Statistical Computing with R: Masters in Data Sciences 503 (S21) Second Batch, SMS, TU, 2023

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Review Preview

- Simple Linear Regression
  - Gradient Decent fit
  - Model Accuracy
  - Model Prediction
  - Model Validation
    - Validation set, Leave one out cross validation, k-folds cross validation, repeated k-folds cross-validation etc.)
- Multiple Linear Regression
  - Simple linear regression +
  - Multicollinearity, its assessment and solutions
  - Regularization
    - Ridge
    - Lasso
    - Elastic Net (Ridge+Lasso)

Simple Linear Regression: Gradient Decent

https://towardsdatascience.com/linear-regression-using-gradient-descent-97a6c8700931

- Linear Regression can also be fitted with Gradient Decent algorithm instead of OLS

- Here we minimize the loss function (E) to find m (slope b) and c (constant a)

$$E = \frac{1}{n}\sum_{i=0}^{n}(y_i - (mx_i + c))^2$$

E = MSE = Mean Sum of Square = Mean Squared Error = Variation

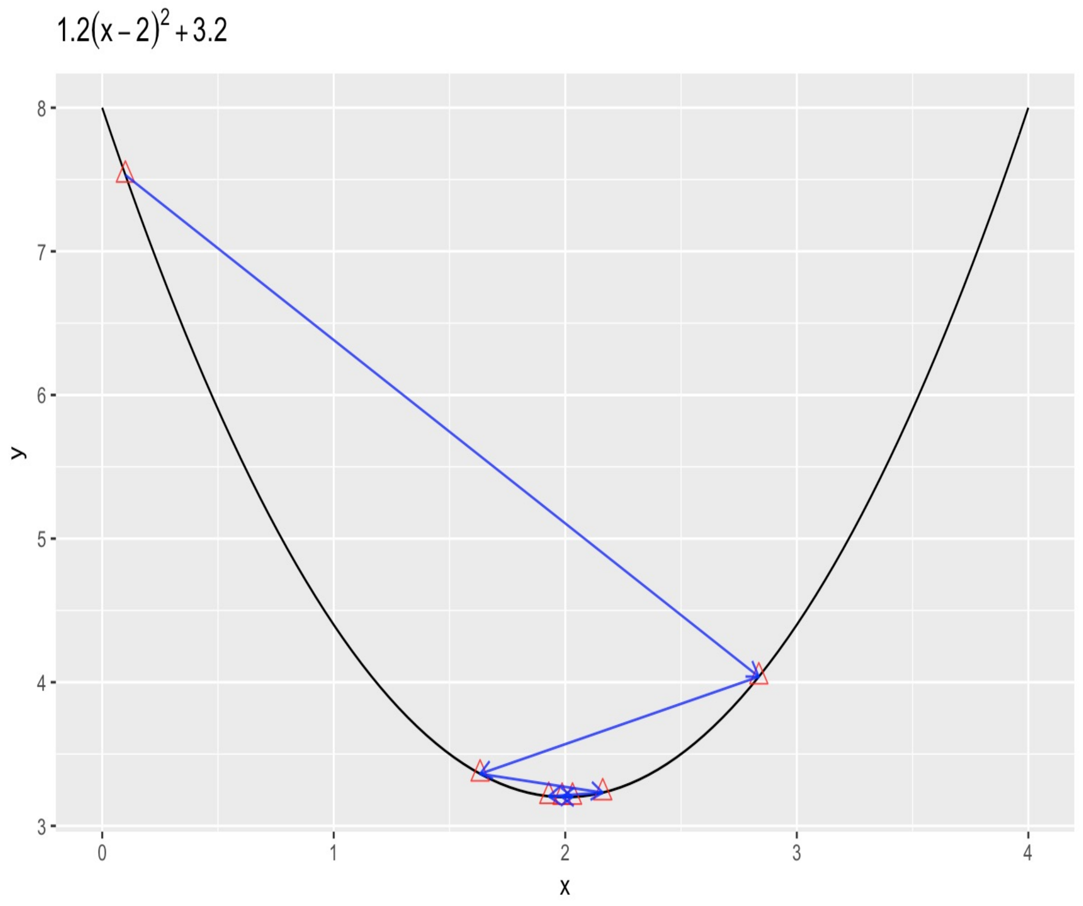
$$D_m = \frac{1}{n}\sum_{i=0}^{n} 2(y_i - (mx_i + c))(-x_i)$$
$$D_m = \frac{-2}{n}\sum_{i=0}^{n} x_i(y_i - \bar{y}_i)$$

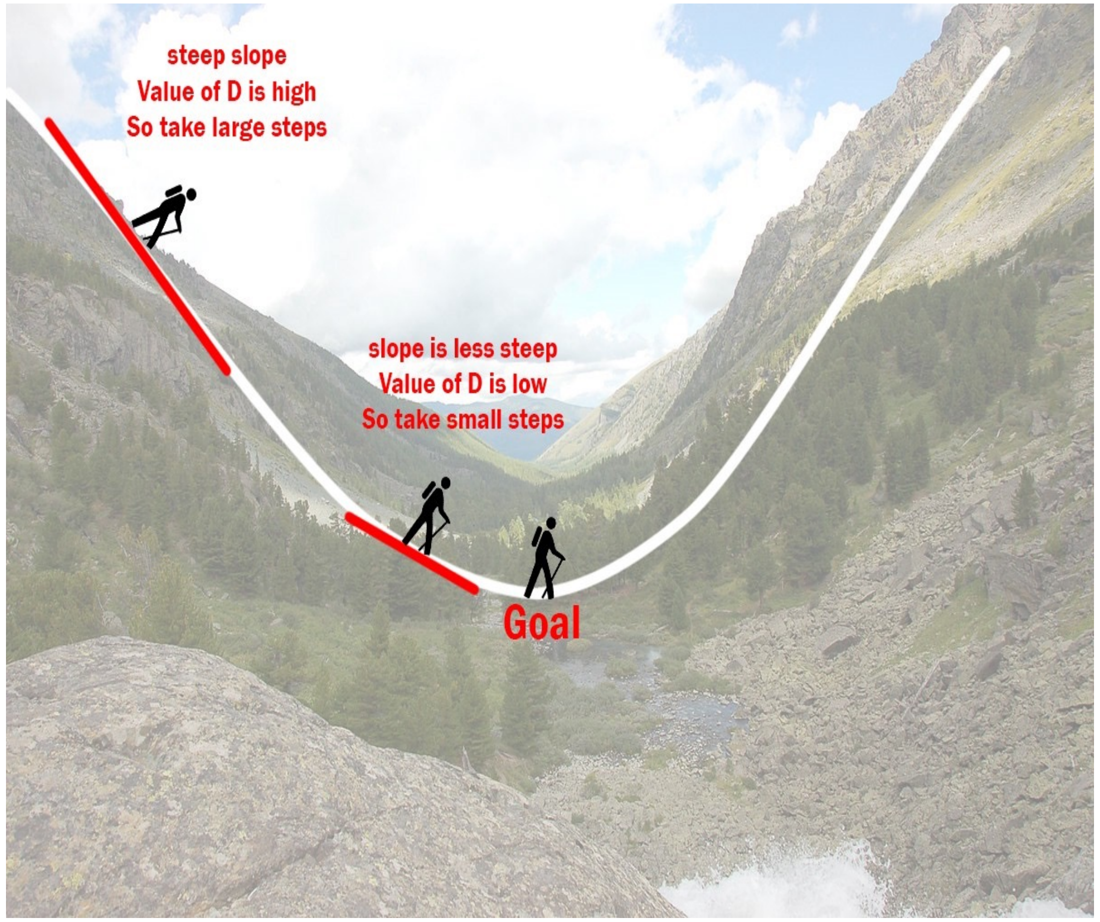
$$D_c = \frac{-2}{n}\sum_{i=0}^{n}(y_i - \bar{y}_i)$$

We can solve these two equations to get the value of m and c. This is an **optimization problem** as we need to MINIMIZE the loss function **MSE** using multiple iterations!

Illustration:

http://ethen8181.github.io/machine-learning/linear_regression/linear_regession.html





How to get MSE of Simple Linear Model? (OLS and Gradient Decent)

- Using the residuals of linear model:

```
lm1 <- lm(mpg ~ wt, data=mtcars)
(mse <- mean(lm1$residuals^2))
```

- Saving predicted values:

```
data <- data.frame(pred =
predict(lm1), actual = mtcars$mpg)
head(data)
mean((data$actual - data$pred)^2)
```

- > (mse <- mean(lm1$residuals^2))
- **[1] 8.697561**

- > mean((data$actual - data$pred)^2)
- **[1] 8.697561**

Model Accuracy of Linear Model:

- **R-square** – Explained variance (higher is better!)

- **RMSE** – Root of MSE (lower is better)
- MAE – Mean Absolute Error (lower is better)

- MAPE – Mean Absolute Percentage Error (lower is better)

$$MAPE = \frac{\overset{\text{Multiplying by 100\% converts to percentage}}{\boxed{100\%}}}{n} \Sigma \left| \frac{\overbrace{y - \hat{y}}^{\text{The residual}}}{\underset{\text{Each residual is scaled against the actual value}}{\boxed{y}}} \right|$$

#Better to use "caret" package

```
Install.packages("caret")
library(caret)
R2 <- R2(data$pred, data$actual)
• 0.7528328
RMSE <- RMSE(data$pred, data$actual)
• 2.949163
MAE <- MAE(data$pred, data$actual)
• 2.340642
```

Get MAPE in R as:

- 12.60733

If LINE is valid after BLUE then we can predict:

(So, we will use "lm1<-lm(mpg~wt, data=mtcars)" model to do it!)

- We need to save independent variable value/values in a new data:

```
new.wt <- data.frame(wt = 6)
```

- We can then use this data to predict the value of the dependent variable based on the fitted model as:

```
predict(lm1, newdata = new.wt)
```

Result = 5.218297

- Interpretation: Cars with 6000 lbs weight will (only) give 5.22 miles per gallon as per the linear regression algorithm!)

Validation & Cross-validation for Predictive Modelling including Linear Model:

- In statistics, we normally use the “full” data to do predictions
- In machine learning, we use validation/cross-validation sets to do the predictions
- Validation/Cross-validation can be done with:
  - Validation set (data split)
  - Leave one out cross-validation (LOOCV)
  - K-fold cross-validation
  - Repeated k-fold validation

Validation: Validation set (widely used!)

- Here the full data is “randomly” divided into two sets:
  - Training set
  - Testing set (validation set)
- Then model is fitted in the training set
- The model fit is then validated in the testing set using prediction
- This is the most widely used cross-validation method in the supervised machine learning

Lets do it for “mtcars” data:

```
#Define the mtcars data as “data”:
data <- mtcars
#Use random seed to replicate the result
set.seed(1234)
#Do random sampling to divide the cases into two independent samples
ind <- sample(2, nrow(mtcars), replace = T, prob = c(0.7, 0.3))
#Data partition
train.data <- data[ind==1,]
test.data <- data[ind==2,]
```

Model Fit, Prediction and Cross-Validation: Validation set approach

```
lm4 <- lm(mpg~wt, data = train.data)
library(dplyr)
library(caret)
predictions <- lm4 %>%
predict(test.data)
data.frame(R2 = R2(predictions,
test.data$mpg),
           RMSE = RMSE(predictions,
           test.data$mpg),
           MAE = MAE(predictions,
           test.data$mpg))
```

Model Accuracy of Training dataset:

summary(lm4)

- **Multiple R-squared: 0.7013**
- MSE = 9.526359 (How?)
- RMSE = SQRT(MSE) = 3.08648

Model Accuracy of Testing dataset:

R2	RMSE	MAE
0.9031085	**2.279303**	**1.698583**

Model Fit, Prediction and Cross-Validation: Leave-One-Out Cross-Validation approach:

```
#Leave one out CV
library(caret)

# Define training control
train.control <- trainControl(method = "LOOCV")

# Train the model
model1 <- train(mpg ~wt, data = mtcars, method =
"lm", trControl = train.control)
#Why mtcars data, why not train.data?

# Summarize the results
print(model1)
```

```
Linear Regression
32 samples
 1 predictor

No pre-processing
Resampling: Leave-One-Out Cross-Validation
Summary of sample sizes: 31, 31, 31, 31, 31, 31, ...
Resampling results:

  RMSE      Rsquared   MAE
  3.201673  0.7104641  2.517436

Tuning parameter 'intercept' was held constant at a
value of TRUE
```

Prediction with LOOCV:

```
predictions1 <- model1 %>% predict(test.data)

data.frame(R2 = R2(predictions1, test.data$mpg),
           RMSE = RMSE(predictions1, test.data$mpg),
           MAE = MAE(predictions1, test.data$mpg))
```

```
         R2          RMSE      MAE
• 0.9031085 2.244232    1.714515
```

Model Fit, Prediction and Cross-Validation: K-folds Cross-Validation approach

```
#k-fold cross validation
library(caret)
# Define training control
set.seed(123)
train.control <- trainControl(method = "cv", number
= 10)

# Train the model
model2 <- train(mpg ~ wt, data = mtcars, method =
"lm",
           trControl = train.control)

# Summarize the results
print(model2)
```

```
Linear Regression
32 samples
 1 predictor

No pre-processing
Resampling: Cross-Validated (10 fold)
Summary of sample sizes: 28, 28, 29, 29, 29, 30, ...
Resampling results:

 RMSE         Rsquared      MAE
 2.85133      0.7346939     2.375068

Tuning parameter 'intercept' was held constant at a
value of TRUE
```

Predictions with k-folds CV:

predictions2 <- model2 %>% predict(test.data)

data.frame(R2 = R2(predictions2, test.data$mpg),

RMSE = RMSE(predictions2, test.data$mpg),

MAE = MAE(predictions2, test.data$mpg))

```
        R2      RMSE          MAE
• 0.9031085 2.244232     1.714515
```

Model Fit, Prediction and Cross-Validation: Repeated K-folds Cross-Validation approach

```
#repeated k-fold cross validation
library(caret)
# Define training control
set.seed(123)
train.control <- trainControl(method = "repeatedcv",
                              number = 10, repeats = 3)
# Train the model
model <- train(mpg ~wt, data = mtcars, method = "lm",
               trControl = train.control)
# Summarize the results
print(model)
```

```
Linear Regression
32 samples
 1 predictor

No pre-processing
Resampling: Cross-Validated (10 fold, repeated 3 times)
Summary of sample sizes: 28, 28, 29, 29, 29, 30, ...
Resampling results:

  RMSE       Rsquared   MAE
  2.975392   0.8351572  2.539797
Tuning parameter 'intercept' was held constant at a value of TRUE
```

Prediction with repeated k-folds CV:

```
predictions3 <- model3 %>%
predict(test.data)

data.frame( R2 = R2(predictions3,
test.data$mpg),
            RMSE = RMSE(predictions3,
test.data$mpg),
            MAE = MAE(predictions3,
test.data$mpg))
```

```
         R2      RMSE           MAE
• 0.9031085 2.244232    1.714515
```

Summary: Which one should be used based on R-squared values of “lm” model?

- R-square for training set: 0.7013
- R-square for training with LOOCV: 0.7104641
- R-square for training with k-folds CV: 0.7346939
- R-square for training with repeated k-folds CV: 0.8351572

- R-square for testing set: 0.9031085
- R-square for testing with LOOCV: 0.9031085
- R-square for testing with k-folds CV: 0.9031085
- R-square for testing with repeated k-folds CV: 0.9031085

Summary: Which one should be used based on RMSE value?

- RMSE for training set: 3.08648
- RMSE for training with LOOCV : 3.201673
- RMSE for training with k-folds CV: 2.85133
- RMSE for training with repeated k-folds CV: 2.975392

- RMSE for testing test: **2.279303**
- RMSE for testing with LOOCV: 2.244232
- RMSE for testing with k-folds CV: 2.244232
- RMSE for testing with repeated k-folds CV: 2.244232

Quick Think!

- Which model must be selected: Based on R-square or based on RMSE?
- Do we need to check the BLUE and LINE assumptions for the fit done with the training data?

- If BLUE and LINE test is a must then which training model should be checked?
- Validation set model?
- LOOCV set model?
- K-fold CV set model?
- Repeated K-fold CV set model?

Question/queries so far?

Multiple linear regression:

- It is an extension of the simple linear regression
- Multiple linear regression have more than one (two or more) independent variables
- Multiple linear regression has one (1) continuous dependent variable so it is a supervised learning
- All the assumptions of the simple linear regression are also applicable here
- There is one more condition:
- Multicollinearity must not be present i.e. correlations between independent variables must not be "high"

Multiple Linear Regression

A multiple linear regression model of Y on X_1, $X_{2,}$ … X_n in stochastic form in statistics is written as:

$$Y = \alpha + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_n X_n + u$$

where α is called y-intercept and and β_1, β_2, …, β_n are called slopes of X_1, X_2, …, X_n respectively, and u is called error or disturbance term, which is <u>erratic or random in nature</u>.

Multiple Linear Regression Estimation

$$\hat{y} = a + b_1 x_1 + b_2 x_2 + \ldots + b_n x_n$$

- where a, b_1, b_2, …, b_n are <u>least square estimates</u> of α and β_1, β_2, …, β_n respectively.

- We need to calculate best solutions of n equations each containing unknown parameters α, $\beta 1$, β_2, …, β_n using Ordinary Least Square (OLS) method using statistical software R

Multiple linear regression process:

- We must fit bi-variate linear regression for all the predictors and can take ONLY the statistically significant predictors in the final model
- However, must must assess the MULTICOLLINEARITY of the predictor variables before taking them into the final model
- Multicollinearity can be assessed using Pearson’s correlation coefficient but it is better to use Variance Inflation Factor (VIF)

Fit simple linear regression models of mpg with all the predictors of “mtcars” data

- What did you find?
- Which predictors can be taken to the final model?
- What to do now?
- What will be your conclusion?

Assessing multicollinearity:

- Pearson correlation coefficients can be used
- We need to get a correlation matrix and flag the correlations with more than 0.75
- These pair/s of independent variables influences the linear model coefficients

- Variance Inflation Factor (VIF) is most commonly used to assess multicollinearity
- We can get the VIF for each independent variable
- Multicollinearity will be confirmed for an independent variable with VIF > 10 for linear models

Fitting multiple linear regression model using "mtcars" data:

- mlr <- lm(mpg ~., data = mtcars)
- summary(mlr)
- library(car)
- vif(mlr)
- We need to drop the independent variable with highest VIF and run the model again until all the VIF <10!

- None of the variables used in the model are statistically significant!

```
> vif(mlr)
      cyl      disp        hp
15.373833  21.620241  9.832037
drat       wt         qsec
3.374620   15.164887  7.527958
vs         am         gear
4.965873   4.648487   5.357452
carb
7.908747
```

Fitting multiple linear regression using “mtcars” data:

#Removing “disp” variable:

```
mlr1 <- lm(mpg ~ cyl+hp+drat+wt+qsec+vs+am+gear+carb, data = mtcars)
summary(mlr1)
vif(mlr1)
```

- We need to drop the independent variable with highest VIF and run the model again until all the VIF <10!

- The “wt” variable is significant

- > vif(mlr1)

```
      cyl        hp        drat
**14.284737**  7.123361  3.329298
       wt      qsec        vs
 6.189050  6.914423  4.916053
       am      gear      carb
 4.645108  5.324402  4.310597
```

Fitting multiple linear regression using “mtcars” data:

#Removing “cyl” variable:

```
mlr2 <- lm(mpg ~
hp+drat+wt+qsec+vs+am+gear+carb,
data = mtcars)
summary(mlr1)
vif(mlr1)
```

- We need to drop the independent variable with highest VIF and run the model again until VIF <10!
- **If all the VIF < 10 then we can interpret the model and do the predictions**

- The “wt” variable is significant, b = -2.60968 (1 unit increase in wt reduces the mpg by 2.61 unit controlling for other independent variables)

- > vif(mlr2)

```
hp              drat            wt
6.015788      3.111501        6.051127
qsec            vs              am
5.918682        4.270956        4.285815
gear     carb
4.690187        4.290468
```

Assignment:

- Use the validation and cross-validation methods for the multiple linear regression (mlr2) model
- Which model is the best model?
- Why?
- Predict the weight of the cars based on the best model identified using the test.data
- Change all the variables (except mpg) as standardized variable using "scale" command in R/R Studio
- Fit the multiple linear regression model with these standardized variables
- **Does it solve the multicollinearity issue?**
- Why? Write conclusions.

Alternative way to deal with multicollinearity in data science/machine learning:

- We can use the "regularization" methods

- The most common ones are:

  - Ridge regression
  - Lasso regression
  - Elastic net regression

- Once the "multicollinearity" problem is fixed then we can do the predictions and use the validation indices to select the best model for our data!

- **I will post a YouTube video link and you can fit these models for the "mtcars" data and learn from them!**

Regularized Regression:

- https://www.datacamp.com/tutorial/tutorial-ridge-lasso-elastic-net
- https://daviddalpiaz.github.io/r4sl/regularization.html
- https://www.r-bloggers.com/2017/07/machine-learning-explained-regularization/
- https://medium.com/edureka/regularization-in-machine-learning-4e041bbbdae

Question/queries?

Next class

- Other regression models used in the supervised learning: polynomial regression, KNN algorithm etc.
- Neural Network, Perceptron
- MLP, neural net regression etc.

Thank you!

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