Modul 3

Regression

Data Science Program

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What is Regression?

- Tool for finding existence of an association relationship between a dependent variable (Y) and one or more independent variables (X_1, X_2, …, X_n)

- Relationship can be linear or non-linear

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Mathematical vs Statistical Relationship

- Mathematical is an exact relationship

$$\boxed{\mathbf{Y} = \beta_0 + \beta_1 \mathbf{X}}$$

- Statistical is NOT an exact relationship

$$\boxed{\mathbf{Y} = \beta_0 + \beta_1 \mathbf{X} + \epsilon}$$

Regression Dictionary

- Dependent variable (*response variable*) measures an outcome of a study (can also be called *outcome variable*)
- Independent variables (*explanatory variables)* explain changes in a response variable
- Given set values of explanatory variable to see how it affects response variable -> predict response variable

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Dependent and Independent Variables

- Terms dependent and independent does not necessarily imply a causal relationship between two variables
- Regression is NOT to capture causality
- Purpose regression: predict the value of dependent variable given the values of independent variables

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Why we need Regression?

- Companies would like to know about factors that have significant impact on their key performance indicators.

- Helps to create new hypothesis that assist companies to improve their performance and hence better decision making

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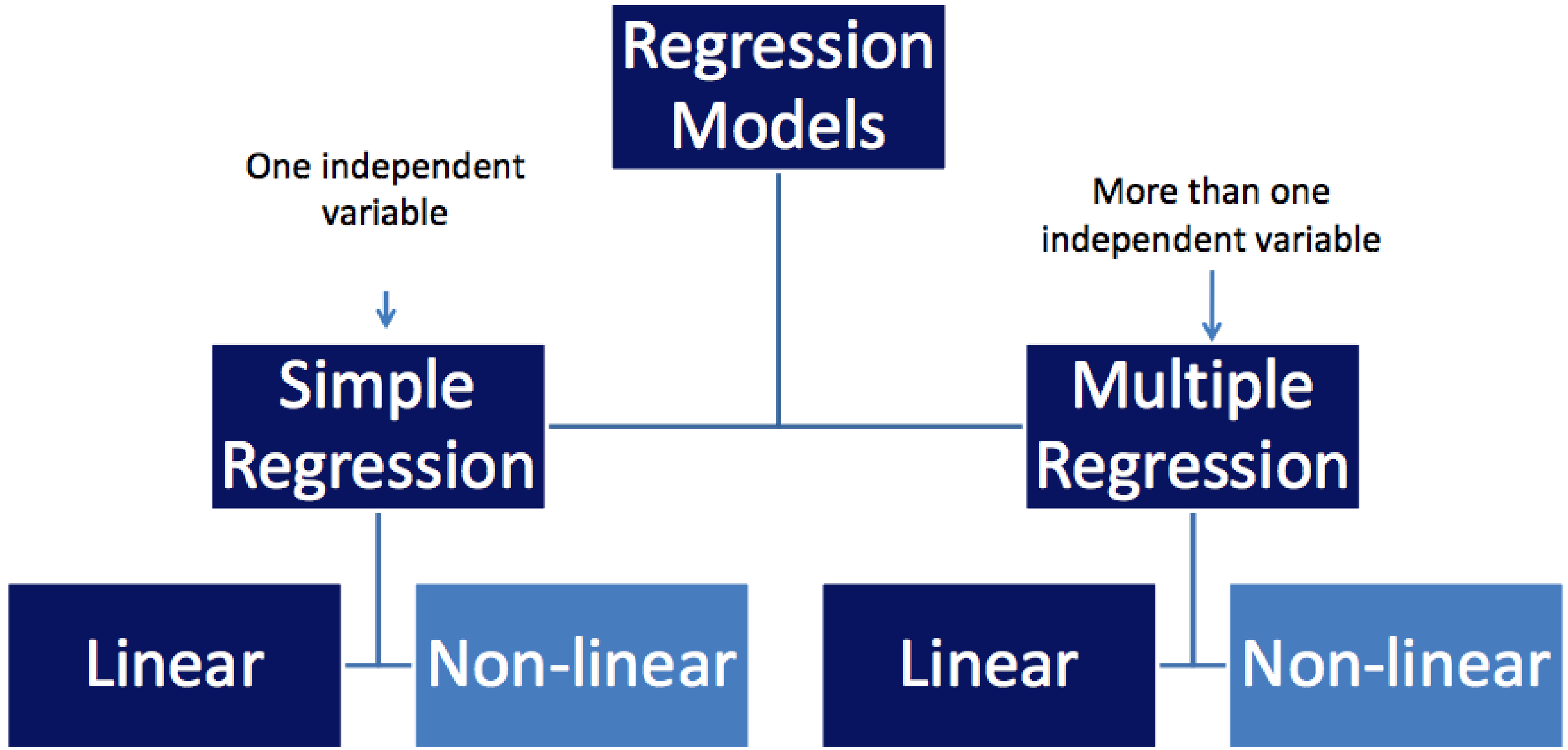
Types of Regression (1)



Types of Regression (2)

- Simple Linear Regression

$$\boxed{\mathbf{Y} = \beta_0 + \beta_1 \mathbf{X} + \epsilon}$$

- Multiple Linear Regression

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_k X_k + \varepsilon$$

- Important task in Regression is to estimate beta values

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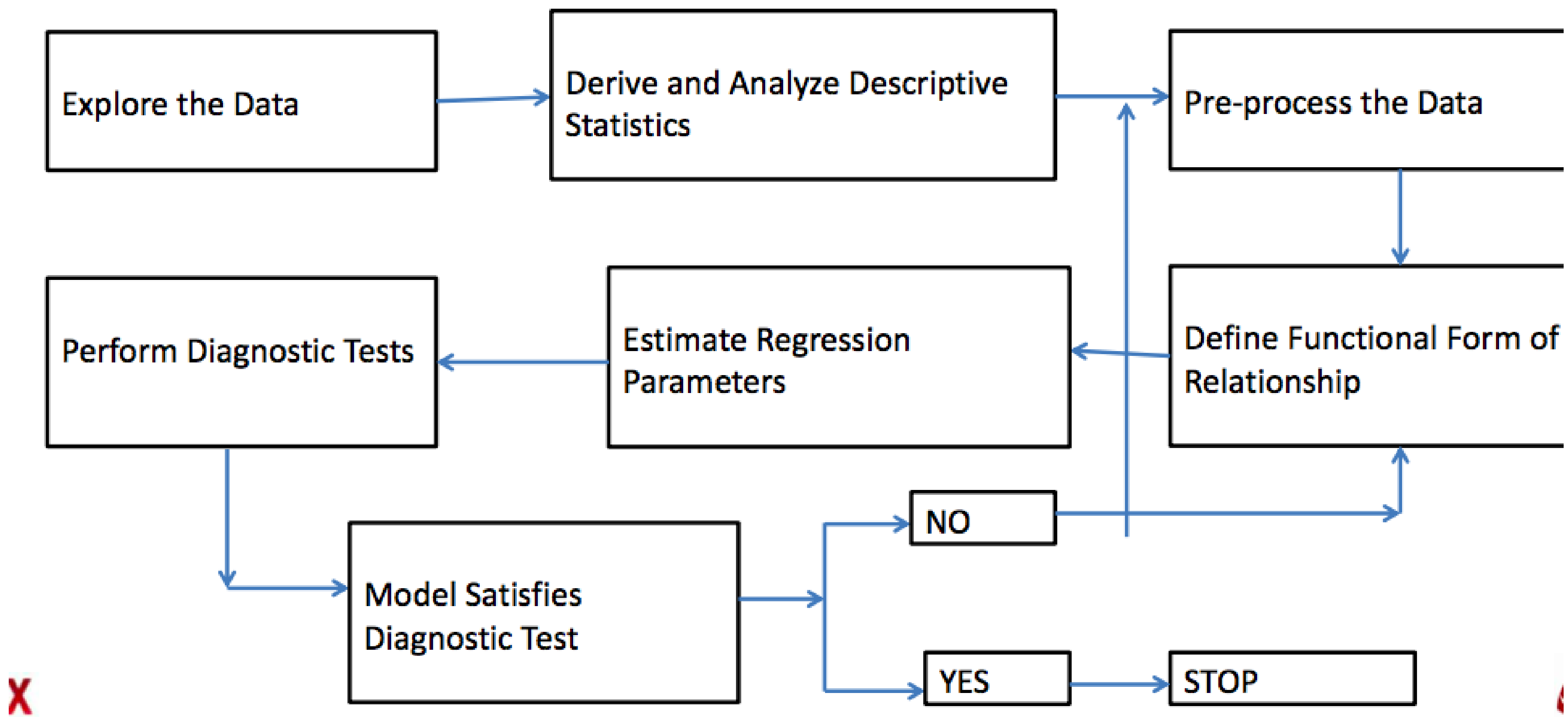
Regression Model Development



Model Building

- Identify explanatory variable
- Specify the nature of relationship between dependent variable and explanatory variables

Linear Regression Model

- Relationship between variables is a linear function

Population Y-Intercept

Population Slope

Random Error

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i$$

Dependent (Response)

Independent (Explanatory)

Linear Regression Model Assumption

Assumptions	Impacts on the Regression Model
Error follows normal distribution	This condition is necessary for reliability of statistical tests (*t and F*).
Homoscedasticity (constant variance)	It is necessary for statistical tests (*F and t*).
Multi-collinearity	Inflates standard error of estimate of regression coefficients (beta coefficients). May *reject* significant variables.
Auto-correlation	Underestimates standard error of estimates of regression coefficients. May *accept* insignificant variables.

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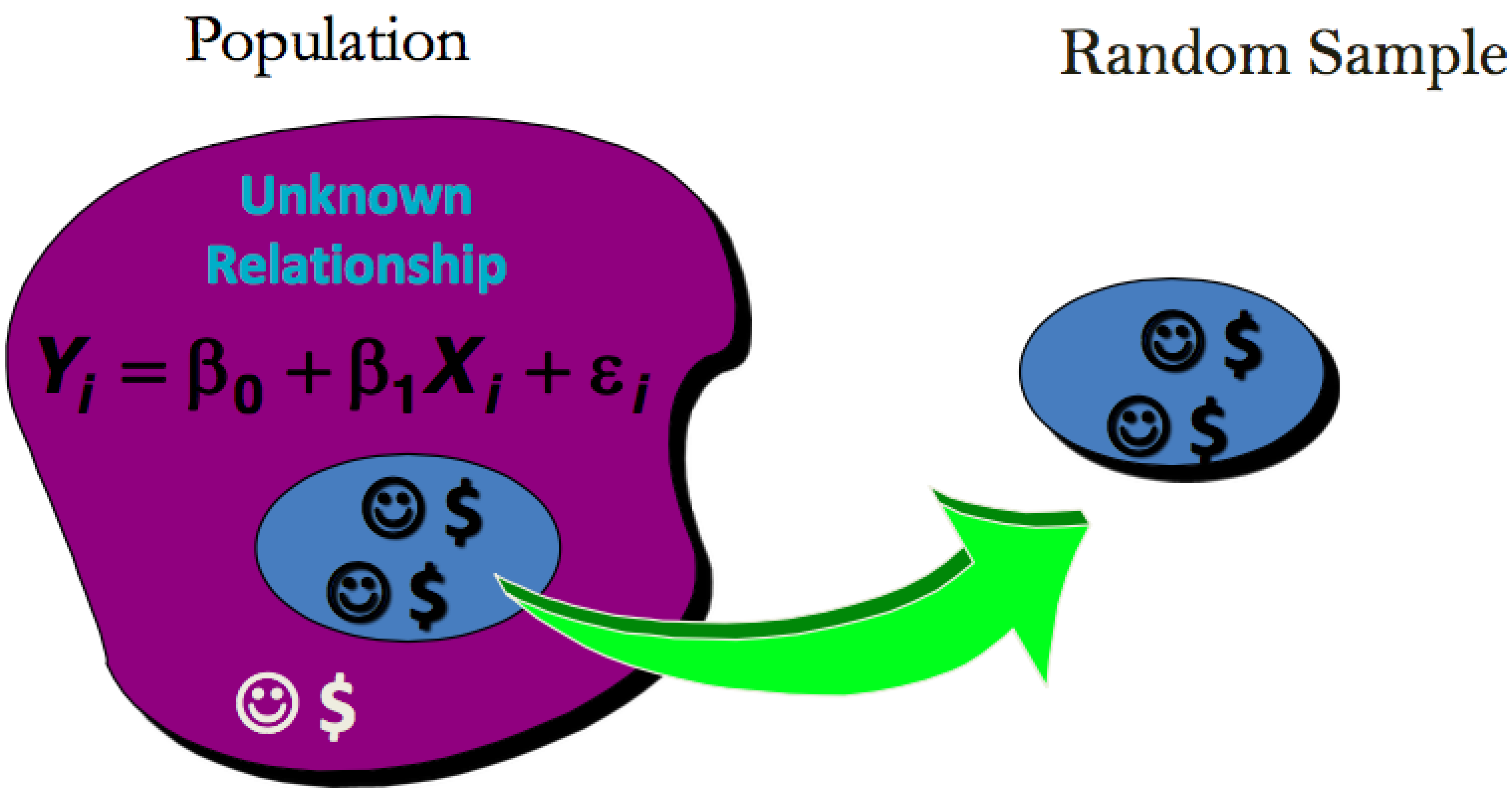
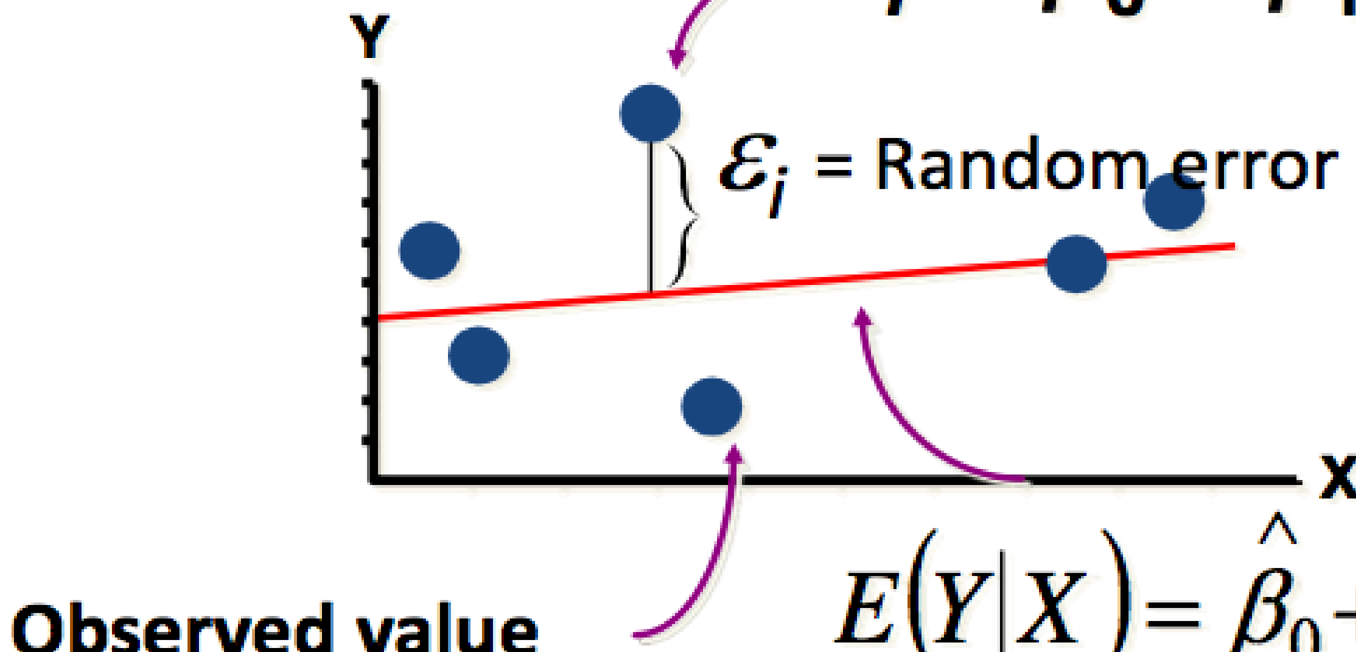
Regression: OLS (Ordinary Least Squares)estimation



Population Linear Regression Model

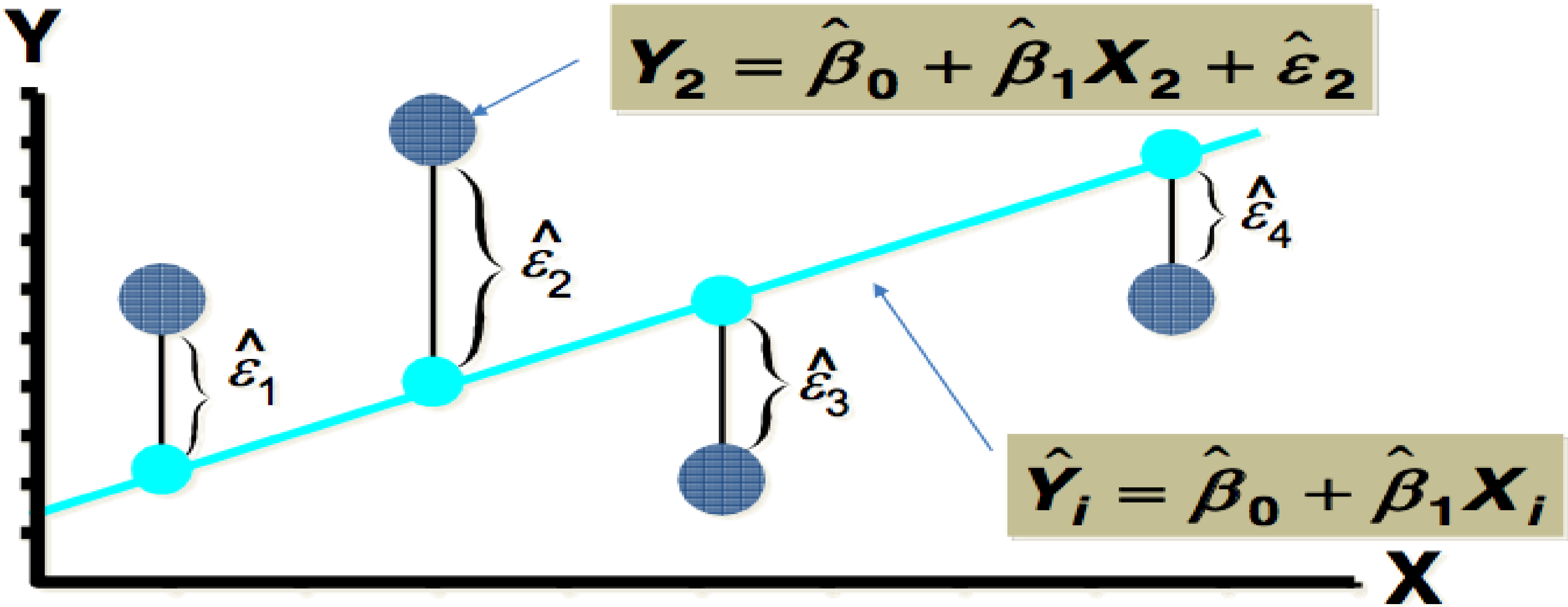
$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i$$



$$E(Y|X) = \hat{\beta}_0 + \hat{\beta}_1 X_i$$

Least Squares

$$\text{LS minimizes} \sum_{i=1}^{n} \hat{\varepsilon}_i^2 = \hat{\varepsilon}_1^2 + \hat{\varepsilon}_2^2 + \hat{\varepsilon}_3^2 + \ldots + \hat{\varepsilon}_n^2$$



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Estimation of Parameters in Regression

- Least squares function is given by:

$$SSE = \sum_{i=1}^{n} \varepsilon_i^2 = \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{k} \beta_j x_{ij} \right)^2$$

Coefficient Equations

- Prediction Equation:

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$$

- Sample Slope:

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

- Sample Y-intercept:

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

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Why Least Squares Estimate?

- OLS beta estimates provided the error terms are uncorrelated (no auto regression) and have equal variance (homoscedasticity)

$$E\left[\beta - \hat{\beta}\right] = 0$$

- it implies that E{Beta-Beta(hat) = 0, where Beta = population parameter, Beta(hat) = parameter that we estimate using sample

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Interpret Beta

- Interpretation depends on the functional form of the relationship between response and explanatory variables.
- Coefficients Interpretation:
  - The intercept, β_0 is the mean value of the dependent variable Y, when the independent variable X = 0
  - The slope, β_1 is the change in the value of dependent variable Y, for unit change in the independent variable X

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Simple Linear Regression

Variable x and y has ***Linear*** relationship	Assumption of the world
$y = \beta_0 + \beta_1 x + \varepsilon$, ***Minimize SSE***	Fitting a model
Is x really related to y? ***Is β_1 statistically significant?***	Validating the model
Predict y for a given x.	Using a model

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Model validation

- Use of co-efficient of determination to check the goodness of fit of regression
- Analysis of Variance (ANOVA) and F-test to check the overall fitness of the regression model
- T-test to validate relationship between dependent and independent variables
- Residual analysis to check the model adequacies

Coefficient of Determination

- Measure of how well the regression line fits the data
- Coefficient of determination (R^2 square) lies between 0 and 1
- Percentage of variation that can be explained by the regression model

Variation in Y (1)

$$\boxed{Y_i = \beta_0 + \beta_1 X + \varepsilon_i}$$

$\boxed{\text{Variation in } Y_i}$ = $\boxed{\text{Systemic Variation}}$ + $\boxed{\text{Random Variation}}$

or

$\boxed{\text{Variation in } Y_i}$ = $\boxed{\text{Explained Variation}}$ + $\boxed{\text{Unexplained Variation}}$

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Variation in Y (2)

$$\underset{\text{Total variation}}{Y_i - \bar{Y}} = \underset{\text{Explained variation}}{\hat{Y}_i - \bar{Y}} + \underset{\text{Unexplained variation}}{Y_i - \hat{Y}_i}$$

$$\underset{SST}{\sum_{i=1}^{n}(Y_i - \bar{Y})^2} = \underset{SSR}{\sum_{i=1}^{n}(\hat{Y}_i - \bar{Y})^2} + \underset{SSE}{\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2}$$

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- SST (Total Sum of Squares):
  - How much error is there in predicting Y without the knowledge of X
- SSE (Sum of Squares Error):
  - How much error is there in predicting Y with the knowledge of X
- SSR (Sum of Squares Regression):
  - Amount of variation explained by the model
- Mathematically, SST = SSR + SSE

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R-square

- What is explained by model over what is total variation

$$R^2 = \frac{SSR}{SST} = 1 - \frac{SSE}{SST}$$

Standard Error of Estimate

- Standard error is the estimate of the standard deviation of the regression errors
- Standard error of estimate, Se, measures the variability or scatter of the observed values around the regression line

Interpretation of SE Estimate

- Smaller SE of Estimate indicates better fit
- Larger SE of Estimate, the greater the scattering of points around the regression line
- Standard error of estimate for regression coefficient measures the amount of sampling error in a regression coefficient.

Standard Error of Estimate

$$S_e = \sqrt{\frac{\sum\left(Y_i - \hat{Y}_i\right)^2}{n-2}}$$

$$S(\beta_0) = \frac{S_e \times \sqrt{\sum x^2}}{\sqrt{nSS_x}}$$

$$S(\beta_1) = \frac{S_e}{\sqrt{SS_x}}$$

$$SS_x = \sum_i (X_i - \bar{X})^2$$

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T-test

- Beta co-efficient is a function of Yi, since Yi follows normal distribution, al β_1 follows normal distribution
- Yi follows normal distribution since we assume that the error term follows normal distribution
- $$\beta_1 = \frac{\sum_{i=1}^{n}(X_i - \bar{X})(Y_i - \bar{Y})}{\sum_{i}(X_i - \bar{X})^2}$$

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T-test

- Check whether the real slope is zero or not,
- In simple linear regression, F-test and t-test check the same hypothesis (H0: = 0) β_1
- Use t-test instead of z-test since standard error is estimated from the sample

T-test Hypothesis

- Two-tailed test

Null hypothesis:

$$H_0\text{: } \beta_1 = 0$$

Alternative hypothesis:

$$H_1\text{: } \beta_1 \neq 0$$

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Test Statistic

- Errors follow normal distribution, thus test statistic follows t-distribution with n-2 degrees of freedom

- Test statistic:

$$t_{(n-2)} = \frac{\text{Estimate value of parameter} - \text{hypotheis parameter}}{\text{Estimated standard error of estimate}} = \frac{\hat{\beta}_1 - \beta_1}{S_e(\hat{\beta}_1)}$$

$$t_{(n-2)} = \frac{\hat{\beta}_1 \sqrt{SS_x}}{S_e}, \text{ where } \beta = 0$$

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Hypothesis testing decision rule

- If significance alpha = 0.05, then we reject null hypothesis.

- (1-alpha)100% is the confidence that we have that the null hypothesis may not be true.

P-value

- if less than 0.05, then we reject null hypothesis, accept alternative hypothesis -> 95% confidence that null hypothesis may not be true

Multiple Linear Regression

- Several independent variables may influence the change in response variable we are trying to study
- Relationship between 1 dependent & 2 or more independent variables is a linear function

Population Y-intercept

Population slopes

Random error

$$Y_i = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \cdots + \beta_k X_{ki} + \varepsilon_i$$

Dependent (response) variable

Independent (explanatory) variables

Multiple Regression Modeling Steps

1. Start with a hypothesis or belief
2. Estimate unknown model parameters (Beta coefficients)
3. Probability distribution of random error term -> assumed to be a normal distribution
4. Check the assumptions of regression (normality, heteroscedasticity and multi-collinearity)
5. Evaluate Model
6. Use Model for Prediction and Estimation

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Prediction Model

- Prediction equation obtained from sample data

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X_{1i} + \hat{\beta}_2 X_{2i} + \cdots + \hat{\beta}_k X_{ki}$$

Model Diagnostics

- Test for overall model fitness (R-square and adjusted R-square)
- Test for overall model statistical significance (F test test)
- Test for portions of the model (Partial F-test)
- Test for statistical significance of individual explanatory variables (t test)
- Test for Normality and Homoscedasticity of residuals
- Test for Multi-collinearity and Auto Correlation

Co-efficient of determination in Multiple Regression

- Coefficient of determination increases as the number of explanatory variables increases.
- In SSR/SST, the numerator, SSR, increases as the number of explanatory variables increases, whereas the denominator, SST, remains constant.
- Increase in R^2 can deceptive, since more number of explanatory variables may over-fit the data.

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Adjusted R-square

- Inclusion of additional explanatory variable will increase R^2 value.
- By introducing an additional explanatory variable, we increase the numerator of the expression for R^2 while the denominator remains the same.
- To correct this defect, we adjust the R^2 by taking into account the degrees of freedom.

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Adjusted R-Square

$$R_A^2 = 1 - \frac{SSE/(n-k-1)}{SST/(n-1)}$$

$$R_A^2 = \text{Adjusted R - Square}$$

$$n = \text{number of observations}$$

$$k = \text{number of explanatory variables}$$

Test for overall significance of model – F Test

- Test for overall significance of multiple regression model.
- Checks if there is a statistically significant relationship between Y and any of the explanatory variables

$$H_0 : \beta_1 = \beta_2 = \ldots\ldots = \beta_k = 0$$

$$H_A : \text{Not all } \beta \text{ values are zero}$$

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F statistic

- Mean square regression over mean square error

- Relationship between F and R^2

$$F = \frac{R^2 / k}{(1 - R^2)/(n - k - 1)}$$

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Testing for Significance of Individual Parameters

- T-test: by rejecting null hypothesis, there is a statistically significant relationship between the response variable Y and explanatory variable Xi.

$$H_0 : \beta_i = 0$$
$$H_A : \beta_i \neq 0$$

$$t = \frac{\hat{\beta}_i}{S_e(\hat{\beta}_i)}$$

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Dummy Variable (1)

- Categorical (qualitative) variables in Regression as explanatory variable
- Qualitative variables (categorical variables) in regression are replaced with dummy variables (or indicator variables) in regression model
- A categorical variable with n levels are replaced with (n-1) dummy variables. The category for which no dummy variable assigned is known as “Base Category”

Dummy variable (2)

- When there are more than one qualitative variable, it is advisable to use (n-1) dummy variables for both qualitative variables along with the intercept.

- Use of n dummy variables along with intercept will result in multi- collinearity, known as dummy variable trap.

Dummy variables in Regression

- The intercept, β_0 is the mean value of the base category.
- The coefficients attached to dummy variables are called differential intercept coefficients -> measure deviation from the base category for that specific dummy variable

Interaction Variables

- A regression model of type:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1 X_2$$

Interaction variable

- Usually an interaction between a quantitative and qualitative variable

Interaction Variable Example

- Predict Gender Discrimination
- Consider a regression model with salary as response variable Y:

$$Y = \beta_0 + \beta_1 \text{ Gender} + \beta_2 \text{ Work Experience} + \boldsymbol{\beta_3} \textbf{ Gender x Work Experience}$$

Let Gender = 1 implies Female:

Then Y for Female is:

$$Y = \beta_0 + \beta_1 + (\boldsymbol{\beta_2 + \beta_3}) \text{ Work Experience}$$

Y for Male is:

$$Y = \beta_0 + \beta_2 \text{ x Work Experience}$$

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Multicollinearity

- High correlation between explanatory variables is called multi-collinearity.
- Multi-collinearity leads to unstable coefficients.
- Always exists; matter of degree.

Things to check of Multi-collinearity

- High R^2 but few significant t ratios.
- F-test rejects the null hypothesis, but none of the individual t-tests are rejected.
- Correlations between pairs of X variables are more than with Y variables.

Effects of Multi-collinearity

- The variances of regression coefficient estimators are inflated.
- Magnitudes of regression coefficient estimates may be different
- Adding and removing variables produce large changes in the coefficient estimates.
- Regression coefficient may have opposite sign.

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Identify Multi-collinearity Variance Inflation Factor (VIF)

- The variance inflation factor (VIF) is a relative measure of the increase in the variance in standard error of beta coefficient because of collinearity.
- A VIF greater than 10 indicates that collinearity is very high. A VIF value of more than 4 is not acceptable.

Variance inflation factor

Variance inflation factor associated with introducing a new variable X_j is given by:

$$\mathrm{VIF}(X_j) = \frac{1}{1 - R_j^2}$$

R_j^2 is the coefficient of determination for the regression of X_j as dependent variable

The standard error of the corresponding Beta is inflated by $\sqrt{VIF}$

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VIF method

- Take particular X as response variable and all other explanatory variables as explanatory variables.
- Run a regression between one of those explanatory variables with remaining explanatory variables.
- Standard error of estimate is inflated by a quantity which is square root of VIF

Regression Model Building

- In *Forward selection* method, the entry variable is the one with smallest p-value based on F-test
- In *Backward elimination* method, all variables are entered into the equation and then sequentially removed starting with the most insignificant variable. At each step, the largest probability of F is removed
- In *Step-wise Regression,* the entry variable is the one with smallest p-value based on F-test. At each step, the independent variable not in the equation that has the smallest probability of F is entered.

Residual Plot

- Residual plot is a plot of error (or standardized error) against one of the following variables:
  - The dependent variable Y.
  - The independent variable X.
  - The standardized independent or dependent variable.

Residual Analysis

- Analysis of residuals reveal whether the assumption of normally distributed errors hold.
- Residual plots are used to check if there is heteroscedasticity problem (non constant variance for the error term).
- Residual analysis could also indicate if there are any missing variables.
- Residual plot can also reveal if the actual relationship is non-linear.

Normality of error terms

- Probability plot is a graphical technique for checking whether or not a data set follows a given distribution.
- The data is plotted against a theoretical distribution in such a way that the points should form a straight line.
- In Regression, we create a probability plot of error against normal distribution.
- If residual do not follow normal distribution, t-test and F-test are not valid

Check for heteroscedasticity

- A graph of the residuals versus independent variable Y or dependent variable X will reveal whether the variance of the errors are constant.
- If the width of the scatter plot of the residuals either increases or decreases as X (or Y) increases, then the assumption of constant variance is not met.

Check for non-linearity

- If the residual plot exhibits a curve when plotted, then the actual relationship is non-linear.

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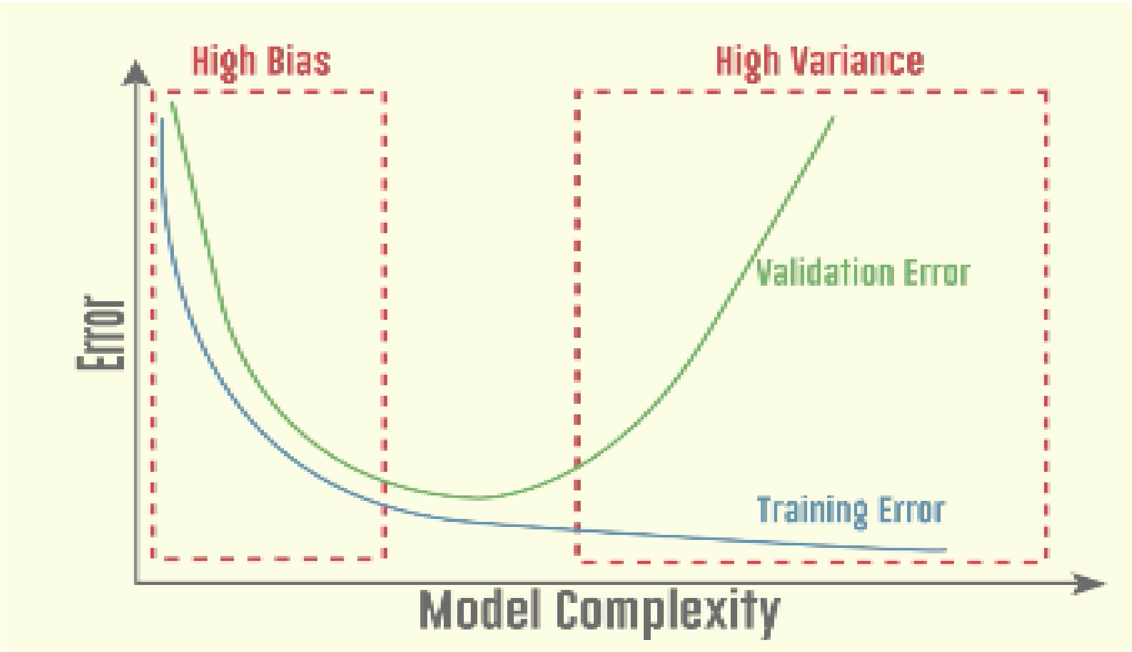
Prediction Error

- Irreducible Error: cannot be reduced

- Reducible Error: can be reduced
  - Bias Error
  - Variance Error



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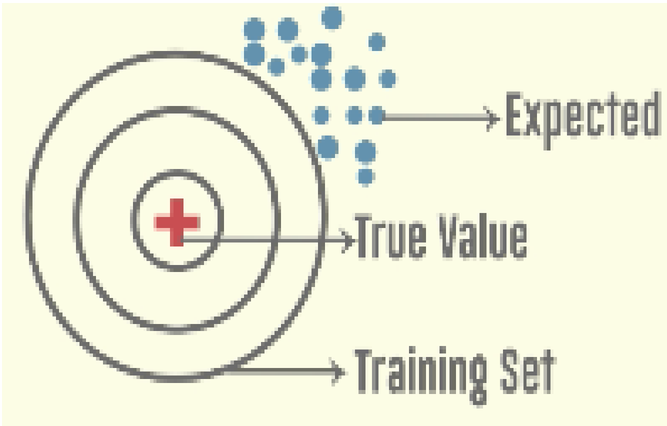
Error due to Bias

- Because of simplifying assumptions
- Less flexible
- Lower predictive performance
- Example – Linear Algorithms



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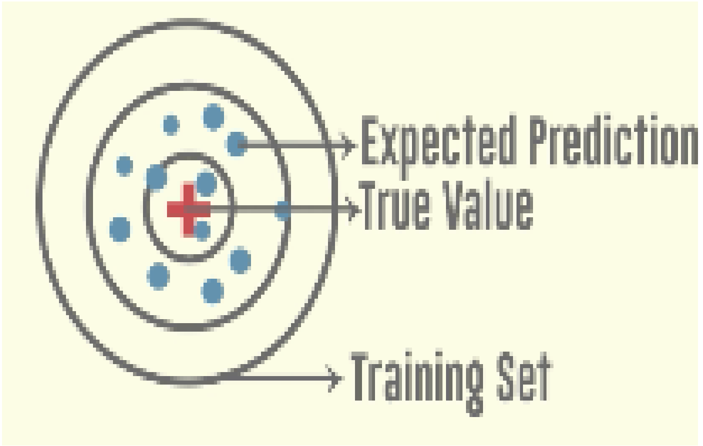
Error due to Variance

- Because of complex algorithms
- Lot of Flexibility
- Example: Decision Trees, Support Vector Machine (SVM)



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How can you know whether model has High Bias or High Variance ?

- High Training Set Error and High Validation Set Error ->
  - High Bias
- Low Training Set Error and High Validation Set Error ->
  - High Variance

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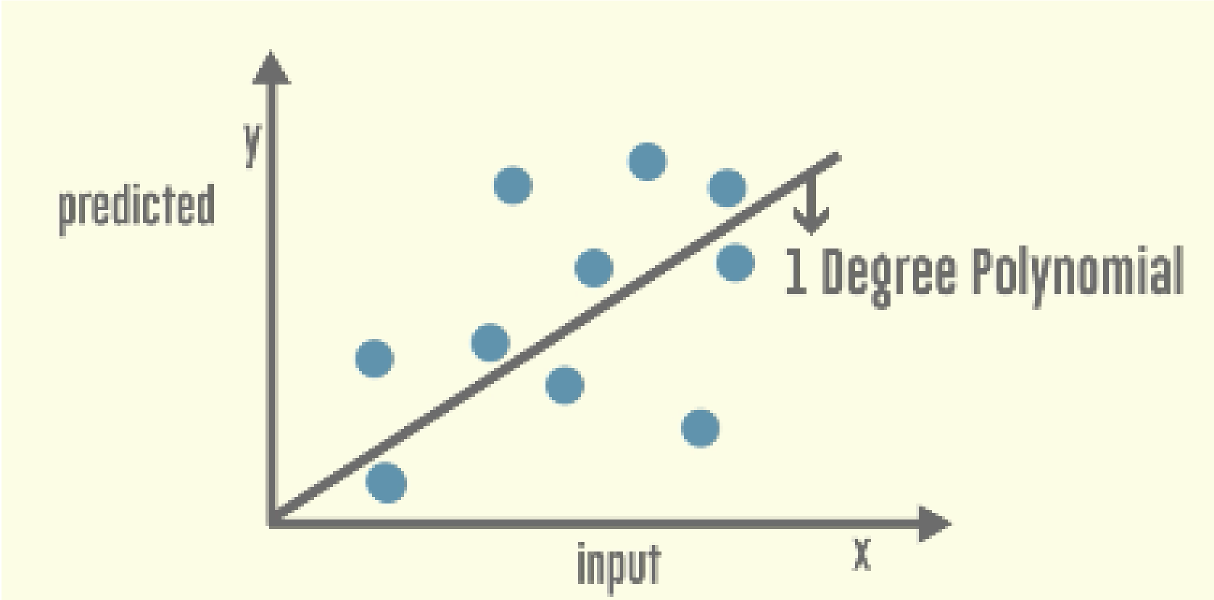
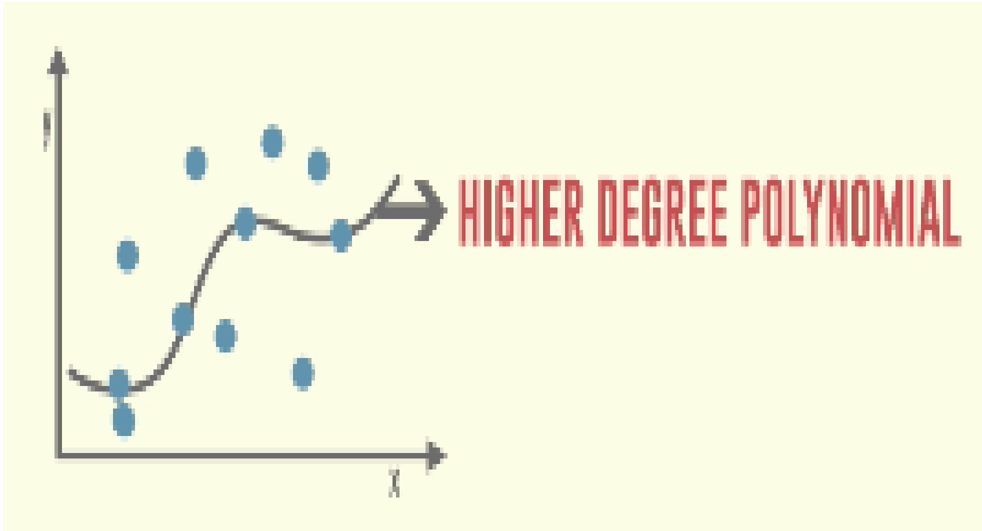
Underfitting



- High Bias and Low Variance
- Simple Model
- Does not capture the underlying trend of the data

Underfitting: How to fix a high bias and underfitting problem

- Train a more complex model
- Obtain more features



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Overfitting

- High Variance and Low Bias
- Too complex
- Firs the data too well
- Learns the noise in the training data which impacts the performance on test data

Overfitting: How to fix high variance and overfitting problem

- Decrease the number of features

- Increasing the number of training examples

Python Application

- Import

- % matplotlib inline -> this allows plots to appear directly in the notebook

Case 1: Advertising Data

- 'http://www-bcf.usc.edu/~gareth/ISL/Advertising.csv’

- #read data into a DataFrame
  - df = pd.read_csv(‘dataset directory/website link’ , index_col = 0)

  - index_col=0 we're explicitly stating to treat the first column as the index

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Exploratory

- Descriptive stats
- Scatter plot

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Build Model using statsmodels

- # this is the standard import if you're using "formula notation" (similar to R)
  - import statsmodels.formula.api as smf

- Fitted model
  - lm = smf.ols(formula= ‘Y variable ~ X variable', data=df).fit()

- Print coefficient: lm.params
- Make predictions: lm.predict
- Print confidence interval: lm.conf_int()
- Print p-values: lm.pvalues
- Print R-squared: lm.rsquared
- Print summary of fitted model: lm.summary()

Build model using scikit-learn

- from sklean.linear_model import LinearRegression

- lm = LinearRegression()

- Model fit: lm.fit

- Print intercept: lm.intercept_
- Print coefficients: lm.coef_
- Calculate r-squared: lm.score

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Case 2: Housing Boston

- Train Test Split

- X_train, X_test, Y_train, Y_test = sklearn.cross_validation.train_test_split(X, Y, test_size=, random_state =)

- Using statsmodel: import statsmodels.api as sm
- Model fit -> sm.OLS(Y, X).fit()

- Test for normality -> Jarque-Bera normality test
  - sm.stats.stattools.jarque_bera(residual data)

    Test to check if the observed skewness and kurtosis matching a normal distribution

- Normal probability plot
  - sm.qqplot(residual data)

    Graphical technique based on comparison between observed distribution and the theoretical distribution under normal assumption

    Null hypothesis (normal dist.) is rejected if the points are not aligned on a straight line

Detection of outliers and influential points

- Detection of outliers and influential points
  - Create object for the analysis of influential point: get_influence()

- Leverage: hat_matrix_diag

- Internally studentized residual: resid_studentized_internal

$$t_i = \frac{\hat{\varepsilon}_i}{\hat{\sigma}_\varepsilon \sqrt{1-h_i}}$$

residuals $\hat{\varepsilon}_i = y_i - \hat{y}_i$, the leverage h_i and the regression standard error $\hat{\sigma}_\varepsilon$

- Externally studentized residual: resid_studentized_external

$$t_i^* = t_i \sqrt{\frac{n-p-2}{n-p-1-t_i^2}}$$

- Automatic detection: Comparison to a threshold value
  - Define threshold values from which a point becomes suspect
  - Leverage: threshold value
    - Observation is suspicious if leverage > threshold value

$$s_h = 2 \times \frac{p+1}{n}$$

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- Externally studentized residual:
  - Probability distribution of externally studentized residual is a student distribution with (n-p-2) degrees of freedom.
  - Threshold value at 5% level

$$s_t = t_{1-0.05/2}(n-p-2)$$

Where $t_{1\text{-}0.05/2}$ is the quantile of the t distribution for a probability 0.975.

An observation is suspicious if

$$|t_i^*| > s_t$$

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- Other criterias:
  - DFFITS

$$|DFFITS_i| > 2\sqrt{\frac{p+1}{n}} \text{ for DFFITS ;}$$

  - Cook’s distance

$$D_i > \frac{4}{n-p-1} \text{ for Cook's distance.}$$

Multicollinearity problem

- Disturbs statistical inference, inflates the estimated SE of coefficients.
- Build correlation matrix -> use corrcoef() from the scipy library
- Variance inflation factor (VIF) ->evaluate relationship of one predictor with all other explanatory variables