assignment_2

2024-10-16

```
library(caTools)
```

```
## Warning: package 'caTools' was built under R version 4.3.3
```

```
library(ggplot2)
```

Problem 1. Regression

```
data <- read.csv("qsar_aquatic_toxicity.csv", sep = ";", header = FALSE)
names(data) <- c(
    "TPSA",
    "SAacc",
    "H050",
    "MLOGP",
    "RDCHI",
    "GATS1p",
    "nN",
    "C040",
    "LC50"
)

head(data)
```

```
##     TPSA   SAacc H050 MLOGP RDCHI GATS1p nN C040  LC50
## 1   0.00   0.000    0 2.419 1.225  0.667  0    0 3.740
## 2   0.00   0.000    0 2.638 1.401  0.632  0    0 4.330
## 3   9.23  11.000    0 5.799 2.930  0.486  0    0 7.019
## 4   9.23  11.000    0 5.453 2.887  0.495  0    0 6.723
## 5   9.23  11.000    0 4.068 2.758  0.695  0    0 5.979
## 6 215.34 327.629    3 0.189 4.677  1.333  0    4 6.064
```

a. Split the data into a training and test set

```
# Use 70% of dataset as training set and remaining 30% as testing set
sample <- sample.split(data$LC50, SplitRatio = 0.7)
train  <- subset(data, sample == TRUE)
test   <- subset(data, sample == FALSE)
```

```r
dim(train)
```

```
## [1] 382   9
```

```r
dim(test)
```

```
## [1] 164   9
```

```r
# Fit linear regression model on training data
model <- lm(LC50 ~ ., data=train)

summary(model)
```

```
##
## Call:
## lm(formula = LC50 ~ ., data = train)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -4.3666 -0.7729 -0.0625  0.6028  5.0378
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  2.462240   0.301036   8.179 4.54e-15 ***
## TPSA         0.025519   0.003346   7.626 2.04e-13 ***
## SAacc       -0.015234   0.002555  -5.963 5.74e-09 ***
## H050         0.095604   0.072157   1.325  0.18600
## MLOGP        0.488611   0.077813   6.279 9.47e-10 ***
## RDCHI        0.511563   0.164988   3.101  0.00208 **
## GATS1p      -0.450424   0.187565  -2.401  0.01682 *
## nN          -0.147462   0.057226  -2.577  0.01035 *
## C040         0.026590   0.090711   0.293  0.76959
## ---
## Signif. codes:  0 ’***’ 0.001 ’**’ 0.01 ’*’ 0.05 ’.’ 0.1 ’ ’ 1
##
## Residual standard error: 1.202 on 373 degrees of freedom
## Multiple R-squared:  0.4954, Adjusted R-squared:  0.4846
## F-statistic: 45.77 on 8 and 373 DF,  p-value: < 2.2e-16
```

```r
# Predict on training and test datasets
pred_train <- predict(model, newdata=train)
pred_test <- predict(model, newdata=test)
```

```r
# Adding predictions columns to the datasets
train$predicted_LC50 <- pred_train
test$predicted_LC50 <- pred_test
```

```r
# Evaluate model: calculate MSE, RMSE, and R-squared for training and test sets
mse_train <- mean((train$LC50 - train$predicted_LC50)^2)
rmse_train <- sqrt(mse_train)
r2_train <- 1 - (sum((train$LC50 - train$predicted_LC50)^2) / sum((train$LC50 - mean(train$LC50))^2))
```

```r
mse_test <- mean((test$LC50 - test$predicted_LC50)^2)
rmse_test <- sqrt(mse_test)
r2_test <- 1 - (sum((test$LC50 - test$predicted_LC50)^2) / sum((test$LC50 - mean(test$LC50))^2))

# Print evaluation metrics
cat("Training Metrics:\n")
```

```
## Training Metrics:
```

```r
cat("MSE (Train): ", mse_train, "\n")
```

```
## MSE (Train):  1.410874
```

```r
cat("RMSE (Train): ", rmse_train, "\n")
```

```
## RMSE (Train):  1.187802
```

```r
cat("R-squared (Train): ", r2_train, "\n\n")
```

```
## R-squared (Train):  0.4953916
```

```r
cat("Test Metrics:\n")
```

```
## Test Metrics:
```

```r
cat("MSE (Test): ", mse_test, "\n")
```

```
## MSE (Test):  1.499417
```

```r
cat("RMSE (Test): ", rmse_test, "\n")
```

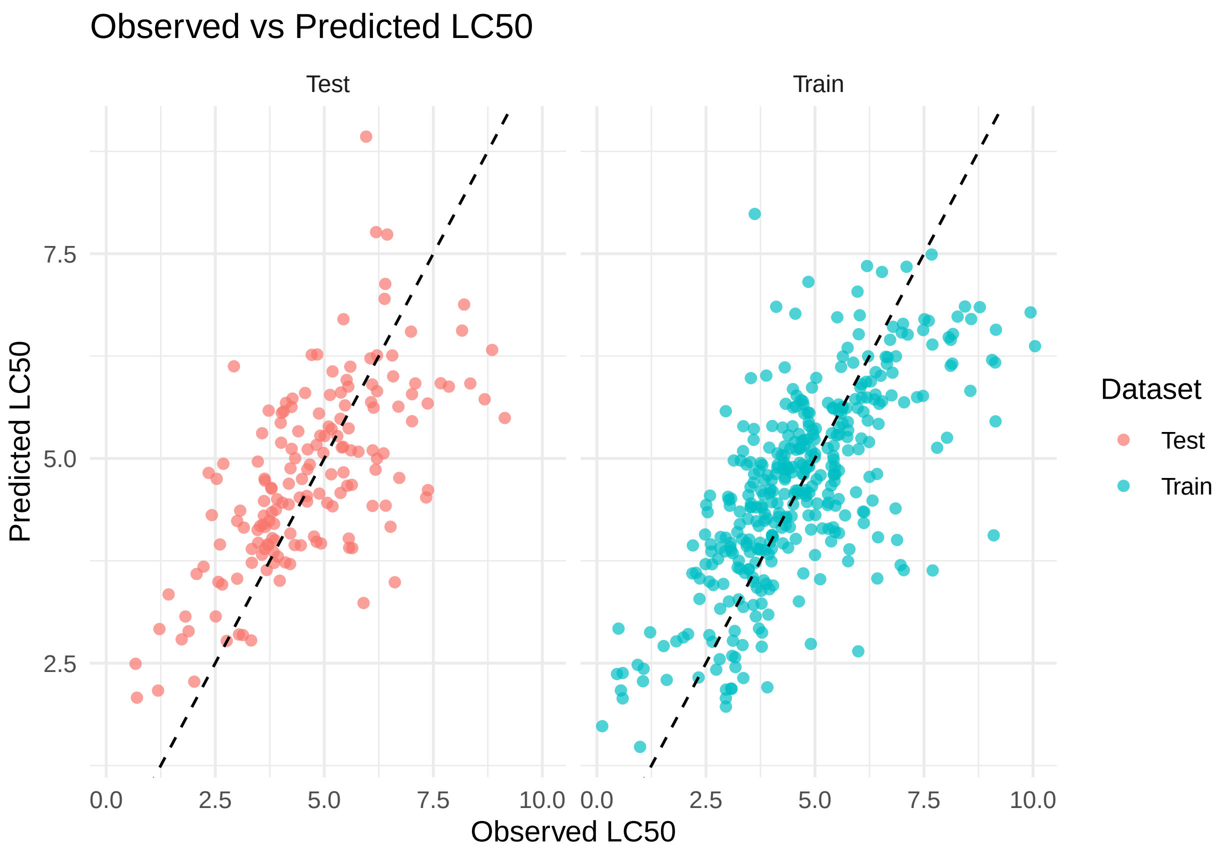
```
## RMSE (Test):  1.224507
```

```r
cat("R-squared (Test): ", r2_test, "\n")
```

```
## R-squared (Test):  0.4450487
```

```r
# Combine data for plotting
train$Dataset <- 'Train'
test$Dataset <- 'Test'
plot_data <- rbind(train, test)

# Plot observed vs predicted LC50 values
ggplot(plot_data, aes(x = LC50, y = predicted_LC50, color = Dataset)) +
  geom_point(alpha = 0.7) +
  geom_abline(intercept = 0, slope = 1, linetype = "dashed") +
  labs(title = "Observed vs Predicted LC50", x = "Observed LC50", y = "Predicted LC50") +
  theme_minimal() +
  facet_wrap(~Dataset)
```


Observed vs Predicted LC50
Test
Train
Predicted LC50
Observed LC50
2.5
5.0
7.5
0.0
2.5
5.0
7.5
10.0
0.0
2.5
5.0
7.5
10.0
Dataset
Test
Train