Unit III: Regression Analysis

Linear multiple regression, Estimation and testing of coefficients, R^2 and adjusted R^2 coefficients Logistic regression, Estimation and Testing of coefficients, K – Nearest Neighbor classifier, random forest, classifycation errors, Ridge Regression and Support Vector Machine.

Linear Regression:

Straight-line regression analysis involves a response variable, y, and a single predictor variable, x. It is the simplest form of regression, and models y as a linear function of x.

That is,

$$y = w_0 + w_1 x.$$

where the variance of y is assumed to be constant, and w_0 and w_1 are regression coefficients specifying the Y-intercept and slope of the line, respectively.

These coefficients can be solved for by the method of least squares, which estimates the best-fitting straight line which minimizes the error between the actual data and the estimate of the line. Let D be a training set consisting of values of predictor variable, x, for some population and their associated values for response variable, y. The training set contains |D| data points of the form (x1, y1), (x2, y2),..., (x|D| , y|D|).12 The regression coefficients can be estimated using this method with the following equations:

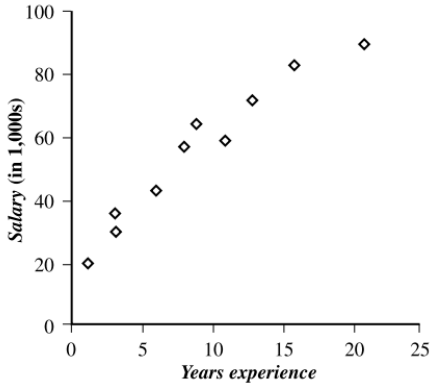
$$w_1 = \frac{\sum_{i=1}^{|D|}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{|D|}(x_i - \bar{x})^2}$$

$$w_0 = \bar{y} - w_1 \bar{x}$$

where $\bar{x}$ is the mean value of $x_1, x_2, \ldots, x_{|D|}$, and $\bar{y}$ is the mean value of $y_1, y_2, \ldots, y_{|D|}$.

Example:

x years experience	y salary (in $1000s)
3	30
8	57
9	64
13	72
3	36
6	43
11	59
21	90
1	20
16	83



We model the relationship that salary may be related to the number of years of work experience with the equation $y = w_0 + w_1 x$.

Given the above data, we compute $\bar{x} = 9.1$ and $\bar{y} = 55.4$. Substituting these values into Equations (6.50) and (6.51), we get

$$w_1 = \frac{(3-9.1)(30-55.4)+(8-9.1)(57-55.4)+\cdots+(16-9.1)(83-55.4)}{(3-9.1)^2+(8-9.1)^2+\cdots+(16-9.1)^2} = 3.5$$

$$w_0 = 55.4-(3.5)(9.1) = 23.6$$

Thus, the equation of the least squares line is estimated by $y = 23.6 + 3.5x$.

we can predict that the salary of a college graduate with, say, 10 years of experience is
=23.6+3.5*10
=58,600.

Multiple linear regression: https://www.statology.org/multiple-linear-regression/

https://www.statology.org/multiple-linear-regression-by-hand/

http://faculty.cas.usf.edu/mbrannick/regression/Reg2IV.html

It is an extension of straight-line regression which involve more than one predictor variable. It allows response variable y to be modeled as a linear function of, say, n predictor variables or attributes, A1, A2,..., An, describing a tuple, X. (That is, X = (x1, x2,..., xn).)

Our training data set, D, contains data of the form (X1, y1), (X2, y2), ... , (X|D| , y|D|), where the Xi are the n-dimensional training tuples with associated class labels, yi .

An example of a multiple linear regression model based on two predictor attributes or variables, A1 and A2, is

$$y = w_0 + w_1 x_1 + w_2 x_2,$$

where x1 and x2 are the values of attributes A1 and A2, respectively, in X. The method of least squares is used to solve for w0, w1, and w2.

For two variable case,

$$w_{1.} = \frac{(\sum x_2^2)(\sum x_1 y) - (\sum x_1 x_2)(\sum x_2 y)}{(\sum x_1^2)(\sum x_2^2) - (\sum x_1 x_2)^2}$$

$$w_{2.} = \frac{(\sum x_1^2)(\sum x_2 y) - (\sum x_1 x_2)(\sum x_1 y)}{(\sum x_1^2)(\sum x_2^2) - (\sum x_1 x_2)^2}$$ and

$$a = \bar{Y} - b_1 \bar{X}_1 - b_2 \bar{X}_2$$ where a= w_0 , B_1=w_1 and b_2= w_2

Example: following dataset with one response variable *y* and two predictor variables X_1 and X_2:

y	X_1	X_2
140	60	22
155	62	25
159	67	24
179	70	20
192	71	15
200	72	14
212	75	14
215	78	11

Step 1: Calculate X_1^2, X_2^2, X_1y, X_2y and X_1X_2.

	y	X_1	X_2
	140	60	22
	155	62	25
	159	67	24
	179	70	20
	192	71	15
	200	72	14
	212	75	14
	215	78	11
Mean	181.5	69.375	18.125
Sum	1452	555	145

X_1^2	X_2^2	X_1y	X_2y	X_1X_2
3600	484	8400	3080	1320
3844	625	9610	3875	1550
4489	576	10653	3816	1608
4900	400	12530	3580	1400
5041	225	13632	2880	1065
5184	196	14400	2800	1008
5625	196	15900	2968	1050
6084	121	16770	2365	858
Sum 38767	2823	101895	25364	9859

Step 2: Calculate Regression Sums.

Next, make the following regression sum calculations:

- $\Sigma x_1^2 = \Sigma X_1^2 - (\Sigma X_1)^2 / n = 38{,}767 - (555)^2 / 8 =$ **263.875**
- $\Sigma x_2^2 = \Sigma X_2^2 - (\Sigma X_2)^2 / n = 2{,}823 - (145)^2 / 8 =$ **194.875**
- $\Sigma x_1 y = \Sigma X_1 y - (\Sigma X_1 \Sigma y) / n = 101{,}895 - (555*1{,}452) / 8 =$ **1,162.5**
- $\Sigma x_2 y = \Sigma X_2 y - (\Sigma X_2 \Sigma y) / n = 25{,}364 - (145*1{,}452) / 8 =$ **-953.5**
- $\Sigma x_1 x_2 = \Sigma X_1 X_2 - (\Sigma X_1 \Sigma X_2) / n = 9{,}859 - (555*145) / 8 =$ **-200.375**

	y	X_1	X_2
	140	60	22
	155	62	25
	159	67	24
	179	70	20
	192	71	15
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38767	2823	101895	25364	9859

Reg Sums	263.875	194.875	1162.5	-953.5	-200.375

The formula to calculate w_1 is: $[(\Sigma x_2^2)(\Sigma x_1 y) - (\Sigma x_1 x_2)(\Sigma x_2 y)] / [(\Sigma x_1^2)(\Sigma x_2^2) - (\Sigma x_1 x_2)^2]$

Thus,

$\mathbf{w_1} = [(194.875)(1162.5) - (-200.375)(-953.5)] / [(263.875)(194.875) - (-200.375)^2] =$ **3.148**

The formula to calculate w_2 is: $[(\Sigma x_1^2)(\Sigma x_2 y) - (\Sigma x_1 x_2)(\Sigma x_1 y)] / [(\Sigma x_1^2)(\Sigma x_2^2) - (\Sigma x_1 x_2)^2]$

Thus,

$\mathbf{w_2} = [(263.875)(-953.5) - (-200.375)(1152.5)] / [(263.875)(194.875) - (-200.375)^2] =$ **-1.656**

The formula to calculate w_0 is: $y - w_1X_1 - w_2X_2$

Thus, $\mathbf{w_0} = 181.5 - 3.148(69.375) - (-1.656)(18.125) =$ **-6.867**

Step 5: Place b_0, b_1, and b_2 in the estimated linear regression equation.

The estimated linear regression equation is:

$\hat{y} = w_0 + w_1*x_1 + w_2*x_2$

In our example, it is $\hat{\mathbf{y}} = \mathbf{-6.867 + 3.148x_1 - 1.656x_2}$

How to Interpret a Multiple Linear Regression Equation

Here is how to interpret this estimated linear regression equation:

$\hat{y} = -6.867 + 3.148x_1 - 1.656x_2$

Example :

x1 Product 1 Sales	x2 Product 2 Sales	Y Weekly Sales
1	4	1
2	5	6
3	8	8
4	2	12

Here, the matrices for Y and X are given as follows:

$$X = \begin{pmatrix} 1 & 1 & 4 \\ 1 & 2 & 5 \\ 1 & 3 & 8 \\ 1 & 4 & 2 \end{pmatrix} \text{ and } Y = \begin{pmatrix} 1 \\ 6 \\ 8 \\ 12 \end{pmatrix}$$

The coefficient of the multiple regression equation is given as

$$a = \begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix}.$$

The regression coefficient for multiple regression is calculated the same way as linear regression:

$$\hat{a} = ((X^T X)^{-1} X^T) Y$$

$$X^T X = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 3 & 4 \\ 4 & 5 & 8 & 2 \end{pmatrix} \begin{pmatrix} 1 & 1 & 4 \\ 1 & 2 & 5 \\ 1 & 3 & 8 \\ 1 & 4 & 2 \end{pmatrix} = \begin{pmatrix} 4 & 10 & 19 \\ 10 & 30 & 46 \\ 19 & 46 & 109 \end{pmatrix}$$

$$(X^T X)^{-1} = \begin{pmatrix} 4 & 10 & 19 \\ 10 & 30 & 46 \\ 19 & 46 & 109 \end{pmatrix}^{-1} = \begin{pmatrix} 3.15 & -0.59 & -0.30 \\ -0.59 & 0.20 & 0.016 \\ -0.30 & 0.016 & 0.054 \end{pmatrix}$$

$$X^T X)^{-1} X^T = \begin{pmatrix} 3.15 & -0.59 & -0.30 \\ -0.59 & 0.20 & 0.016 \\ -0.30 & 0.016 & 0.054 \end{pmatrix} \times \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 3 & 4 \\ 4 & 5 & 8 & 2 \end{pmatrix} = \begin{pmatrix} 0.05 & 0.47 & -1.02 & 0.19 \\ -0.32 & -0.098 & 0.155 & 0.26 \\ -0.065 & 0.005 & 0.185 & -0.125 \end{pmatrix}$$

$$\hat{a} = ((X^T X)^{-1} X^T) Y = \begin{pmatrix} 0.05 & 0.47 & -1.02 & 0.19 \\ -0.32 & -0.098 & 0.155 & 0.26 \\ -0.065 & 0.005 & 0.185 & -0.125 \end{pmatrix} \times \begin{pmatrix} 1 \\ 6 \\ 8 \\ 12 \end{pmatrix} = \begin{pmatrix} -1.69 \\ 3.48 \\ -0.05 \end{pmatrix}$$

$$a_0 = -1.69$$
$$a_1 = 3.48$$
$$a_2 = -0.05$$

- $y = a_0 + a_1 x_1 + a_2 x_2$
- Hence, the constructed model is:
- $y = -1.69 + 3.48 x_1 - 0.05 x_2$

R^2- R-squared:

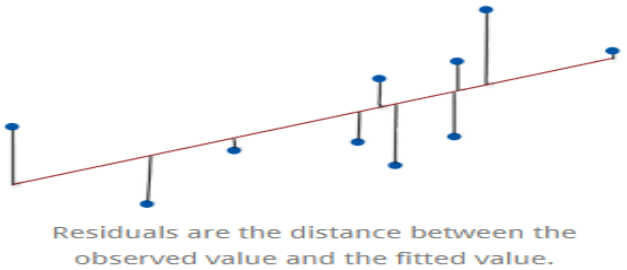
https://statisticsbyjim.com/regression/interpret-r-squared-regression/

R-squared is a goodness-of-fit measure for linear regression models. This statistic indicates the percentage of the variance in the dependent variable that the independent variables explain collectively. R-squared measures the strength of the relationship between your model and the dependent variable on a convenient 0 – 100% scale.

After fitting a linear regression model, it is need to determine how well the model fits the data. There are several key goodness-of-fit statistics for regression analysis, **R-squared** is one of them.

Linear regression identifies the equation that produces the smallest difference between all the observed values and their fitted values. Linear regression finds the smallest sum of squared residuals that is possible for the dataset. regression model fits the data well if the differences between the observations and the predicted values are small and unbiased. Unbiased means that the fitted values are not systematically too high or too low anywhere in the observation space. R-squared evaluates the scatter of the data points around the fitted regression line. It is also called the coefficient of determination, or the coefficient of multiple determination for multiple regression. For the same data set, higher R-squared values represent smaller differences between the observed data and the fitted values. R-squared is the percentage of the dependent variable variation that a linear model explains.

$$R^2 = \frac{\text{Variance explained by the model}}{\text{Total variance}}$$



Residuals are the distance between the observed value and the fitted value.

R-squared is always between 0 and 100%. Usually, the larger the R^2, the better the regression model fits the observations. Linear regression uses the sum of squares for your model to find R-squared. Consider the following formula for the given provlem.

$$R^2 = 1 - \frac{\text{sum squared regression (SSR)}}{\text{total sum of squares (SST)}}$$
$$= 1 - \frac{\sum(y_i - \hat{y}_i)^2}{\sum(y_i - \bar{y})^2}.$$

Example:

y	X_1	X_2
140	60	22
155	62	25
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179	70	20
192	71	15
200	72	14
212	75	14
215	78	11

$\hat{y} = -6.867 + 3.148x_1 - 1.656x_2$

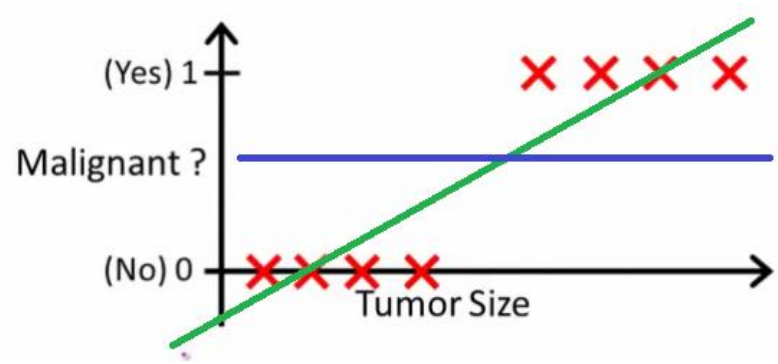
Adjusted r-squared: It can be defined as the proportion of variance explained by the model while taking into account both the number of predictor variables and the number of samples used in the regression analysis. The adjusted r-squared increases only when adding an additional variable to the model improves its predictive capability more than expected by chance alone. Adjusted R-squared is always less than or equal to R-squared.
The idea behind adjusted R-squared is to account for the addition of variables that do not significantly improve the model. When more and more predictor variables are added to the model, the R-squared will generally increase (even if those variables are only weakly associated with the response). This can give a misleading impression of improving model fit. Adjusted R-squared controls for this by penalizing the addition of uninformative predictors.

Mathematically, adjusted r-squared can be calculated as the function of R-squared in the following manner:

$$Adjusted\ R^2 = 1 - \frac{(1 - R^2)(N - 1)}{N - p - 1}$$ where,

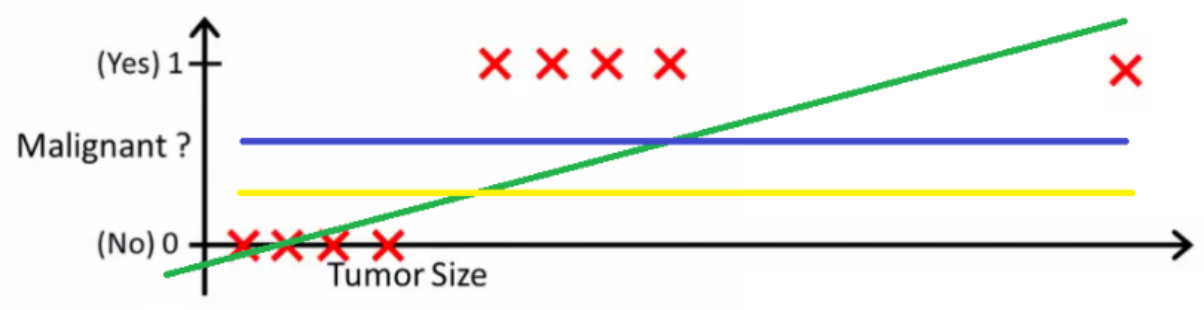
P: is the number of predictor variables.
N: is the number of records.
R^2: r-squared value of the dataset.

Logistic regression :
if we use linear regression to find the best fit line which aims at minimizing the distance between the predicted value and actual value, the line will be like this:



Here the threshold value is 0.5, which means if the value of h(x) is greater than 0.5 then we predict malignant tumour (1) and if it is less than 0.5 then we predict benign tumour (0).

If we add some outliers in our dataset, now this best fit line will shift to that point. Hence the line will be somewhat like this:

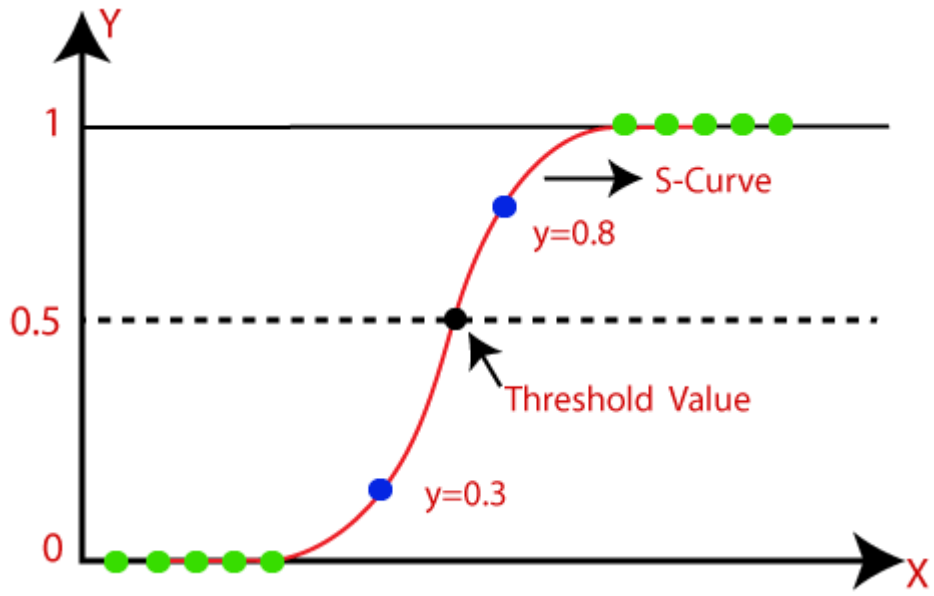


The blue line represents the old threshold and the yellow line represents the new threshold which is maybe 0.2 here. To keep our predictions right we had to lower our threshold value.
Hence, we can say that linear regression is prone to outliers.
Another problem with linear regression is that the predicted values may be out of range. We know that probability can be between 0 and 1, but if we use linear regression this probability may exceed 1 or go below 0.
To overcome these problems we use Logistic Regression, which converts this straight best fit line in linear regression to an S-curve using the sigmoid function, which will always give values between 0 and 1.

Logistic regression is the appropriate regression analysis to conduct when the dependent variable is dichotomous (binary). Like all regression analyses, logistic regression is a predictive analysis. Logistic regression is used to describe data and to explain the relationship between one dependent binary variable and one or more nominal, ordinal, interval or ratio-level independent variables.

- Logistic regression is one of the most popular Machine Learning algorithms, which comes under the Supervised Learning technique. It is used for predicting the categorical dependent variable using a given set of independent variables.
- Logistic regression predicts the output of a categorical dependent variable. Therefore the outcome must be a categorical or discrete value. It can be either Yes or No, 0 or 1, true or False, etc. but instead of giving the exact value as 0 and 1, **it gives the probabilistic values which lie between 0 and 1**.
- Logistic Regression is much similar to the Linear Regression except that how they are used. Linear Regression is used for solving Regression problems, whereas **Logistic regression is used for solving the classification problems**.
- In Logistic regression, instead of fitting a regression line, we fit an "S" shaped logistic function, which predicts two maximum values (0 or 1).

The below image is showing the logistic function:



- The sigmoid function is a mathematical function used to map the predicted values to probabilities.
- It maps any real value into another value within a range of 0 and 1.
- In logistic regression, we use the concept of the threshold value, which defines the probability of either 0 or 1. Such as values above the threshold value tends to 1, and a value below the threshold values tends to 0.

$$P = \frac{1}{1 + e^{-(\beta_0 + \beta_1 x)}}$$

The three main types of logistic regression are:
1. **Binary Logistic Regression:** Used for binary classification, where the dependent variable has only two possible outcomes.
2. **Multinomial Logistic Regression:** Applied when the dependent variable has more than two categories, but they are not ordered.
3. **Ordinal Logistic Regression:** Used when the dependent variable is ordinal, meaning it has ordered categories, but the intervals between them are not necessarily equal.