Practical Machine Learning with R

Lecture 5 : Regression and Regression Trees

Objectives:

- ❖ Comprehend Regression in context of predictive scope of machine learning algorithms.
- ❖ Perceive Ordinary Linear Regression and the estimation of regression coefficients.
- ❖ Adaptation of classification Trees to depict regression trees for the purpose of quantification of the prediction.

Regression Methods for Forecasting:

- These methods help quantify the numeric relationship between the attributes of interest.
- Numerical predictions are inherently more insightful and substantive
- Regression entails elucidating relationships between one or multiple independent variable and a dependent variable. The relationship therefore can depicted by a technique called Simple Regression or Multiple Regression.
- The inherent premise/assumption for Simple Regression is that the relationship between the Independent and Dependent variable is linear ie follows a straight line pattern.
- Simple Linear Regression is a scientific paradigm introduced by the genetic scientist Sir Francis Galton. He empirically proved that son's height regresses to the mean of the father's and mother's height.
- Regression technique, although a simple technique can model complex relationships that facilitate ascertaining the strength, direction as well as numerical quantification of the response variable including futuristically achieving extrapolation.
- This methodology can be used for a spectrum of domain areas including but not limited to insurance claims, crime rates, election results, profit projection etc.
- Regression encompasses a family of algorithms addressing different combination of Categorical and Quantitative data.
- In context of Simple or Multiple Regression the dependent (response variable) variables are quantitative and the independent variable can be categorical or quantitative.
- If the dependent variable is a binary categorical variable and independent variable is nominal, ordinal, interval or ratio then for classification purposes the technique titled Logistic Regression is used whereas multinomial Logistic regression is used if the classification entails a categorical dependent response variable and multiple independent variable is is nominal, ordinal, interval or ratio.
- Poisson Regression is used for modelling integer count data enumerated as 0,1,2,3…. Unlike Logistic Regression, Poisson Regression is not constrained to specific values.

Simple Linear Regression For representing the regression equation between a dependent and independent variable the following equation is used:

Population:

$y = \alpha + \beta x + \varepsilon$ Epsilion is the error term

Alpha α is the y intercept and Beta β is slope of the line

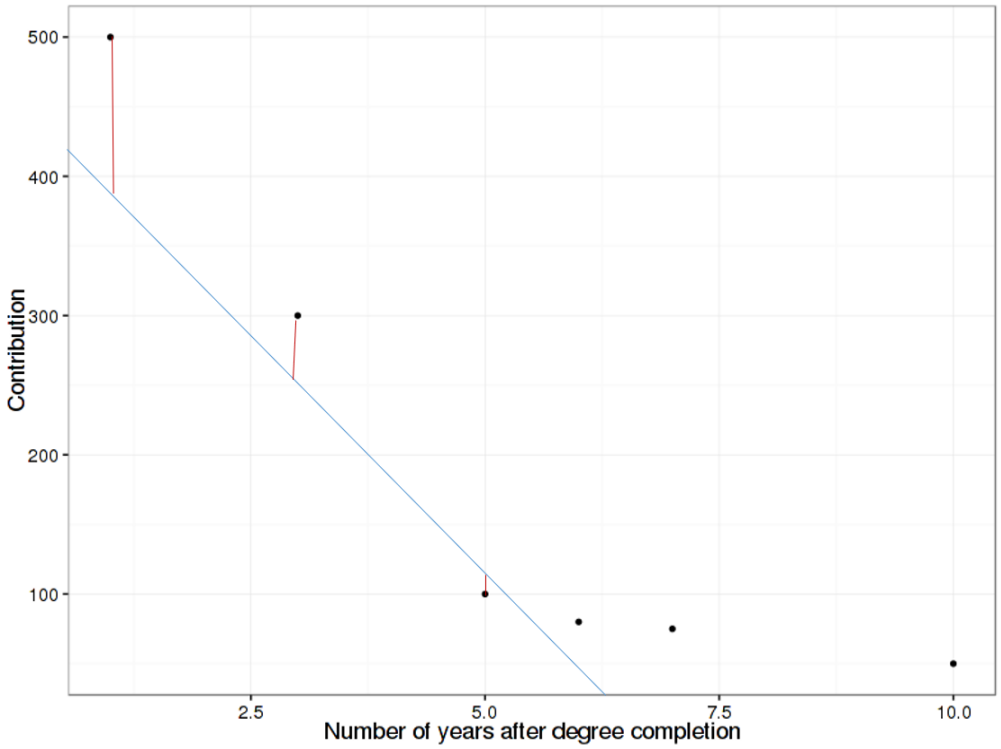
Sample:

$\hat{y} = a + bx$ where this is the Line of Best Fit which estimates the real response variable y.

Where a and b are the estimates of α and β

Example: Information regarding the amount of contribution and the years in college are given as follows:

Years out of college	1	5	3	10	7	6
Amount of contribution (1000 Dollars)	500	100	300	50	75	80



Ordinary Least Squares Estimation is a process of ascertaining the line of best fit that minimizes cumulative residual error.

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

- The line of best fit is found by computing a and b by minimizing the error.

$$\sum (y_i - \hat{y}_i)^2 = \sum {e_i}^2$$

This is minimized by using calculus and the value of a and b are derived as follows:

$$a = \bar{y} - b\bar{x} \quad \text{and} \quad b = \frac{\sum(x_i - \bar{x})(y_i - \bar{y})}{\sum(x_i - \bar{x})^2}$$

The value of b can be transformed by the following formula of variance and covariance:

$$Var(x) = \frac{\sum(x_i - \bar{x})^2}{n}$$

And

$$Cov(x, y) = \frac{\sum(x_i - \bar{x})(y_i - \bar{y})}{n}$$

$$b = \frac{Cov(x, y)}{Var(x)}$$

a and b estimates α and β

Correlation The correlation between two variables determines the strength and direction of a relationship between two variables. This quantified by a measure called Pearson's correlation coefficient named after a scientist called Karl Pearson. Pearson correlation ranges from – to 1 where 0 signifies no correlation.

Conventionally 0--.49 Weak .5---.69 Moderate .7---1.0 Strong

$$\rho_{x,y} = Corr(x, y) = \frac{Cov(x, y)}{\sqrt{Var(x)}\sqrt{Var(y)}} = \frac{Cov(x, y)}{\sigma_x \sigma_y}$$

Multiple Linear Regression If there are several independent /predictor variables for an outcome /response variable then Multiple Linear Regression is very useful.

This a good technique that can model any numeric data though the model formulation must be specified by the user.

This technique works intrinsically for numeric data and requires additional processing for categorical data.

The algorithm makes strong assumptions of the underlying data, does not handle missing data.

$$Y = \alpha + \beta X + \varepsilon$$

$$Y = \alpha + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 \ldots\ldots\ldots\ldots \beta_i X_i + \varepsilon$$

This can also be represented as

$$Y = \beta_0 X_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 \ldots\ldots\ldots\ldots \beta_i X_i + \varepsilon$$

Where $\alpha = \beta_0$

Therefore

$$Y = \beta X + \varepsilon$$

β_0	β_1	β_2	β_3

Y

Xo	X_1	X_2	X_3

ε

Each row is an example , X_i s are features Y is the outcome and betas are the regression coefficients.

This can be depicted in vector notation as:

$$\boldsymbol{Y = \beta X + \varepsilon}$$

The model for the multiple regression equation is

$$\boldsymbol{\widehat{Y} = \widehat{\beta} X}$$

Where

$$\boldsymbol{\widehat{\beta} = (X^T X)^{-1}(X^T Y)}$$

Regression Trees and Model Trees

- If the classification tree is adjusted the tree can be used to make numeric predictions.
- There two types of trees used for numeric predictions: Regression trees and Model trees.
- Paradoxically Regression trees (CART package) use the average value of the examples that reach the leaf rather than linear regression techniques to make predictions.
- Model trees are more powerful and these use Regression techniques. Specifically at each leaf node a multiple Regression model is built from the examples reaching the nodes. These might be more accurate but sometimes could possible be very cumbersome if they are too many leaves.
- Regression trees and model trees are less known as compared to Linear regression.
- Trees require significantly large data for training the algorithm.
- The tree automatically chooses the features for the final prediction to create a multiple regression framework but this comes with the tradeoff of not being able to ascertain effect of individual features.
- Even though the regression tree might fit the data to a greater extent the trees are more challenging to interpret as compared to a conventional regression model.
- Model Trees using the regression model are better for scenarios where there are multiple features and these showcase non linear relationships between features and outcomes . Trees also do not need to satisfy distribution constraints like normality for the outcome data which are the inherent assumptions for Regression models.
- The data is partitioned using the Divide and Conquer strategy.
- Unlike Trees which uses Entropy to access the homogeneity trees use a measure called Standard Deviation reduction.

$$\boldsymbol{SDR = sd(T) - \sum_i \frac{|T_i|}{|T|} * sd(T_i)}$$

sd(T) is the Standard deviation in the set T and T_i are the standard deviations resulting from split i. |T| is the number of observations in set T. This formula measures the reduction of SD pre-split versus post-split.

For example, consider the following case in which a tree is deciding whether or not to perform a split on binary feature A or B:

original data	1	1	1	2	2	3	4	5	5	6	6	7	7	7	7
split on feature A	1	1	1	2	2	3	4	5	5	6	6	7	7	7	7
split on feature B	1	1	1	2	2	3	4	5	5	6	6	7	7	7	7
							T_1							T_2	

In this formula, the $sd(T)$ function refers to the standard deviation of the values in set T, while T_1, T_2, ..., T_n are the sets of values resulting from a split on a feature. The $|T|$ term refers to the number of observations in set T. Essentially, the formula measures the reduction in standard deviation by comparing the standard deviation pre-split to the weighted standard deviation post-split.

For example, consider the following case in which a tree is deciding whether or not to perform a split on binary feature A or B:

original data	1	1	1	2	2	3	4	5	5	6	6	7	7	7	7
split on feature A	1	1	1	2	2	3	4	5	5	6	6	7	7	7	7
split on feature B	1	1	1	2	2	3	4	5	5	6	6	7	7	7	7
				T_1						T_2					

Let's compare the SDR of A against the SDR of B:

```
> sdr_a
[1] 1.202815
> sdr_b
[1] 1.392751
```

Since the SD for tree split by feature A has decreased as compared to B therefore the split as per A precedes as it creates more homogeneous grouping.

Using the groups that would result from the proposed splits, we can compute the SDR for A and B as follows. The `length()` function used here returns the number of elements in a vector. Note that the overall group T is named `tee` to avoid overwriting R's built-in `T()` and `t()` functions:

```
> tee <- c(1, 1, 1, 2, 2, 3, 4, 5, 5, 6, 6, 7, 7, 7, 7)
> at1 <- c(1, 1, 1, 2, 2, 3, 4, 5, 5)
> at2 <- c(6, 6, 7, 7, 7, 7)
> bt1 <- c(1, 1, 1, 2, 2, 3, 4)
> bt2 <- c(5, 5, 6, 6, 7, 7, 7, 7)
> sdr_a <- sd(tee) - (length(at1) / length(tee) * sd(at1) +
              length(at2) / length(tee) * sd(at2))
> sdr_b <- sd(tee) - (length(bt1) / length(tee) * sd(bt1) +
              length(bt2) / length(tee) * sd(bt2))
```

Let's compare the SDR of A against the SDR of B:

```
> sdr_a
[1] 1.202815
> sdr_b
[1] 1.392751
```

The SDR for the split on feature A was about 1.2 versus 1.4 for the split on feature B. Since the standard deviation was reduced more for the split on B, the decision tree would use B first. It results in slightly more homogeneous sets than with A.

Suppose that the tree stopped growing here using this one and only split. A regression tree's work is done. It can make predictions for new examples depending on whether the example's value on feature B places the example into group T_1 or T_2. If the example ends up in T_1, the model would predict *mean(bt1) = 2*, otherwise it would predict *mean(bt2) = 6.25*.