

Presentation on Linear Regression and its Cousins

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# AN INTRODUCTION TO REGRESSION

- Regression refers to the technique which is used to find the relation between **dependent or response** variable with one or more **independent or predictor variables**. The relation between dependent and independent variables might be linear or non-linear.
- If we have data in the form  $(x_1, y_1), (x_2, y_2), \dots (x_n, y_n)$  then expected value  $E(Y|X=x) = \beta_0 + \beta_1 x$
- There might be random error which cannot be predicted thus  $Y_i = \beta_0 + \beta_1 x + e_i$
- But the linear regression model has the form  $\hat{y} = b_0 + bx$ , where  $b_0$  and  $b_1$  are unbiased estimates of  $\beta_0$  and  $\beta_1$  respectively. Slope refers to the rise in y for each unit increment in x, and  $\hat{y}$  is known as an estimate of y or expected value of y.
- For each value of x, we get an estimate for y or we can write  $model(x_i) \Rightarrow \hat{y}_i$  or we get a pair  $(x_i, \hat{y}_i)$  from the model for each input x and joining all the points gives us a straight line called as the **Best fit line** that is why the regression is known as the **Linear Regression**.
- The difference  $(y \hat{y})$  is termed as an error or residual  $e_i$ . Sum of all the residuals is always zero. Thus, the Residual Sum of Squares (RSS) is calculated and minimized to get the **Best fit line**.

### MATHEMATICAL TREATMENT OF RESIDUALS

• Residual Sum of Squares,  $RSS = \sum e_i^2 = \sum (y_i - \hat{y}_i)^2$ 

$$RSS = \sum_{i=1}^{n} (y_i - b_0 - b_1 x)^2$$

• For RSS to be a minimum, It must be partially differentiated with respect to  $b_0$  and  $b_1$ 

$$\frac{\partial (RSS)}{\partial b_0} = -2\sum_{i=1}^{n} (y_i - b_0 - b_1 x) = 0$$

$$\frac{\partial (RSS)}{\partial b_1} = -2\sum_{i=1}^{n} x_i (y_i - b_0 - b_1 x) = 0$$

## MATHEMATICAL TREATMENT OF RESIDUALS

Rearranging and solving these two gives us

$$b_1 = \hat{\beta}_1 = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sum (x_i - \bar{x})^2} = \frac{S_{xy}}{S_{xx}}$$

$$b_0 = \bar{y} - b_1 \,\bar{x}$$

- **Assumptions** for the single predictor:
- 1. y is related to x and shows a linear trend on the scatter plot of  $(x_i, y_i)$
- 2. The errors  $e_1, e_2, e_3, \dots e_n$  are independent of each other
- 3. The errors have a common variance which is constant.
- 4. The errors are normally distributed with mean 0 and variance  $\sigma^2$

- Scatter plot and the line of best fit
- The diagram shows that the dots referring to data points are scattered around the line of the best fit.

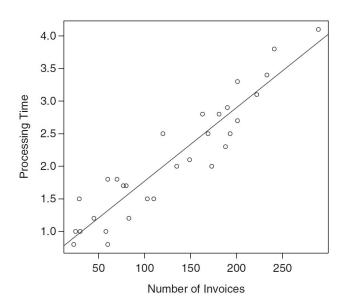


Figure 1: A typical scatter plot with line of best fit (Source: A modern approach to regression with R)

# VALIDITY OF A REGRESSION MODEL

- A regression model is considered to be valid if all the four assumptions are satisfied else the regression model is not valid for any inference.
- **Assumption 1**. There should be a valid linear trend in the data which can be viewed in scatter plot.

In the figure on right, it can be seen that the Data set 1 gives valid linear regression while other data set do not give a valid linear regression. Data set 2 is not linear, Data set 3 has an outlier and Data set 4 also does not give a valid linear regression.

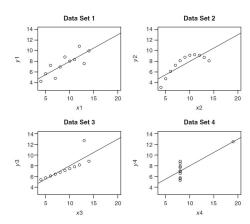


Figure 2: Plot showing trends

# VALIDITY OF A REGRESSION MODEL

• Assumption 2. Homoscedasticity of Residuals or equal variances

First plot shows uniform variance Second plot shows non-uniform Variance. Thus, first plot will give valid linear regression model and Second will not give valid linear regression model.

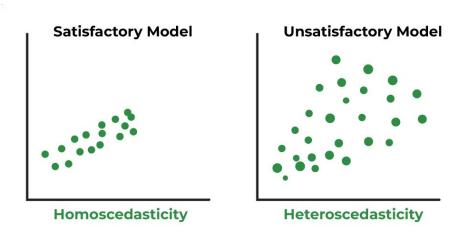


Figure 3: Plot showing homoscedasticity and heteroscedasticity

# VALIDITY OF A REGRESSION MODEL

• **Assumption 3**. Number of samples must be greater than the number of predictor variables.

This assumption is critical for the inference of the result obtained from the linear regression. If the number of predictor variables are more than the number of samples (number of rows less than the number of columns) then the result obtained from the linear regression becomes invalid. This assumption needs to be checked even before the split of the dataset. Suppose, we have a data frame such that X has 100 rows and 80 columns so that 100 samples and 80 predictor variable for Y and if we split the data set in the ratio of 70:30 such that the training set has 70 rows and test set has 30 rows. Since 70 is less than 80 hence the number of samples becomes less than the number of predictor variables. Thus, the regression model becomes invalid for any interpretation.

• **Assumption 4.** The residuals must be a white noise. If there is any trend in the residuals then the regression model becomes invalid. The coefficients will not be able to capture the trend and make predictions.

Hence, there is need to check the assumptions before drawing any conclusions.

# MULTIPLE LINEAR REGRESSION MODEL

• When the number of predictor variables are more than one then the linear regression is termed as the multiple linear regression. It has mathematical form as:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_n x_n + error$$

- But mathematically by minimizing the residuals we get estimates for coefficients  $\beta_0, \beta_1, \dots \beta_n$  written as  $b_0, b_1, b_2 \dots b_n$ .
- Multiple linear regression is valid when there is no multicollinearity among the predictors. If multicollinearity or autocorrelation is found among the variables then there is need to transform the data before running any multiple regression model.
- The transformations such as log transformation, Box-Cox transformation have wide range of applications to make data suitable for further regression.
- The suitable transformation is found by looking the nature of the data and relation between response and predictor variables.

# **COUSINS OF REGRESSION**

- The "cousins" of linear regression share the same purpose, methodology, and principles as linear regression.
- Some "cousins" may include logistic regression and polynomial regression.
- Logistic regression shares some of the same assumptions as linear regression and also involves estimating coefficients to explain the relationship between predictor variables and response variables. Logistic regression is a form of a **Generalized Linear Model** which basically allows for a different type of response variable (binary or categorical instead of continuous).
- Polynomial regression allows for a curved relationship between predictors and response rather than a straight line.
- Other "cousins" include **Penalized Regression Models** such as **lasso** and **ridge** regression which can be used to address collinearity and overfitting for linear models.

# CAUSE OF COUSINS OF REGRESSION

- If any of the assumptions of the linear regression is violated, it causes a problem to the inferences of the result and leading to the formulation of the cousins of the regression. To address the issue resulted due to the violation of any of the assumptions there is need to modify the technique of the linear regression leading to a new type of model which is known as cousin of linear regression.
- For example if multicollinearity is found among the predictors then there are two options to address this problem: (a) remove the predictors which have the correlation among them leading to Partial regression (b) to add bias so that the model has reduced the root mean squared error (RMSE) leading to the Ridge regression.
- The problem of multicollinearity can be addressed by using the dimensional reduction technique such as **Principal Component Analysis (PCA)** or **Partial Least Squares (PLS)**.
- PLS is based on the Herman Wold's Non Linear Iterative Partial Least Squares (NIPALS) algorithm (Wold 1982). This algorithm handles correlated predictors efficiently when sample size is less than 2500.
- If response variable is not continuous numeric then there is need to use Bayesian Probabilistic model which can handle binary or categorical response variable leading to logistic regression etc.

• The algorithm Simple PLS (SIMPLS) developed by de Jong (1993) through statistics, deflates the covariance matrix at each iteration making it more efficient than NIPALS.

### • R Implementations:

Let us assume that the data frame containing predictor variables are X\_train, and response variable is y\_train, then the R function lm() can be used to get the linear regression model as follows:

If the we have predictors as well as response in a data frame df\_train then we can get the model as:

$$model \leftarrow lm(y\sim., data = df_train)$$

Here the '.' refers to all the variables except y in the data frame df\_train. The summary of the model can be found using the function summary()

```
summary(model)
```

#### **Prediction based on the model:**

```
pred <- predict(model, X_test)
head(pred)</pre>
```

The observed and predicted test values can be collected into a data frame then defaultSumary() from caret can be used to estimate the test set performances.

```
df_Ob_Pred <- data.frame(obs=y_test,pred= pred)
defaultSummary(df_Ob_Pred)</pre>
```

Robust linear regression model can be generated using rlm() from MASS package. The argument of rlm are similar to lm(). It will produce result with crossvalidation equals to 10

Regression model without highly correlated predictors:

```
threshold <- 0.8
high_cor <- findCorrelation(cor(X_train), threshold)
var_to_rm <-names(X_train)[high_cor]
X_train <- X_train[, -var_to_rm]
X_test <- X_test[, -var_to_rm]
Now X_train can be used to build the regression model. It will be just like PLS.
set.seed(100)
filtered_model <- train(X_train, y_train, method="lm", + trControl=ctrl)
summary(filtered_model)</pre>
```

This model will drop the any possible highly correlated variable whose correlation between then is more than 0.80

Robust Regression model without highly correlated predictors using train():

This will produce summary of the robust model with 10 fold cross-validations.

# PARTIAL LEAST SQUARES (PLS)

The package pls has functions for PLS and PCR. The main function in this package is plsr(). This function has arguments for keyword method as 'oscorespls', 'simpls', 'widekernelpls'

```
plsr(y~., data = df_train)
Or

pls.fit <- plsr(y_train~ X_train)
    pred <- predict(pls.fit, X_test, ncomp =1:2)</pre>
```

The function plsr has options for K-fold, PLS algorithm to be used by method argument. Fine tune the model:

# PENALIZED REGRESSION MODELS

Ridge regression model can be created using lm.ridge() from MASS package or enet() from elasticnet package. Lambda argument in enet() specify the penalty for the ridge regression.

```
ridgeModel <- enet(x=as.matrix(X_train), y=y_train, lambda = 0.001)
```

• The function enet() has both ridge penalty as well as lasso penalty. The predict function for enet generates predictions for one or more value of lasso penalty using s and mode arguments. For the ridge regression, we have s=1 and mode="fraction"

• The lasso model can be generated using lars() from package lars, enet() from elasticnet and glmnet() from glmnet package.

# USE CASE: CAR PRICE PREDICTION MULTIPLE LINEAR REGRESSION

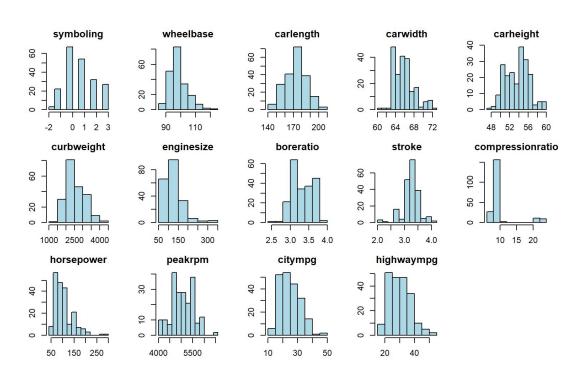
- Each entry corresponds to a car
- 205 entries
- 25 variables
  - o 24 predictor variables
  - 1 response variable **price**
- **GOAL:** Predict the price of the car based on the numerous features of the car (the engine size, horsepower, make, model, miles per gallon, etc.)

- Preview data using glimpse()
- Data made up of numeric and non-numeric variables
- No missing values

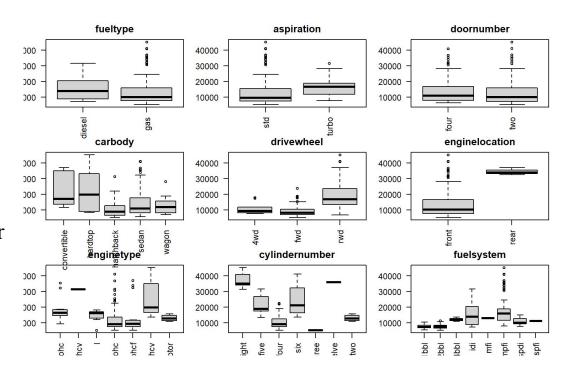
			To 13
symboling	CarName	fueltype	aspiration
0			0
doornumber	carbody	drivewheel	enginelocation
0			0
wheelbase	carlength	carwidth	carheight
0			0
curbweight	enginetype	cylindernumber	enginesize
0			0
fuelsystem	boreratio	stroke	compressionratio
0			0
horsepower	peakrpm	citympg	highwaympg
0			0
price			
0			

```
Rows: 205
Columns: 25
$ symboling
                                         <int> 3, 3, 1, 2, 2, 2, 1, 1, 1, 0, 2, 0, 0, 0, 1, 0, 0, ...
$ CarName
                                         <chr> "alfa-romero giulia", "alfa-romero stelvio", "alfa-rom.
$ fueltype
                                                                    "gas", "gas",
                                                                                                  "gas",
                                                                                                                 "gas",
$ aspiration
                                         <chr> "std". "std". "std". "std". "std". "std".
                                         <chr> "two", "two", "two", "four", "four", "two", "four"
$ doornumber
                                         <chr> "convertible", "convertible", "hatchback", "sedan", "s...
$ carbody
 $ drivewheel
                                         <chr> "rwd", "rwd", "rwd", "fwd", "4wd", "fwd", "fwd", "fwd"...
$ enginelocation
                                         <chr> "front", "front", "front", "front", "front", "front", ...
$ wheelbase
                                         <db7> 88.6, 88.6, 94.5, 99.8, 99.4, 99.8, 105.8, 105.8, 105...
$ carlength
                                         <db7> 168.8, 168.8, 171.2, 176.6, 176.6, 177.3, 192.7, 192.7...
 $ carwidth
                                         <db7> 64.1, 64.1, 65.5, 66.2, 66.4, 66.3, 71.4, 71.4, 71.4, ...
$ carheight
                                         <db7> 48.8, 48.8, 52.4, 54.3, 54.3, 53.1, 55.7, 55.7, 55.9, ...
$ curbweight
                                         <int> 2548, 2548, 2823, 2337, 2824, 2507, 2844, 2954, 3086, ...
                                         <chr> "dohc", "dohc", "ohcv", "ohc", 
$ enginetype
                                         <chr> "four", "four", "six", "four", "five", "five", "five", "
$ cylindernumber
$ enginesize
                                         <int> 130, 130, 152, 109, 136, 136, 136, 136, 131, 131, 108,...
$ fuelsvstem
                                         <chr> "mpfi", "mpfi", "mpfi", "mpfi", "mpfi", "mpfi",
$ boreratio
                                         <db1> 3.47, 3.47, 2.68, 3.19, 3.19, 3.19, 3.19, 3.19, 3.13, ...
$ stroke
                                         <db7> 2.68, 2.68, 3.47, 3.40, 3.40, 3.40, 3.40, 3.40, 3.40, ...
$ compressionratio <db1> 9.00, 9.00, 9.00, 10.00, 8.00, 8.50, 8.50, 8.50, 8.30,...
$ horsepower
                                         <int> 111, 111, 154, 102, 115, 110, 110, 110, 140, 160, 101,...
$ peakrpm
                                         <int> 5000, 5000, 5000, 5500, 5500, 5500, 5500, 5500, 5500, ...
$ citympq
                                         <int> 21, 21, 19, 24, 18, 19, 19, 19, 17, 16, 23, 23, 21, 21...
$ highwaympg
                                         <int> 27, 27, 26, 30, 22, 25, 25, 25, 20, 22, 29, 29, 28, 28...
$ price
                                         <db7> 13495.00, 16500.00, 16500.00, 13950.00, 17450.00, 1525...
```

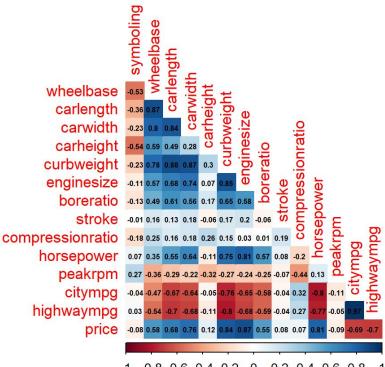
- Distributions of numerical predictors
- enginesize and horsepower have a left skew



- Distributions of categorical variables
- Diesel cars priced higher than gas
- Turbo cars price higher than standard
- Convertible and hardtops priced higher but also more varied
- Rear wheel drive priced higher
- Rear engines priced higher
- Eight cylinder engines priced high

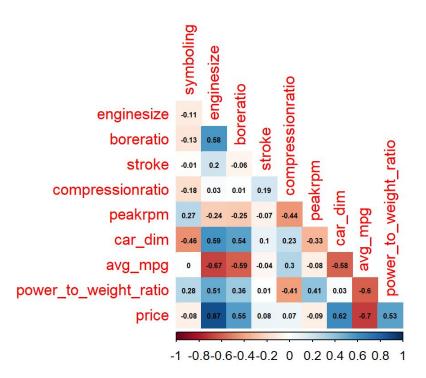


- Correlations of numeric variables
- Price positively correlated with wheelbase, carlength, carwidth, curbweight, enginesize, horsepower
- Price negatively correlated with citympg, highwaympg
- Many highly correlated predictor variables (ex: carwidth, wheelbase, carlength, carheight; citympg, highwaympg)



# DATA PREPARATION

- New variables to deal with collinearity:
  - car\_dim =
    carlength\*carwidth\*carheight
  - avg\_mpg = (citympg + highwaympg) / 2
  - power\_to\_weight\_ratio = horsepower / curbweight
- Remove cylindernumber singularity errors



# MODEL BUILDING

• "Stepwise" method:

```
model <- lm(price~., car_price)
model_updated <- step(model)
```

```
Residuals:
            10 Median
                                   Max
-6618.7 -1313.3
                -167.5 1107.3 10359.1
Coefficients:
                    Estimate Std. Error t value Pr(>|t|)
(Intercept)
                   -1.868e+03 8.138e+03 -0.230 0.818737
aspirationturbo
                   2.385e+03 6.889e+02
carbodyhardtop
                   -4.648e+03 1.413e+03
carbodyhatchback
                  -4.324e+03 1.184e+03
carbodysedan
                   -4.105e+03 1.216e+03
                                        -3.375 0.000909 ***
carbodywagon
                   -5.682e+03 1.374e+03
                                        -4.134 5.50e-05 ***
drivewheelfwd
                   -6.180e+02 1.017e+03
                                        -0.608 0.544217
drivewheelrwd
                                          1.298 0.196055
enginelocationrear 8.112e+03 2.135e+03
                                          3.800 0.000199 ***
enginetypedohcv
                                         2.955 0.003556 **
enginetypel
                   -4.899e+02 1.281e+03
                                         -0.382 0.702607
                                          3.167 0.001816 **
enginetypeohc
enginetypeohcf
                   2.728e+03 1.581e+03
                                          1.725 0.086325 .
enginetypeohcv
                                        -2.622 0.009518 **
enginetyperotor
                                         4.966 1.61e-06 ***
                   1.360e+04 2.739e+03
                                        16.301 < 2e-16 ***
enginesize
fuelsystem2bbl
                   3.880e+02 9.239e+02
                                         0.420 0.675060
fuelsystem4bbl
                                        -0.338 0.735752
fuelsystemidi
                   1.904e+04 5.983e+03
                                          3.182 0.001727 **
fuelsystemmfi
fuelsystemmpfi
                   7.354e+02 9.752e+02
                                          0.754 0.451802
fuelsystemspdi
fuelsystemspfi
boreratio
stroke
                   -4.016e+03 9.033e+02 -4.446 1.55e-05
compressionratio
                  -1.372e+03 4.310e+02 -3.184 0.001718
peakrpm
                   2.774e+00 5.897e-01
                                          4.704 5.13e-06
car_dim
                   2.680e-02 5.215e-03
                                         5.139 7.28e-07 ***
avg_mpg
                   1.483e+02 7.021e+01 2.112 0.036070
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' '
Residual standard error: 2441 on 176 degrees of freedom
Multiple R-squared: 0.9195, Adjusted R-squared: 0.9067
```

F-statistic: 71.78 on 28 and 176 DF, p-value: < 2.2e-16

Significance of variable

Model's ability to capture variability

# VARIANCE INFLATION FACTOR

- car packagecar::vif(model\_updated)
- VIF > 5 shows a high multicollinearity issue

			R AND COMMON CONTRACTOR
	GVIF	Df	$GVIF^{(1/(2*Df))}$
aspiration	2.415550	1	1.554204
carbody	3.496517	4	1.169377
drivewheel	4.759044	2	1.476998
enginelocation	2.261583	1	1.503856
enginetype	91.460718	6	1.456922
enginesize	7.478188	1	2.734628
fuelsystem	2465.098287	7	1.746923
boreratio	3.547939	1	1.883597
stroke	2.748372	1	1.657821
compressionratio	100.368942	1	10.018430
peakrpm	2.709323	1	1.646002
car_dim	5.880626	1	2.425000
avg_mpg	7.501759	1	2.738934

#### Residuals: 1Q Median Max -6618.7 -1313.3 -167.5 1107.3 10359.1 Coefficients: Estimate Std. Error t value Pr(>|t|) (Intercept) -1.868e+03 8.138e+03 -0.230 0.818737 aspirationturbo 2.385e+03 6.889e+02 3.463 0.000671 \*\*\* carbodyhardtop -4.648e+03 1.413e+03 -3.289 0.001214 \*\* carbodyhatchback -4.324e+03 1.184e+03 -3.653 0.000341 \*\*\* carbodysedan -4.105e+03 1.216e+03 -3.375 0.000909 \*\*\* -5.682e+03 1.374e+03 -4.134 5.50e-05 \*\*\* carbodywagon drivewheelfwd -6.180e+02 1.017e+03 -0.608 0.544217 drivewheelrwd 1.498e+03 1.155e+03 1.298 0.196055 enginelocationrear 8.112e+03 2.135e+03 3.800 0.000199 \*\*\* 8.023e+03 2.715e+03 2.955 0.003556 \*\* enginetypedohcv enginetypel -4.899e+02 1.281e+03 -0.382 0.702607 enginetypeohc 2.756e+03 8.703e+02 3.167 0.001816 \*\* enginetypeohcf 2.728e+03 1.581e+03 1.725 0.086325 . enginetypeohcy -3.000e+03 1.144e+03 -2.622 0.009518 \*\* 1.360e+04 2.739e+03 4.966 1.61e-06 \*\*\* enginetyperotor enginesize 1.829e+02 1.122e+01 16.301 < 2e-16 \*\*\* fuelsystem2bbl 3.880e+02 9.239e+02 0.420 0.675060 fuelsvstem4bbl -1.010e+03 2.987e+03 -0.338 0.735752 fuelsystemidi 1.904e+04 5.983e+03 3.182 0.001727 fuelsystemmfi -2.810e+03 2.766e+03 -1.016 0.311075 fuelsystemmpfi 7.354e+02 9.752e+02 0.754 0.451802 fuelsystemspdi -2.529e+03 1.375e+03 -1.838 0.067685 fuelsystemspfi 9.792e+02 2.663e+03 0.368 0.713494 boreratio -5.092e+03 1.188e+03 -4.285 3.00e-05 \*\*\* stroke -4.016e+03 9.033e+02 -4.446 1.55e-05 \*\*\*

compressionratio

peakrpm

car\_dim

avg\_mpg

-1.372e+03 4.310e+02 -3.184 0.001718 \*\*

1.483e+02 7.021e+01 2.112 0.036070 \*

Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 2441 on 176 degrees of freedom

F-statistic: 71.78 on 28 and 176 DF, p-value: < 2.2e-16

Multiple R-squared: 0.9195. Adjusted R-squared: 0.9067

2.774e+00 5.897e-01 4.704 5.13e-06 \*\*\*

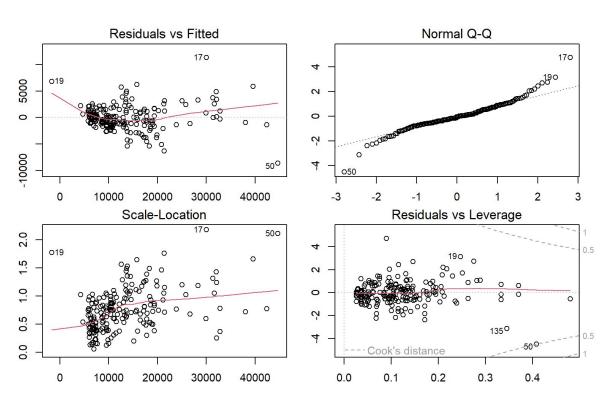
2.680e-02 5.215e-03 5.139 7.28e-07 \*\*\*

remove compressionratio

# DIAGNOSTICS

```
Residuals:
            10 Median
-8626.9 -1246.9 -47.2 1226.1 11357.7
Coefficients:
                    Estimate Std. Error t value Pr(>|t|)
(Intercept)
                  -1.330e+04 7.488e+03 -1.776 0.077410 .
                   3.110e+03 6.667e+02
                                         4.665 6.07e-06 ***
aspirationturbo
carbodyhardtop
                   -5.162e+03 1.440e+03 -3.585 0.000435 ***
carbodyhatchback
                  -4.586e+03 1.211e+03 -3.787 0.000208
carbodysedan
                   -4.452e+03 1.242e+03 -3.584 0.000437 ***
carbodywagon
                   -6.112e+03 1.402e+03 -4.358 2.22e-05 ***
drivewheelfwd
                  -1.086e+03 1.032e+03 -1.052 0.294080
drivewheelrwd
                   9.586e+02 1.171e+03
                                         0.818 0.414189
enginelocationrear 7.429e+03 2.178e+03
                                          3.411 0.000802
enginetypedohcv
                   7.131e+03 2.769e+03
                                         2.575 0.010840
enginetype1
                   8.779e+02 1.238e+03
                                          0.709 0.479083
                   3.132e+03 8.843e+02
enginetypeohc
                                          3.542 0.000509 ***
                   3.414e+03 1.607e+03
                                         2.125 0.034975 *
enginetypeohcf
enginetypeohcy
                   -2.778e+03
                             1.171e+03
                                        -2.372 0.018782
enginetyperotor
                   1.304e+04 2.803e+03
                                         4.651 6.45e-06 ***
enginesize
                   1.806e+02 1.148e+01 15.730 < 2e-16 ***
fuelsystem2bbl
                   5.373e+02 9.463e+02
                                          0.568 0.570895
fuelsvstem4bbl
                   -1.004e+03 3.063e+03
                                         -0.328 0.743516
fuelsystemidi
                   4.562e+02 1.349e+03
                                         0.338 0.735637
fuelsystemmfi
                  -1.797e+03 2.817e+03 -0.638 0.524383
fuelsystemmpfi
                   7.314e+02 1.000e+03
                                         0.731 0.465507
fuelsystemspdi
                  -1.372e+03 1.360e+03 -1.009 0.314439
fuelsystemspfi
                   5.905e+02 2.728e+03
                                         0.216 0.828870
boreratio
                  -5.079e+03 1.219e+03 -4.167 4.81e-05
                  -3.154e+03 8.837e+02
                                        -3.568 0.000462 ***
stroke
peakrpm
                   2.500e+00 5.982e-01
                                         4.179 4.60e-05 ***
car_dim
                   2.707e-02 5.347e-03
                                          5.063 1.03e-06 ***
avg_mpg
                   8.322e+01 6.888e+01 1.208 0.228607
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Residual standard error: 2503 on 177 degrees of freedom
Multiple R-squared: 0.9148. Adjusted R-squared: 0.9018
F-statistic: 70.42 on 27 and 177 DF. p-value: < 2.2e-16
```

# **DIAGNOSTICS**



# REFERENCES

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