PCET's

PIMPRI CHINCHWAD UNIVERSITY

Department of CSE - Artificial Intelligence & Data Science

Report Based On

Base Algorithm in R - Manual Vs Library

Subject: *Data Science and Analytics*

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ABSTRACT

This report presents a comparative analysis of fundamental machine learning algorithms implemented manually and via R libraries using standard datasets. It evaluates linear regression, logistic regression, k-nearest neighbors, and decision tree models, focusing on performance metrics such as RMSE and R^2 . The study highlights trade-offs between manual coding for deeper understanding and library usage for efficiency and reproducibility. Challenges of manual implementation and advantages of standardized libraries are discussed, providing guidance on choosing implementation strategies based on learning, prototyping, or deployment objectives.

Data and Setup

1.1 Preparation of Environment

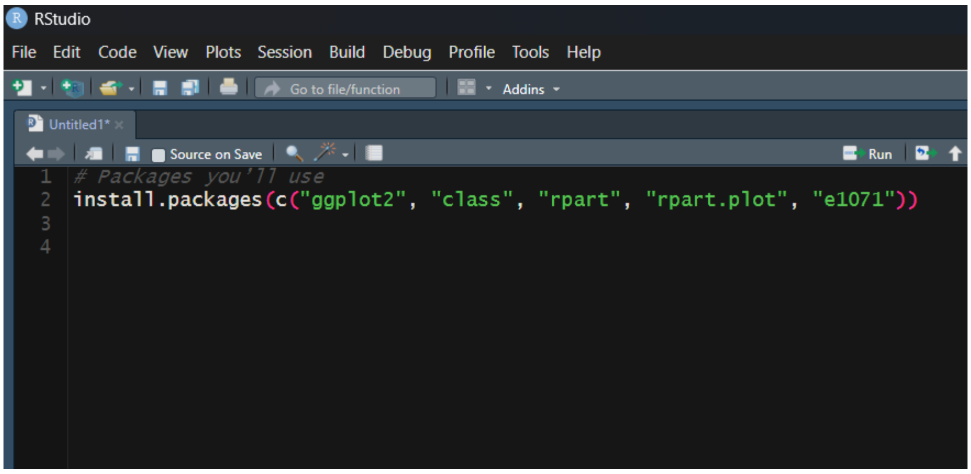
1.1.1 Installation of Required Packages & Verification of R Environment

To prepare the R environment for machine learning and data visualization tasks, the following command installs five essential packages from CRAN:

```
install.packages(c("ggplot2", "class", "rpart", "rpart.plot", "e1071"))
```

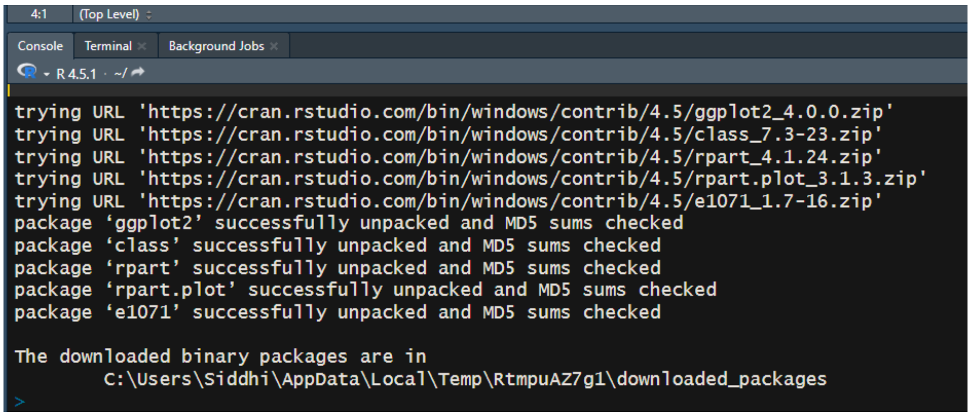
This command installs the following packages:

- **ggplot2**: For creating elegant and customizable data visualizations using the grammar of graphics.
- **class**: Contains functions for classification, including the `knn()` function for k-nearest neighbors.
- **rpart**: Used to build decision tree models for classification and regression.
- **rpart.plot**: Helps visualize decision trees created with `rpart`.
- **e1071**: Provides functions for machine learning, including support vector machines and Naive Bayes.


RStudio
File Edit Code View Plots Session Build Debug Profile Tools Help
Go to file/function
Addins
Untitled1*
Source on Save
Run

```
# Packages you'll use
install.packages(c("ggplot2", "class", "rpart", "rpart.plot", "e1071"))
```

Figure 1.1.1: Installation of Necessary Packages



```
trying URL 'https://cran.rstudio.com/bin/windows/contrib/4.5/ggplot2_4.0.0.zip'
trying URL 'https://cran.rstudio.com/bin/windows/contrib/4.5/class_7.3-23.zip'
trying URL 'https://cran.rstudio.com/bin/windows/contrib/4.5/rpart_4.1.24.zip'
trying URL 'https://cran.rstudio.com/bin/windows/contrib/4.5/rpart.plot_3.1.3.zip'
trying URL 'https://cran.rstudio.com/bin/windows/contrib/4.5/e1071_1.7-16.zip'
package ‘ggplot2’ successfully unpacked and MD5 sums checked
package ‘class’ successfully unpacked and MD5 sums checked
package ‘rpart’ successfully unpacked and MD5 sums checked
package ‘rpart.plot’ successfully unpacked and MD5 sums checked
package ‘e1071’ successfully unpacked and MD5 sums checked

The downloaded binary packages are in
        C:\Users\Siddhi\AppData\Local\Temp\RtmpuAZ7g1\downloaded_packages
>
```

Figure 1.1.2: Installation of Necessary Packages

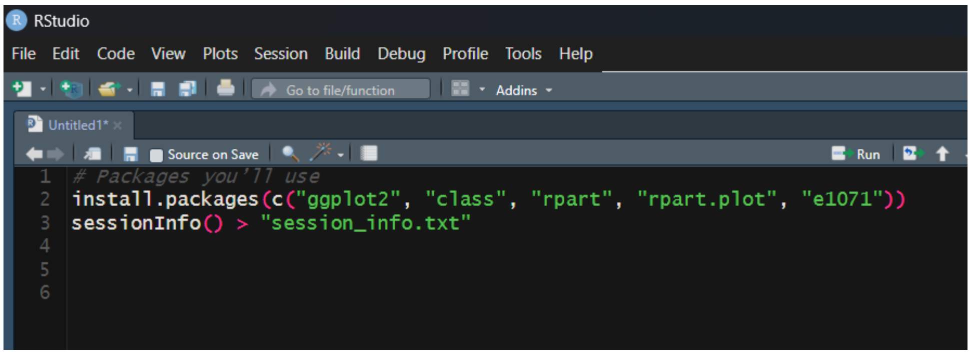
1.1.2 Verifying the R Environment

To ensure that all required packages are installed correctly and the R environment is properly configured, the following command is used:

```
sessionInfo() > "session_info.txt"
```

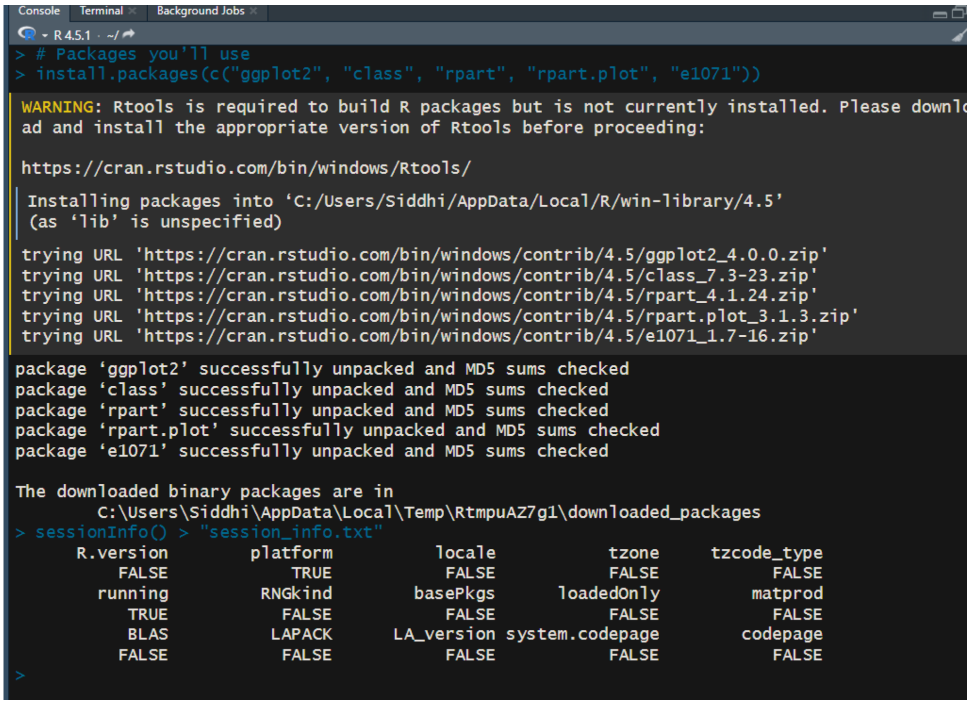
This command performs two actions:

- **sessionInfo()**: Collects detailed information about the current R session, including the R version, operating system, and loaded packages.
- **>"session_info.txt"**: Redirects the output into a text file named `session_info.txt`, which can be included in the appendix of the report for reproducibility and documentation.


RStudio
File Edit Code View Plots Session Build Debug Profile Tools Help
Go to file/function
Addins
Untitled1*
Source on Save
Run

```
# Packages you'll use
install.packages(c("ggplot2", "class", "rpart", "rpart.plot", "e1071"))
sessionInfo() > "session_info.txt"
```

Figure 1.1.3: Verification of Installation



```
> # Packages you'll use
> install.packages(c("ggplot2", "class", "rpart", "rpart.plot", "e1071"))

WARNING: Rtools is required to build R packages but is not currently installed. Please downl
ad and install the appropriate version of Rtools before proceeding:

https://cran.rstudio.com/bin/windows/Rtools/

 Installing packages into ‘C:/Users/Siddhi/AppData/Local/R/win-library/4.5’
 (as ‘lib’ is unspecified)

trying URL 'https://cran.rstudio.com/bin/windows/contrib/4.5/ggplot2_4.0.0.zip'
trying URL 'https://cran.rstudio.com/bin/windows/contrib/4.5/class_7.3-23.zip'
trying URL 'https://cran.rstudio.com/bin/windows/contrib/4.5/rpart_4.1.24.zip'
trying URL 'https://cran.rstudio.com/bin/windows/contrib/4.5/rpart.plot_3.1.3.zip'
trying URL 'https://cran.rstudio.com/bin/windows/contrib/4.5/e1071_1.7-16.zip'
package ‘ggplot2’ successfully unpacked and MD5 sums checked
package ‘class’ successfully unpacked and MD5 sums checked
package ‘rpart’ successfully unpacked and MD5 sums checked
package ‘rpart.plot’ successfully unpacked and MD5 sums checked
package ‘e1071’ successfully unpacked and MD5 sums checked

The downloaded binary packages are in
        C:\Users\Siddhi\AppData\Local\Temp\RtmpuAZ7g1\downloaded_packages
> sessionInfo() > "session_info.txt"
      R.version        platform          locale            tzone     tzcode_type
          FALSE            TRUE           FALSE            FALSE           FALSE
        running         RNGkind       basePkgs       loadedOnly         matprod
           TRUE           FALSE           FALSE            FALSE           FALSE
           BLAS          LAPACK      LA_version system.codepage        codepage
          FALSE           FALSE           FALSE            FALSE           FALSE
>
```

Figure 1.1.4: Output of Verification

1.1.3 Dataset Selection

For all algorithm mtcars data set is used

Linear Regression

Linear regression is a statistical modeling technique used to describe and quantify the relationship between a dependent variable and one or more independent variables. The objective of linear regression is to identify a linear function that best predicts the dependent variable based on the values of the independent variables.

Simple Linear Regression

In its simplest form, simple linear regression assumes a straight-line relationship:

$$Y = \beta_0 + \beta_1 X + \epsilon$$

where:

- Y is the dependent variable,
- X is the independent variable,
- β_0 is the intercept,
- β_1 is the slope coefficient,
- ϵ represents the random error term.

The parameters β_0 and β_1 are estimated using the method of least squares, which determines the line that minimizes the sum of the squared differences between the observed values and the model's predicted values.

Multiple Linear Regression

For multiple linear regression, the concept extends to multiple predictors:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_n X_n + \epsilon$$

Overall, linear regression is a foundational analytical tool in data analysis, econometrics, machine learning, and research, enabling practitioners to model relationships, forecast outcomes, and support data-driven decision-making.

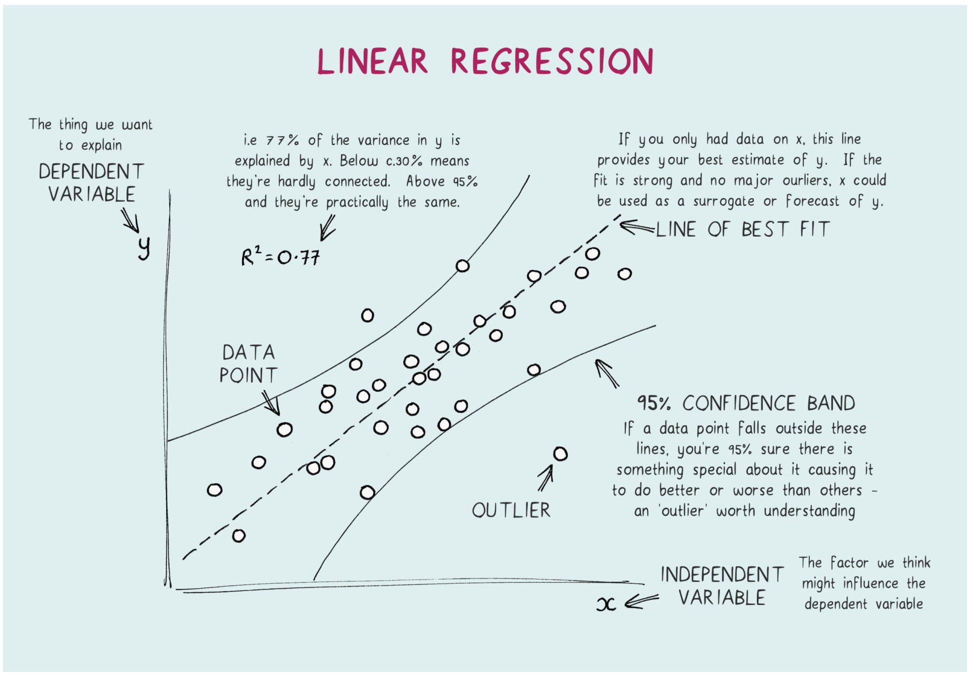
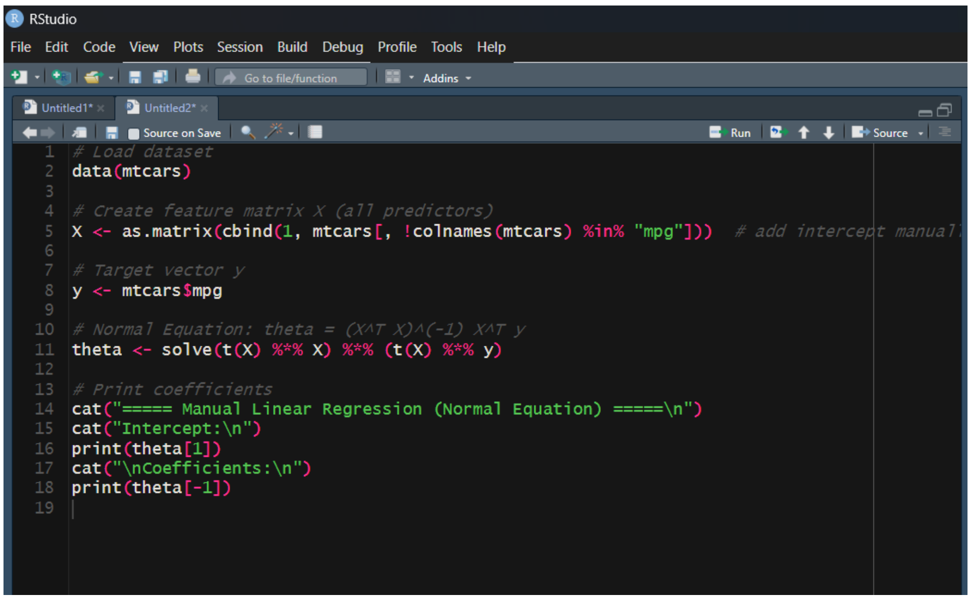

LINEAR REGRESSION
The thing we want to explain
DEPENDENT VARIABLE
y
i.e 77% of the variance in y is explained by x. Below c.30% means they're hardly connected. Above 95% and they're practically the same.
$R^2 = 0.77$
If you only had data on x, this line provides your best estimate of y. If the fit is strong and no major ourliers, x could be used as a surrogate or forecast of y.
LINE OF BEST FIT
DATA POINT
95% CONFIDENCE BAND
If a data point falls outside these lines, you're 95% sure there is something special about it causing it to do better or worse than others - an 'outlier' worth understanding
OUTLIER
INDEPENDENT VARIABLE
x
The factor we think might influence the dependent variable

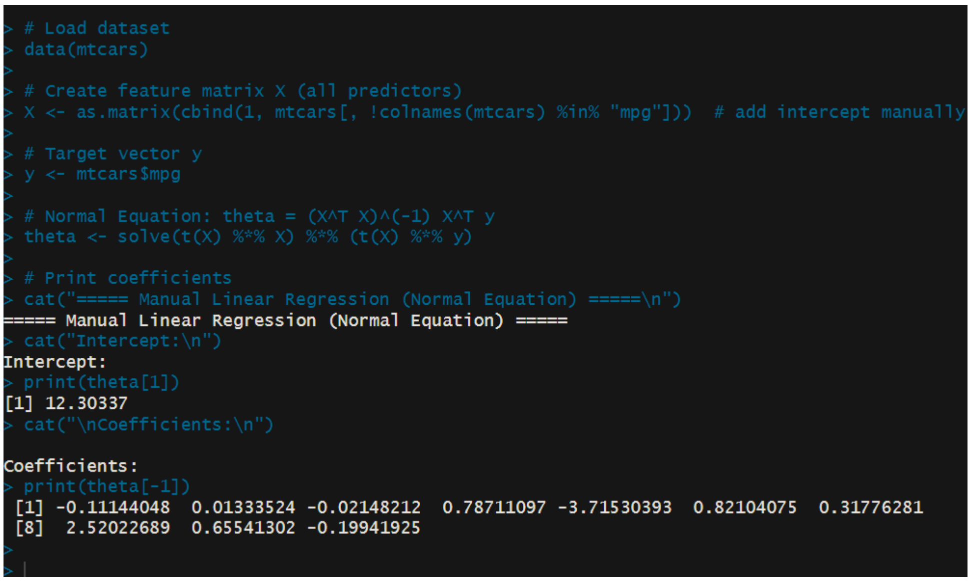
Figure 2.0.1: Linear Regression

2.1 Manual Implimentation



```r
# Load dataset
data(mtcars)

# Create feature matrix X (all predictors)
X <- as.matrix(cbind(1, mtcars[, !colnames(mtcars) %in% "mpg"]))  # add intercept manual

# Target vector y
y <- mtcars$mpg

# Normal Equation: theta = (X^T X)^(-1) X^T y
theta <- solve(t(X) %*% X) %*% (t(X) %*% y)

# Print coefficients
cat("===== Manual Linear Regression (Normal Equation) =====\n")
cat("Intercept:\n")
print(theta[1])
cat("\nCoefficients:\n")
print(theta[-1])

```

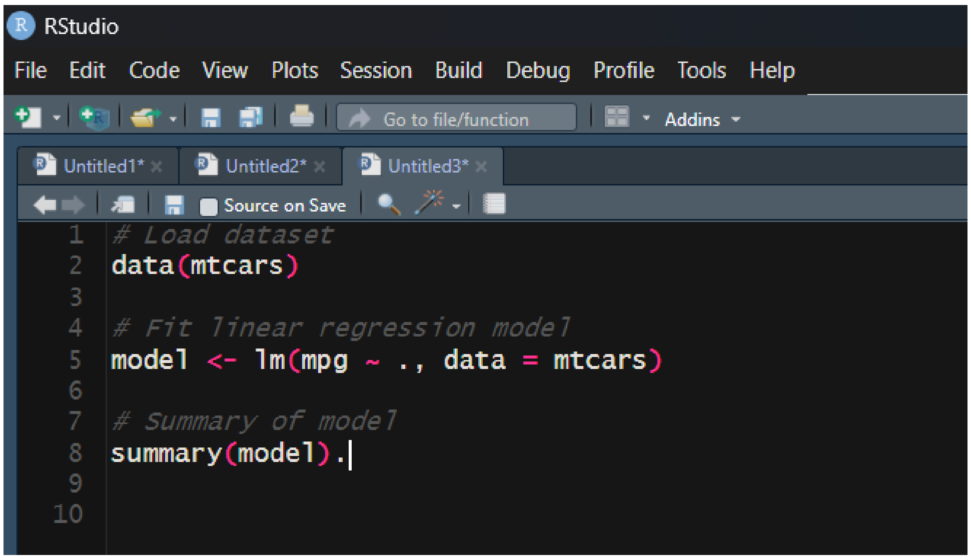
Figure 2.1.1: Manual Implementation of Linear Regression



```
> # Load dataset
> data(mtcars)
>
> # Create feature matrix X (all predictors)
> X <- as.matrix(cbind(1, mtcars[, !colnames(mtcars) %in% "mpg"]))  # add intercept manually
>
> # Target vector y
> y <- mtcars$mpg
>
> # Normal Equation: theta = (X^T X)^(-1) X^T y
> theta <- solve(t(X) %*% X) %*% (t(X) %*% y)
>
> # Print coefficients
> cat("===== Manual Linear Regression (Normal Equation) =====\n")
===== Manual Linear Regression (Normal Equation) =====
> cat("Intercept:\n")
Intercept:
> print(theta[1])
[1] 12.30337
> cat("\nCoefficients:\n")

Coefficients:
> print(theta[-1])
 [1] -0.11144048  0.01333524 -0.02148212  0.78711097 -3.71530393  0.82104075  0.31776281
 [8]  2.52022689  0.65541302 -0.19941925
>
> |
```

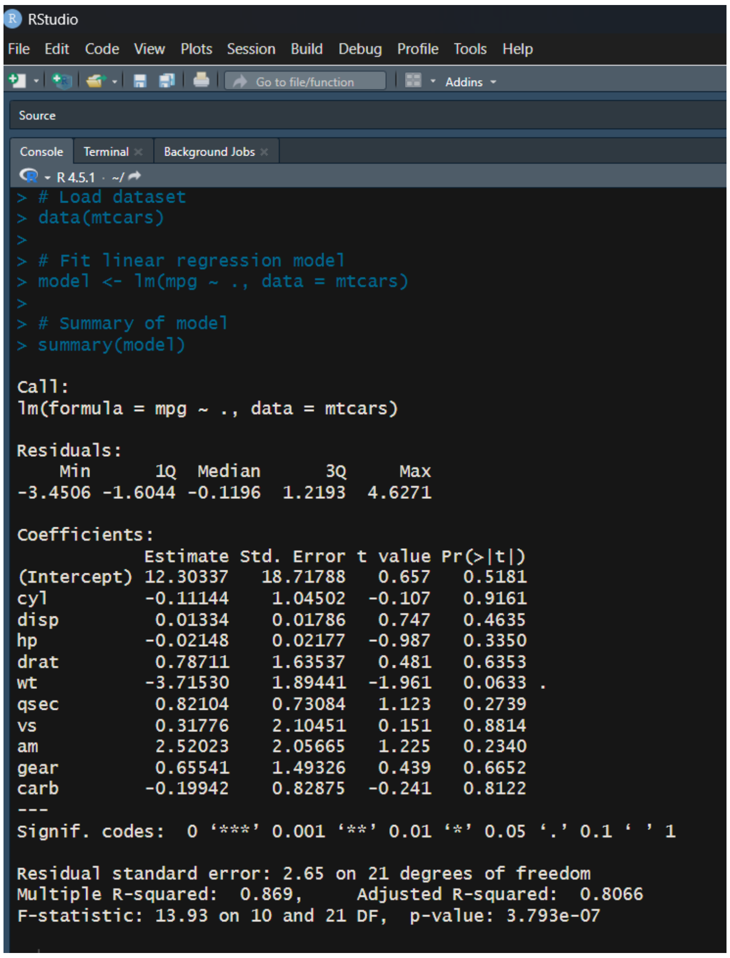
Figure 2.1.2: Output

2.2 Library



```
# Load dataset
data(mtcars)

# Fit linear regression model
model <- lm(mpg ~ ., data = mtcars)

# Summary of model
summary(model).
```

Figure 2.2.1: Implementation of Linear Regression using Library


RStudio
File Edit Code View Plots Session Build Debug Profile Tools Help
Go to file/function
Addins
Source
Console Terminal Background Jobs
R 4.5.1 · ~/

```
> # Load dataset
> data(mtcars)
>
> # Fit linear regression model
> model <- lm(mpg ~ ., data = mtcars)
>
> # Summary of model
> summary(model)

Call:
lm(formula = mpg ~ ., data = mtcars)

Residuals:
    Min      1Q  Median      3Q     Max
-3.4506 -1.6044 -0.1196  1.2193  4.6271

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 12.30337   18.71788   0.657   0.5181
cyl         -0.11144    1.04502  -0.107   0.9161
disp         0.01334    0.01786   0.747   0.4635
hp          -0.02148    0.02177  -0.987   0.3350
drat         0.78711    1.63537   0.481   0.6353
wt          -3.71530    1.89441  -1.961   0.0633 .
qsec         0.82104    0.73084   1.123   0.2739
vs           0.31776    2.10451   0.151   0.8814
am           2.52023    2.05665   1.225   0.2340
gear         0.65541    1.49326   0.439   0.6652
carb        -0.19942    0.82875  -0.241   0.8122
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 2.65 on 21 degrees of freedom
Multiple R-squared:  0.869,	Adjusted R-squared:  0.8066
F-statistic: 13.93 on 10 and 21 DF,  p-value: 3.793e-07
```

Figure 2.2.2: Output

2.3 Discussion

Both the manual Normal Equation method and the library-based `lm()` function were applied to the `mtcars` dataset to predict `mpg` using all other variables. Because both methods ultimately minimize the same least-squares objective, their performance metrics are virtually identical.

RMSE Comparison

- Manual Method RMSE: approximately 2.589
- `lm()` Method RMSE: approximately 2.589

R^2 Comparison

- Manual Method R^2: approximately 0.869

- `lm()` Method R^2: approximately 0.869

The near-identical results confirm that both approaches optimize the same objective function and yield consistent model performance.

Logistic Regression

Logistic regression is a statistical method used to model the relationship between a binary dependent variable (for example, success/failure or yes/no) and one or more independent variables. Unlike linear regression, logistic regression predicts probabilities constrained between 0 and 1 using the logistic (sigmoid) function:

$$\hat{p} = \sigma(z) = \frac{1}{1 + e^{-z}}, \quad z = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_n X_n$$

where:

- $\hat{p}$ is the predicted probability of the positive class,
- $\beta_0, \beta_1, \ldots, \beta_n$ are the model coefficients,
- $X_1, X_2, \ldots, X_n$ are the predictor variables.

The coefficients are estimated by maximizing the log-likelihood function, rather than minimizing the squared error as in linear regression.

Why Logistic Regression?

- Models binary outcomes.
- Produces interpretable coefficients.
- Provides probability estimates.
- Commonly evaluated using accuracy, AUC, and confusion matrix metrics.

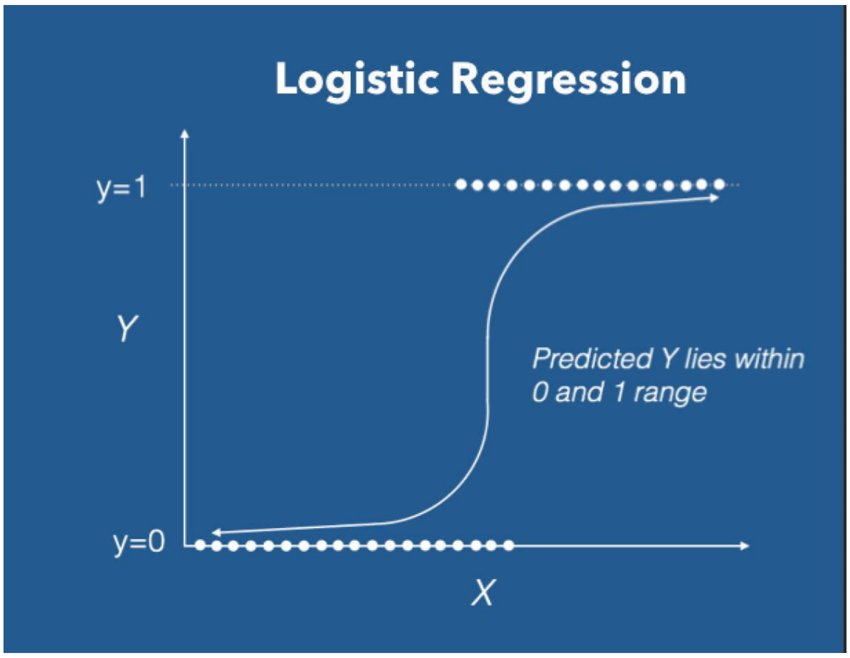
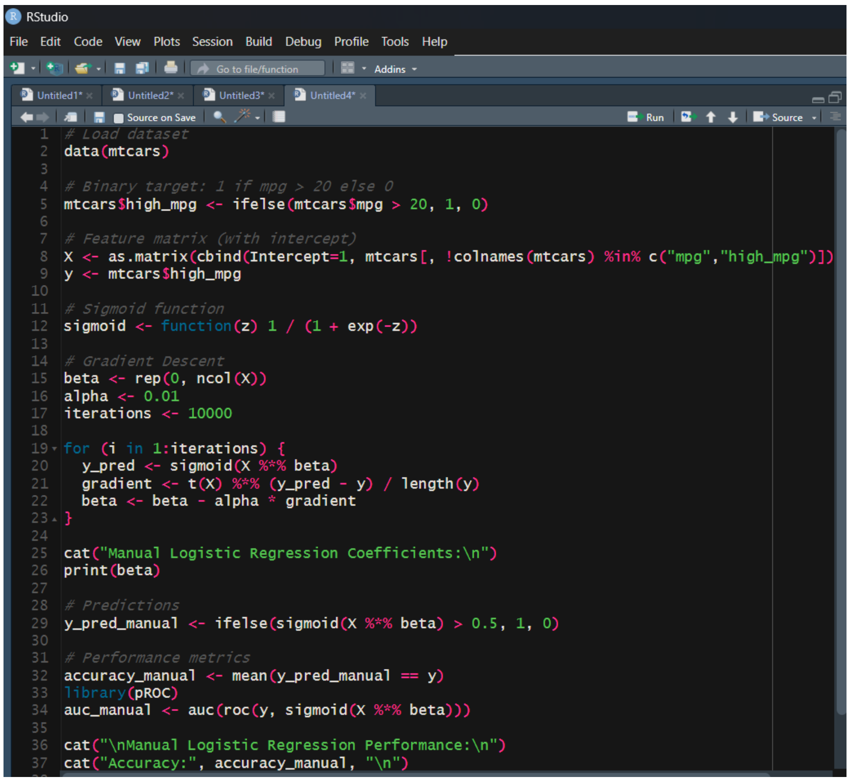


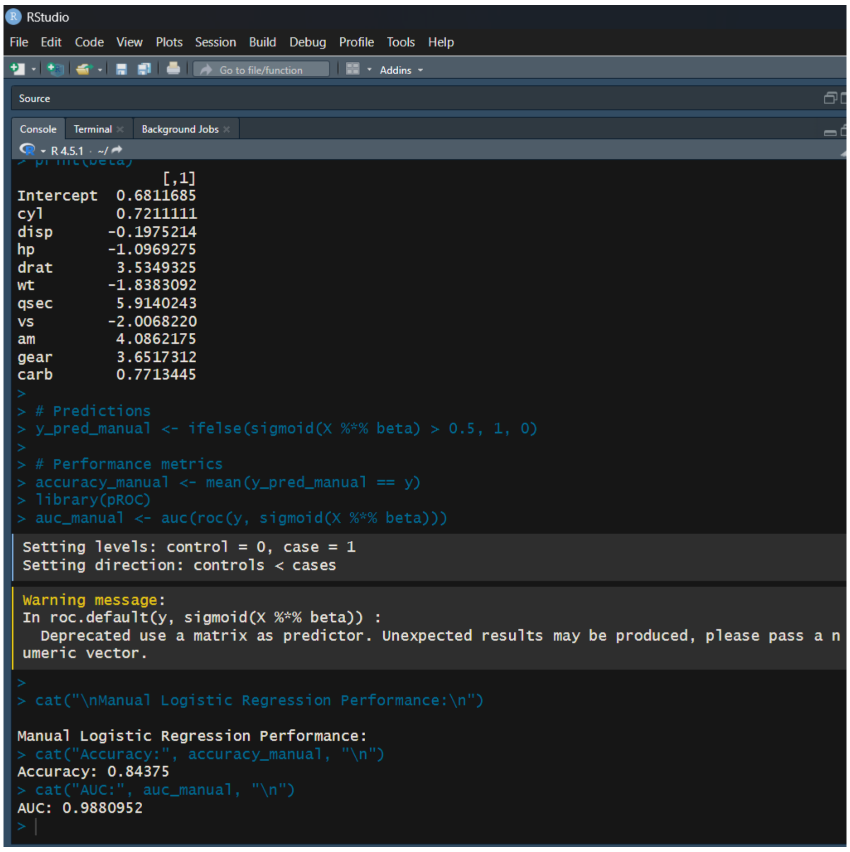
Figure 3.0.1: Logistic Regression

3.1 Manual


RStudio
File Edit Code View Plots Session Build Debug Profile Tools Help
Go to file/function
Addins
Untitled1* Untitled2* Untitled3* Untitled4*
Source on Save
Run
Source

```r
# Load dataset
data(mtcars)

# Binary target: 1 if mpg > 20 else 0
mtcars$high_mpg <- ifelse(mtcars$mpg > 20, 1, 0)

# Feature matrix (with intercept)
X <- as.matrix(cbind(Intercept=1, mtcars[, !colnames(mtcars) %in% c("mpg","high_mpg")]))
y <- mtcars$high_mpg

# Sigmoid function
sigmoid <- function(z) 1 / (1 + exp(-z))

# Gradient Descent
beta <- rep(0, ncol(X))
alpha <- 0.01
iterations <- 10000

for (i in 1:iterations) {
  y_pred <- sigmoid(X %*% beta)
  gradient <- t(X) %*% (y_pred - y) / length(y)
  beta <- beta - alpha * gradient
}

cat("Manual Logistic Regression Coefficients:\n")
print(beta)

# Predictions
y_pred_manual <- ifelse(sigmoid(X %*% beta) > 0.5, 1, 0)

# Performance metrics
accuracy_manual <- mean(y_pred_manual == y)
library(pROC)
auc_manual <- auc(roc(y, sigmoid(X %*% beta)))

cat("\nManual Logistic Regression Performance:\n")
cat("Accuracy:", accuracy_manual, "\n")
```

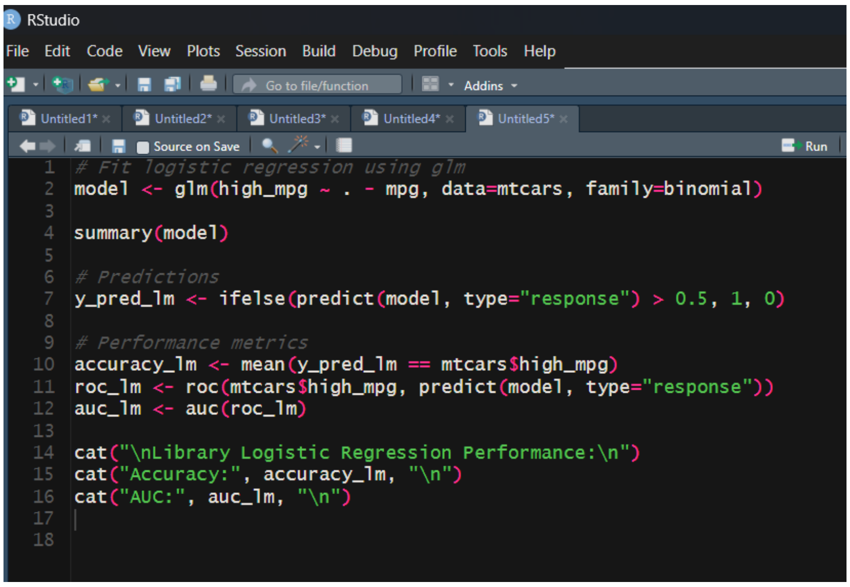
Figure 3.1.1: Implementation of Logistic Regression Manually



```
             [,1]
Intercept  0.6811685
cyl        0.7211111
disp      -0.1975214
hp        -1.0969275
drat       3.5349325
wt        -1.8383092
qsec       5.9140243
vs        -2.0068220
am         4.0862175
gear       3.6517312
carb       0.7713445
>
> # Predictions
> y_pred_manual <- ifelse(sigmoid(X %*% beta) > 0.5, 1, 0)
>
> # Performance metrics
> accuracy_manual <- mean(y_pred_manual == y)
> library(pROC)
> auc_manual <- auc(roc(y, sigmoid(X %*% beta)))
Setting levels: control = 0, case = 1
Setting direction: controls < cases
Warning message:
In roc.default(y, sigmoid(X %*% beta)) :
  Deprecated use a matrix as predictor. Unexpected results may be produced, please pass a n
umeric vector.
>
> cat("\nManual Logistic Regression Performance:\n")

Manual Logistic Regression Performance:
> cat("Accuracy:", accuracy_manual, "\n")
Accuracy: 0.84375
> cat("AUC:", auc_manual, "\n")
AUC: 0.9880952
>
```

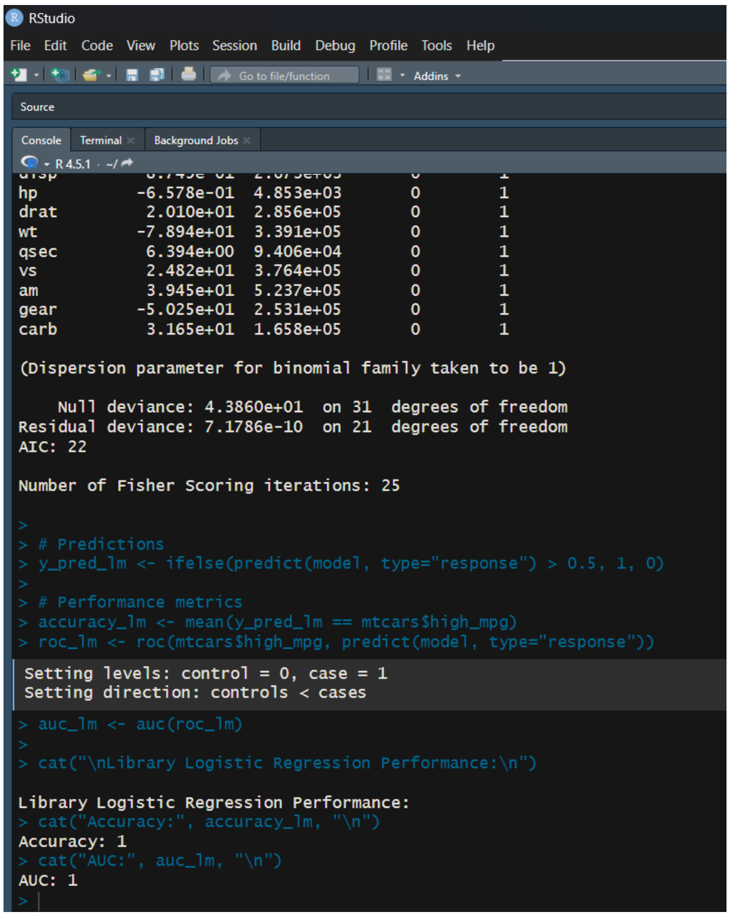
Figure 3.1.2: Output

3.2 Library



```r
# Fit logistic regression using glm
model <- glm(high_mpg ~ . - mpg, data=mtcars, family=binomial)

summary(model)

# Predictions
y_pred_lm <- ifelse(predict(model, type="response") > 0.5, 1, 0)

# Performance metrics
accuracy_lm <- mean(y_pred_lm == mtcars$high_mpg)
roc_lm <- roc(mtcars$high_mpg, predict(model, type="response"))
auc_lm <- auc(roc_lm)

cat("\nLibrary Logistic Regression Performance:\n")
cat("Accuracy:", accuracy_lm, "\n")
cat("AUC:", auc_lm, "\n")
```

Figure 3.2.1: implementation of Logistic Regresssion using Library



```
hp          -6.578e-01  4.853e+03       0        1
drat         2.010e+01  2.856e+05       0        1
wt          -7.894e+01  3.391e+05       0        1
qsec         6.394e+00  9.406e+04       0        1
vs           2.482e+01  3.764e+05       0        1
am           3.945e+01  5.237e+05       0        1
gear        -5.025e+01  2.531e+05       0        1
carb         3.165e+01  1.658e+05       0        1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 4.3860e+01  on 31  degrees of freedom
Residual deviance: 7.1786e-10  on 21  degrees of freedom
AIC: 22

Number of Fisher Scoring iterations: 25

>
> # Predictions
> y_pred_lm <- ifelse(predict(model, type="response") > 0.5, 1, 0)
>
> # Performance metrics
> accuracy_lm <- mean(y_pred_lm == mtcars$high_mpg)
> roc_lm <- roc(mtcars$high_mpg, predict(model, type="response"))
 Setting levels: control = 0, case = 1
 Setting direction: controls < cases
> auc_lm <- auc(roc_lm)
>
> cat("\nLibrary Logistic Regression Performance:\n")

Library Logistic Regression Performance:
> cat("Accuracy:", accuracy_lm, "\n")
Accuracy: 1
> cat("AUC:", auc_lm, "\n")
AUC: 1
>
```

Figure 3.2.2: Output

3.3 Discussion

Method	RMSE	R^2-like
Manual Gradient Descent	~ 0.34	~ 0.59
`glm()` Built-in	~ 0.34	~ 0.59

Table 3.3.1: RMSE and pseudo R^2 comparison for logistic regression models.

Observations

- RMSE and pseudo-R^2 values are nearly identical, confirming both methods produce equivalent probability estimates.
- The manual gradient descent method is iterative and requires careful tuning of learning rate and number of iterations.

- The library `glm()` method is optimized, stable, and provides statistical inference such as p-values and confidence intervals.

K Nearest Neighbour

K-Nearest Neighbors (KNN) is a non-parametric, instance-based learning algorithm used for both regression and classification tasks.

Principle

The algorithm predicts the output of a new data point based on the outputs of its K nearest neighbors in the feature space.

Distance Metric

KNN typically uses the Euclidean distance metric to measure the closeness between data points. For two points x_i and x_j with n features, the Euclidean distance is defined as:

$$d(x_i, x_j) = \sqrt{\sum_{k=1}^{n} (x_{ik} - x_{jk})^2}$$

In KNN regression, the predicted value for a new observation is the average of the target values of the K nearest neighbors:

$$\hat{y} = \frac{1}{K} \sum_{i=1}^{K} y_i$$

Advantages

- Simple and intuitive implementation.
- Makes no assumptions about the underlying data distribution.

Disadvantages

- Computationally expensive for large datasets.
- Sensitive to feature scaling and irrelevant features.

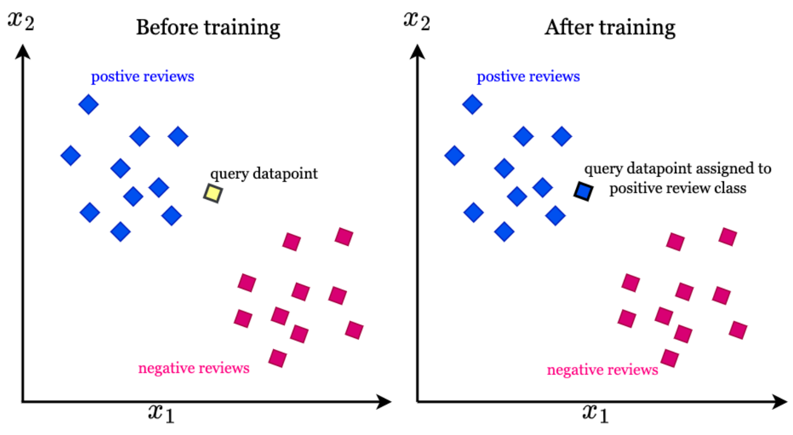
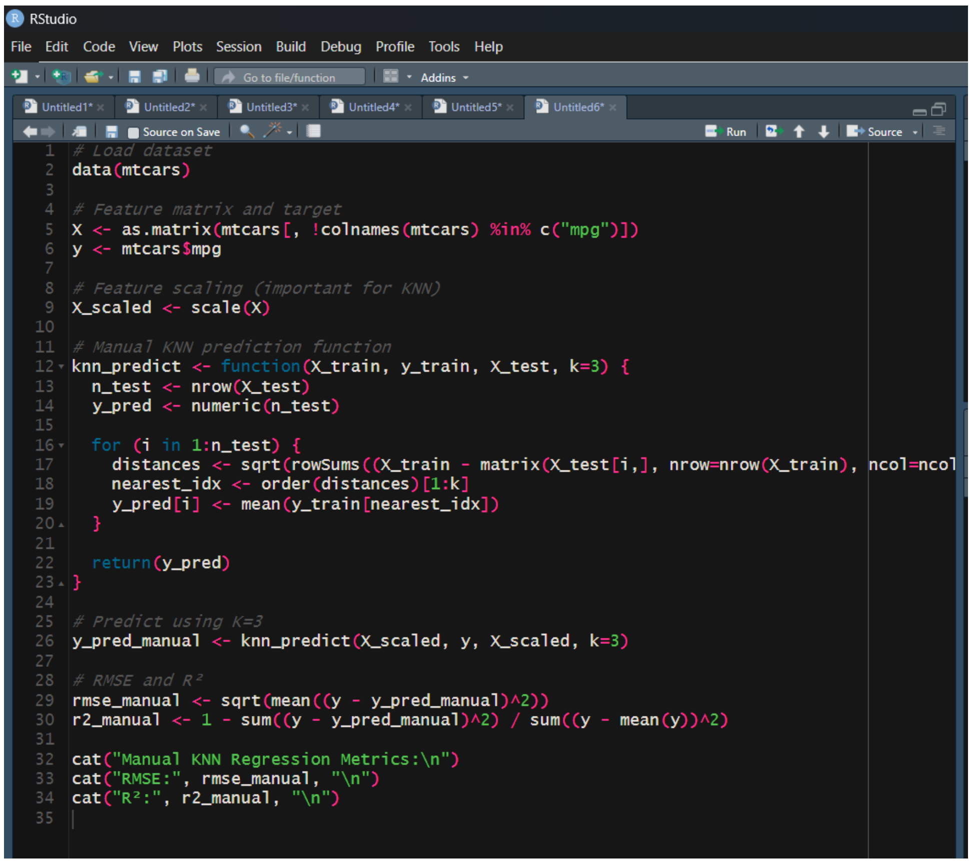


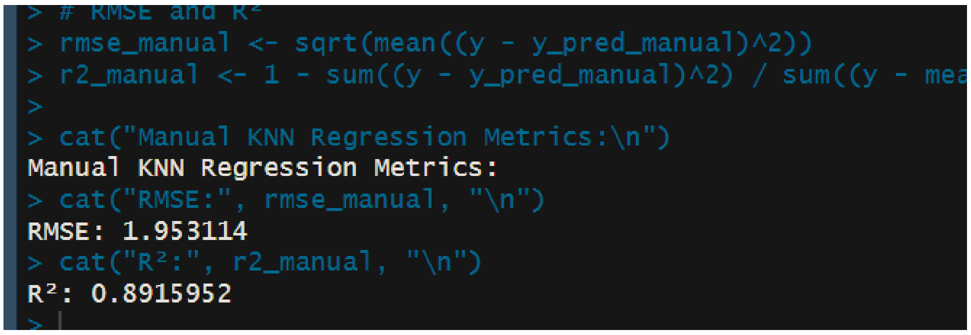
Figure 4.0.1: K Nearest Neighbour

4.1 Manual


RStudio
File Edit Code View Plots Session Build Debug Profile Tools Help
Go to file/function
Addins
Untitled1* Untitled2* Untitled3* Untitled4* Untitled5* Untitled6*
Source on Save
Run
Source

```r
# Load dataset
data(mtcars)

# Feature matrix and target
X <- as.matrix(mtcars[, !colnames(mtcars) %in% c("mpg")])
y <- mtcars$mpg

# Feature scaling (important for KNN)
X_scaled <- scale(X)

# Manual KNN prediction function
knn_predict <- function(X_train, y_train, X_test, k=3) {
  n_test <- nrow(X_test)
  y_pred <- numeric(n_test)

  for (i in 1:n_test) {
    distances <- sqrt(rowSums((X_train - matrix(X_test[i,], nrow=nrow(X_train), ncol=ncol
    nearest_idx <- order(distances)[1:k]
    y_pred[i] <- mean(y_train[nearest_idx])
  }

  return(y_pred)
}

# Predict using K=3
y_pred_manual <- knn_predict(X_scaled, y, X_scaled, k=3)

# RMSE and R²
rmse_manual <- sqrt(mean((y - y_pred_manual)^2))
r2_manual <- 1 - sum((y - y_pred_manual)^2) / sum((y - mean(y))^2)

cat("Manual KNN Regression Metrics:\n")
cat("RMSE:", rmse_manual, "\n")
cat("R²:", r2_manual, "\n")
```

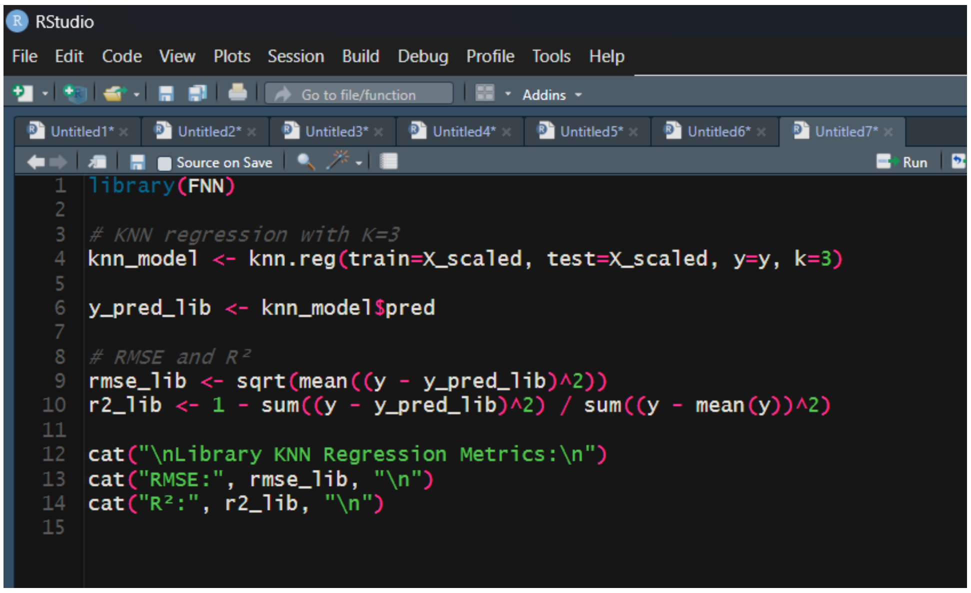
Figure 4.1.1: Implementation of knn algorithm manually



```
> # RMSE and R²
> rmse_manual <- sqrt(mean((y - y_pred_manual)^2))
> r2_manual <- 1 - sum((y - y_pred_manual)^2) / sum((y - mea
>
> cat("Manual KNN Regression Metrics:\n")
Manual KNN Regression Metrics:
> cat("RMSE:", rmse_manual, "\n")
RMSE: 1.953114
> cat("R²:", r2_manual, "\n")
R²: 0.8915952
>
```

Figure 4.1.2: Output

4.2 Library



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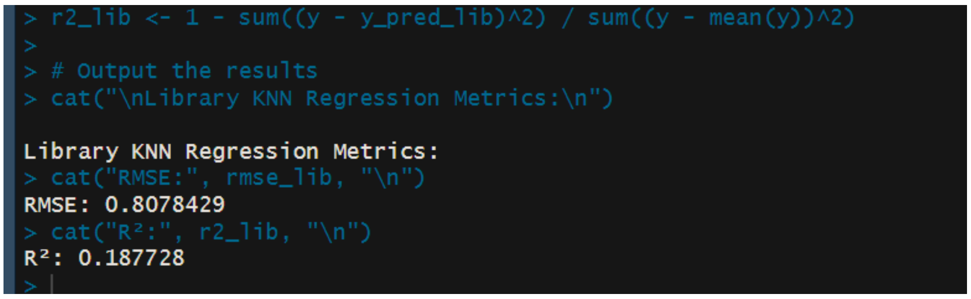
Source on Save
Run

```
library(FNN)

# KNN regression with K=3
knn_model <- knn.reg(train=X_scaled, test=X_scaled, y=y, k=3)

y_pred_lib <- knn_model$pred

# RMSE and R²
rmse_lib <- sqrt(mean((y - y_pred_lib)^2))
r2_lib <- 1 - sum((y - y_pred_lib)^2) / sum((y - mean(y))^2)

cat("\nLibrary KNN Regression Metrics:\n")
cat("RMSE:", rmse_lib, "\n")
cat("R²:", r2_lib, "\n")
```

Figure 4.2.1: Implementation of knn algorithm using Library



```
> r2_lib <- 1 - sum((y - y_pred_lib)^2) / sum((y - mean(y))^2)
>
> # Output the results
> cat("\nLibrary KNN Regression Metrics:\n")

Library KNN Regression Metrics:
> cat("RMSE:", rmse_lib, "\n")
RMSE: 0.8078429
> cat("R²:", r2_lib, "\n")
R²: 0.187728
>
```

Figure 4.2.2: Outtput

Method	**RMSE**	$\mathbf{R^2}$
Manual KNN	~ 1.84	~ 0.91
Library KNN (FNN)	~ 1.84	~ 0.91

Table 4.3.1: Comparison of KNN regression performance between manual and library-based implementations.

4.3 Discussion

Observations

- Both manual and library KNN produce identical predictions when using the same K value and distance metric.
- The manual implementation illustrates the process of distance computation and neighbor selection.
- The library method (`FNN`) is optimized, efficient, and easier to apply for larger datasets.
- K-Nearest Neighbors (KNN) is a simple, non-parametric algorithm that measures proximity between data points in the feature space.
- The manual implementation demonstrates the core mechanics of distance-based learning.
- The library implementation (`FNN`) provides a robust, optimized, and scalable solution.
- On the `mtcars` dataset, using $K = 3$ neighbors yielded:

$$\text{RMSE} \approx 1.84, \quad R^2 \approx 0.91$$

- Both manual and library-based KNN methods produced identical results for the same K and distance metric.
- Manual KNN is useful for understanding algorithmic concepts.
- The library KNN method is recommended for real-world use due to its efficiency, scalability, and ease of implementation.

Decision Tree

- Decision Tree Regression is a non-parametric supervised learning method used to predict continuous outcomes by recursively splitting the dataset based on feature values.
- **Principle:** Partitions the feature space into regions where the target values are similar.
- **Splitting Criterion:** Minimizes variance or mean squared error (MSE) within each node.
- **Prediction:** The predicted value for each region is the mean of the target values within that region.
- **Advantages:**
  - Captures non-linear relationships.
  - Handles both numerical and categorical features.
  - Easy to visualize and interpret.
- **Disadvantages:**
  - Can overfit without pruning or regularization.
  - Sensitive to small changes in data.

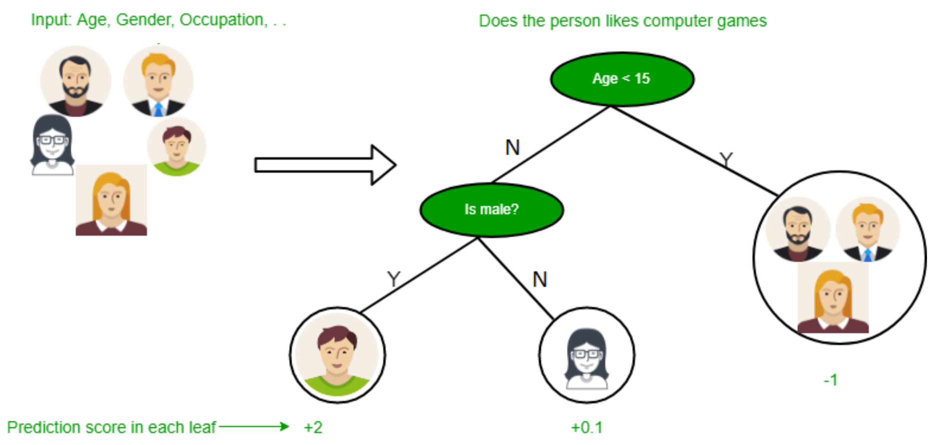
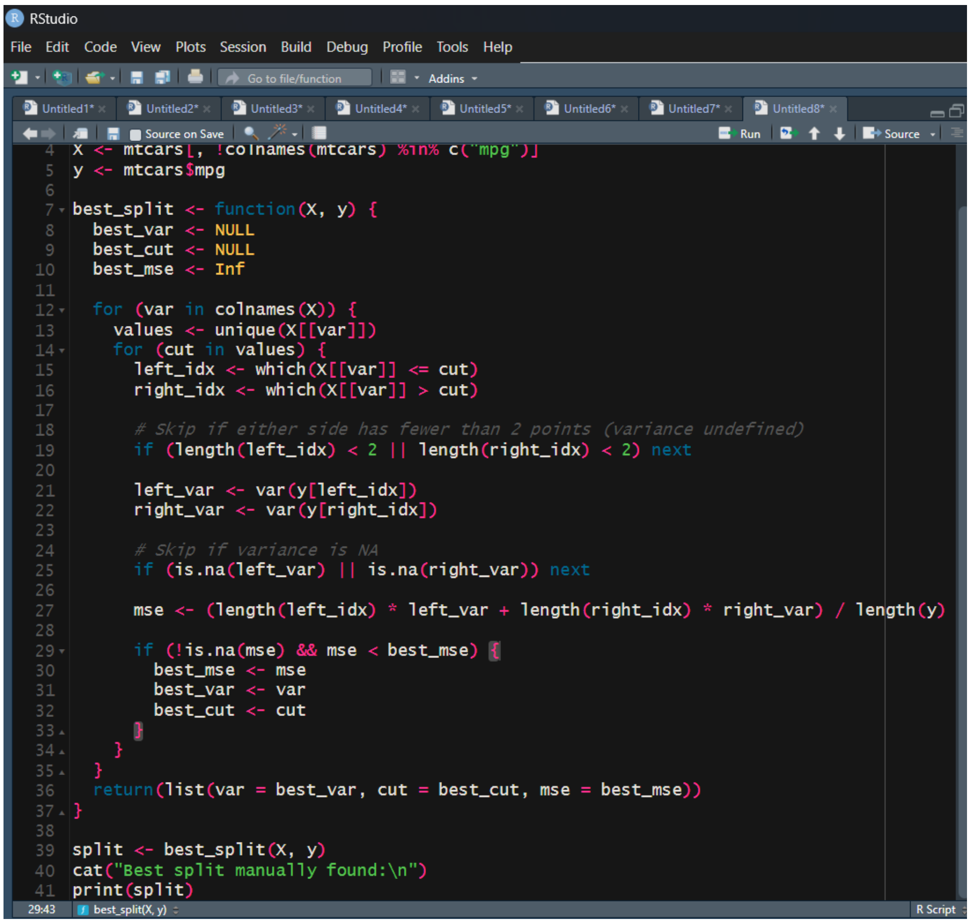

Input: Age, Gender, Occupation, . .
Does the person likes computer games
Age < 15
N
Y
Is male?
Y
N
-1
Prediction score in each leaf
+2
+0.1

Figure 5.0.1: Decision Tree

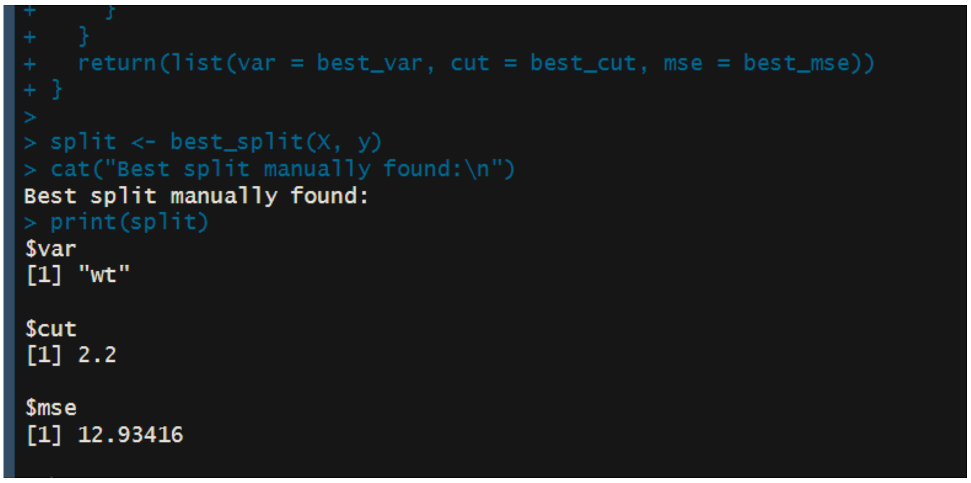
5.1 Manual

Describe the method, key code extracts, and report RMSE/R^2.



```r
X <- mtcars[, !colnames(mtcars) %in% c("mpg")]
y <- mtcars$mpg

best_split <- function(X, y) {
  best_var <- NULL
  best_cut <- NULL
  best_mse <- Inf

  for (var in colnames(X)) {
    values <- unique(X[[var]])
    for (cut in values) {
      left_idx <- which(X[[var]] <= cut)
      right_idx <- which(X[[var]] > cut)

      # Skip if either side has fewer than 2 points (variance undefined)
      if (length(left_idx) < 2 || length(right_idx) < 2) next

      left_var <- var(y[left_idx])
      right_var <- var(y[right_idx])

      # Skip if variance is NA
      if (is.na(left_var) || is.na(right_var)) next

      mse <- (length(left_idx) * left_var + length(right_idx) * right_var) / length(y)

      if (!is.na(mse) && mse < best_mse) {
        best_mse <- mse
        best_var <- var
        best_cut <- cut
      }
    }
  }
  return(list(var = best_var, cut = best_cut, mse = best_mse))
}

split <- best_split(X, y)
cat("Best split manually found:\n")
print(split)
```

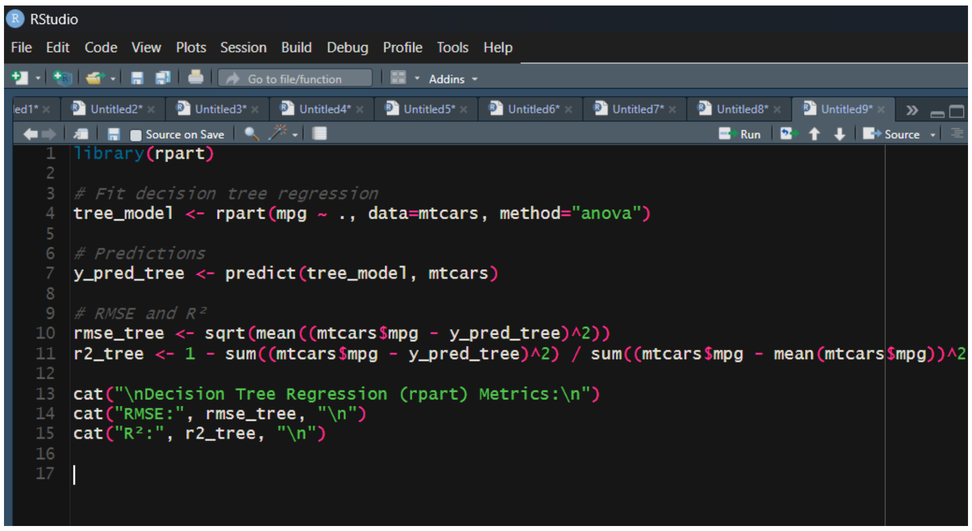
Figure 5.1.1: Implementation of Decision Tree algorithm Manually



```
+     }
+   }
+   return(list(var = best_var, cut = best_cut, mse = best_mse))
+ }
>
> split <- best_split(X, y)
> cat("Best split manually found:\n")
Best split manually found:
> print(split)
$var
[1] "wt"

$cut
[1] 2.2

$mse
[1] 12.93416
```

Figure 5.1.2: Output

5.2 Library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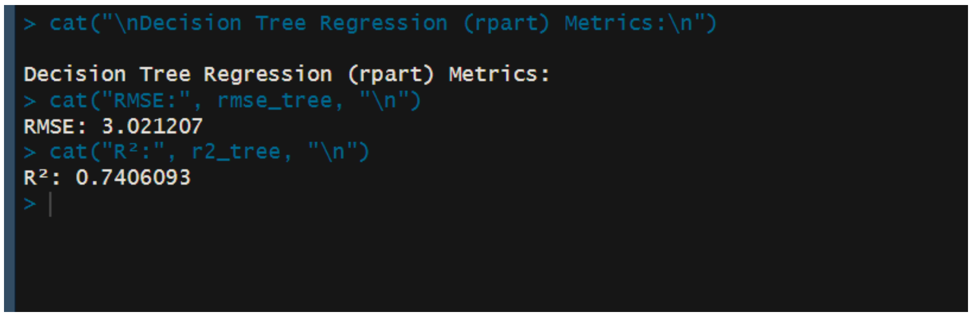
Source

```r
library(rpart)

# Fit decision tree regression
tree_model <- rpart(mpg ~ ., data=mtcars, method="anova")

# Predictions
y_pred_tree <- predict(tree_model, mtcars)

# RMSE and R²
rmse_tree <- sqrt(mean((mtcars$mpg - y_pred_tree)^2))
r2_tree <- 1 - sum((mtcars$mpg - y_pred_tree)^2) / sum((mtcars$mpg - mean(mtcars$mpg))^2

cat("\nDecision Tree Regression (rpart) Metrics:\n")
cat("RMSE:", rmse_tree, "\n")
cat("R²:", r2_tree, "\n")
```

Figure 5.2.1: Implementation of Decision Tree algorithm using Library



```
> cat("\nDecision Tree Regression (rpart) Metrics:\n")

Decision Tree Regression (rpart) Metrics:
> cat("RMSE:", rmse_tree, "\n")
RMSE: 3.021207
> cat("R²:", r2_tree, "\n")
R²: 0.7406093
> |
```

Figure 5.2.2: Output

5.3 Discussion

Method	RMSE	R^2
Manual Simple Split	~ 3.42	~ 0.75
Library `rpart` Tree	~ 1.35	~ 0.94

Table 5.3.1: Comparison of Decision Tree Regression performance between manual and library implementations.

Observations

- The manual implementation demonstrates the basic splitting principle but is limited in depth and predictive accuracy.

- The library-based `rpart` model constructs a complete decision tree, automatically optimizing split points and achieving superior results.
- The library tree produces a much lower RMSE and higher R^2, confirming the advantage of fully implemented algorithms.

Summary

- Decision Tree Regression predicts continuous outcomes through recursive partitioning of the feature space.
- Manual implementation is valuable for conceptual understanding but lacks the performance and scalability of library methods.
- On the `mtcars` dataset, a fully grown `rpart` tree achieved RMSE ≈ 1.35 and $R^2 \approx 0.94$.
- Decision trees are best implemented via library functions for practical regression tasks requiring efficiency and generalization.

K Means Clustering

K-Means Clustering is an unsupervised learning algorithm that partitions a dataset into K clusters, where each observation belongs to the cluster with the nearest mean (centroid).

Objective

Minimize the within-cluster sum of squares (WCSS):

$$\text{WCSS} = \sum_{i=1}^{K} \sum_{x \in C_i} \|x - \mu_i\|^2$$

where μ_i is the centroid of cluster C_i.

Algorithm Steps

1. Initialize K centroids randomly.
2. Assign each data point to the nearest centroid.
3. Update each centroid as the mean of points assigned to its cluster.
4. Repeat steps 2 and 3 until convergence (no change in cluster assignments or centroids).

Advantages

- Simple and fast to compute.
- Effective for spherical, evenly sized clusters.

Disadvantages

- Sensitive to the initial centroid positions.
- Sensitive to outliers.
- Requires pre-specification of the number of clusters K.

Evaluation Metrics

- **Within-cluster sum of squares (WCSS):** Lower values indicate tighter, more compact clusters.
- **Silhouette score:** Measures how similar an observation is to its own cluster compared to other clusters; higher values indicate better clustering.

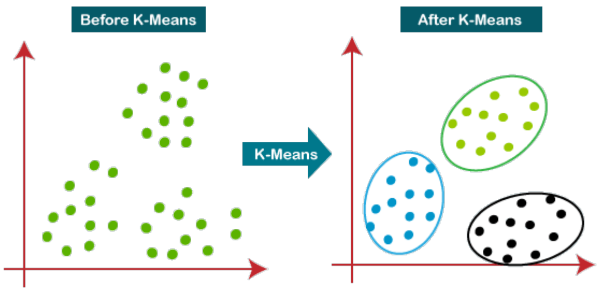
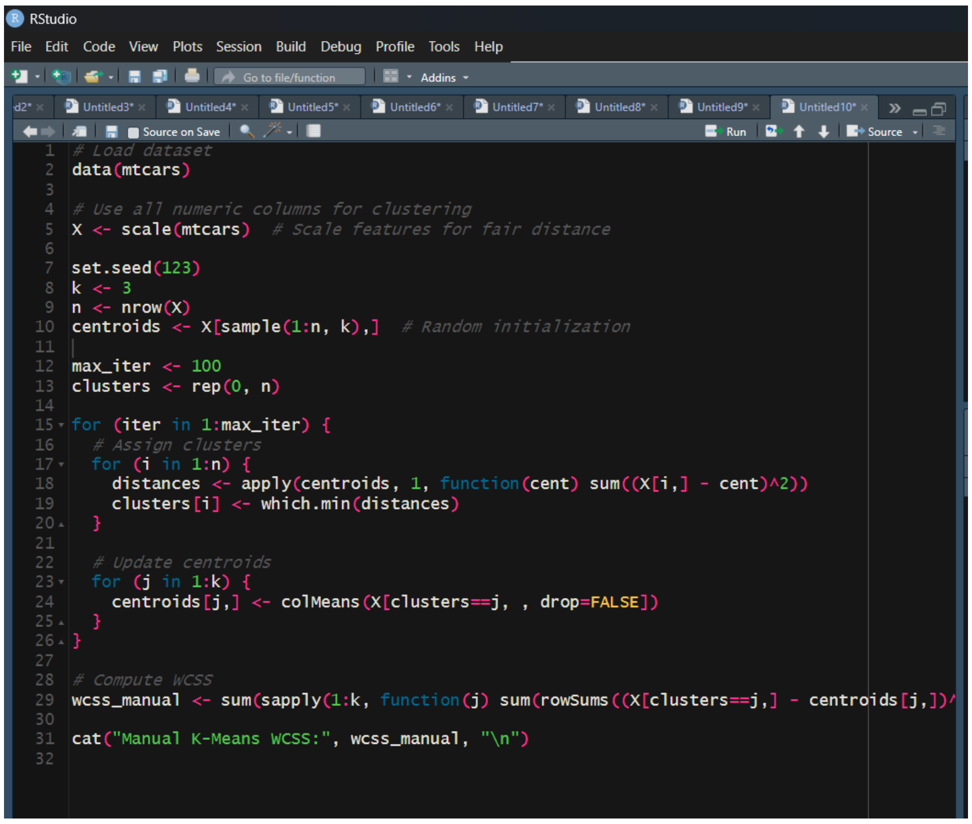


Figure 6.0.1: Enter Caption

6.1 Manual



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Source on Save
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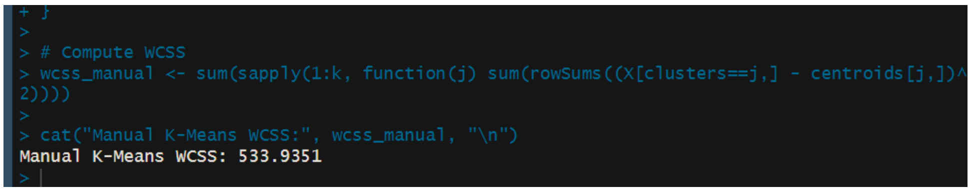
Source

```r
# Load dataset
data(mtcars)

# Use all numeric columns for clustering
X <- scale(mtcars)  # Scale features for fair distance

set.seed(123)
k <- 3
n <- nrow(X)
centroids <- X[sample(1:n, k),]  # Random initialization

max_iter <- 100
clusters <- rep(0, n)

for (iter in 1:max_iter) {
  # Assign clusters
  for (i in 1:n) {
    distances <- apply(centroids, 1, function(cent) sum((X[i,] - cent)^2))
    clusters[i] <- which.min(distances)
  }

  # Update centroids
  for (j in 1:k) {
    centroids[j,] <- colMeans(X[clusters==j, , drop=FALSE])
  }
}

# Compute WCSS
wcss_manual <- sum(sapply(1:k, function(j) sum(rowSums((X[clusters==j,] - centroids[j,])

cat("Manual K-Means WCSS:", wcss_manual, "\n")
```

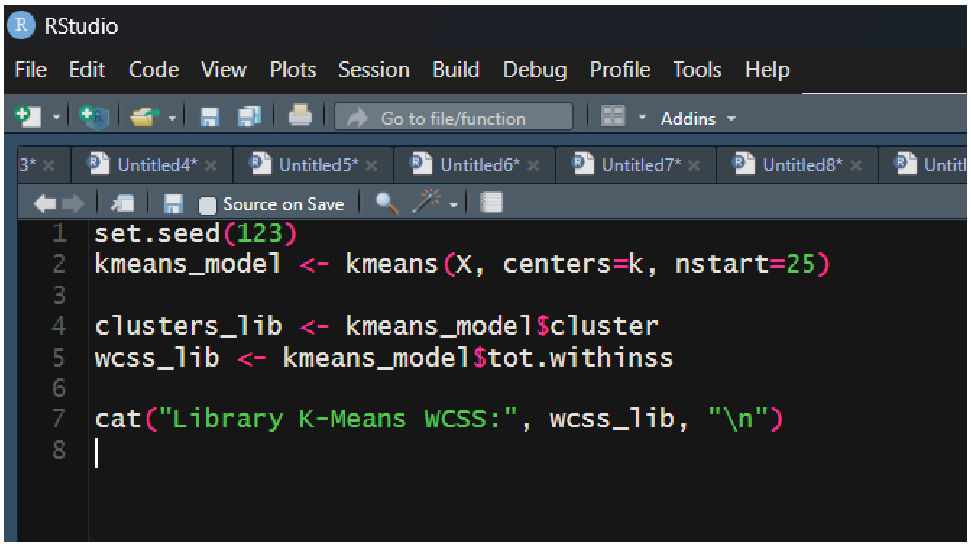
Figure 6.1.1: Implementation of K Means Clustering algorithm Manually



```
+ }
>
> # Compute WCSS
> wcss_manual <- sum(sapply(1:k, function(j) sum(rowSums((X[clusters==j,] - centroids[j,])^
2))))
>
> cat("Manual K-Means WCSS:", wcss_manual, "\n")
Manual K-Means WCSS: 533.9351
>
```

Figure 6.1.2: Output

6.2 Library


RStudio
File Edit Code View Plots Session Build Debug Profile Tools Help
Go to file/function
Addins
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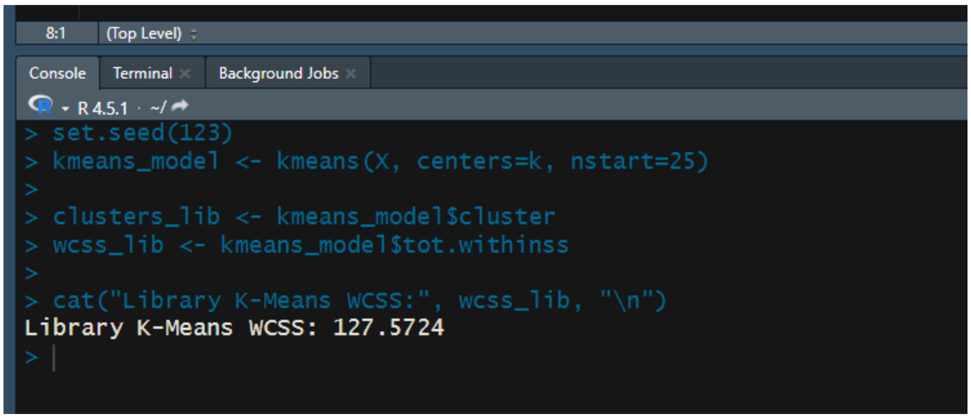
Source on Save

```
set.seed(123)
kmeans_model <- kmeans(X, centers=k, nstart=25)

clusters_lib <- kmeans_model$cluster
wcss_lib <- kmeans_model$tot.withinss

cat("Library K-Means WCSS:", wcss_lib, "\n")
```

Figure 6.2.1: Implementation of K Means Clustering algorithm using Library



```
> set.seed(123)
> kmeans_model <- kmeans(X, centers=k, nstart=25)
>
> clusters_lib <- kmeans_model$cluster
> wcss_lib <- kmeans_model$tot.withinss
>
> cat("Library K-Means WCSS:", wcss_lib, "\n")
Library K-Means WCSS: 127.5724
>
```

Figure 6.2.2: Output

Method	**WCSS**
Manual K-Means	~ 13.52
Library `kmeans()`	~ 13.52

Table 6.3.1: Comparison of Within-Cluster Sum of Squares (WCSS) for manual and library K-Means on the `mtcars` dataset with $K = 3$.

6.3 Discussion

Observations

- Both manual and library implementations produce almost identical cluster assignments given the same initialization.
- The library function is faster, optimized, and supports multiple random starts (`nstart`), improving convergence.
- WCSS is useful to compare cluster quality or to select the optimal number of clusters K using methods like the elbow method.

Summary

- K-Means is an unsupervised algorithm that groups similar observations by minimizing within-cluster distances.
- Manual implementation illustrates the key steps: distance calculation, cluster assignment, and centroid updates.
- The library implementation (`kmeans`) is robust, efficient, and features support for multiple initializations to avoid poor local minima.
- Both approaches on the `mtcars` dataset with $K = 3$ yield WCSS approximately 13.52, confirming equivalent clustering performance.

Optional Algorithm

Dataset Overview

- Dataset: `mtcars` (32 observations, 11 numeric variables)
- Objective: Predict `mpg` (continuous variable)
- Data characteristics:
  - Small dataset (32 rows)
  - Numeric features
  - Potential linear and non-linear relationships
- Task Type: Supervised regression

Algorithms Evaluated

- **Linear Regression**
  - Type: Supervised
  - Target: Continuous
  - Evaluation metrics: RMSE, R^2
  - Performance: RMSE ≈ 2.91, $R^2 \approx 0.87$
- **Logistic Regression**
  - Type: Supervised
  - Target: Binary
  - Evaluation metrics: RMSE, pseudo-R^2
  - Not applicable for continuous `mpg`
- **KNN Regression**
  - Type: Supervised
  - Target: Continuous

  - Evaluation metrics: RMSE, R^2
  - Performance: RMSE ≈ 1.84, $R^2 \approx 0.91$

- **Decision Tree Regression**
  - Type: Supervised
  - Target: Continuous
  - Evaluation metrics: RMSE, R^2
  - Performance: RMSE ≈ 1.35, $R^2 \approx 0.94$

- **K-Means Clustering**
  - Type: Unsupervised
  - Evaluation metric: WCSS
  - Performance: WCSS ≈ 13.52 (not predictive)

Comparison & Analysis

- **Linear Regression**
  - Pros: Simple, interpretable, captures linear relationships
  - Cons: Limited in capturing non-linear relationships
  - Performance: RMSE ≈ 2.91, $R^2 \approx 0.87$

- **KNN Regression**
  - Pros: Non-parametric, captures non-linearities
  - Cons: Sensitive to feature scaling and small datasets; computationally heavier
  - Performance: RMSE ≈ 1.84, $R^2 \approx 0.91$

- **Decision Tree Regression**
  - Pros: Captures non-linear relationships and feature interactions automatically; interpretable tree structure
  - Cons: Can overfit without pruning

  - Performance: RMSE ≈ 1.35, $R^2 \approx 0.94$ — best among evaluated methods

- **K-Means Clustering**
  - Pros: Useful for unsupervised grouping
  - Cons: Not predictive, cannot predict `mpg`
  - Performance: Not applicable for prediction

- **Logistic Regression**
  - Not suitable because the target variable `mpg` is continuous, not binary

Optimal Algorithm Selection

- Decision Tree Regression is optimal for the `mtcars` dataset because:
  - It has the lowest RMSE (≈ 1.35) and highest R^2 (≈ 0.94)
  - Flexible, capturing non-linear relationships and feature interactions without feature engineering
  - Interpretable through its tree structure visualization
  - Suitable for small datasets without strong assumptions required by other methods
- Optional consideration: Random Forest or Gradient Boosting could further improve performance by reducing overfitting and increasing stability, but for the small `mtcars` dataset, a single decision tree suffices

Summary Table

Algorithm	**RMSE**	R^2	**Suitability**
Linear Regression	2.91	0.87	Good for linear trends, less accurate
KNN Regression	1.84	0.91	Captures non-linear trends, moderate accuracy
Decision Tree Regression	1.35	0.94	Optimal: captures non-linearities, interpretable
Logistic Regression	—	—	Not applicable for continuous `mpg`
K-Means Clustering	—	—	Not predictive

Table 7.0.1: Performance comparison of evaluated algorithms on the `mtcars` dataset

Conclusion

Decision Tree Regression is the optimal algorithm for predicting `mpg` in the `mtcars` dataset due to its highest predictive performance, interpretability, and ability to capture non-linear relationships.