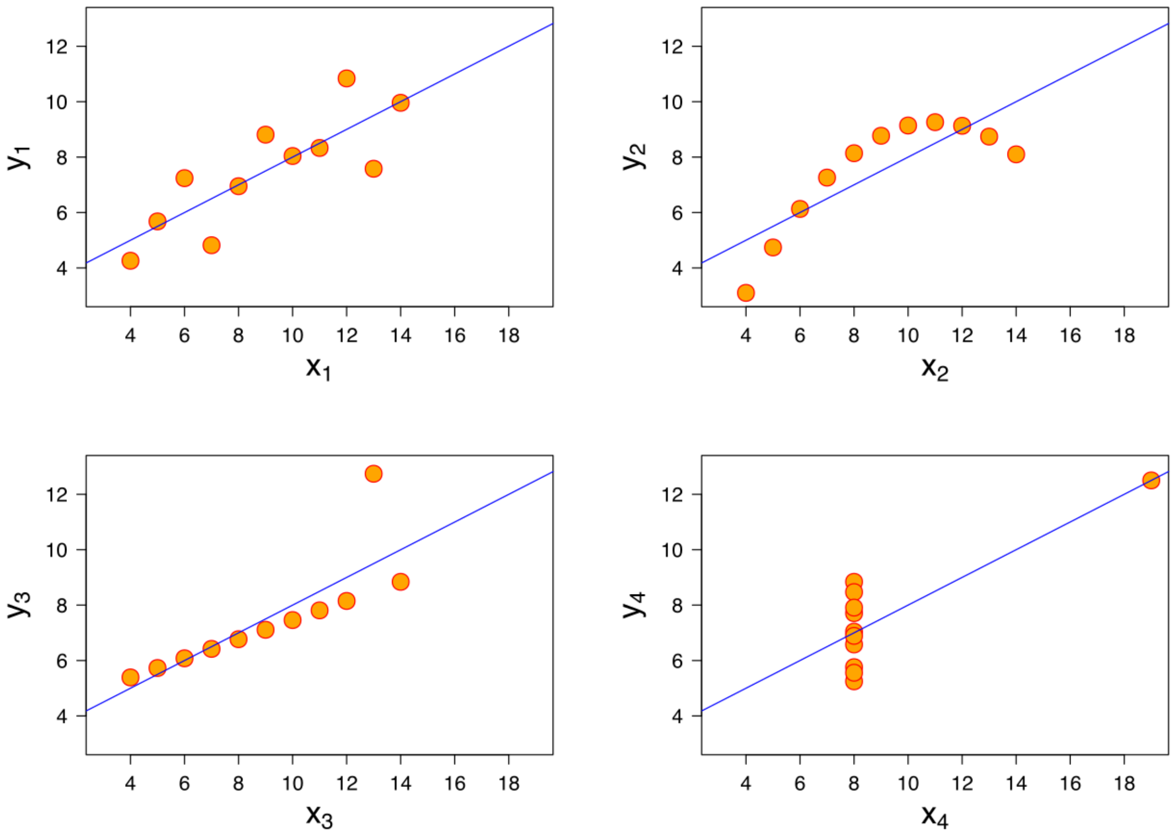
$$y = \beta_0 + \beta_1 x + \epsilon$$
$$\epsilon \sim N(0, \sigma^2)$$



http://reliawiki.org/index.php/Simple_Linear_Regression_Analysis

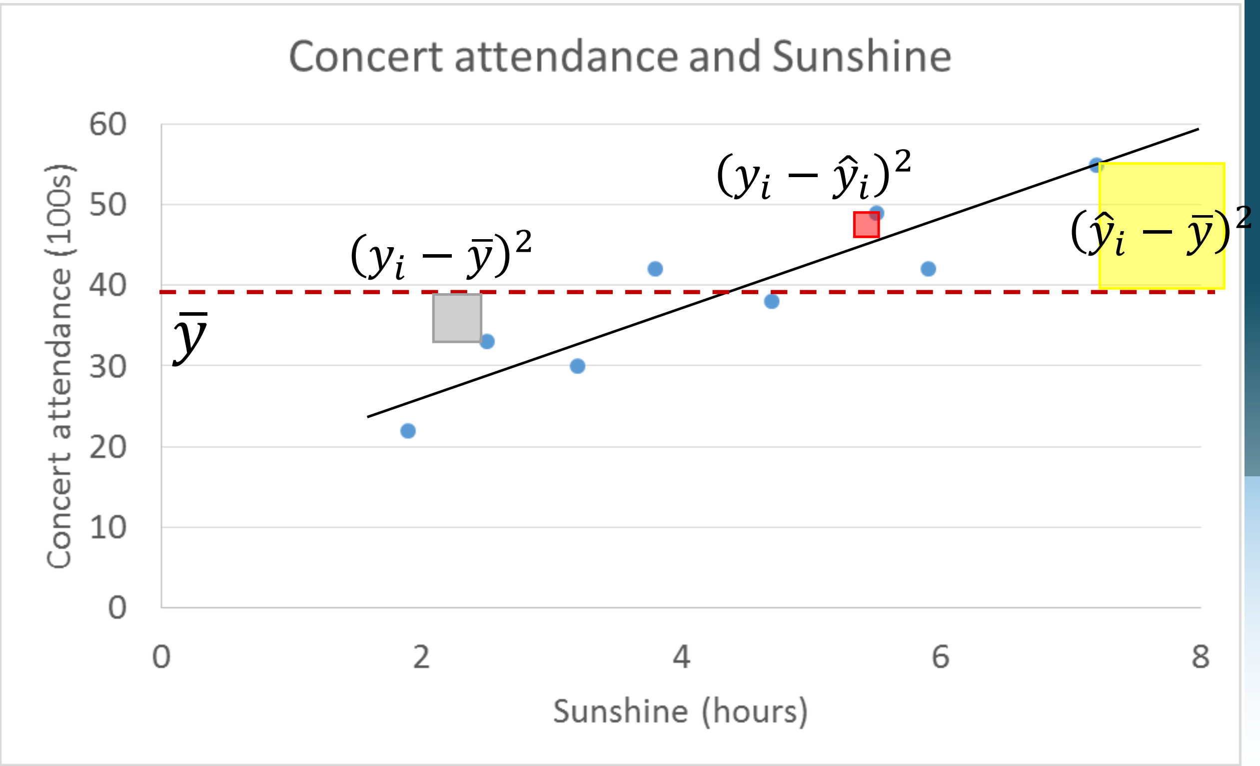
How good is your line?

- Among all possible lines, LR selects one that minimize the RSS
    - Is this good enough?
    - Visual comparison
    - Quantification



How good is your line? : Quantify.

- How good is your line / fit / model?
  - What would be the best line?
  - RSS = 0 : Not always possible : over-specified problem 2 variables, n data points
- Goodness of line = RSS?
  - Depends on the units of y
  - What is big? What is small?
  - Interpretability? Model comparison?
- Coefficient of Determination R-sq (R^2)
  - Intuition: P(Y|X) should have low variance
  - $TSS = \sum(y_i - \bar{y})^2$
  - $ESS = \sum(\hat{y}_i - \bar{y})^2$
  - $RSS = \sum(y_i - \hat{y}_i)^2$
  - $TSS = ESS + RSS$
  - $R^2 = \frac{ESS}{TSS} = \frac{TSS-RSS}{TSS} = 1 - \frac{RSS}{TSS}$
  - = Square of the pearson correlation (for simple LR)

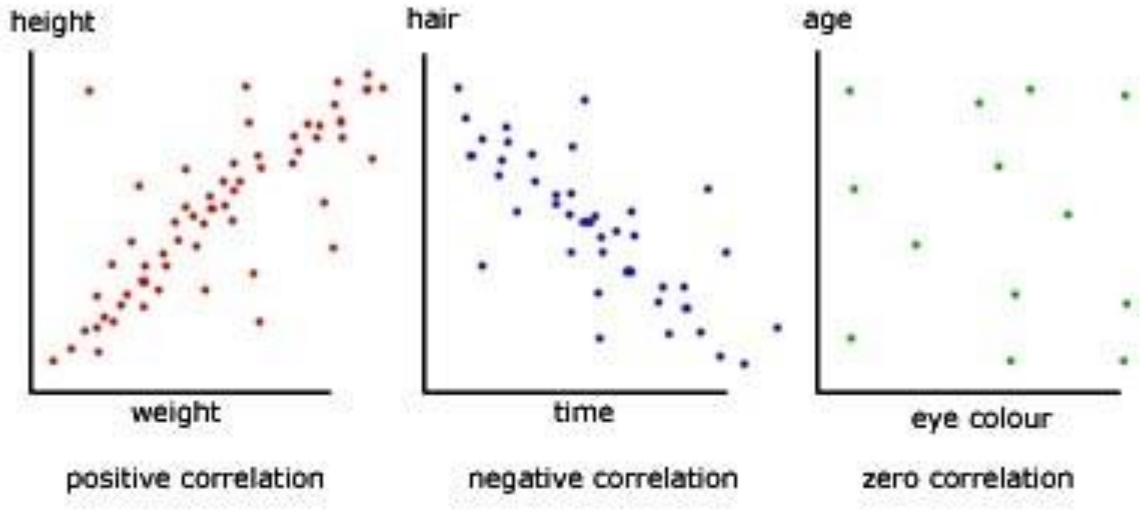


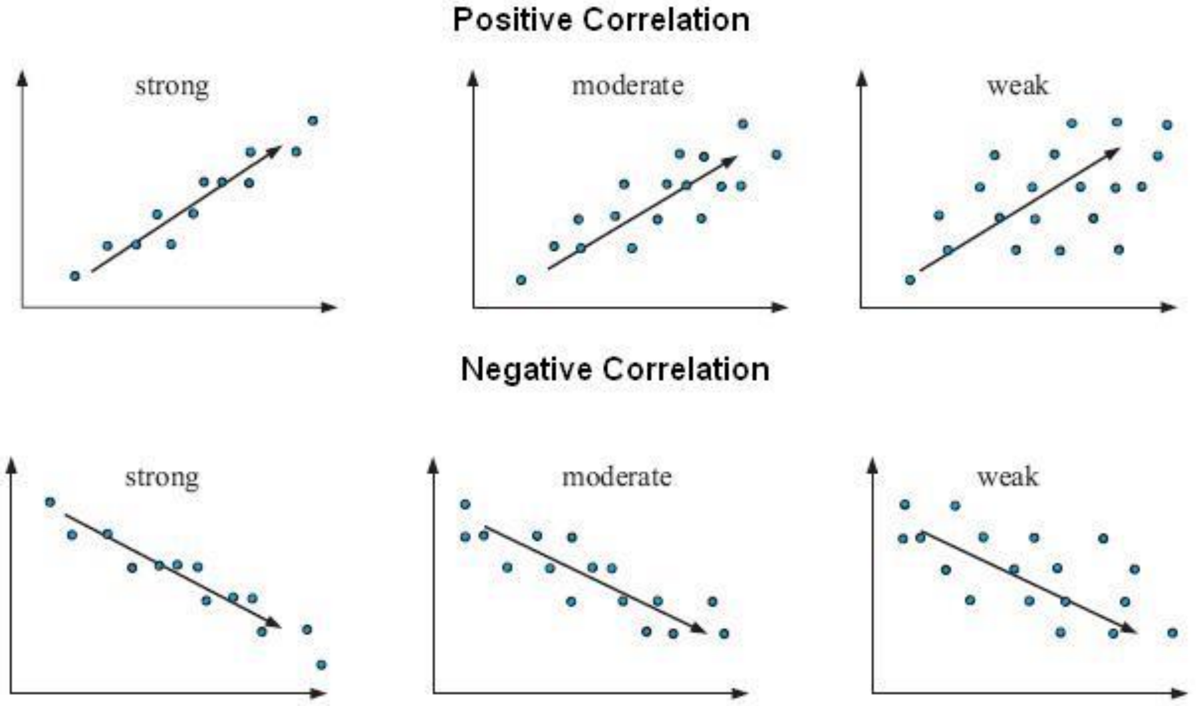
$$1 = \frac{ESS}{TSS} + \frac{RSS}{TSS} = \frac{\sum(\hat{Y}_i - \bar{Y})^2}{\sum(Y_i - \bar{Y})^2} + \frac{\sum(Y_i - \hat{Y}_i)^2}{\sum(Y_i - \bar{Y})^2}$$

Coefficient of Determination : Correlation

- Coefficient of Determination R-sq (R^2)
  - $1 - \frac{SSE}{SST} = R^2$
  - = Square of the pearson correlation (for simple LR)

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





LR: Statistics?

Data : Sample or Population

- Different lines for different samples of the data
  - Estimated parameters depend on the data set

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2} \qquad \hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

- Prediction (Model)
  - For a given x, predict y : use given (sample) data to establish a relationship
  - For a given x, predict y : use given (sample) data to build a model
  - Use given (sample) data to build a model which can be applied on population (future data points)
  - A regression line provides a point estimate from a sample.

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x$$

- Estimated parameters
  - Are sample statistics
  - Are random variables
  - Will create a sampling distribution

Inferential Statistics on model parameters

- Sampling Distribution of model parameters
  - Standard Error (s.d. of the sampling distribution)

$$SE(\hat{\beta}_1) = \sqrt{\frac{\sigma^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2}} \qquad SE(\hat{\beta}_0) = \sqrt{\sigma^2\left(\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2}\right)}$$

- Variance of the population
  - Unknown
  - Estimate (Residual Standard Error)
  - Assume large enough sample

$$\hat{\sigma}^2 = RSE = \sqrt{\frac{RSS}{(n-2)}} = \sqrt{\frac{\sum_{i=1}^{n}(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2}{n-2}}$$

- Confidence Interval
  - In which the true (population) parameters lie

$$95\%\ \text{C.I.}:\ \hat{\beta}_1 \pm 2SE(\hat{\beta}_1)$$
$$95\%\ \text{C.I.}:\ \hat{\beta}_0 \pm 2SE(\hat{\beta}_0)$$

Inferential Statistics on model parameters : Hypothesis Testing

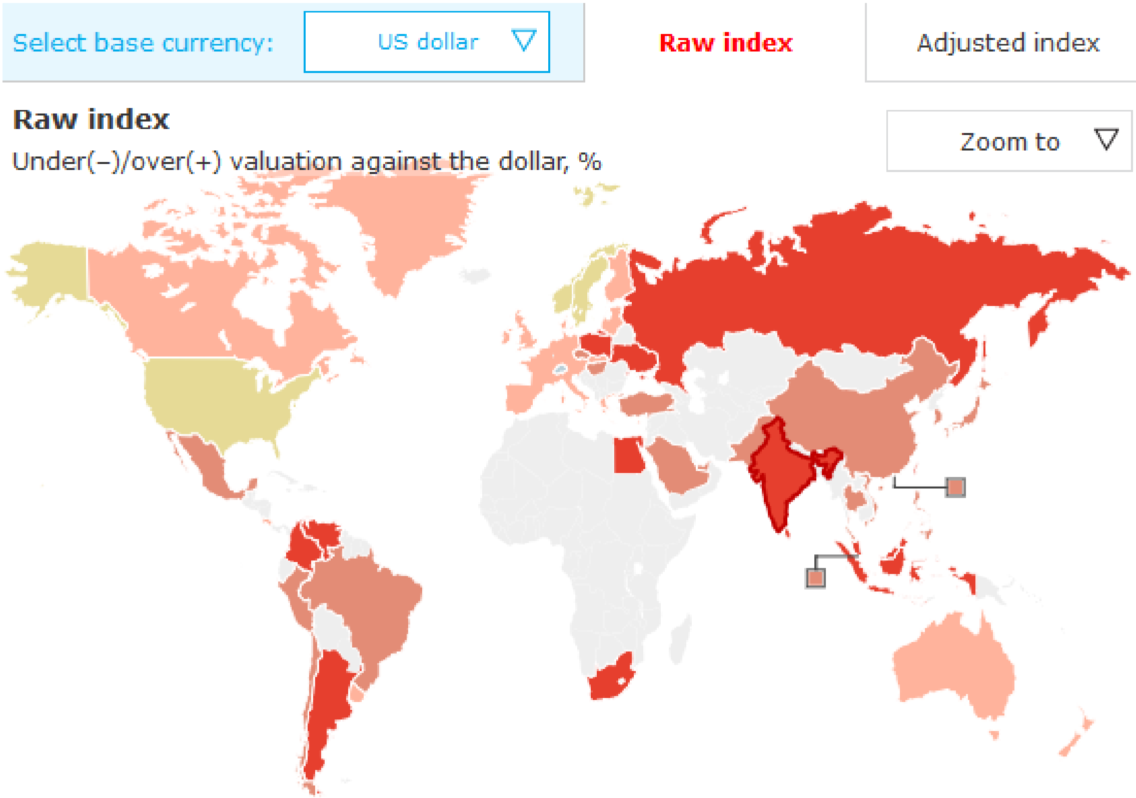
- State the Hypothesis
  - $H_0: \beta_1 = 0$ *(No correlation between x and y)*
  - $H_1: \beta_1 \neq 0$

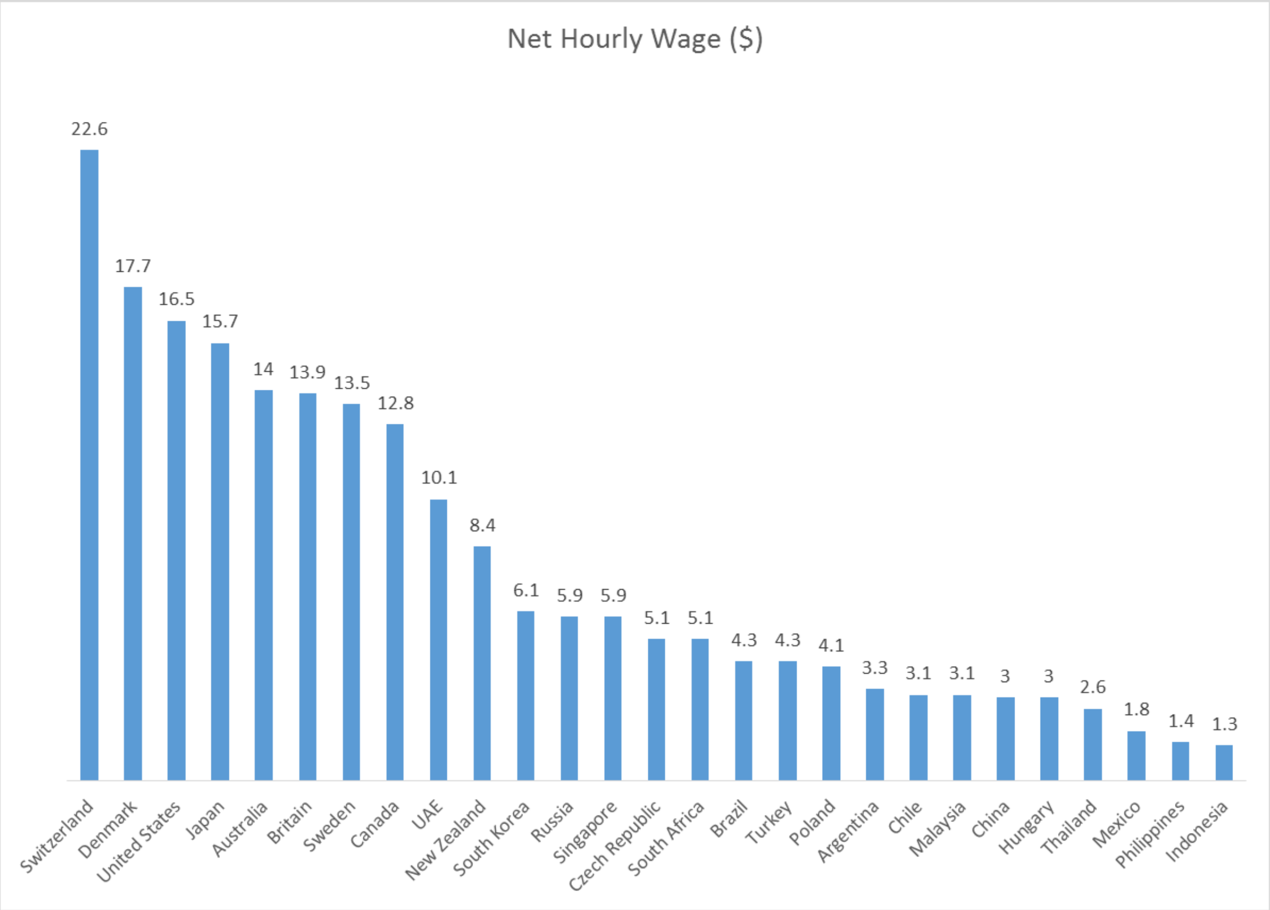
- Define the test statistic
  - Assume Null hypothesis true

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

- Can we reject the null hypothesis?
  - Could we have obtained this coefficient by chance?
  - How far is the observed value of the coefficient from zero?
  - How far is the observed value of the coefficient from zero in terms of the standard error?
  - How large is the t-statistic?
  - What is the p-value for the observed t-statistic (Probability of observing this t by chance?)

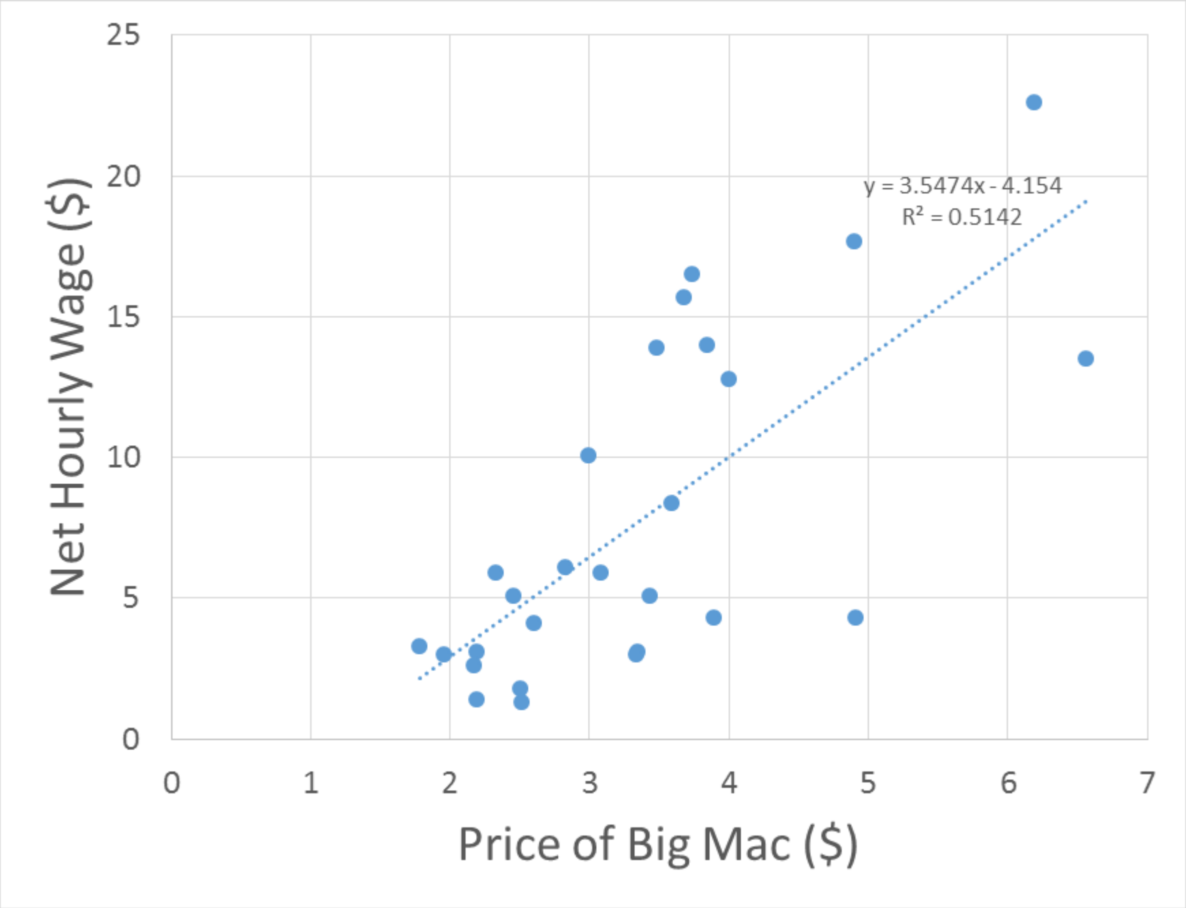
Example : Burgerprice vs. Net Hourly wage





Example (cont'd)

	Coefficients	Standard Error	t Stat	P-value
Intercept	-4.154014573	2.447784673	-1.697050651	0.102104456
Big Mac Price ($)	3.547427488	0.689658599	5.143744297	2.57053E-05

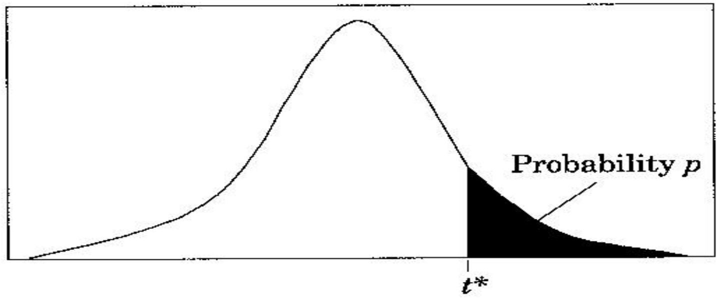


$$\hat{\sigma}^2 = RSE = \sqrt{\frac{RSS}{(n-2)}} = \sqrt{\frac{\sum_{i=1}^{n}\left(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i\right)^2}{n-2}}$$

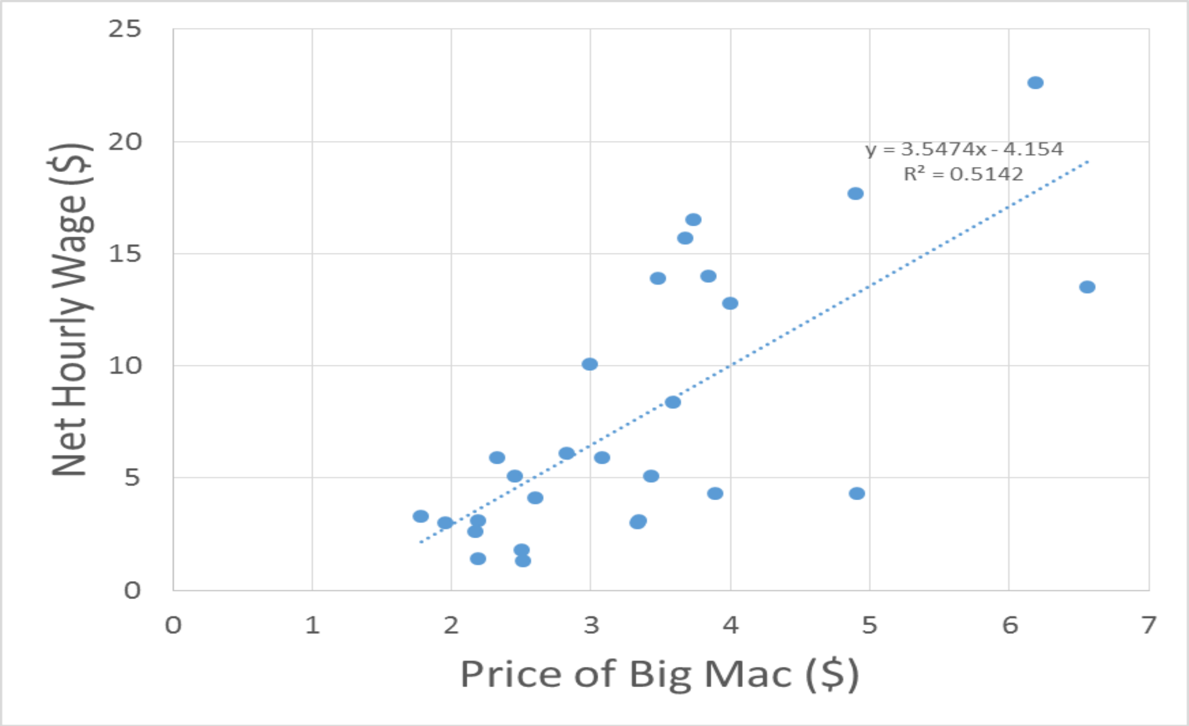
$$SE(\hat{\beta}_1) = \sqrt{\frac{\sigma^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2}} \qquad SE(\hat{\beta}_0) = \sqrt{\sigma^2\left(\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2}\right)}$$

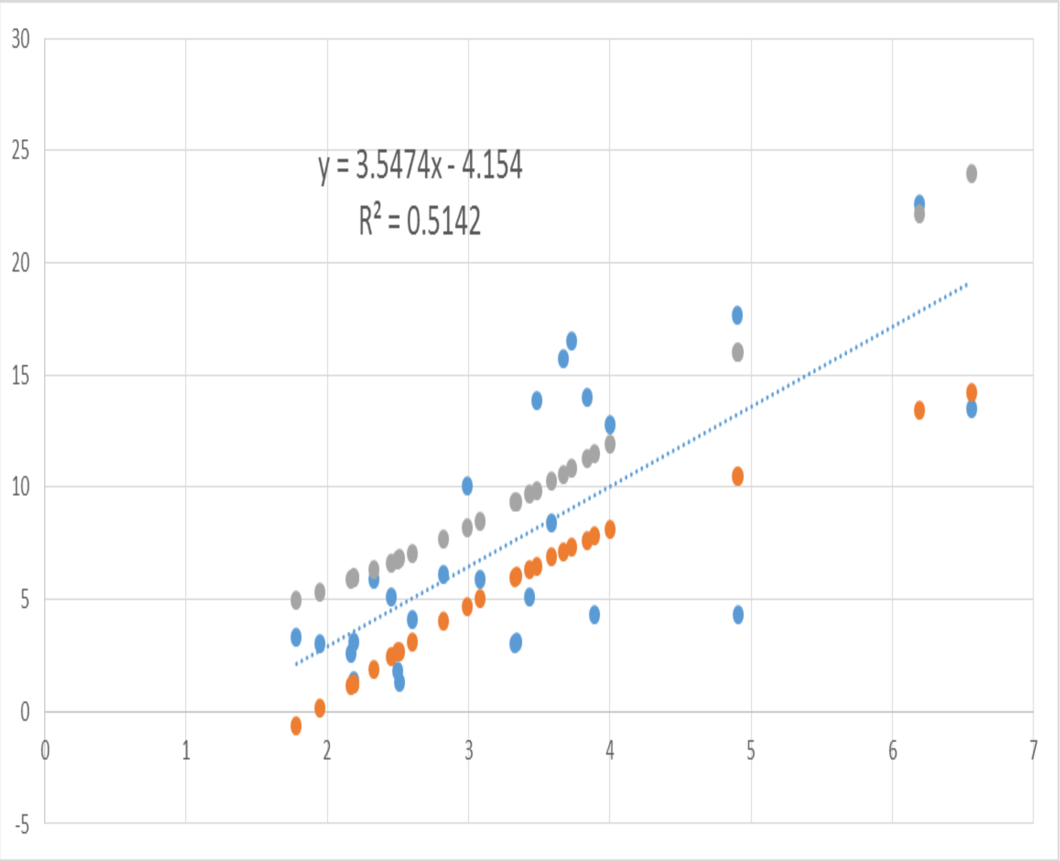
$$t = \frac{\hat{\beta}_1 - 0}{SE(\hat{\beta}_1)}$$

- $t = 5.1437$



Example (cont'd)





	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	-4.154014573	2.447784673	-1.697050651	0.102104456	-9.195321476	0.88729233
Big Mac Price ($)	3.547427488	0.689658599	5.143744297	2.57053E-05	2.127049014	4.967805962

$$95\% \text{ C.I. : } \hat{\beta}_1 \pm 2SE(\hat{\beta}_1)$$

$$95\% \text{ C.I. : } \hat{\beta}_0 \pm 2SE(\hat{\beta}_0)$$

LR: (In)validating assumptions

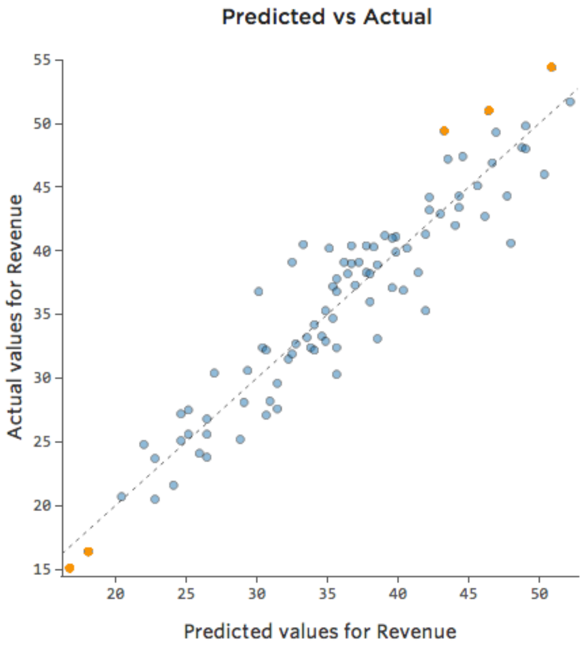
LR: Assumptions

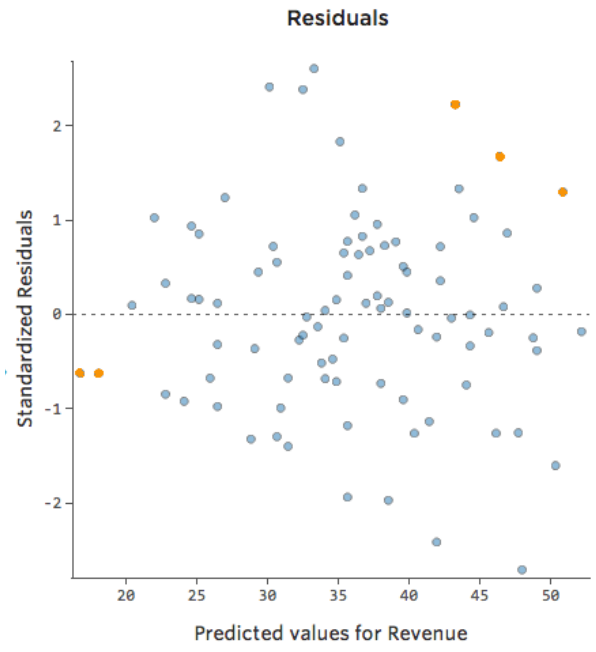
- Assume i.i.d. normally distributed
  - CLT : Additive noise
- Errors: Mean 0
  - CLT: Sample mean is an unbiased estimator of the mean
  - By Design (Intercept term is chosen)
- Errors: Assume fixed variance
  - Simplification
- Assume linearity
  - Linear correlation between x and y

$$y = \beta_0 + \beta_1 x + \epsilon$$
$$\epsilon \sim N(0, \sigma^2)$$

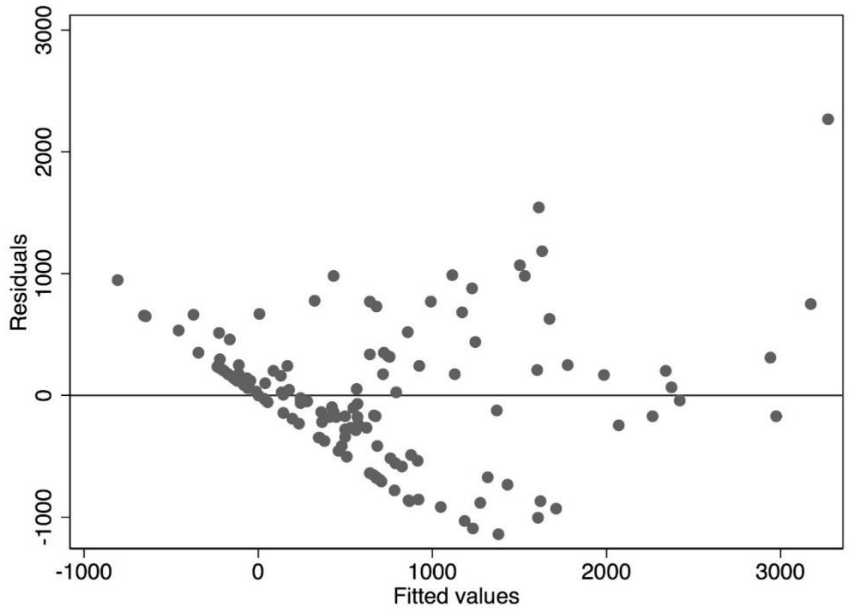
Linear correlation between x and y?

- Is there a non-linear relationship?
  - Linear ➔ Plot between y & $(\beta_0 + \beta_1 x)$ would be linear
  - Linear ➔ Errors (Residuals) will not show any pattern
- Residual Plots
  - Graphical tool for identifying non-linearity
  - Plot residuals vs. fitted values
- Interpretation
  - No discernible pattern ➔ Linearity
  - U shape ➔ Non-linearity
- What next?
  - Feature Transformations (later)



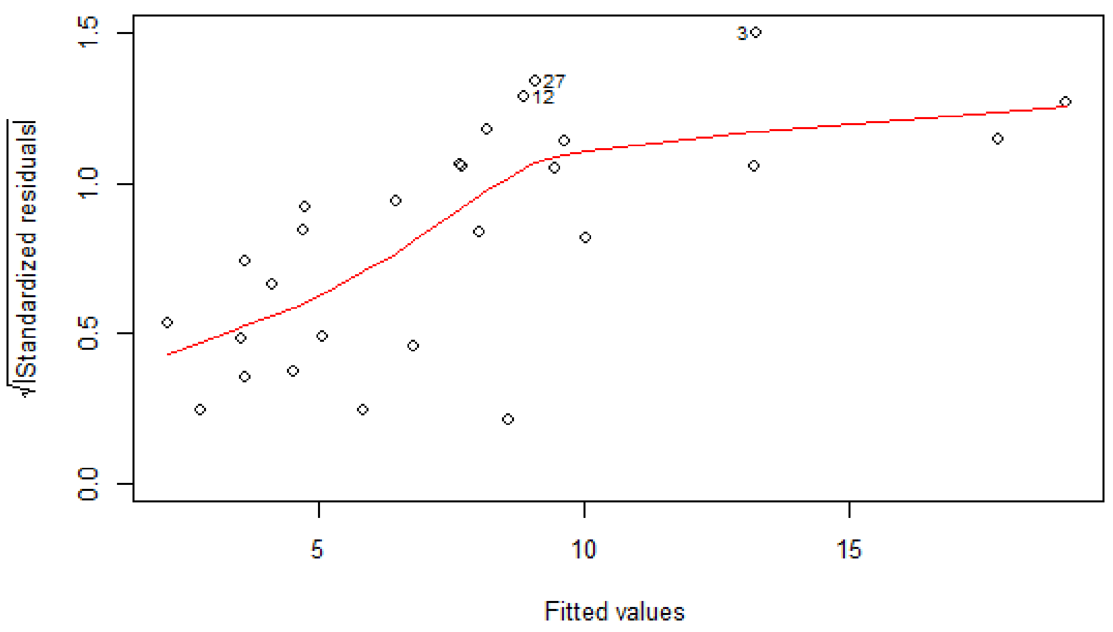


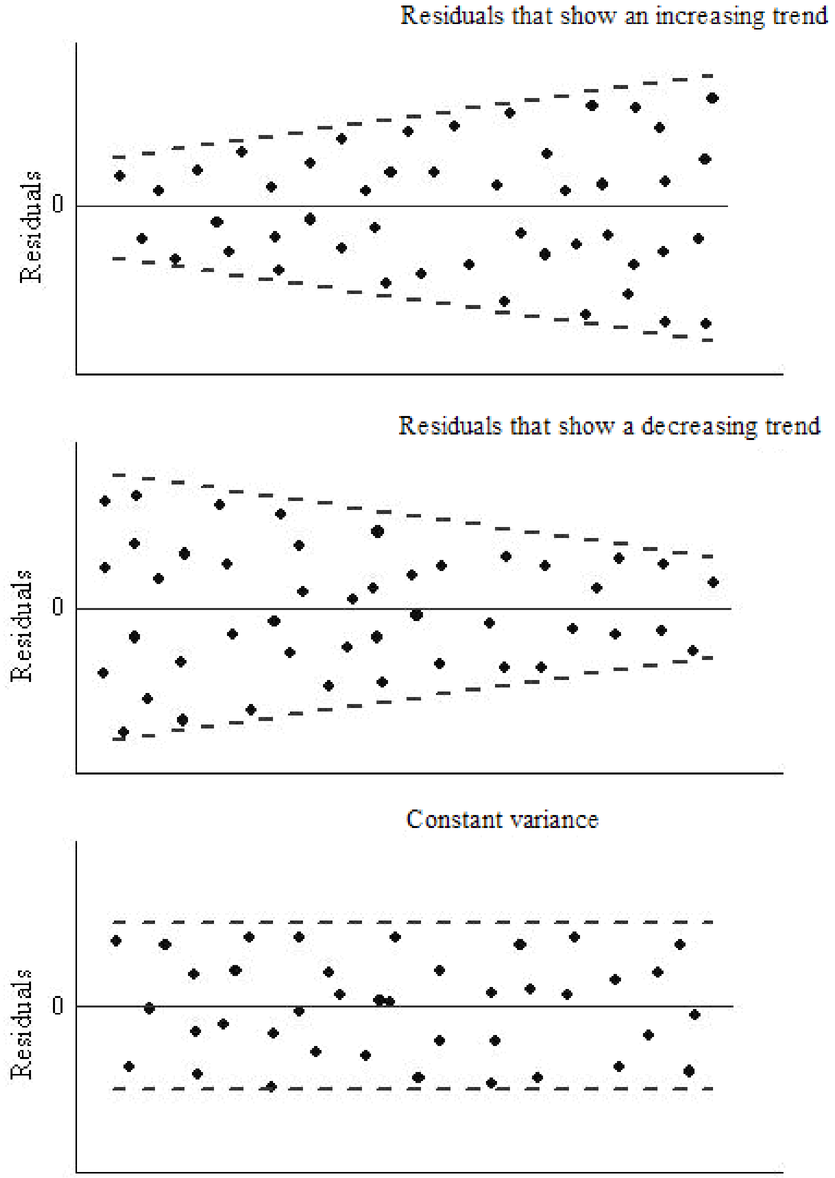
http://docs.statwing.com/interpreting-residual-plots-to-improve-your-regression/



Noise has fixed variance

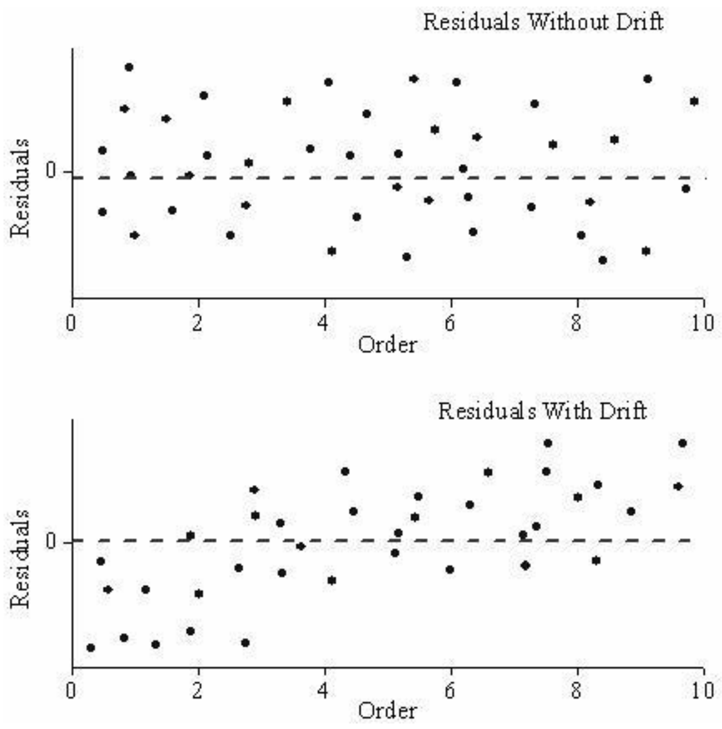
- The error terms have constant variances : homoscedasticity
  - What if variance depends on the predictor variable?
  - Need to check for heteroscedasticity
- What next?
  - Feature Transformations (later)

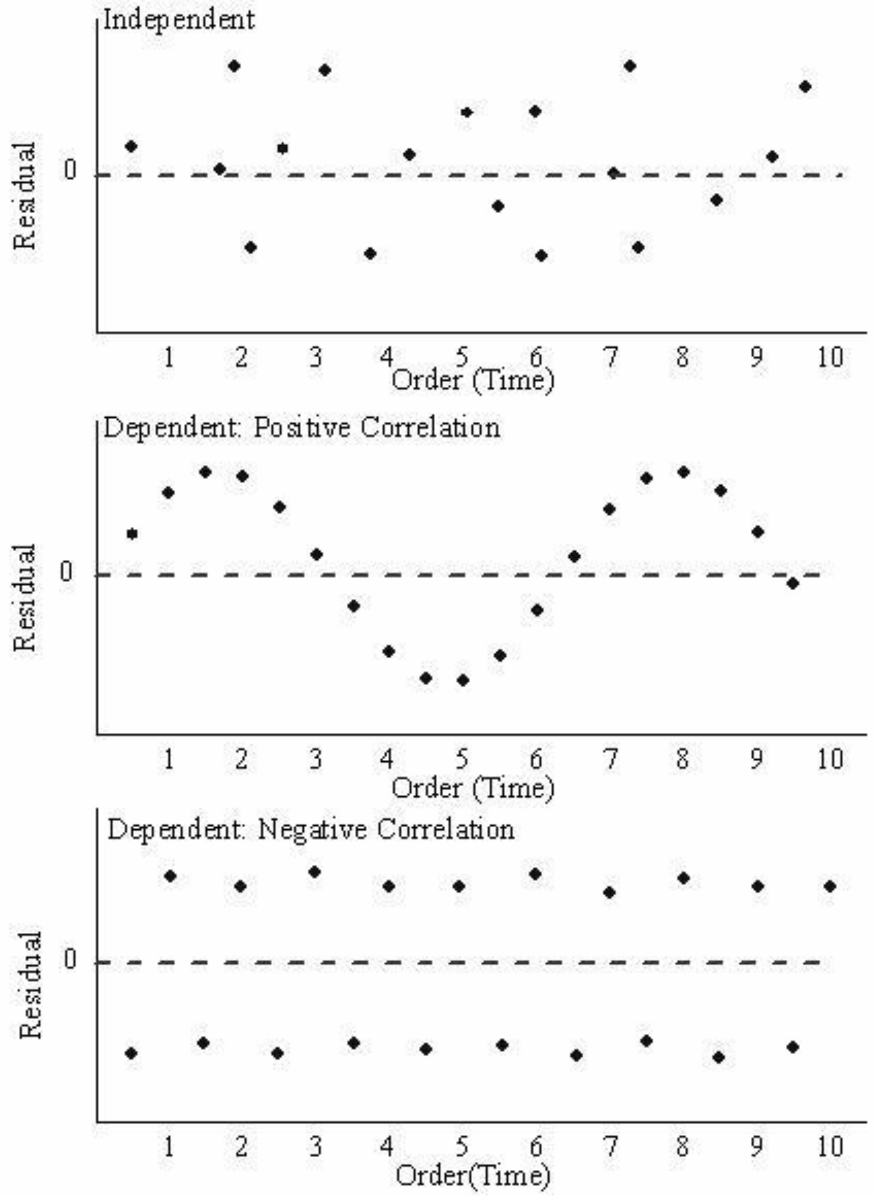




Noise (residuals) independent (i.i.d.) ?

- Are error terms correlated?
  - Are "successive" residuals correlated?
  - ϵ_i is positive provides no information about the sign of ϵ_{i+1}
- Successive?
  - Temporal
  - Any sequence… (e.g. spatial)
- Source
  - Sampling error!
  - Design of Experiment error!



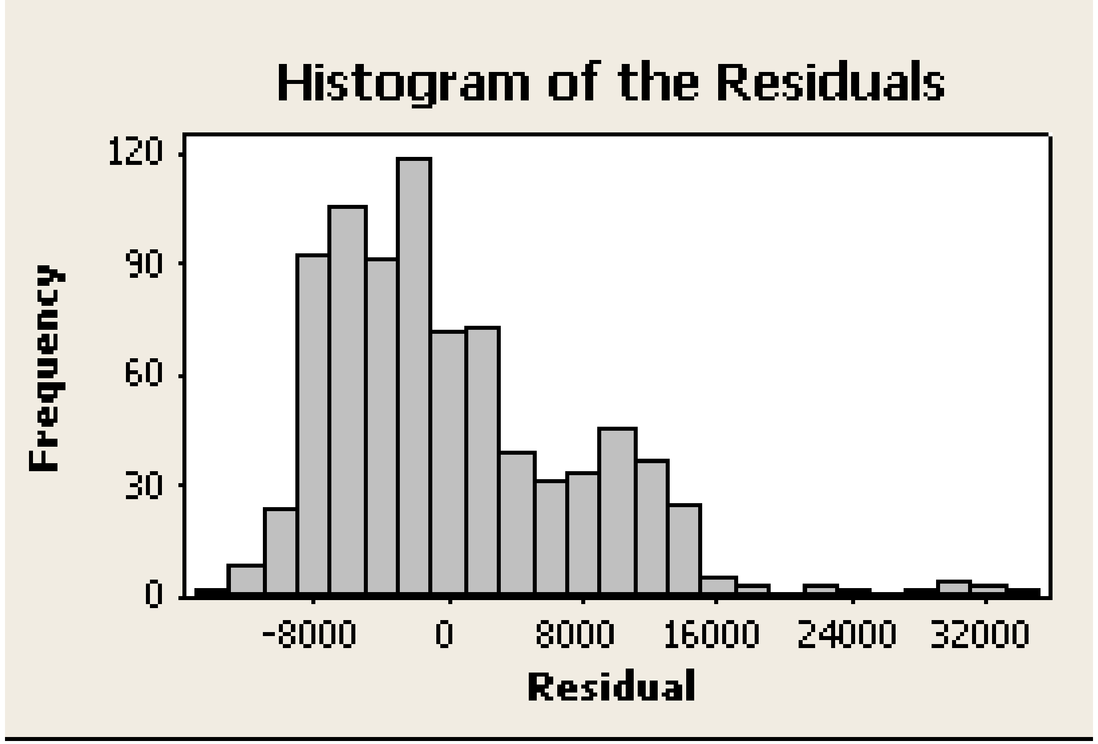


http://www.originlab.com/doc/en/UserGuide/images/Graphic_Residual_Analysis/Graphic_Residual_Analysis-4.jpg

Noise (residuals) normally distributed?

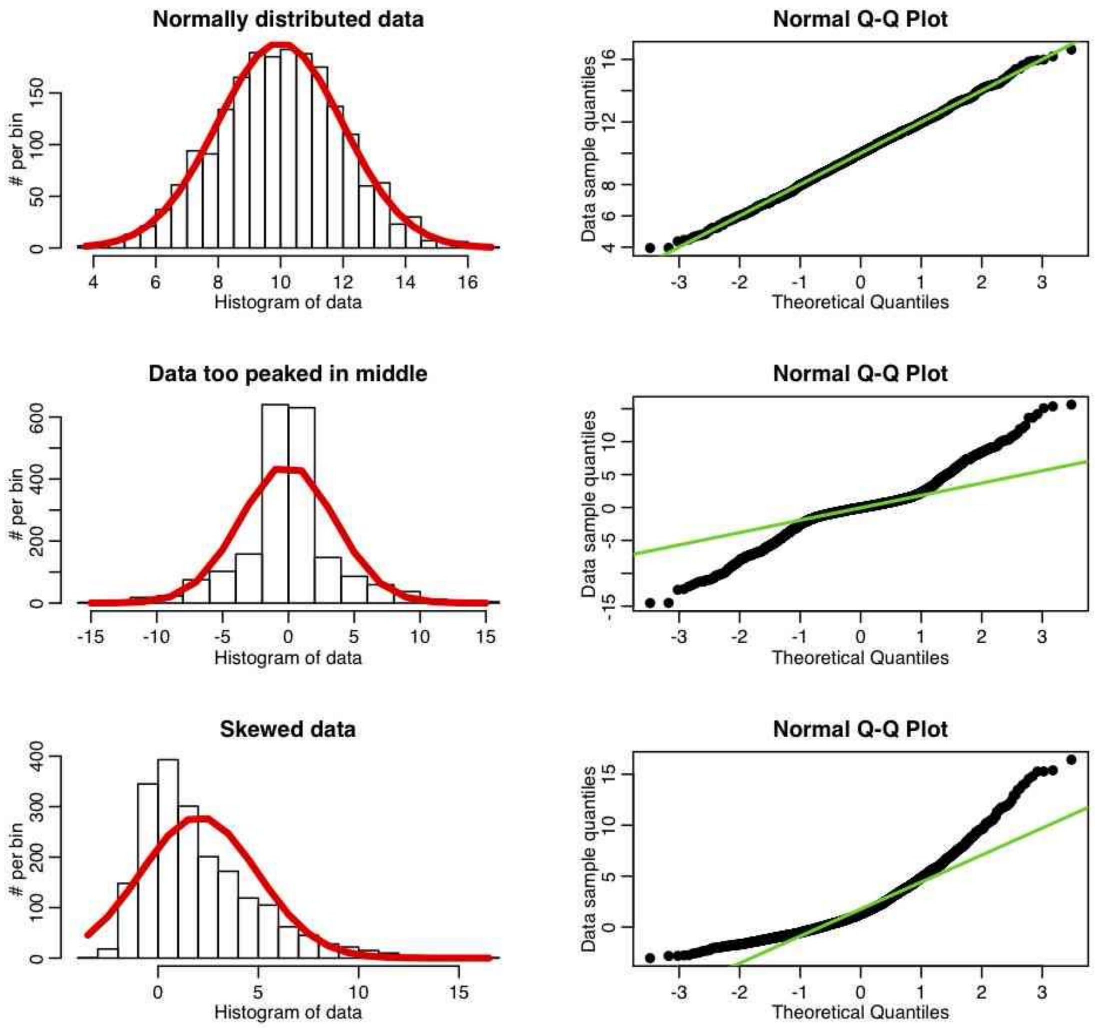
- Residual distribution is normal?
  - Plot & check

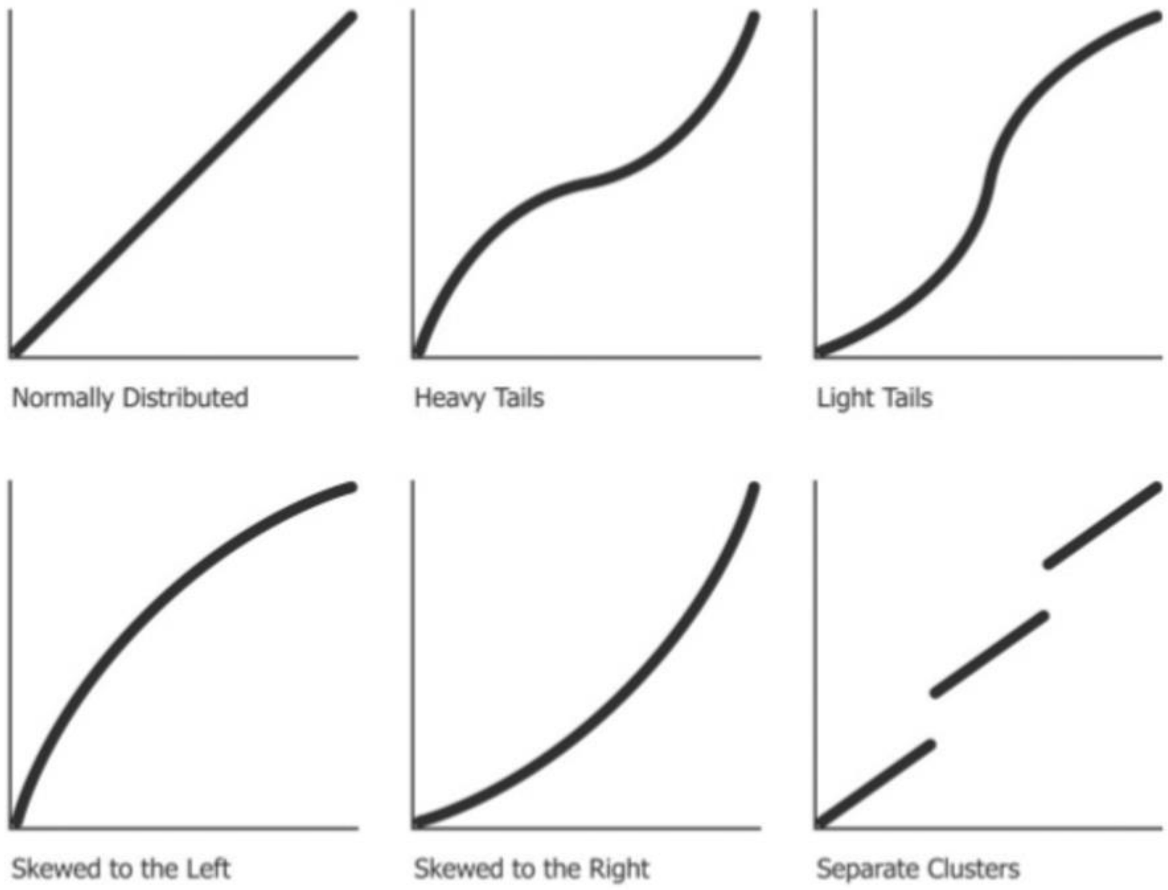
- Q-Q plot
  - Used to validate distributional assumptions of a data set.
  - Normality ➔ z-scores of the residuals should be equal to the expected z-scores at corresponding quantiles.



http://sherrytowers.com/wp-content/uploads/2013/08/qqplot_examples.jpg

Noise (residuals) normally distributed? (cont'd)

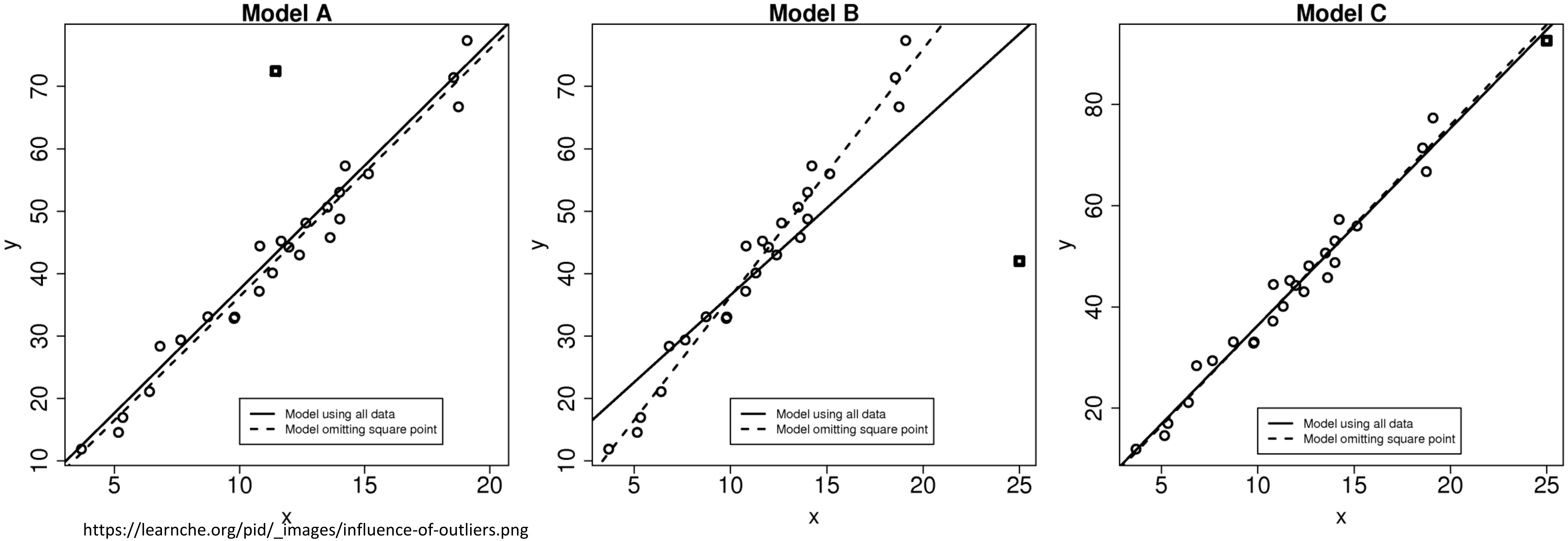




LR: Sample to Population

Sample vs. Population: Preparing for generalization

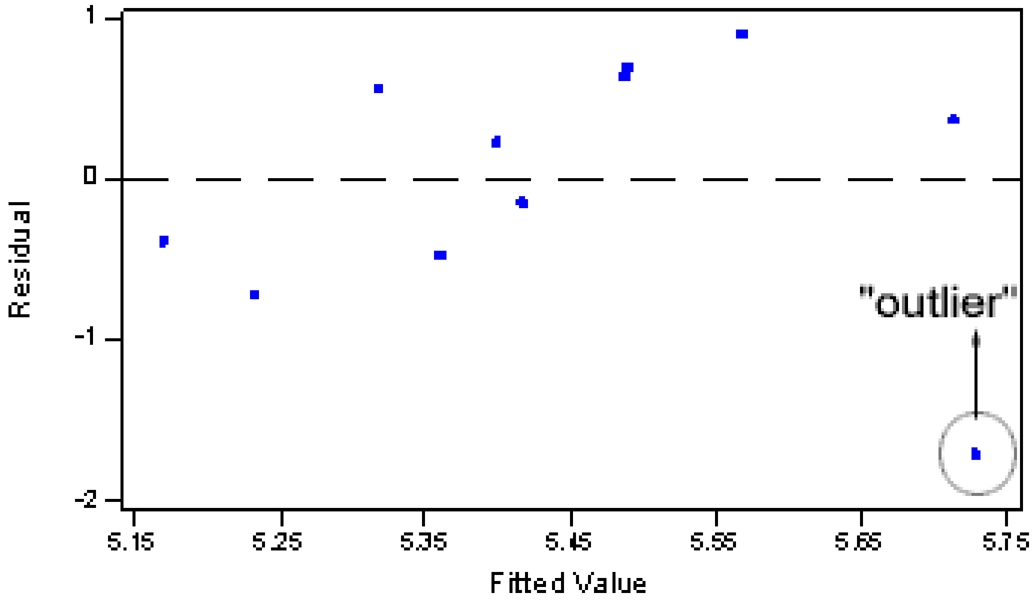
- How much does a single data point impact the model?
  - Linear regression : Steel rod and weights interpretation
- Guard against overfitting
  - Guard against sampling bias
  - Outliers, High Leverage data points, Extrapolation

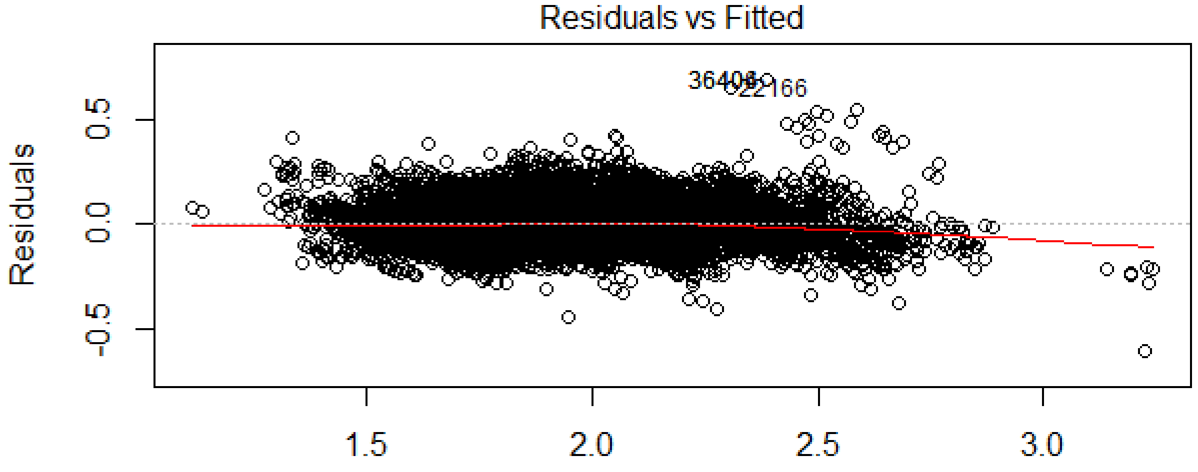


https://learnche.org/pid/_images/influence-of-outliers.png

Outliers

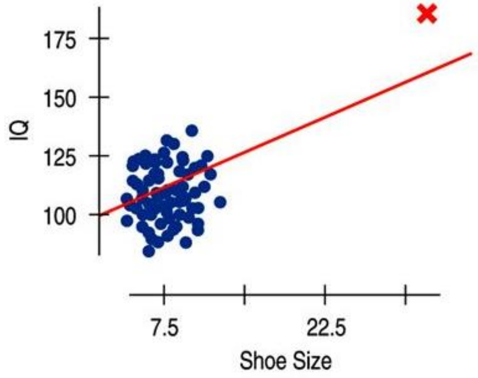
- Outlier
  - A data point for which y_i is far from the value predicted
- What next?
  - Remove outliers & build a new model
- Impact of removing the outliers
  - RSE will reduce significantly
  - CI will shrink
  - p-values will reduce
  - The model (LR equation) may not change much (Leverage much more important)

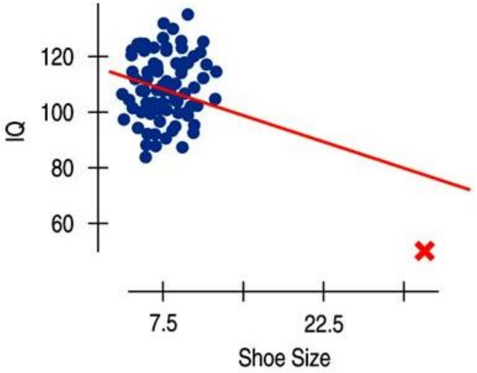




https://i.stack.imgur.com/DjhnO.png

High Leverage data points



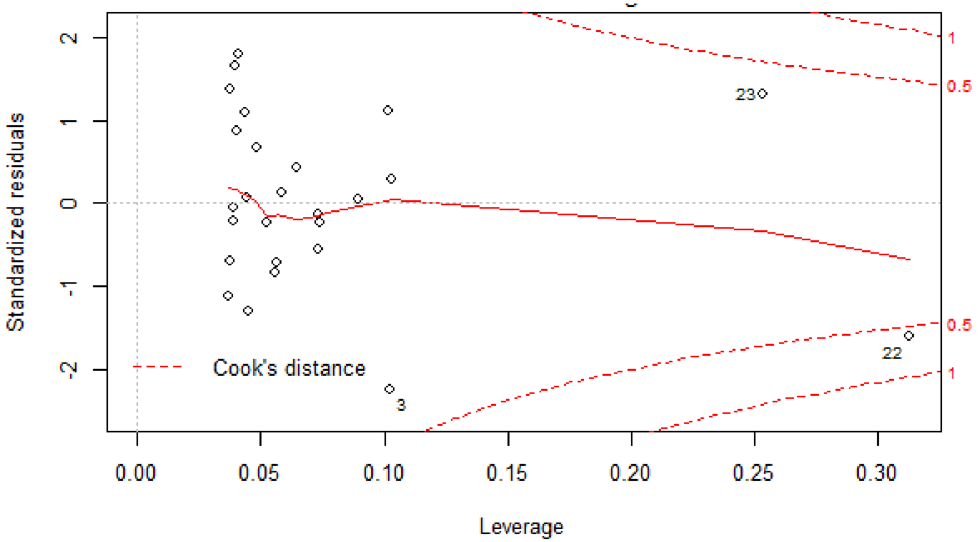


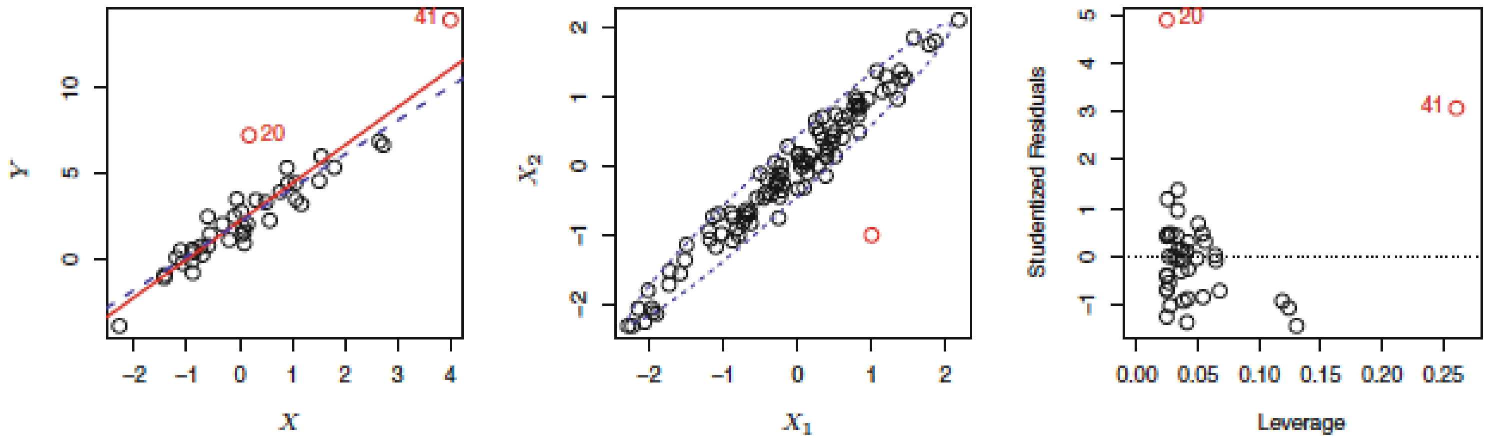
- High Leverage : a data point which has an unusual x_i value
  - Can have significant impact on the model (parameters)
- Quantify using leverage statistic
  - h_i >> (p+1)/n ➔ High leverage

$$h_i = \frac{1}{n} + \frac{(x_i - \bar{x}^2)}{\sum_{j \neq i}(x_j - \bar{x})^2}$$

- Quantify using Cooks D distance
  - Calculated by removing the i^{th} data point and recalculating the regression.
  - Summarizes how much all the values in the regression model change when the i^{th} observation is removed

$$D_i = \frac{\sum_{j=1}^{n}(\hat{Y}_j - \hat{Y}_{j(i)})^2}{(p+1)\,\hat{\sigma}^2}$$





http://bravojackielee.blogspot.in/2016/07/studentized-residualsoutliers-points_70.html

Point 20 is an outlier but does not have leverage ➔ its influence is low
Point 41 is an outlier and has high leverage ➔ its influence is high

Linear Regression

Putting it all together

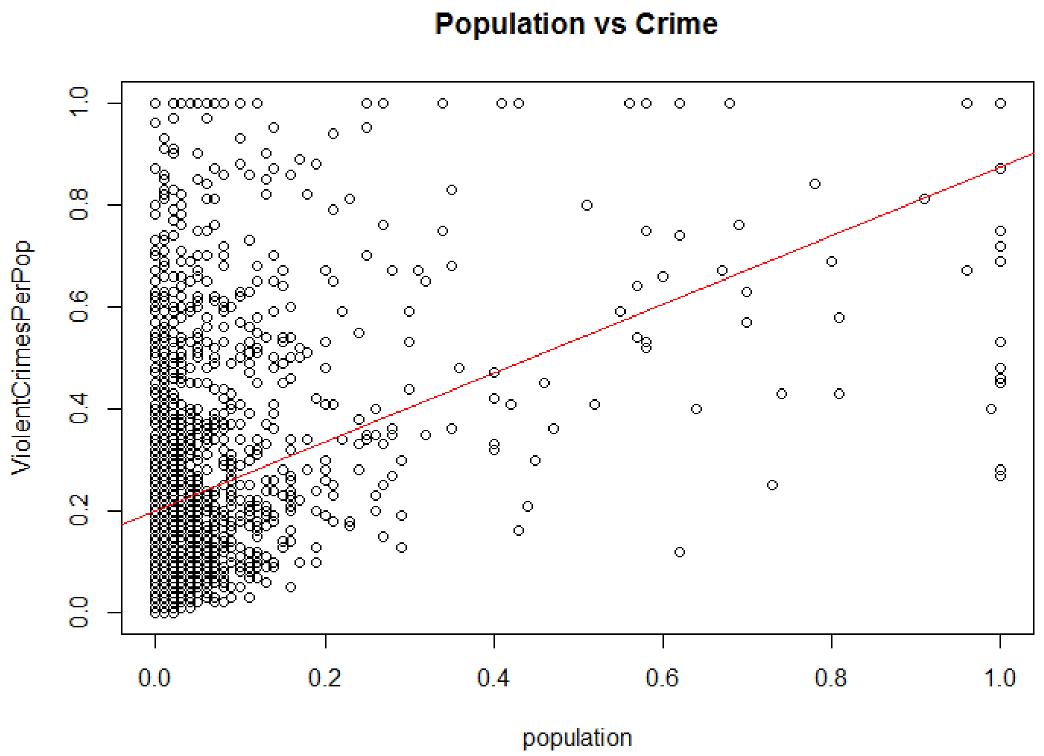
Example

- Residual (Noise) distribution
  - ~Quartiles
- Coefficients
  - Slope
- Inferential statistics
  - SE, t, p (* Significance at 0.05)
- Goodness of fit
  - R2
- Interpretation
  - Good enough?
  - R-Sq suggests that 15% of variation in *y* can be explained by variation in *x*.
  - *t* test shows that coefficient is significant and null hypothesis should be rejected.
  - ***Statistical significance*** **doesn't necessarily mean** ***practical significance***.
  - Vice-versa

```
Call:
lm(formula = ROLL ~ UNEM, data = datavar)

Residuals:
    Min      1Q  Median      3Q     Max
-7640.0 -1046.5   602.8  1934.3  4187.2

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   3957.0     4000.1   0.989   0.3313
UNEM          1133.8      513.1   2.210   0.0358 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 3049 on 27 degrees of freedom
Multiple R-squared: 0.1531, Adjusted R-squared: 0.1218
F-statistic: 4.883 on 1 and 27 DF,  p-value: 0.03579
```

http://rtutorialseries.blogspot.in/2009/11/r-tutorial-series-simple-linear.html

Example

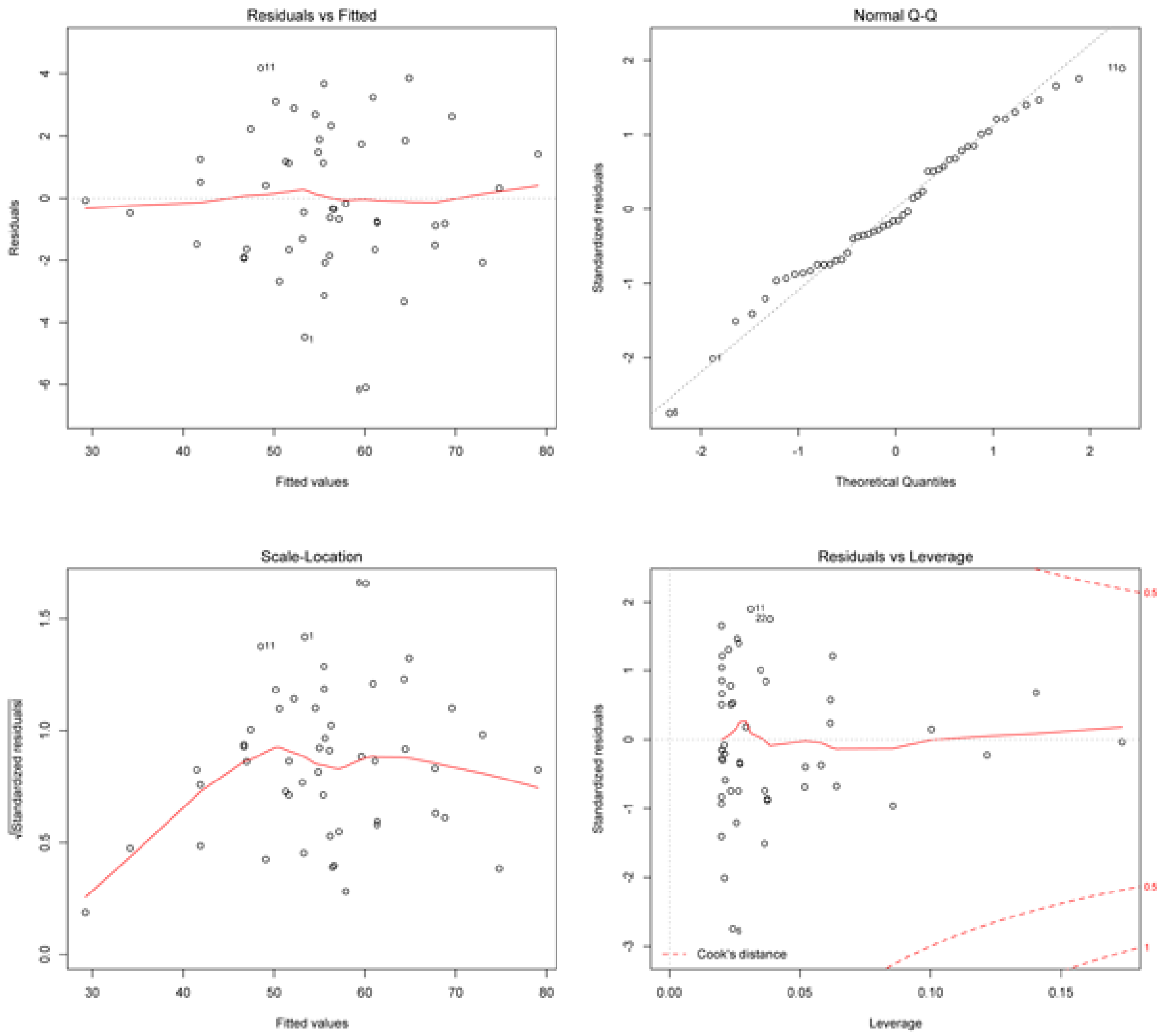



```
Call:
lm(formula = ViolentCrimesPerPop ~ population, data = crimeData)

Residuals:
    Min      1Q  Median      3Q     Max 
-0.5850 -0.1549 -0.0749  0.0851  0.7786 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept) 0.208435   0.006224   33.49   <2e-16 ***
population  0.646540   0.040125   16.11   <2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.2217 on 1607 degrees of freedom
Multiple R-squared:  0.1391,	Adjusted R-squared:  0.1386 
F-statistic: 259.6 on 1 and 1607 DF,  p-value: < 2.2e-16
```

https://medium.com/humansystemsdata/linear-regression-learning-the-r-way-33b7cc7dee65

Example

- Is this a good model?
  - Heteroscedascity?
  - Outliers?



Evaluating a Regression Model

- Residuals
  - Error between actual and predicted
- Residual Sum of Squares (RSS)
  - Measure of total error
  - R-sq.
    - Normalized by Total Sum of Squares
    - Unitless
  - Mean Square Error (MSE)
    - Normalized by number of observations
    - Squared Units of dependent variable
  - Root Mean Square Error (RMSE)
    - Normalized by number of observations
    - Units of dependent variable
- Mean Absolute Error (MAE)
    - Normalized by number of observations
    - Units of dependent variable
- Mean Absolute Percentage Error (MAPE)
    - Normalized by number of observations
    - Unitless
- Inferential Statistics (t, p) + Validate assumptions

$$RSS = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

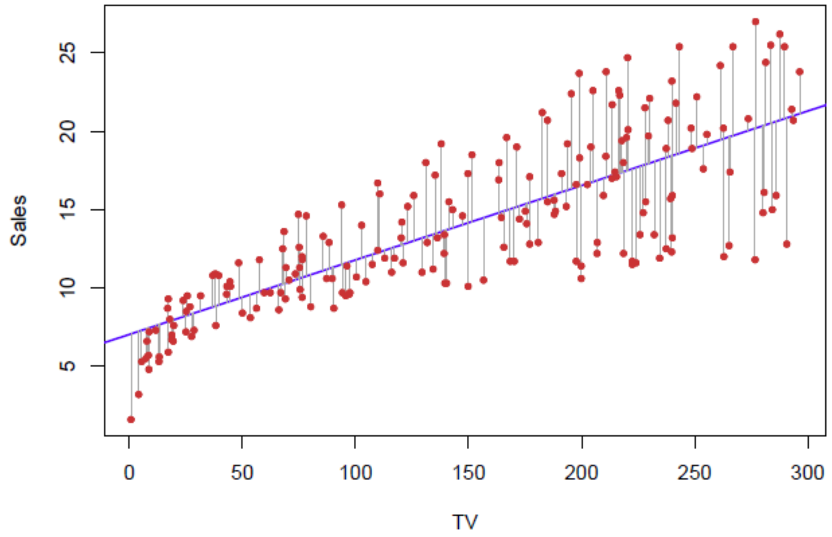
$$R^2 = \frac{TSS-RSS}{TSS} = 1 - \frac{RSS}{TSS}$$

$$MSE = \frac{RSS}{n} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

$$RMSE = \sqrt{\frac{RSS}{n}} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i|$$

$$MAPE = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{y_i-\hat{y}_i}{y_i}\right|$$



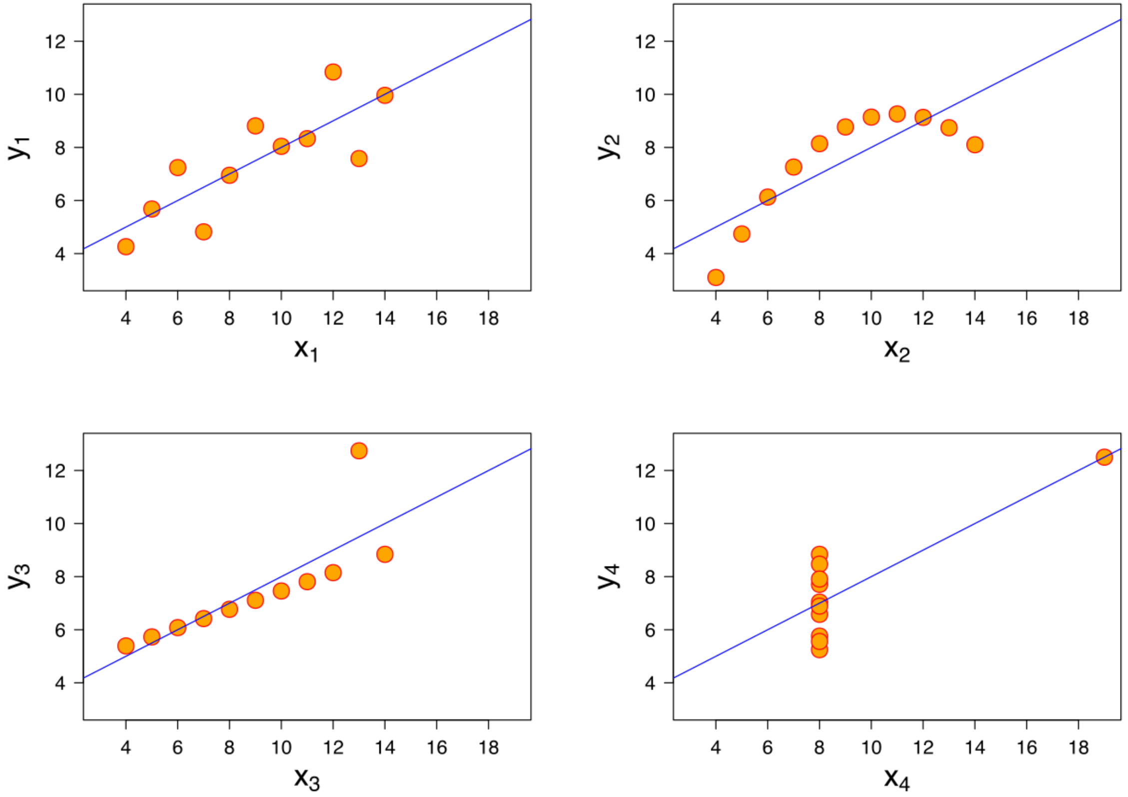
LR: Beyond Linearity

Linear Regression

- Among all possible **lines**, LR selects one that minimize the RSS
  - What if the relationship is not linear?

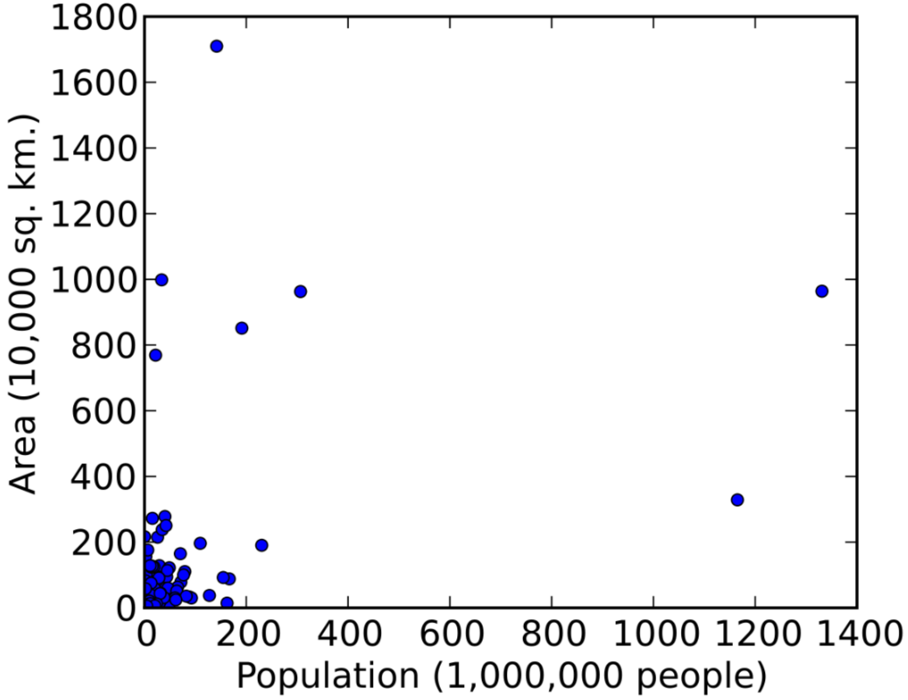
- Transformation of data
  - square root, logarithm, etc
  - Can improve model fit/ correct normality / heteroscedasticity
  - Often, a transformation that fixes one, fixes all.

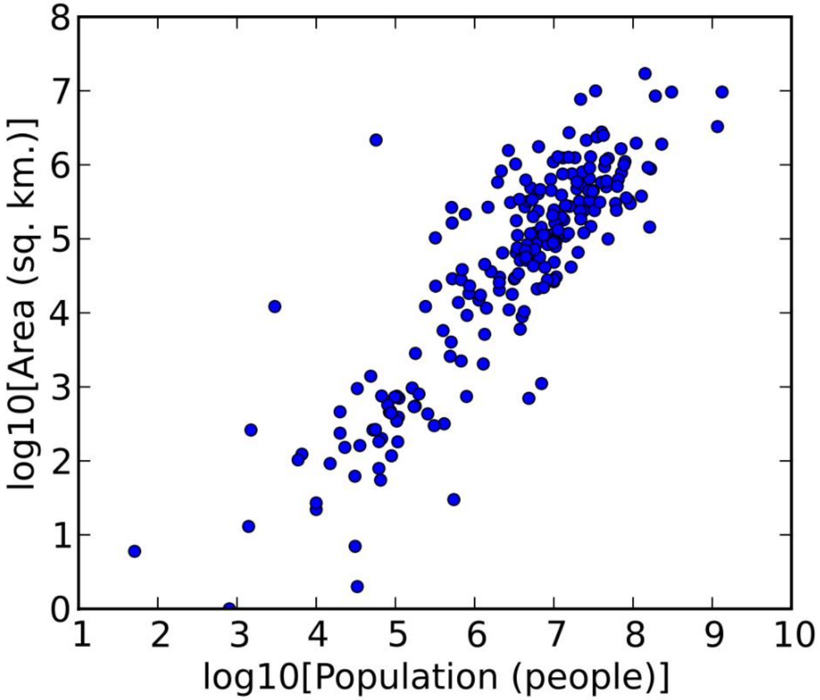
- Approach to determine whether to transform X or Y to achieve linearity, homoscedasticity and normality:
  - In general, transforming both is not required, although sometimes it is.
- A general rule of thumb:
  - Transform Y first to remove heteroscedasticity.
  - Then transform X to remove non-linearity.



Annacombes Quartet

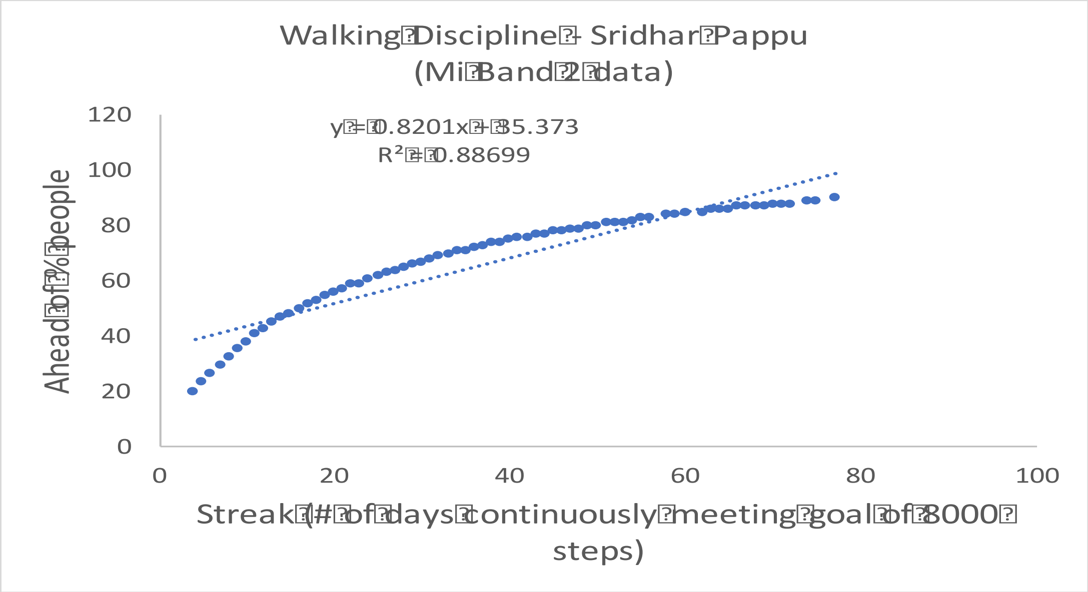
Example : Data Transformation improves fit

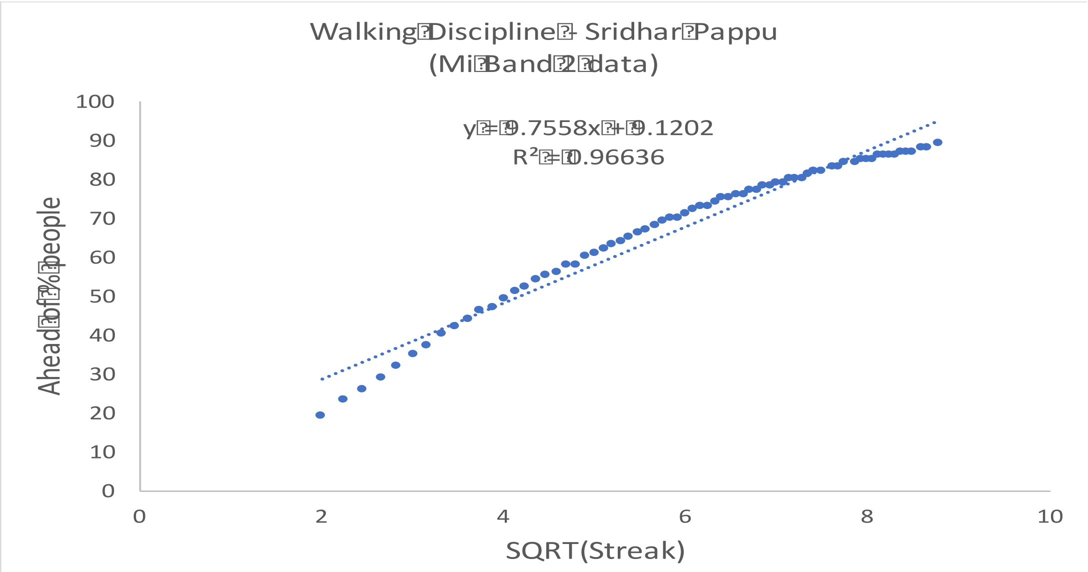


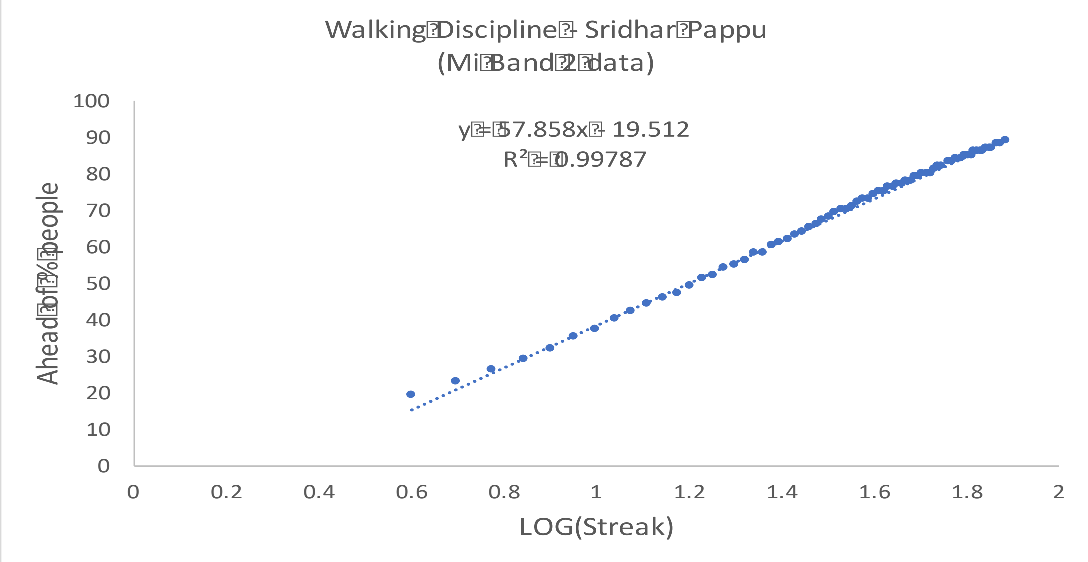


https://en.wikipedia.org/wiki/Data_transformation_(statistics)

Example (Dr. Sridhar's walking discipline)

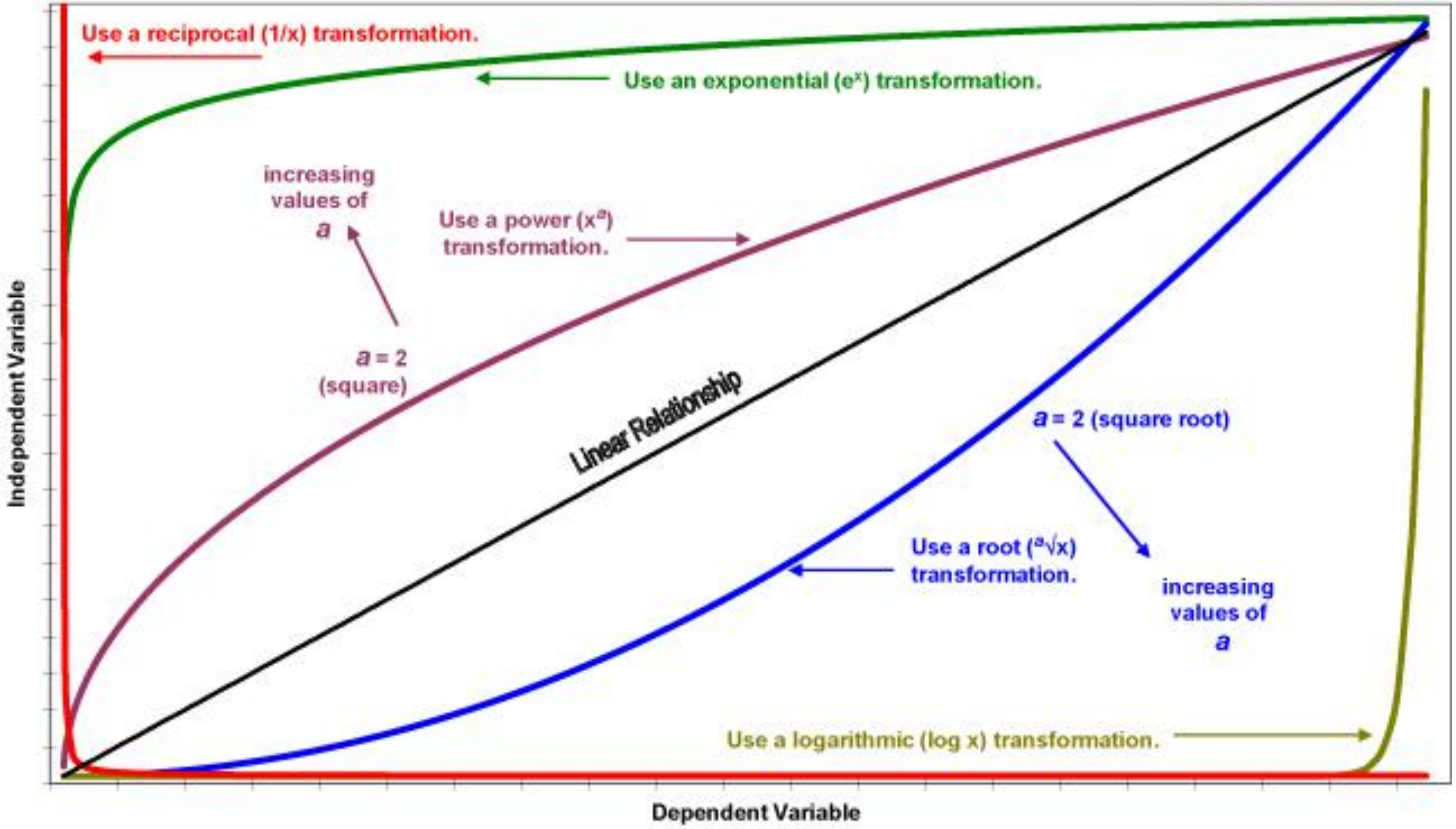






Data	Equation	R-Squared	Ahead of % People (Prediction for Day 78)
Original	0.8201x + 35.373	88.7%	99.34
Square Root on X	9.7558x + 9.1202	96.6%	95.28
Log on X	57.858x – 19.512	99.8%	89.96

Data Transformation cheat sheet



https://statswithcats.wordpress.com/2010/11/21/fifty-ways-to-fix-your-data/

Linear Regression: Summary

Get familiar with data

- Plots
- Descriptive stats

Formulate a linear model and fit to data

- Do regression

Inadequate fit

Check model and assumptions

- Look at residual plots
- Look at unusual observations
- Look at R-Squared
- Look at p-values

Good fit

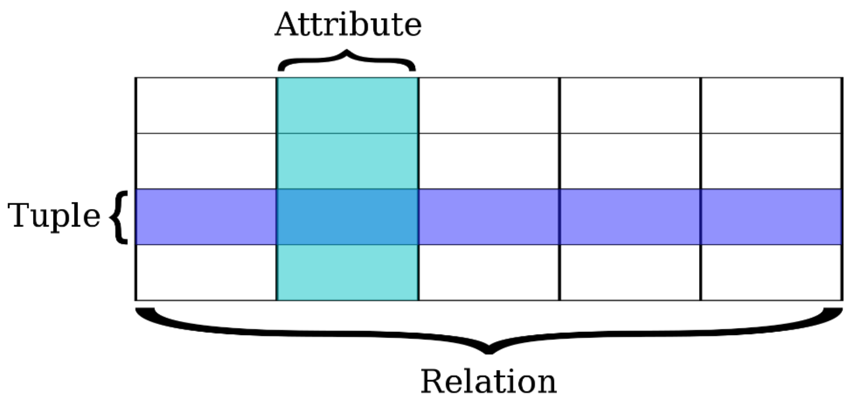
Report results and equation

- Make predictions for values of interest

Multiple Linear Regression

Praphul Chandra

From 1 to many

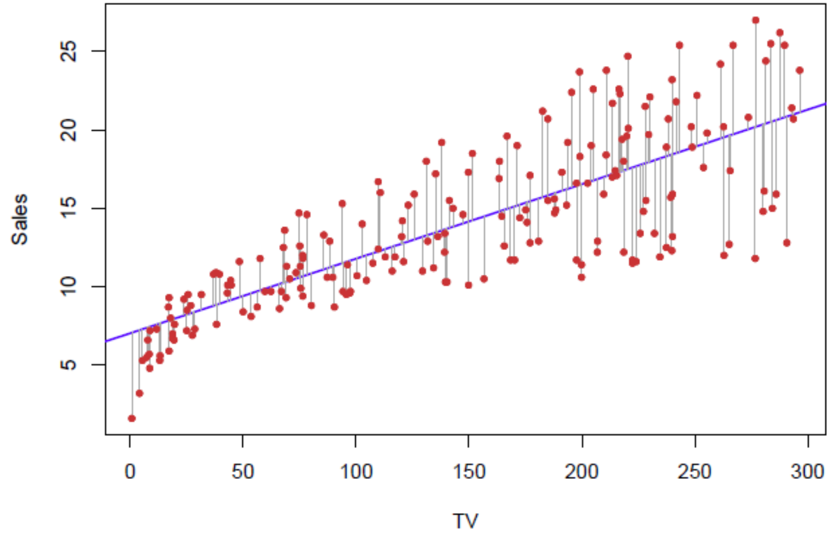


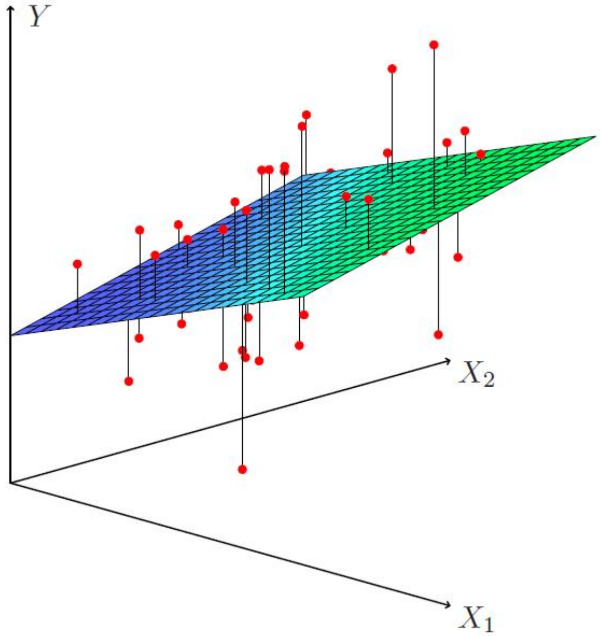
- Independent random variable.
  - Predictor variables, explanatory variables, feature, dimension, attributes
- Simple Linear Regression → Multiple Linear Regression
  - 1 independent r.v. → Multiple independent r.v.
  - Models the effect of several independent variables, x_1, x_2 etc., on one dependent variable, y
  - The different x variables are combined in a linear way and each has its own regression coefficient
  - Same assumptions: Linearity, Noise is i.i.d. Normal with mean 0 and fixed variance

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots .. + \beta_p x_p + \varepsilon$$

- Independence assumption (new!)
  - Independence among predictor variables : hence the name.
  - β parameters reflect the independent contribution of each variable, x, on the value of the dependent variable, y.
  - A coefficient is the slope of the linear relationship between the dependent variable (DV) and the independent contribution of the independent variable (IV),
    - i.e., that part of the IV that is independent of (or uncorrelated with) all other IVs.

Multiple Linear Regression : Visualization





p=1

$$y = \beta_0 + \beta_1 x_1 + \varepsilon$$

p=2

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

p > 2 ?

Simple LR → Multiple LR

- Multiple Linear Regression
  - Dependent variable is numeric
  - Fit a ~~line~~ plane / hyper-plane

- ~~Line~~ Hyperplane Fitting
  - More than p+1 data points → Over-specified problem
  - Criteria : Minimize error (sum of squared residuals)

- Optimization problem
  - Solve (using matrix manipulation)
  - Find coefficients (line) which minimizes the Residual Sum of Squares

- Use estimated coefficients ("model") to make predictions

Multiple Linear Regression : Math

$$y = \beta_0 + \beta_1 x + \epsilon$$
$$\epsilon \sim N(0, \sigma^2)$$

$$RSS = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2$$

$$\min_{\beta} RSS$$

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2}$$

$$\bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$$

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x$$

$$y = \beta_0 + \beta_1 x_1 + + \beta_2 x_2 + \ldots + \beta_p x_p + \epsilon$$
$$\epsilon \sim N(0, \sigma^2)$$

$$RSS = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2$$

$$\min_{\beta} RSS$$

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

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \ldots + \hat{\beta}_p x_p$$

More is better …. Or is it?

- More is better
  - More explanatory variables ➔ More (potential) explanation ➔ Higher R^2 (Better Fit)

- But
  - Multi-collinearity
  - Model comparison
  - Feature selection

- Assumptions (as in simple linear regression)
  - Linearity
  - Homoscedasticity (constant variance)
  - Independence of errors
  - Normality of errors

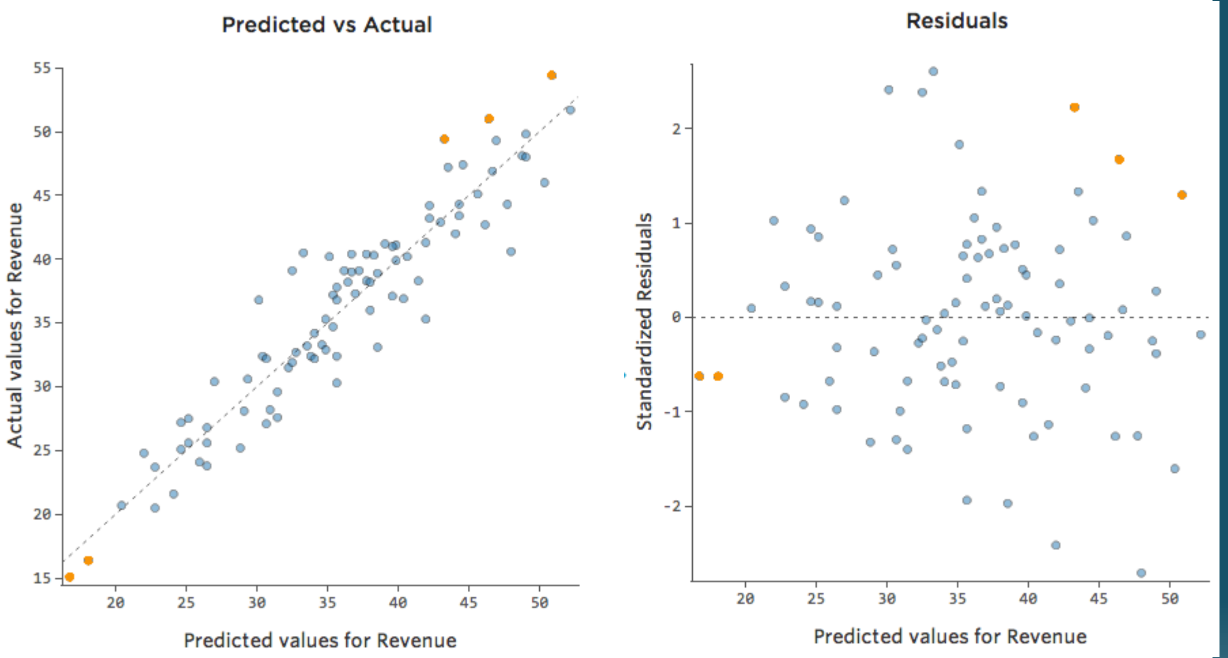
Linear correlation between x and y?

- Is there a non-linear relationship?
  - Linear ➔ Plot between y & $(\beta_0 + \beta_1 x)$ would be linear
  - Linear ➔ Errors (Residuals) will not show any pattern

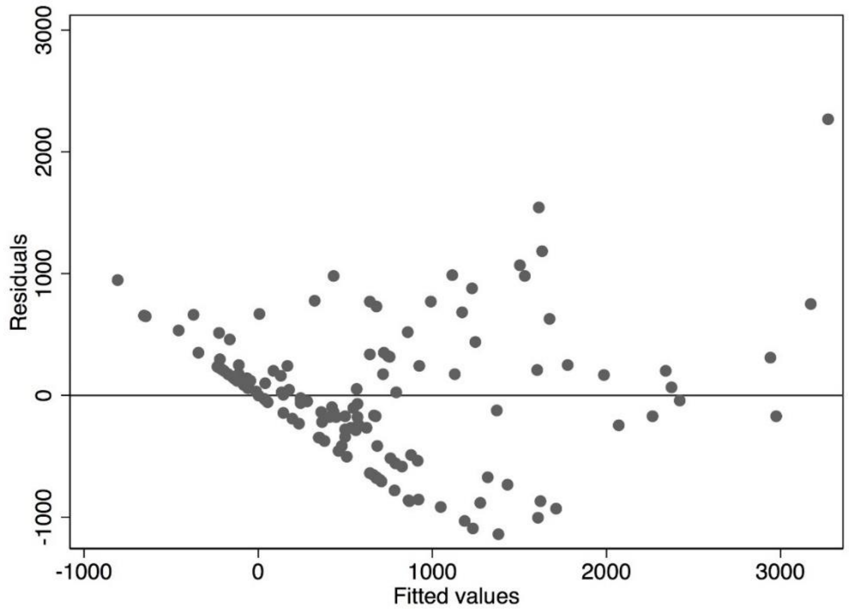
- Residual Plots
  - Graphical tool for identifying non-linearity
  - Plot residuals vs. fitted values

- Interpretation
  - No discernible pattern ➔ Linearity
  - U shape ➔ Non-linearity

- What next?
  - Feature Transformations (later)

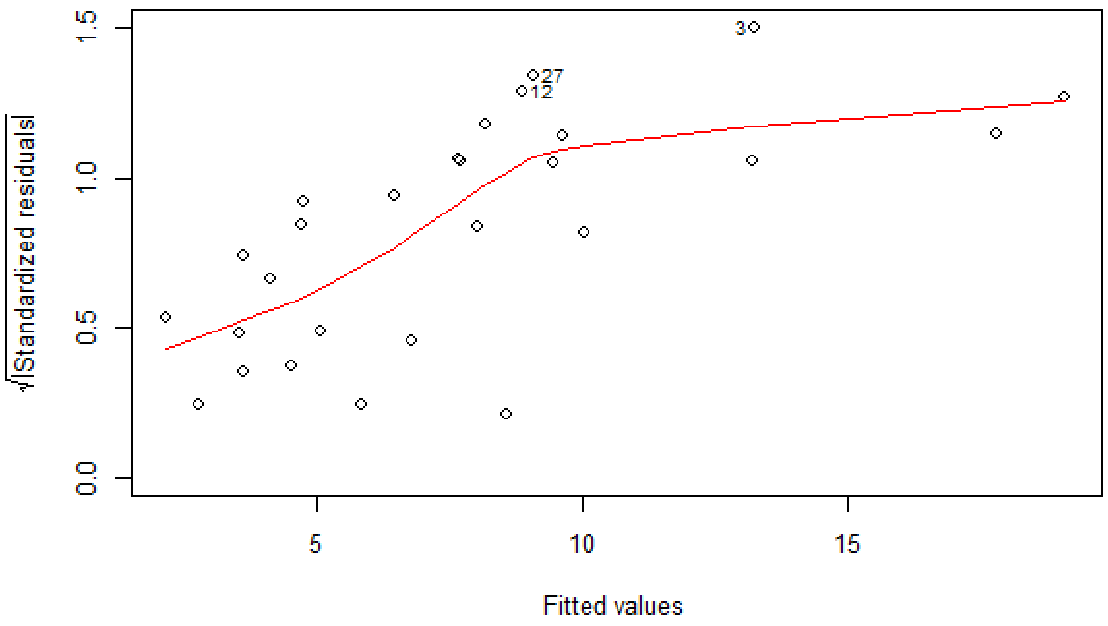


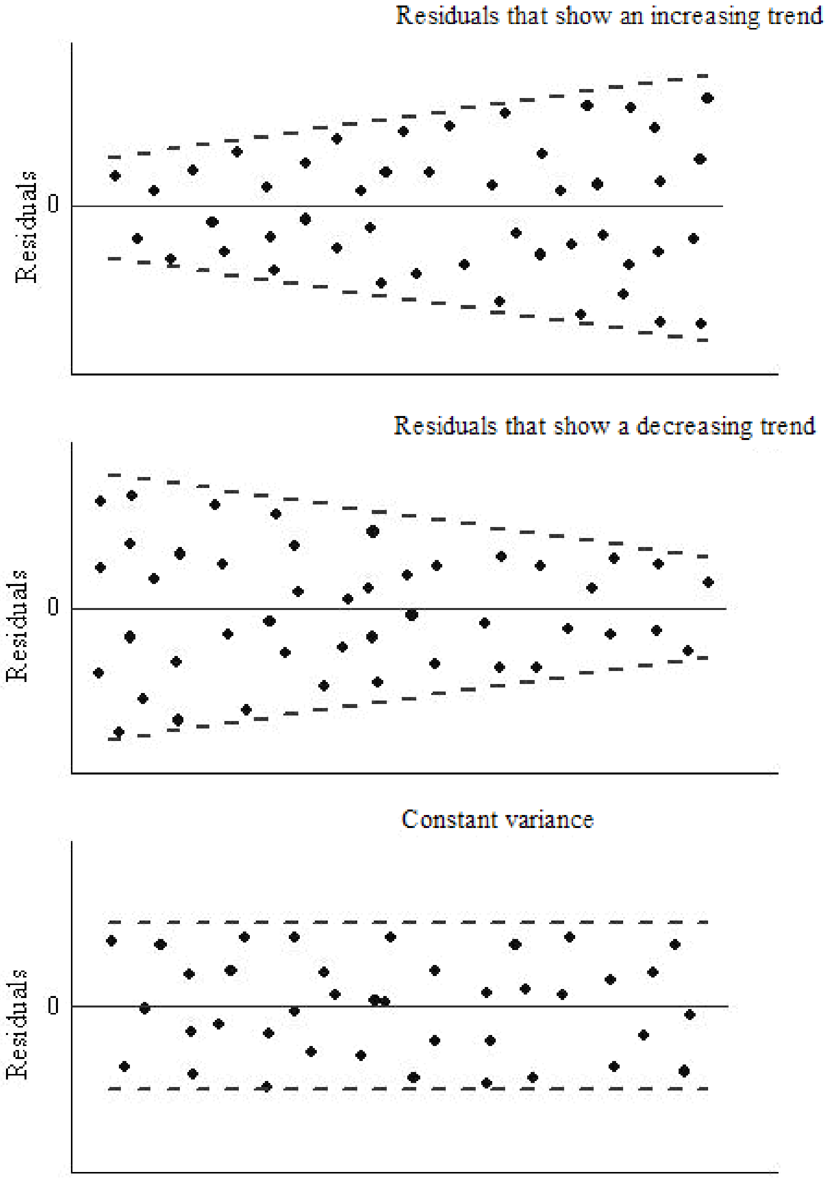
http://docs.statwing.com/interpreting-residual-plots-to-improve-your-regression/



Noise has fixed variance

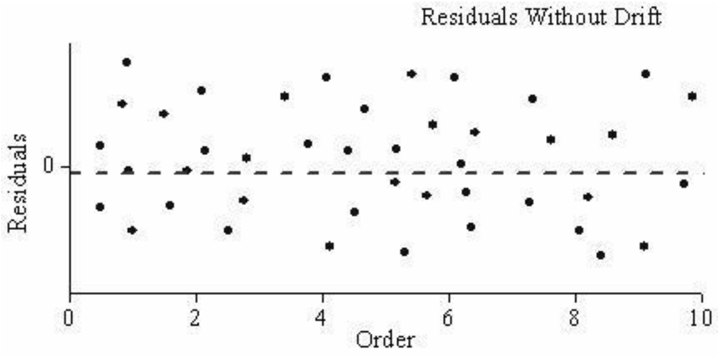
- The error terms have constant variances : homoscedasticity
  - What if variance depends on the predictor variable?
  - Need to check for heteroscedasticity
- What next?
  - Feature Transformations (later)

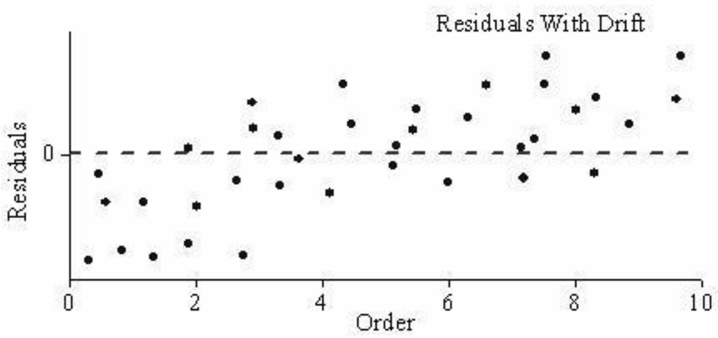


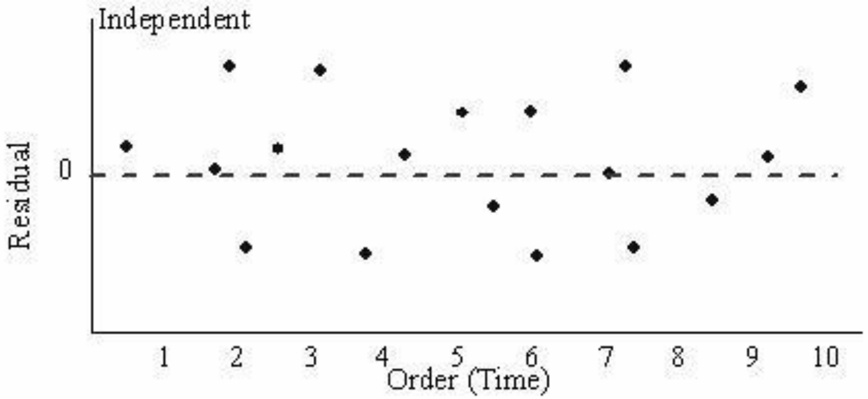


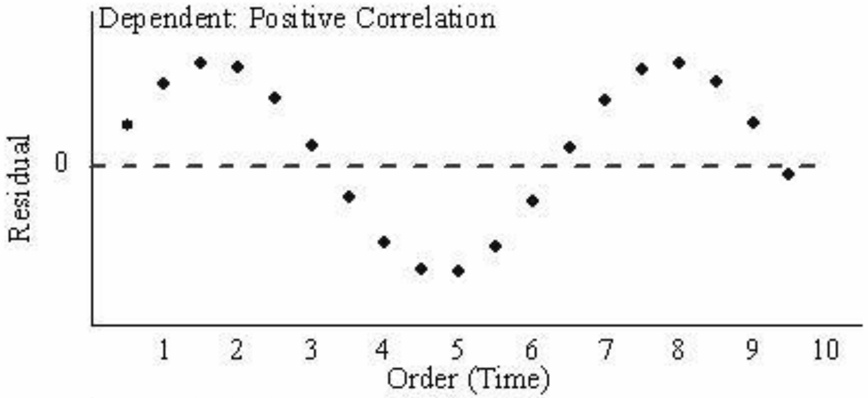
Noise (residuals) independent (i.i.d.) ?

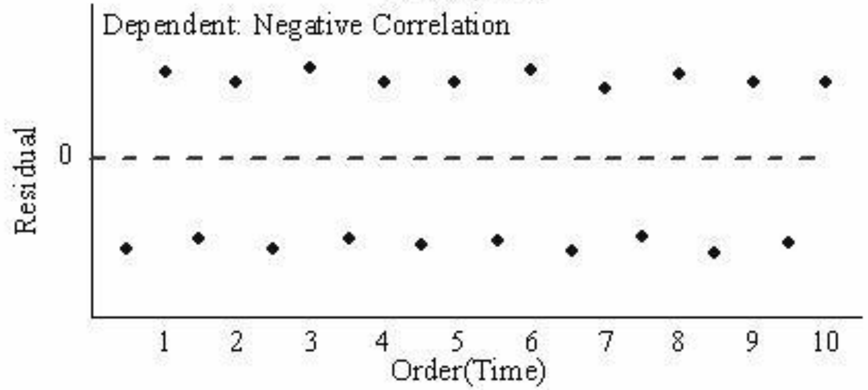
- Are error terms correlated?
  - Are "successive" residuals correlated?
  - ϵ_i is positive provides no information about the sign of ϵ_{i+1}
- Successive?
  - Temporal
  - Any sequence… (e.g. spatial)
- Source
  - Sampling error!
  - Design of Experiment error!









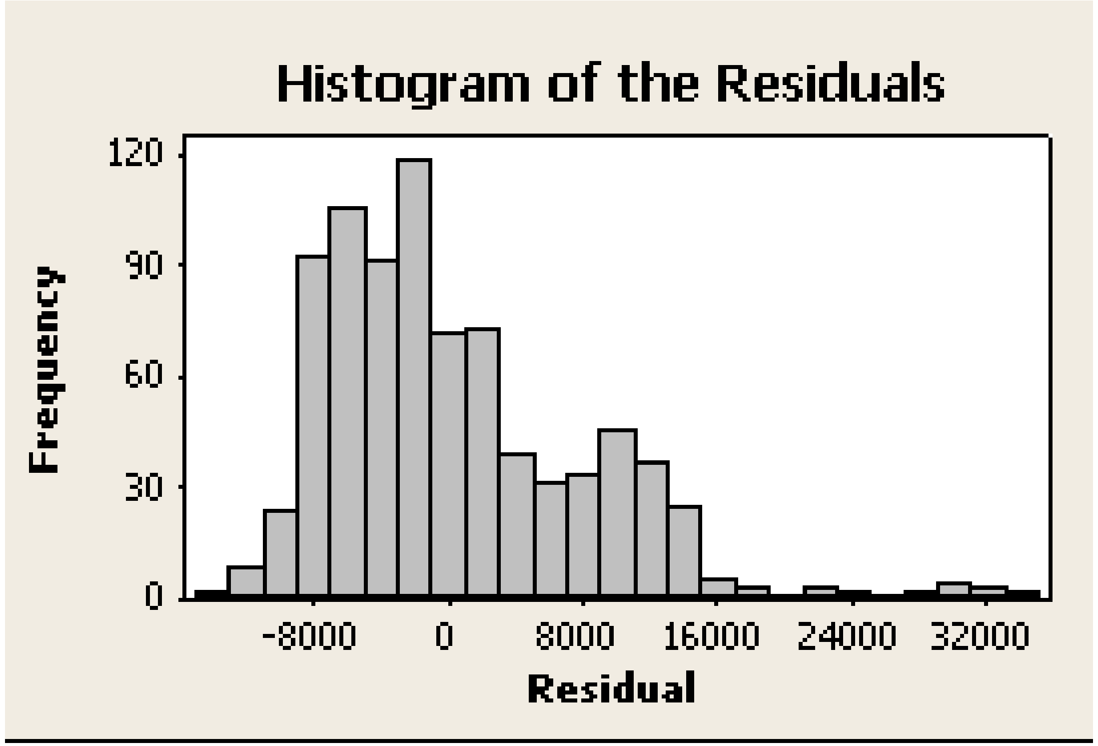


http://www.originlab.com/doc/en/UserGuide/images/Graphic_Residual_Analysis/Graphic_Residual_Analysis-4.jpg

Noise (residuals) normally distributed?

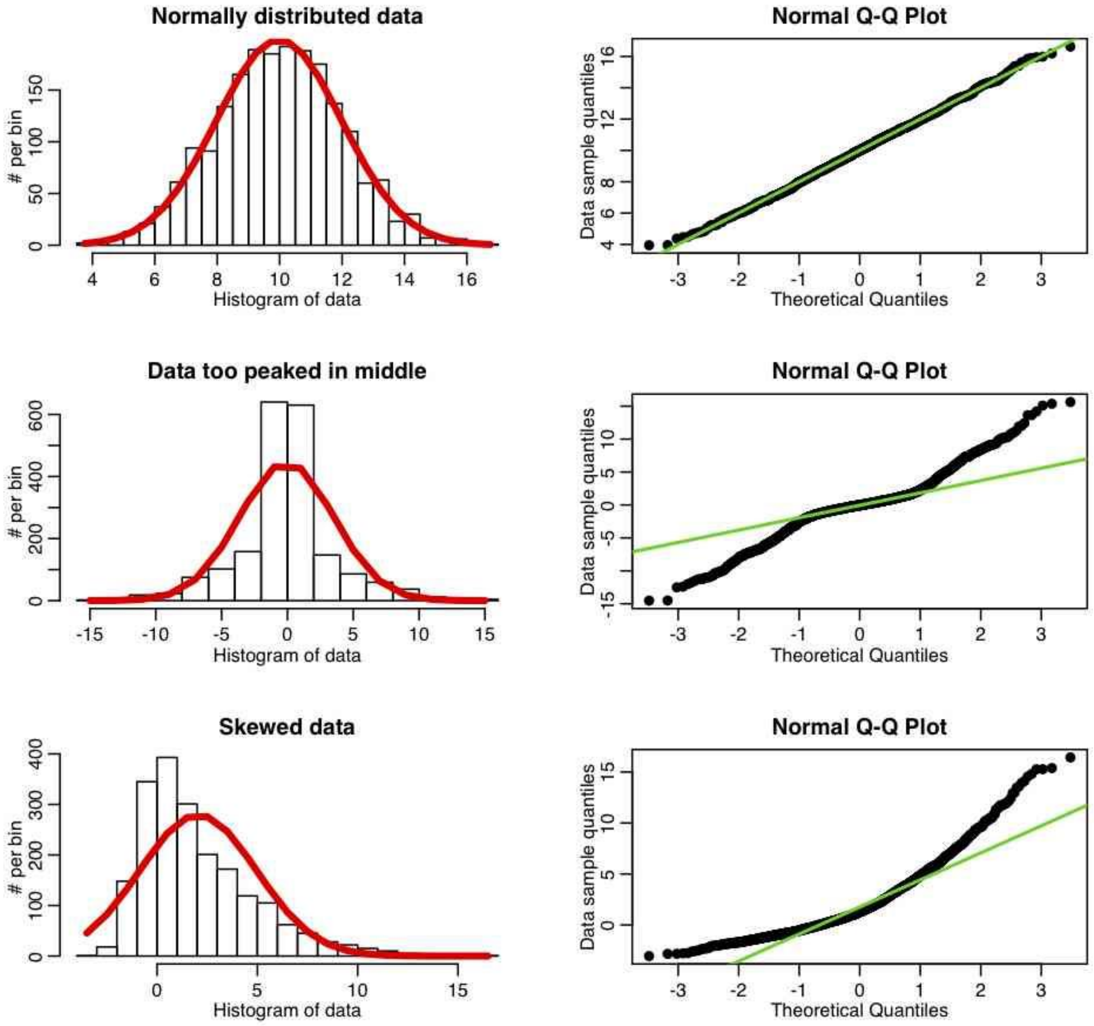
- Residual distribution is normal?
  - Plot & check

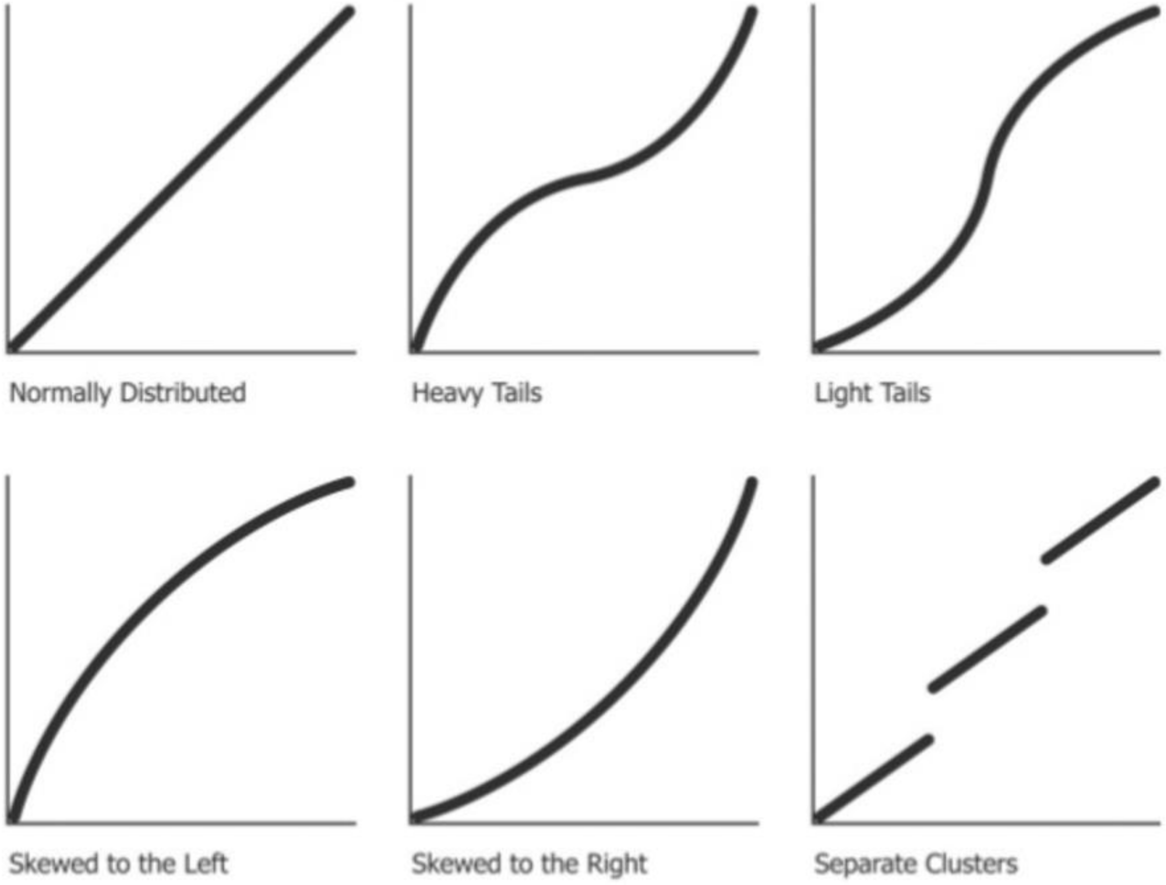
- Q-Q plot
  - Used to validate distributional assumptions of a data set.
  - Normality ➔ z-scores of the residuals should be equal to the expected z-scores at corresponding quantiles.



http://sherrytowers.com/wp-content/uploads/2013/08/qqplot_examples.jpg

Noise (residuals) normally distributed? (cont'd)





Example

- In a real estate study, multiple variables were explored to determine the price of a house.
  - # of bedrooms
  - # of bathrooms
  - Age of the house
  - # of square feet of living space
  - Total # of square feet of space
  - # of garages
- Predict the price of the house by total square feet and age of the house.

$$\hat{y} = 57.35 + 0.0177Area - 0.666Age$$

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	57.35074586	10.00715186	5.73097587	1.31298E-05	36.47619286	78.22529885
Area (sq ft) (x1)	0.017718036	0.00314562	5.632605205	1.63535E-05	0.011156388	0.024279685
Age of House (years) (x2)	-0.666347946	0.227996703	-2.922620973	0.008417613	-1.141940734	-0.190755157

Inferential statistic : Caution!

- p-value for a regression coefficient
  - Probability of obtaining a t-statistic very far from 0 by chance
  - Expected number of coefficient for which this will happen by chance?
  - What if number of dimensions =10? 100? 1000?
  - p-value=0.05, number of dimensions = 100 ➔ 5 predictor variables may show up as “significant” by chance!

- F-statistic for k-dimensional multiple regression model
  - Tests that at least one of the regression coefficients is different from 0. (Null hypothesis : All coefficients 0)
  - $R^2 = \frac{ESS}{TSS} = \frac{TSS-RSS}{TSS} = 1 - \frac{RSS}{TSS}$
  - $F = \frac{ESS/k}{TSS/(n-k-1)} = \frac{(TSS-RSS)/k}{TSS/(n-k-1)}$
  - F-test: Comparing “the variance explained by the model” to “the variance not explained by the model”
  - When there is no relationship between the dependent variables and the predictors F is close to 1
  - If F is large, there is a relationship

(Multi)-collinearity

More isn't always better

(Multi)-collinearity

	Energy consumption	Nuclear	Coal	Dry gas	Fuel rate
Energy consumption	1				
Nuclear	0.856	1			
Coal	0.791	0.952	1		
Dry gas	0.057	-0.404	-0.448	1	
Fuel rate	0.791	0.972	0.968	-0.423	1

- Violation of "independence" among predictor variables
  - Predictor variables are correlated
  - Which coefficient should be higher in the model?
- Impact
  - Impacts the interpretability of the model (not necessarily predictive power)
  - A variable which is in fact important may end with a lower coefficient (correlated variable gets a higher coefficient)
  - A regression coefficient which should be +ve ends up –ve (correlated variable gets a high +ve coefficient)
  - Removing one independent variable drastically changes the coefficient of others
- For example, fuel rate and coal production are highly correlated (0.968).
  - $\hat{y}=44.869+0.7838(fuel\ rate)$
  - $\hat{y}=45.072+0.0157(coal)$
  - $\hat{y}=45.806+0.0277(coal)-0.3934(fuel\ rate)$

http://circabook.com/multicollinearity-in-regression-models-penn-state-eberly-/

(Multi)-collinearity

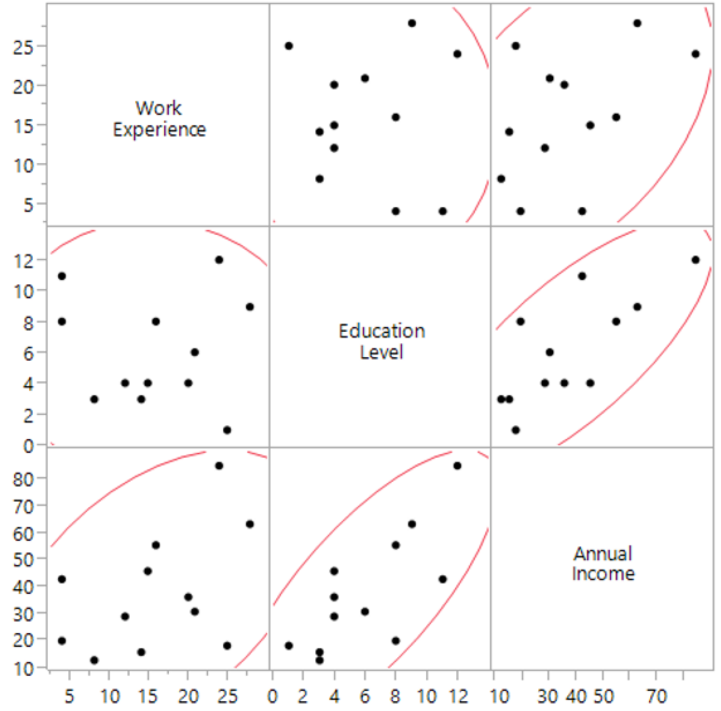
- What next?
  - Check for correlation among predictor variables.
  - Ideally before building the model
  - Drop correlated predictor variables
  - Feature transformation: PCA, PLS

- Inferential Statistics Explanation
  - Challenge: Which coefficient should be higher in the model?
  - ➔ Reduces the accuracy of the estimates of the model coefficients
  - ➔ Sampling distribution variance increases
  - ➔ Standard Errors of the coefficients increases
  - ➔ t-statistic decreases
  - ➔ p-value increases

Multivariate Correlations

	Work Experience	Education Level	Annual Income
Work Experience	1.0000	-0.0423	0.4628
Education Level	-0.0423	1.0000	0.7551
Annual Income	0.4628	0.7551	1.0000

Scatterplot Matrix



http://circabook.com/multicollinearity-in-regression-models-penn-state-eberly-/

Example

- A drug precursor molecule is extracted from a type of nut, which is commonly contaminated by a fungal toxin that is difficult to remove during the purification process. The suspected predictors of the amount of fungus are:
  - Rainfall (cm/week)
  - Noon temperature (oC)
  - Sunshine (h/day)
  - Wind speed (km/h)
  - The fungal toxin concentration is measured in µg/100 g.

```
> correlation
                Toxin         Rain    NoonTemp   Sunshine    WindSpeed
Toxin      1.00000000  0.868734134 -0.07319548 -0.05169949 -0.270555628
Rain       0.86873413  1.000000000  0.11691043  0.16841144 -0.002180167
NoonTemp  -0.07319548  0.116910426  1.00000000  0.50082303 -0.368972511
Sunshine  -0.05169949  0.168411437  0.50082303  1.00000000 -0.018439486
WindSpeed -0.27055563 -0.002180167 -0.36897251 -0.01843949  1.000000000
```

```
Call:
lm(formula = ToxinConc$Toxin ~ ToxinConc$Rain + ToxinConc$NoonTemp +
    ToxinConc$Sunshine + ToxinConc$WindSpeed, data = ToxinConc)

Residuals:
      1       2       3       4       5       6       7       8
-1.8818  2.0498 -0.6314  0.4787 -0.5805  1.2508 -0.1921 -0.1813
      9      10
-1.1552  0.8429

Coefficients:
                    Estimate Std. Error t value Pr(>|t|)
(Intercept)          31.6084     7.1051   4.449  0.00671 **
ToxinConc$Rain        7.0676     1.0031   7.046  0.00089 ***
ToxinConc$NoonTemp   -0.4201     0.2413  -1.741  0.14215
ToxinConc$Sunshine   -0.2375     0.5086  -0.467  0.66018
ToxinConc$WindSpeed  -0.7936     0.2977  -2.666  0.04458 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.574 on 5 degrees of freedom
Multiple R-squared:  0.9186,    Adjusted R-squared:  0.8535
F-statistic: 14.11 on 4 and 5 DF,  p-value: 0.006232
```

Example (cont'd)

- Remove one of the correlated variables
- Rebuild model
- Business Implication
  - Toxin concentrations increase with increasing rainfall and decrease in drier climates characterized by higher temperatures and wind speeds.
  - The business can take a decision to rent farms in drier climates if the cost benefits of saved nuts versus higher rents are high.

```
Call:
lm(formula = ToxinConc$Toxin ~ ToxinConc$Rain + ToxinConc$NoonTemp +
    ToxinConc$WindSpeed, data = ToxinConc)

Residuals:
    Min      1Q  Median      3Q     Max
-1.6394 -0.9308  0.1394  0.6545  2.0909

Coefficients:
                    Estimate Std. Error t value Pr(>|t|)
(Intercept)          31.5651     6.6253   4.764  0.00311 **
ToxinConc$Rain        7.0108     0.9285   7.551  0.00028 ***
ToxinConc$NoonTemp   -0.4790     0.1919  -2.495  0.04682 *
ToxinConc$WindSpeed  -0.8218     0.2718  -3.023  0.02331 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.468 on 6 degrees of freedom
Multiple R-squared:  0.915,     Adjusted R-squared:  0.8726
F-statistic: 21.54 on 3 and 6 DF,  p-value: 0.001298
```

Multicollinearity

- Testing for pair-wise correlation not enough
  - A predictor variable may be correlated with two other variables taken together

- Variance Inflation Factor (VIF)
  - Intuition : Regress each predictor variable w.r.t. other predictors.
  - Predict an independent variable by the other independent variables.
  - The independent variable being predicted becomes the dependent variable in this analysis.
  - A “large” VIF (>> 10) indicates multicollinearity.

$$VIF(\hat{\beta}_j) = \frac{1}{1-R^2_{X_j|X_{-j}}}$$

- Stepwise regression prevents this problem to a great extent.

Checking for multi-collinearity in R

```
Call:
lm(formula = model0, data = regData)

Residuals:
     Min       1Q   Median       3Q      Max 
-0.25843 -0.11727 -0.00533  0.07364  0.49503 

Coefficients:
                Estimate Std. Error t value Pr(>|t|)    
(Intercept)     10.85028    3.07946   3.523  0.00182 ** 
log(Miles)       0.42533    0.22528   1.888  0.07170 .  
log(Speed)      -0.75004    0.73563  -1.020  0.31853    
log(Hours)      -0.45601    0.18423  -2.475  0.02111 *  
log(Population)  0.02401    0.04341   0.553  0.58559    
LoadFactor      -5.82500    0.49084 -11.867 2.76e-11 ***
log(Capacity)   -1.80998    0.14851 -12.187 1.62e-11 ***
log(AdjAsset)    0.11555    0.07611   1.518  0.14259    
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.1747 on 23 degrees of freedom
Multiple R-squared:  0.9898, Adjusted R-squared:  0.9868 
F-statistic: 320.3 on 7 and 23 DF,  p-value: < 2.2e-16
```

```
> vif(fit)
     log(Miles)      log(Speed)      log(Hours) log(Population)      LoadFactor   log(Capacity)   log(AdjAsset) 
      15.437923       14.227428        2.600507        3.761584        4.586951        6.951357       18.006015 
```

http://subhasis4analytics.blogspot.in/2014/09/linear-regression-analysis-with-r-and.html

Feature (Model) Selection

Feature engineering

Feature Selection

- Best subset selection
  - Brute force : Try all possible combinations from the available set of predictors
  - Number of models to try 2^p
  - Computational load?

- Forward subset selection
  - p simple linear regression models; Select the best one.
  - Greedy approach: May not find THE best model but often good enough

- Backward subset selection
  - Start will all variables in.
  - Remove insignificant variables one-by-one

- Hybrid subset selection
  - Grown & prune

Forward (Hybrid) subset selection

- Starts a model with a single predictor and then adds or deletes predictors one step at a time.
- Step 1
  - Simple regression model for each of the independent variables one at a time.
  - Model with largest absolute value of t selected and the corresponding independent variable considered the best single predictor, denoted x1.
  - If no variable produces a significant t, the search stops with no model.
- Step 2
  - All possible two-predictor regression models with x1 as one variable.
  - Model with largest absolute t value in conjunction with x1 and one of the other k-1 variables denoted x2.
  - Occasionally, if x1 becomes insignificant, it is dropped and search continued with x2.
  - If no other variables are significant, procedure stops.
  - The above process continues with the 3rd variable added to the above 2 selected and so on.

Example: Feature (Model) selection

- Suppose a model to predict the world crude oil production (barrels per day) is to be developed and the predictors used are:
  - US energy consumption (BTUs)
  - Gross US nuclear electricity generation (kWh)
  - US coal production (short-tons)
  - Total US dry gas (natural gas) production (cubic feet)
  - Fuel rate of US-owned automobiles (miles per gallon)
- What does your intuition say about how each of these variables would affect the oil production?
- Search procedures help choose the more attractive model.
  - If 3 variables can explain the variation nearly as well as 5 variables, the simpler model is better.
  - All variables used in all combinations ➔ search among 31 models
  - Tedious, Time-Consuming, Inefficient, Overwhelming.
  - Use Forward subset selection

Example (cont'd)

Dependent Variable	Independent Variable	*t* Ratio	*p*-value	R^2
Oil production	Energy consumption	11.77	1.86e-11	85.2%
Oil production	Nuclear	4.43	0.000176	45.0
Oil production	Coal	3.91	0.000662	38.9
Oil production	Dry gas	1.08	0.292870	4.6
Oil production	Fuel rate	3.54	0.00169	34.2

$$y = 13.075 + 0.580x_1$$

$$y = 7.14 + 0.772x_1 - 0.517x_2$$

Dependent Variable, *y*	Independent Variable, x_1	Independent Variable, x_2	*t* Ratio of x_2	*p*-value	R^2
Oil production	Energy consumption	Nuclear	-3.60	0.00152	90.6%
Oil production	Energy consumption	Coal	-2.44	0.0227	88.3
Oil production	Energy consumption	Dry gas	2.23	0.0357	87.9
Oil production	Energy consumption	Fuel rate	-3.75	0.00106	90.8

Example (cont'd)

Dependent Variable, *y*	**Independent Variable, x_1**	**Independent Variable, x_2**	**Independent Variable, x_3**	***t* Ratio of x_3**	***p*-value**
Oil production	Energy consumption	Fuel rate	Nuclear	-0.43	0.672
Oil production	Energy consumption	Fuel rate	Coal	1.71	0.102
Oil production	Energy consumption	Fuel rate	Dry gas	-0.46	0.650

- No *t* ratio is significant at $\alpha = 0.05$. No new variables are added to the model.

Categorical Predictor Variables

Dealing with categorical variables

- Type of r.v. (Till now: Assume all numeric)
  - If dependent r.v. categorical : Logistic regression
  - If independent r.v. categorical : One hot encoding
- Categorical Predictor variables
  - Gender, geographic region, occupation, marital status, level of education, economic class, buying/renting a home, etc
- Replace with Indicator (Dummy) random variables
  - If a survey question asks about the region of country your office is located in, with North, South, East and West as the options, the **recoding** can be done as follows:
  - If there are *n* categories, *n-1* dummy variables need to be inserted into the regression analysis.

Region
North
East
South
West

→

North	West	South
1	0	0
0	0	0
0	0	1
0	1	0

Example

- Consider the issue of gender discrimination in the salary earnings of workers in some industries. If there is discrimination, how much is one gender earning more than the other?

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	1.732060612	0.235584356	7.352189	8.83E-06	1.218766395	2.245354829
Age (10 years)	0.111220164	0.072083424	1.542937	0.148796	-0.045836124	0.268276453
Gender (1=Male, 0=Female)	0.458684065	0.053458498	8.58019	1.82E-06	0.342208003	0.575160126

  - Interpret as two equations.

Example

```r
# creating the factor variable
hsb2$race.f <- factor(hsb2$race)
```

```r
hsb2$race.f[1:15]
```

```
##  [1] 4 4 4 4 4 4 3 1 4 3 4 4 4 4 3
## Levels: 1 2 3 4
```

```
##
## Call:
## lm(formula = write ~ race.f, data = hsb2)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -23.055  -5.458   0.972   7.000  18.800
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)    46.46       1.84   25.22  < 2e-16 ***
## race.f2        11.54       3.29    3.51  0.00055 ***
## race.f3         1.74       2.73    0.64  0.52461
## race.f4         7.60       1.99    3.82  0.00018 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 9.03 on 196 degrees of freedom
## Multiple R-squared:  0.107,  Adjusted R-squared:  0.0934
## F-statistic: 7.83 on 3 and 196 DF,  p-value: 5.78e-05
```

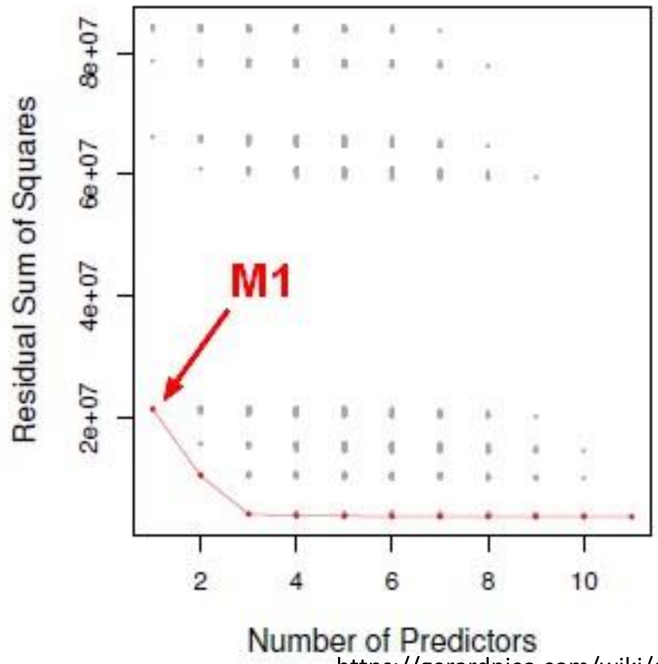
https://stats.idre.ucla.edu/r/modules/coding-for-categorical-variables-in-regression-models/

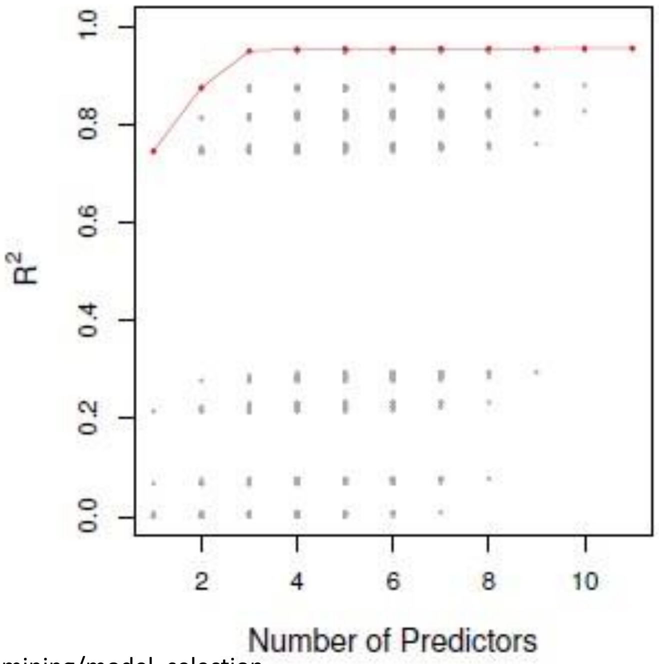
Model Comparison

Apples & Oranges

Model Comparison : Challenge

- Comparing two models with the same number of predictor variables
  - Higher R^2 better
- Comparing two models with different number of predictor variables
  - Apples & Oranges
  - More predictor variables ➔ More “flexibility” in the model
  - However, sometimes these variables are insignificant and add no real value, yet inflating the R2 value.





https://gerardnico.com/wiki/data_mining/model_selection

Model Comparison : Challenge

- Comparing two models with different number of predictor variables
  - Apples & Oranges
  - More predictor variables ➔ More "flexibility" in the model
  - Potential of overfitting

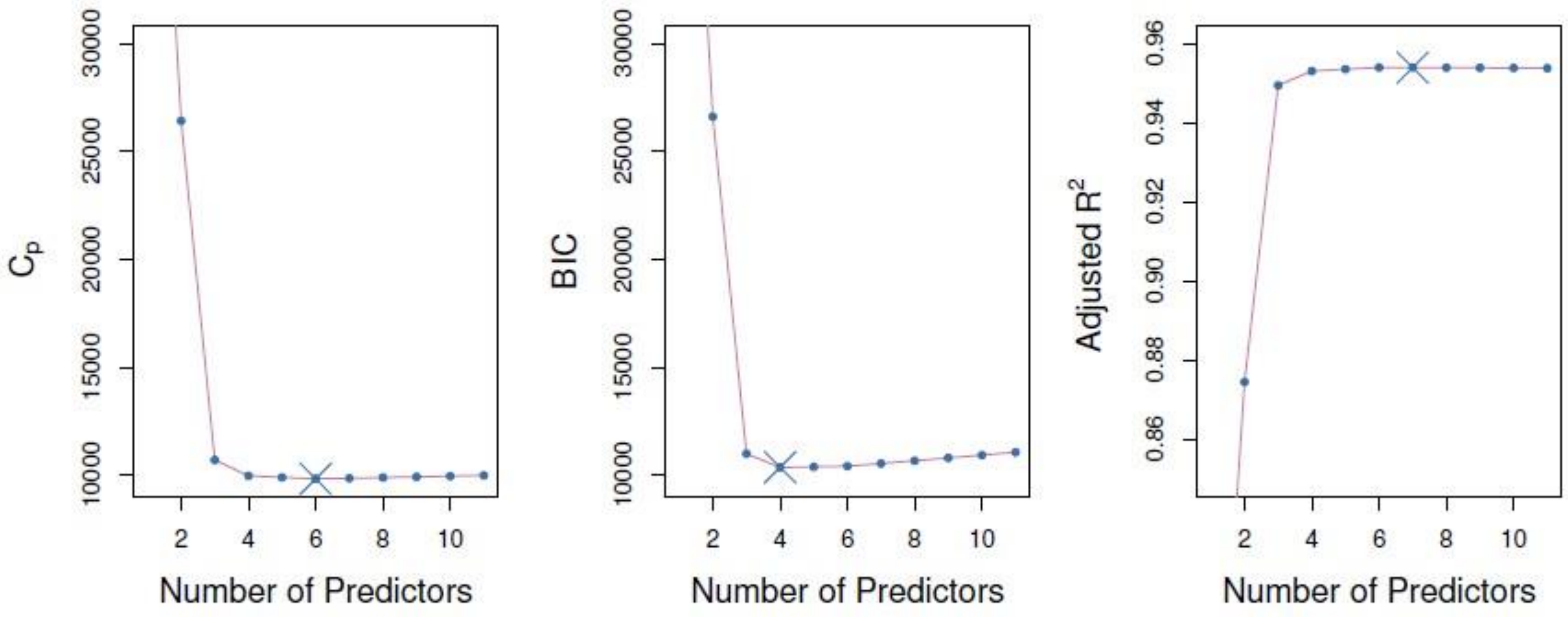
- Generalization Error (BIG Idea)
  - Sample vs. Population

- Two considerations in model building:
  - Explaining most variation in dependent variable
  - Keeping the model simple AND economical
  - Quite often, the above two considerations are in conflict of each other.

Model Comparison : Statistics

- Key Idea
  - Penalize models for using more parameters (predictor variables)
  - $Adjusted\ R^2 = 1 - \frac{\frac{RSS}{(n-d-1)}}{\frac{TSS}{n-1}}$
  - Cp, AIC, BIC
  - Aim to estimate the performance of the model learnt from sample on the population (train-test)

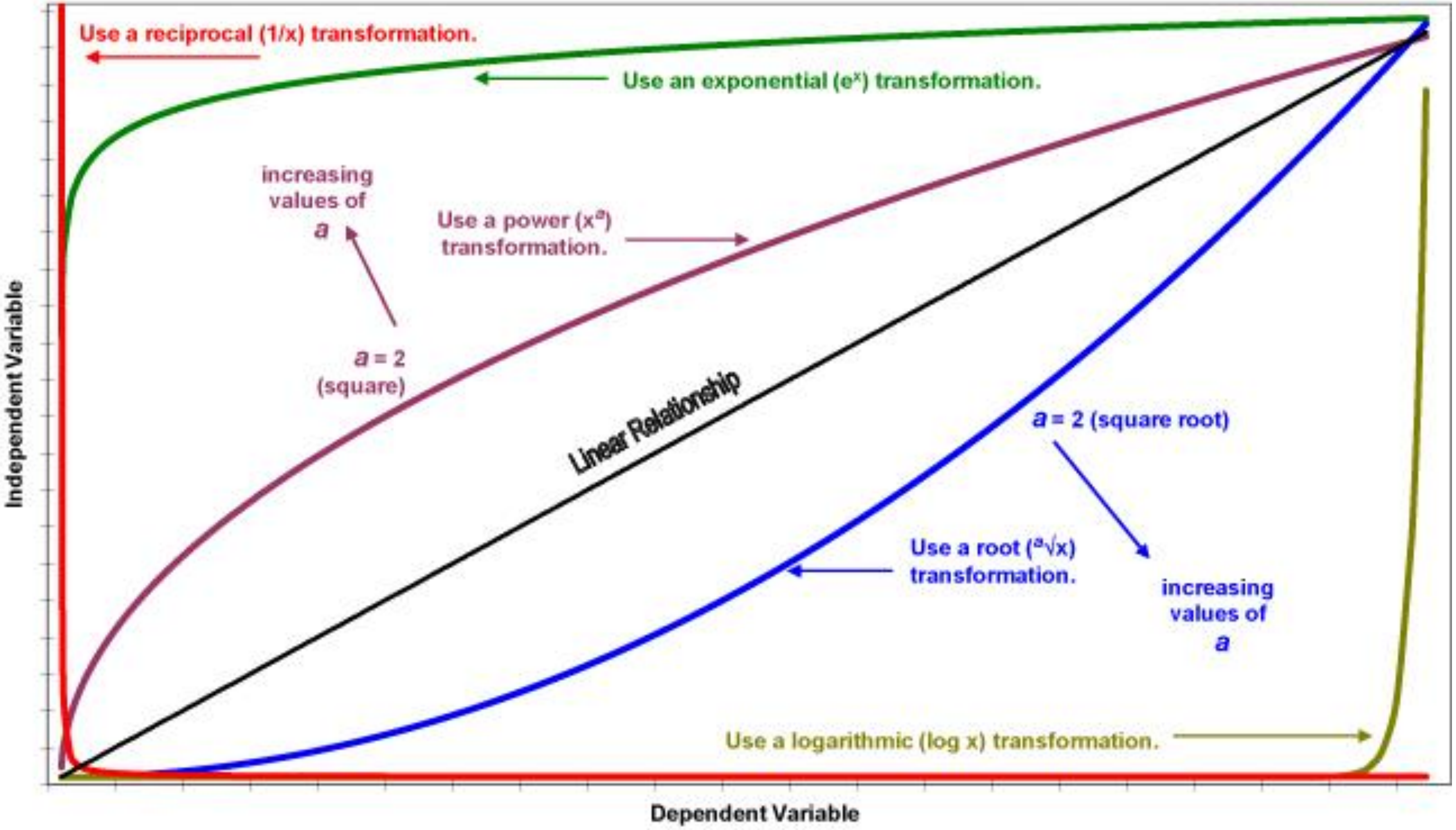
$$C_p = \frac{1}{n}(RSS + 2d\hat{\sigma}^2)$$
$$AIC = \frac{1}{n\hat{\sigma}^2}(RSS + 2d\hat{\sigma}^2)$$
$$BIC = \frac{1}{n}(RSS + \log(n)d\hat{\sigma}^2)$$



Moving beyond Linearity

Feature engineering

Data Transformation cheat sheet



https://statswithcats.wordpress.com/2010/11/21/fifty-ways-to-fix-your-data/

Other tricks in Multiple Linear Regression

- Interaction Terms
- Interaction can be examined as a separate independent variable in regression.
- For example, $y=\beta\_0+\beta\_1\ x\_1+\beta\_2\ x\_2+\beta\_3\ x\_1\ x\_2+\varepsilon$

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	50.85548009	3.790993168	13.41481713	1.38402E-08	42.59561554	59.11534464
Stock 2 ($)	-0.118999968	0.19308237	-0.616317112	0.54919854	-0.539690313	0.301690376
Stock 3 ($)	-0.07076195	0.198984841	-0.35561478	0.728301903	-0.504312675	0.362788775

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	12.04617703	9.312399791	1.29356313	0.222319528	-8.450276718	32.54263077
Stock 2 ($)	0.878777607	0.26187309	3.355738482	0.006412092	0.302398821	1.455156393
Stock 3 ($)	0.220492727	0.143521894	1.536300286	0.152714573	-0.095396832	0.536382286
Stock 2*Stock 3	-0.009984949	0.002314083	-4.314862356	0.00122514	-0.015078211	-0.00489169

Q?

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