

Regression and Classification: A Comprehensive Analysis

Gabriele Durante

In this report, we aim to explore various statistical learning methodologies applied to regression and classification problems.

In the first part of the report, we examine linear regression models applied to aquatic toxicity data. This involves both traditional linear effects and alternative representations using dummy encoding, providing insight into how these transformations impact model fit and predictive accuracy. We apply techniques such as backward elimination and forward selection to perform variable selection, comparing criteria like AIC and BIC. Moreover, we introduce regularization techniques, specifically ridge regression, to address potential overfitting, followed by a discussion on parameter optimization via cross-validation and bootstrap methods. To extend our analysis to non-linear modeling, we apply generalized additive models (GAMs) with smoothing splines to capture more complex relationships within the data. Regression trees are explored, where we employ cost-complexity pruning to optimize tree size, emphasizing the balance between model complexity and prediction accuracy.

In the second part, we shift to a classification problem using the Pima Indians Diabetes dataset. Here, we experiment with k-nearest neighbors (k-NN), generalized additive models, classification trees, bagged trees, random forests, and neural networks. Each method is rigorously evaluated, using cross-validation techniques to assess generalization error and performance trade-offs. The report concludes with a comparative analysis of these models, offering insights into the advantages and limitations of different statistical learning approaches within the context of high-dimensional data.

Regression Model Comparison for Predicting Aquatic Toxicity

In this study, we investigate the acute aquatic toxicity of various organic molecules, as quantified by the lethal concentration (LC50) that induces mortality in 50% of the planktonic crustacean *Daphnia magna* over a 48-hour exposure period. The objective is to develop predictive models that leverage molecular descriptors to ascertain the toxicity levels of these compounds. To this end, we utilize a dataset comprising 546 observations, which is sourced from the UCI Machine Learning Repository. The dataset encompasses eight key molecular descriptors identified as significant predictors of LC50:

- TPSA: Topological Polar Surface Area, calculated via a contribution method considering the presence of nitrogen, oxygen, potassium, and sulfur.
- SAacc: Van der Waals Surface Area (VSA) of hydrogen bond acceptor atoms.
- H050: The count of hydrogen atoms bonded to heteroatoms.
- MLOGP: A measure of lipophilicity, serving as a critical determinant of narcosis.
- RDCHI: A topological index encapsulating information related to molecular size and branching.
- GATS1p: An indicator of molecular polarizability.
- nN: The total number of nitrogen atoms within the molecule.
- C040: The count of specific carbon atom types, including those found in esters, carboxylic acids, thioesters, carbamic acids, and nitriles.

```
summary(data)
```

| ## | TPSA | SAacc | H050 | MLOGP |
|----|----------------|----------------|-----------------|----------------|
| ## | Min. : 0.00 | Min. : 0.00 | Min. : 0.0000 | Min. : -6.446 |
| ## | 1st Qu.: 15.79 | 1st Qu.: 11.00 | 1st Qu.: 0.0000 | 1st Qu.: 1.232 |

```
## Median : 40.46      Median : 42.68      Median : 0.0000      Median : 2.273
## Mean   : 48.47      Mean   : 58.87      Mean   : 0.9377      Mean   : 2.313
## 3rd Qu.: 70.02      3rd Qu.: 77.49      3rd Qu.: 1.0000      3rd Qu.: 3.393
## Max.   :347.32      Max.   :571.95      Max.   :18.0000      Max.   : 9.148
##      RDCHI          GATS1p          nN          C040
## Min.   :1.000      Min.   :0.281      Min.   : 0.000      Min.   : 0.0000
## 1st Qu.:1.975      1st Qu.:0.737      1st Qu.: 0.000      1st Qu.: 0.0000
## Median :2.344      Median :1.020      Median : 1.000      Median : 0.0000
## Mean   :2.492      Mean   :1.046      Mean   : 1.004      Mean   : 0.3535
## 3rd Qu.:2.911      3rd Qu.:1.266      3rd Qu.: 2.000      3rd Qu.: 0.0000
## Max.   :6.439      Max.   :2.500      Max.   :11.000      Max.   :11.0000
##      LC50
## Min.   : 0.122
## 1st Qu.: 3.602
## Median : 4.516
## Mean   : 4.658
## 3rd Qu.: 5.607
## Max.   :10.047
```

```
colSums(is.na(data))
```

```
##      TPSA      SAacc      H050      MLOGP      RDCHI      GATS1p      nN      C040      LC50
##       0         0         0         0         0         0         0         0         0
```

With a complete dataset comprising 546 observations, we can ensure that our modeling efforts are not hindered by data gaps. This completeness facilitates a more accurate assessment of the relationships between the molecular descriptors and LC50, allowing for a more confident interpretation of the findings and their implications in predicting aquatic toxicity.

Linear and Dummy Encoding Approach

To evaluate the predictive models effectively, we partition the dataset into training and testing subsets. A random seed is set using `set.seed(2024)` to ensure reproducibility. The training set is constructed by sampling approximately two-thirds of the total observations with the command `index <- sample(1:nrow(data), size = round(2/3 * nrow(data)))`.

- Training Data: `trainData <- data[index,]` comprises the selected observations for model fitting.
- Testing Data: `testData <- data[-index,]` contains the remaining observations for model evaluation.

```
# build the dataset for the training
set.seed(2024)
index <- sample(1:nrow(data), size = round(2/3 * nrow(data)))
trainData <- data[index, ]
testData <- data[-index, ]
```

Linear Model

First we fitted a linear regression model to predict LC50 using molecular descriptors from the training dataset. The model's performance is summarized as follows:

```
set.seed(2024)
### Modeling Count Variables Directly as Linear Effects
modell1 <- lm(LC50 ~., data = trainData)

pred_model1_train <- predict(modell1, newdata = trainData)
pred_model1_test  <- predict(modell1, newdata = testData)
```

```
error_train <- mean((pred_model1_train - trainData$LC50)^2)
error_test <- mean((pred_model1_test - testData$LC50)^2)
```

```
cat("Training Error (Linear):", error_train, "\n")
```

```
## Training Error (Linear): 1.377162
```

```
cat("Test Error (Linear):", error_test, "\n")
```

```
## Test Error (Linear): 1.556978
```

```
summary(model1)
```

```
##
## Call:
## lm(formula = LC50 ~ ., data = trainData)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -4.1890 -0.7482 -0.1153  0.6079  3.7987
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  2.875587   0.298304   9.640 < 2e-16 ***
## TPSA         0.026589   0.003220   8.258 2.96e-15 ***
## SAacc        -0.012127   0.002522  -4.809 2.25e-06 ***
## H050          0.031343   0.070945   0.442  0.65891
## MLOGP         0.496920   0.077134   6.442 3.83e-10 ***
## RDCHI         0.308016   0.166170   1.854  0.06462 .
## GATS1p        -0.537871   0.187291  -2.872  0.00433 **
## nN            -0.198318   0.057041  -3.477  0.00057 ***
## C040          -0.055902   0.090200  -0.620  0.53582
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.188 on 355 degrees of freedom
## Multiple R-squared:  0.4721, Adjusted R-squared:  0.4602
## F-statistic: 39.68 on 8 and 355 DF, p-value: < 2.2e-16
```

The R-squared value of 0.472 indicates that while the linear model captures some of the variability in the data, it leaves a considerable amount unexplained. Highly significant predictors, such as TPSA ($p < 2e-16$) and MLOGP ($p < 3.83e-10$), reveal strong relationships with LC50, indicating that increased topological polar surface area and greater lipophilicity correlate with higher toxicity levels.

Dummy Linear Model

After, model dummy encoding was applied to the count variables nN, C040, and H050 in both the training and test datasets to transform these continuous variables into binary indicators. Specifically, values greater than zero were recoded to 1, while values of zero were recoded to 0. This approach allows the linear model to assess the presence or absence of these variables as factors influencing acute aquatic toxicity. Predictions were generated for both the training and test datasets, enabling the calculation of the training error and test error.

```
### Dummy Encoding for Count Variables
```

```
train_dummy <- trainData
```

```
test_dummy <- testData
```

```
# dummy encoding
```

```

train_dummy$nN <- ifelse(train_dummy$nN > 0, 1, 0)
test_dummy$nN <- ifelse(test_dummy$nN > 0, 1, 0)
test_dummy$C040 <- ifelse(test_dummy$C040 > 0, 1, 0)
train_dummy$C040 <- ifelse(train_dummy$C040 > 0, 1, 0)
test_dummy$H050 <- ifelse(test_dummy$H050 > 0, 1, 0)
train_dummy$H050 <- ifelse(train_dummy$H050 > 0, 1, 0)

model2 <- lm(train_dummy$LC50 ~ ., data = train_dummy)

pred_model2_train <- predict(model2, newdata = train_dummy)
pred_model2_test <- predict(model2, newdata = test_dummy)

error_train_dummy <- mean((pred_model2_train - train_dummy$LC50)^2)
error_test_dummy <- mean((pred_model2_test - test_dummy$LC50)^2)

cat("Training Error (Dummy):", error_train_dummy, "\n")

## Training Error (Dummy): 1.424236

cat("Test Error (Dummy):", error_test_dummy, "\n")

## Test Error (Dummy): 1.616825

summary(model2)

##
## Call:
## lm(formula = train_dummy$LC50 ~ ., data = train_dummy)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -4.0143 -0.7807 -0.1313  0.6313  3.7856
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  3.007963   0.305982   9.831 < 2e-16 ***
## TPSA         0.022380   0.003185   7.026 1.09e-11 ***
## SAacc        -0.010184   0.002193  -4.643 4.83e-06 ***
## H050         -0.097746   0.154467  -0.633 0.52727
## MLOGP        0.502377   0.076886   6.534 2.22e-10 ***
## RDCHI        0.262639   0.167774   1.565 0.11837
## GATS1p       -0.559217   0.185302  -3.018 0.00273 **
## nN           -0.054983   0.149020  -0.369 0.71237
## C040         -0.162055   0.162002  -1.000 0.31783
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.208 on 355 degrees of freedom
## Multiple R-squared:  0.454, Adjusted R-squared:  0.4417
## F-statistic: 36.9 on 8 and 355 DF, p-value: < 2.2e-16

```

The training error for the dummy-encoded model is 1.424, while the test error is 1.617. Compared to the previous linear model, which yielded a training error of 1.377 and a test error of 1.557, this model exhibits slightly higher error rates on both the training and test datasets. This increase suggests that the dummy encoding may not have improved the model's predictive performance. This could indicate a potential loss of information due to the transformation of continuous variables into binary indicators, which could limit the

model's ability to capture the nuances of the underlying relationships between predictors and the response variable.

The overall model performance is reflected in the Multiple R-squared value of 0.454, while the adjusted R-squared of 0.4417 accounts for the number of predictors in the model. The F-statistic (36.9) with a p-value $< 2.2\text{e-}16$ indicates that the model is statistically significant.

Empirical Error Distribution Analysis in Regression Models

The function `perform_analysis` is defined to conduct repeated evaluations of the two linear models defined before on the same dataset and returns the values of error test and train. The analysis is repeated 200 times using the `replicate` function, enabling the computation of average test errors for both models. The results are then visualized using a density plot, illustrating the empirical distribution of test errors for each model.

```
library(ggplot2)

perform_analysis <- function(data) {
  index <- sample(1:nrow(data), size = round(2/3 * nrow(data)))
  trainData <- data[index, ]
  testData <- data[-index, ]

  # model 1
  model1 <- lm(LC50 ~., data = trainData)
  pred_model1_train_200 <- predict(model1, newdata = trainData)
  pred_model1_test_200 <- predict(model1, newdata = testData)
  error_train_200_lm <- mean((pred_model1_train_200 - trainData$LC50)^2)
  error_test_200_lm <- mean((pred_model1_test_200 - testData$LC50)^2)

  # model 2
  train_dummy <- trainData
  test_dummy <- testData

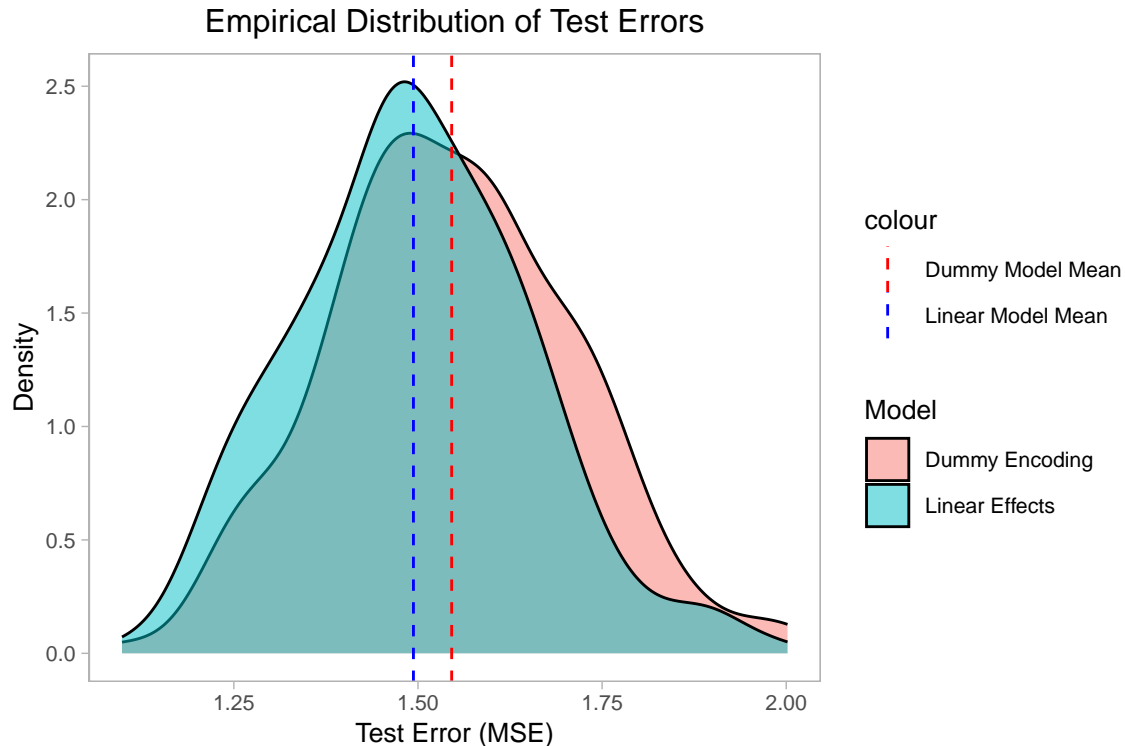
  # dummy encoding
  train_dummy$nN <- ifelse(train_dummy$nN > 0, 1, 0)
  test_dummy$nN <- ifelse(test_dummy$nN > 0, 1, 0)
  test_dummy$C040 <- ifelse(test_dummy$C040 > 0, 1, 0)
  train_dummy$C040 <- ifelse(train_dummy$C040 > 0, 1, 0)
  test_dummy$H050 <- ifelse(test_dummy$H050 > 0, 1, 0)
  train_dummy$H050 <- ifelse(train_dummy$H050 > 0, 1, 0)

  model2 <- lm(train_dummy$LC50 ~ ., data = train_dummy)

  pred_model2_train <- predict(model2, newdata = train_dummy)
  pred_model2_test <- predict(model2, newdata = test_dummy)

  error_train_200_dummy <- mean((pred_model2_train - train_dummy$LC50)^2)
  error_test_200_dummy <- mean((pred_model2_test - test_dummy$LC50)^2)

  return(c(error_test_200_lm, error_test_200_dummy))
}
```



The graph presents a density plot comparing the test error distributions for the two models. The aim should be illustrate the performance of the models on unseen data and their reliability, focusing on the variability and central tendency of their respective errors. The Linear Model exhibits a narrower distribution centered around a lower MSE compared to the Dummy Model, whose distribution appears wider and shifted slightly to the right, indicating higher average test error. Basically, the tighter distribution and lower mean MSE of the Linear Model suggest that it generalize better to the test set compared to the dummy model.

Variable Selection Methods in Linear Regression

In this section we will look at model selection, which involves evaluating a trade-off between the goodness of fit of the model, which reflects the ability to fit the observed data, and the complexity of the model, which refers to the number of parameters used. To do this, various model selection criteria have been developed to guide the choice of parsimonious models that offer good generalization. Two of these widely used criteria are the Akaike Information Criterion (AIC) and the Bayesian Information Criterion (BIC). The AIC estimates the loss of information when a candidate model is used to represent the real data generation process, aiming to minimize this loss. On the other hand, the BIC is derived from a Bayesian perspective and approaches model selection as choosing the model with the highest posterior probability given the observed data. Both the AIC and BIC take into consideration the goodness of fit of the model and penalize model complexity, although the BIC imposes a stricter penalty for complexity, favoring simpler models than the AIC. The Forward Selection method starts with a model containing only one intercept and iteratively adds variables one at a time, selecting at each step the variable that leads to the maximum reduction in AIC or BIC. In contrast, the Backward method starts with a complete model and iteratively removes variables that contribute less significantly to the model, evaluated again by the AIC or BIC. Both the Stepwise and Backward methods provide systematic strategies for model selection, guided by the goal of finding a model that balances goodness of fit and complexity as quantified by the AIC or BIC.

```
summary(backward_aic)
```

```
##  
## Call:
```

```
## lm(formula = LC50 ~ TPSA + SAacc + MLOGP + RDCHI + GATS1p + nN,
##     data = trainData)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -4.1632 -0.7485 -0.1143  0.6156  3.8169
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  2.970390   0.278237  10.676 < 2e-16 ***
## TPSA         0.026358   0.003125   8.435 8.35e-16 ***
## SAacc       -0.011638   0.001946  -5.980 5.40e-09 ***
## MLOGP        0.487552   0.073711   6.614 1.37e-10 ***
## RDCHI        0.290699   0.162996   1.783 0.075358 .
## GATS1p      -0.573581   0.179110  -3.202 0.001485 **
## nN          -0.197504   0.054796  -3.604 0.000357 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.187 on 357 degrees of freedom
## Multiple R-squared:  0.4707, Adjusted R-squared:  0.4618
## F-statistic: 52.91 on 6 and 357 DF, p-value: < 2.2e-16
```

```
summary(backward_bic)
```

```
##
## Call:
## lm(formula = LC50 ~ TPSA + SAacc + MLOGP + GATS1p + nN, data = trainData)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -4.0473 -0.7751 -0.0928  0.5879  3.7865
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  3.123831   0.265406  11.770 < 2e-16 ***
## TPSA         0.028625   0.002863   9.997 < 2e-16 ***
## SAacc       -0.010068   0.001741  -5.783 1.6e-08 ***
## MLOGP        0.594639   0.042886  13.866 < 2e-16 ***
## GATS1p      -0.466421   0.169244  -2.756 0.006152 **
## nN          -0.187790   0.054690  -3.434 0.000665 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.19 on 358 degrees of freedom
## Multiple R-squared:  0.466, Adjusted R-squared:  0.4585
## F-statistic: 62.47 on 5 and 358 DF, p-value: < 2.2e-16
```

```
summary(forward_aic)
```

```
##
## Call:
## lm(formula = LC50 ~ MLOGP + TPSA + SAacc + nN + GATS1p + RDCHI,
##     data = trainData)
##
```

```
## Residuals:
##      Min       1Q   Median       3Q      Max
## -4.1632 -0.7485 -0.1143  0.6156  3.8169
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  2.970390   0.278237  10.676 < 2e-16 ***
## MLOGP        0.487552   0.073711   6.614 1.37e-10 ***
## TPSA         0.026358   0.003125   8.435 8.35e-16 ***
## SAacc        -0.011638   0.001946  -5.980 5.40e-09 ***
## nN           -0.197504   0.054796  -3.604 0.000357 ***
## GATS1p       -0.573581   0.179110  -3.202 0.001485 **
## RDCHI        0.290699   0.162996   1.783 0.075358 .
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.187 on 357 degrees of freedom
## Multiple R-squared:  0.4707, Adjusted R-squared:  0.4618
## F-statistic: 52.91 on 6 and 357 DF,  p-value: < 2.2e-16
```

```
summary(forward_bic)
```

```
##
## Call:
## lm(formula = LC50 ~ MLOGP + TPSA + SAacc + nN + GATS1p, data = trainData)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -4.0473 -0.7751 -0.0928  0.5879  3.7865
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  3.123831   0.265406  11.770 < 2e-16 ***
## MLOGP        0.594639   0.042886  13.866 < 2e-16 ***
## TPSA         0.028625   0.002863   9.997 < 2e-16 ***
## SAacc        -0.010068   0.001741  -5.783 1.6e-08 ***
## nN           -0.187790   0.054690  -3.434 0.000665 ***
## GATS1p       -0.466421   0.169244  -2.756 0.006152 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.19 on 358 degrees of freedom
## Multiple R-squared:  0.466, Adjusted R-squared:  0.4585
## F-statistic: 62.47 on 5 and 358 DF,  p-value: < 2.2e-16
```

```
# Compare Models
```

```
print(backward_aic$call)
```

```
lm(formula = LC50 ~ TPSA + SAacc + MLOGP + RDCHI + GATS1p + nN, data = trainData)
```

```
print(backward_bic$call)
```

```
lm(formula = LC50 ~ TPSA + SAacc + MLOGP + GATS1p + nN, data = trainData)
```

```
print(forward_aic$call)
```

```
lm(formula = LC50 ~ MLOGP + TPSA + SAacc + nN + GATS1p + RDCHI, data = trainData)
```



```
print(forward_bic$call)
```

```
lm(formula = LC50 ~ MLOGP + TPSA + SAacc + nN + GATS1p, data = trainData)
```

```
# Model Comparisons
```

```
cat(paste(
  "AIC Backward:", AIC(backward_aic), "\n",
  "AIC Forward:", AIC(forward_aic), "\n",
  "BIC Backward:", BIC(backward_bic), "\n",
  "BIC Forward:", BIC(forward_bic), "\n"
))
```

```
## AIC Backward: 1166.42136187616
## AIC Forward: 1166.42136187616
## BIC Backward: 1194.93024571721
## BIC Forward: 1194.93024571721
```

Both the AIC and BIC values are identical between the forward and backward procedures, suggesting that the model selection methods converge on the same models based on the respective criterion. The AIC favors slightly more complex models by retaining RDCHI, while the BIC prefers more parsimonious models by excluding it.

Ridge Regression Model Optimization

In this section, we apply Ridge regression to predict the target variable and utilize two methods: cross-validation and bootstrapping to determine the optimal regularization parameter λ . We are doing this because Ridge regression is particularly useful in reducing model complexity and handling multicollinearity by penalizing large coefficients and could improve our current situation. We explore a grid of λ values and contrast the outcomes of the two methods, each aimed at finding the best balance between bias and variance.

The cross-validation method used is 10-fold and the bootstrap procedure resample the training data 100 times. Both techniques are applied to a manually chosen grid of candidate λ values ranging from 10^3 to 10^{-2} .

```
library(glmnet)
library(boot)

index <- sample(seq_len(nrow(data)), size = 2/3 * nrow(data))
trainData <- data[index, ]
testData <- data[-index, ]

X_train <- as.matrix(trainData[, -ncol(trainData)])
y_train <- trainData$LC50
X_test <- as.matrix(testData[, -ncol(testData)])
y_test <- testData$LC50

lambda_grid <- 10^seq(3, -2, length = 100)

# Ridge regression (CV)
cv_ridge <- cv.glmnet(X_train, y_train, alpha = 0,
  lambda = lambda_grid, nfolds = 10)
optimal_lambda_cv <- cv_ridge$lambda.min
```

Optimal lambda from Cross-Validation: 0.01

```
ridge_model <- glmnet(X_train, y_train, alpha = 0,
  lambda = optimal_lambda_cv)
```

```
train_predictions_ridge <- predict(ridge_model, newx = X_train)
test_predictions_ridge <- predict(ridge_model, newx = X_test)

mse_train_ridge <- mean((y_train - train_predictions_ridge)^2)
mse_test_ridge <- mean((y_test - test_predictions_ridge)^2)
```

```
cat("Training Error (Ridge):", mse_train_ridge, "\n")
```

```
## Training Error (Ridge): 1.377282
```

```
cat("Test Error (Ridge):", mse_test_ridge, "\n")
```

```
## Test Error (Ridge): 1.554029
```

The cross-validation process identifies the optimal λ by splitting the dataset into 10 folds and measuring the model's performance on different subsets. This approach tends to balance bias and variance by repeatedly testing the model on different parts of the data. The result showed an optimal λ of 0.01 with a corresponding training error (MSE) of 1.377282 and a test error of 1.554029. These errors indicate that the model performs well on both the training and test sets, demonstrating low variance and good generalization.

```
# Ridge regression (bootstrap)
bootstrap_mse <- function(data, indices, lambda) {
  # Create sample
  bootstrap_sample <- data[indices, ]
  X_bootstrap <- as.matrix(bootstrap_sample[, -ncol(bootstrap_sample)])
  y_bootstrap <- bootstrap_sample$LC50

  model <- glmnet(X_bootstrap, y_bootstrap, alpha = 0, lambda = lambda)
  y_pred <- predict(model, s = lambda, newx = X_test)
  mse <- mean((y_test - y_pred)^2)
  return(mse)
}

# Bootstrap for multiple lambda values
bootstrap_results <- sapply(lambda_grid, function(lambda) {
  mse_values <- replicate(100, boot(trainData, bootstrap_mse, R = 1,
                                   lambda = lambda)$t)

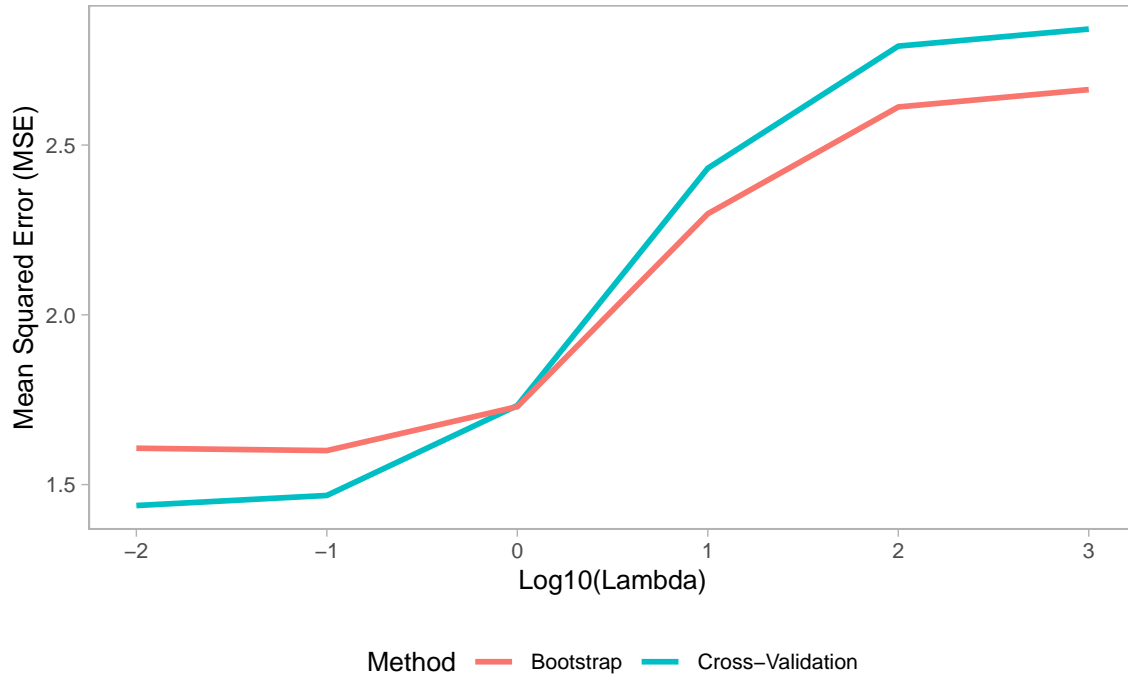
  return(mean(mse_values))
})
```

```
# Optimal Lambda from Bootstrap
optimal_lambda_bootstrap <- lambda_grid[which.min(bootstrap_results)]
cat("Optimal lambda from Bootstrap:", optimal_lambda_bootstrap, "\n")
```

```
## Optimal lambda from Bootstrap: 0.1
```

The bootstrap method resamples the dataset 100 times to evaluate the stability of the model and its performance under various random samples. The key advantage of this approach is that it generates different training datasets to capture variability. The bootstrap results across multiple λ values yielded an optimal λ of 0.1.

Comparison of MSE from Cross-Validation and Bootstrap



The results of the two methods are contrasted using a plot, where the MSE curves are plotted against $\log_{10}(\lambda)$. Both curves exhibit a similar trend, showing a U-shape where error decreases initially with decreasing λ (left-hand side of the plot) before rising as λ increases.

The optimal λ for cross-validation is slightly lower ($\log_{10}(\lambda) = -2$) compared to that of bootstrap ($\log_{10}(\lambda) = -1$). The Cross-Validation method may prefer a model with more regularization compared to Bootstrap, which tends to allow slightly more complexity (i.e., a higher λ). So in this case, Cross-Validation seems to provide a more stable and slightly better performance estimate, as shown by the lower MSE values.

Non-linear Modeling Using Generalized Additive Models

Generalized Additive Models (GAMs) offer a useful compromise between linear models and fully non-parametric models. They allow fitting a non-linear function f_j to each X_j , enabling the automatic modeling of non-linear relationships that standard linear regression would not detect. Since the model is additive, we can still examine the effect of each X_j on Y individually, keeping all other variables fixed. The smoothness of the function f_j for the variable X_j can be summarized by the degrees of freedom. The main limitation of GAMs is that the model is constrained to be additive. With many variables, it is possible to miss important interactions. However, as with linear regression, we can manually add interaction terms to the GAM model by including additional predictors in the form of $X_j \times X_k$. We can also add low-dimensional interaction functions in the form of $f_{jk}(X_j, X_k)$ to the model. Such terms can be fitted using two-dimensional smoothers, such as local regression or two-dimensional splines.

```
sapply(trainData, function(x) length(unique(x)))
```

```
##   TPSA   SAacc   H050   MLOGP   RDCHI   GATS1p   nN   C040   LC50
##   171    160     9    283    259    289     9     6    347
```

```
# GAM less complexity (k = -1)
```

```
k = 1
```

```
gam_model_1 <- gam(LC50 ~ s(TPSA, k=k) + s(SAacc, k=k) + s(H050, k=k) +
                    s(MLOGP, k=k) + s(RDCHI, k=k) + s(GATS1p, k=k) +
```

```

      s(nN, k=k) + s(C040, k=k), data = trainData)

pred_gam_train_1 <- predict(gam_model_1, newdata = trainData)
pred_gam_test_1 <- predict(gam_model_1, newdata = testData)
mse_train_gam_1 <- mean((y_train - pred_gam_train_1)^2)
mse_test_gam_1 <- mean((y_test - pred_gam_test_1)^2)

cat("Training Error (GAM - k=1):", "\t", mse_train_gam_1, "\n")

## Training Error (GAM - k=1):    1.300005

cat("Test Error (GAM - k=1):", "\t", mse_test_gam_1, "\n")

## Test Error (GAM - k=1):    1.565394

# GAM more complexity (k = 6)
k = 6
gam_model_2 <- gam(LC50 ~ s(TPSA, k=k) + s(SAacc, k=k) + s(H050, k=k) +
      s(MLOGP, k=k) + s(RDCHI, k=k) + s(GATS1p, k=k) +
      s(nN, k=k) + s(C040, k=k), data = trainData)

pred_gam_train_2 <- predict(gam_model_2, newdata = trainData)
pred_gam_test_2 <- predict(gam_model_2, newdata = testData)
mse_train_gam_2 <- mean((y_train - pred_gam_train_2)^2)
mse_test_gam_2 <- mean((y_test - pred_gam_test_2)^2)

cat("Training Error (GAM - k=6):", "\t", mse_train_gam_2, "\n")

## Training Error (GAM - k=6):    1.147883

cat("Test Error (GAM - k=6):", "\t", mse_test_gam_2, "\n")

## Test Error (GAM - k=6):    1.634775

```

The first model (`gam_model_1`) is specified with $k = 1$, indicating a lower complexity where each smooth term is linear. The second model (`gam_model_2`) is specified with $k = 6$ (higher value for the model due to unique values for each variable), allowing for more flexibility and complexity in the smooth terms.

`gam_model_2` has a lower training error, its increased complexity results in higher test error compared to `gam_model_1`. Therefore, despite `gam_model_1`'s higher test error, it may be preferable due to its generalization capability.

Regression Tree Model with Cost-Complexity Pruning

```

library(rpart)
library(rpart.plot)

tree_model <- rpart(LC50 ~ ., data = trainData, method = "anova")

train_predictions_tree1 <- predict(tree_model, newdata = trainData)
test_predictions_tree1 <- predict(tree_model, newdata = testData)

mse_train_tree1 <- mean((trainData$LC50 - train_predictions_tree1)^2)
mse_test_tree1 <- mean((testData$LC50 - test_predictions_tree1)^2)

printcp(tree_model)

```

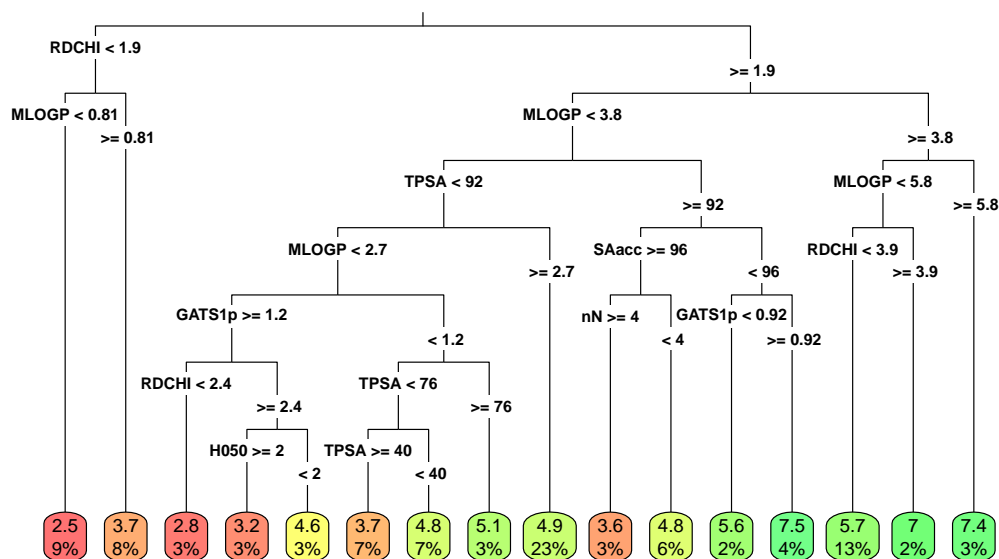
```
##
## Regression tree:
## rpart(formula = LC50 ~ ., data = trainData, method = "anova")
##
## Variables actually used in tree construction:
## [1] GATS1p H050 MLOGP nN RDCHI SAacc TPSA
##
## Root node error: 949.5/364 = 2.6085
##
## n= 364
##
##      CP nsplit rel error  xerror   xstd
## 1  0.202576      0  1.00000 1.00521 0.081444
## 2  0.120003      1  0.79742 0.89217 0.074688
## 3  0.055504      2  0.67742 0.71621 0.060411
## 4  0.029750      4  0.56641 0.68528 0.057679
## 5  0.024807      5  0.53666 0.69253 0.060911
## 6  0.019644      6  0.51186 0.69168 0.061473
## 7  0.018758      7  0.49221 0.68003 0.061525
## 8  0.018127      8  0.47345 0.68003 0.061525
## 9  0.012598      9  0.45533 0.68531 0.063366
## 10 0.011999     10  0.44273 0.70330 0.069257
## 11 0.011431     11  0.43073 0.70041 0.069312
## 12 0.011033     13  0.40787 0.69407 0.069352
## 13 0.010592     14  0.39684 0.69141 0.068352
## 14 0.010000     15  0.38625 0.68556 0.068029

cat("Training Error (Tree):", mse_train_tree1, "\n")

## Training Error (Tree): 1.007531
cat("Test Error (Tree):", mse_test_tree1, "\n")

## Test Error (Tree): 2.053224
```

Customized Regression Tree for LC50



```
optimal_cp <- tree_model$cptable[which.min(tree_model$cptable[, "xerror"]), "CP"]
```

```
pruned_tree <- prune(tree_model, cp = optimal_cp)
train_predictions_tree <- predict(pruned_tree, newdata = trainData)
test_predictions_tree <- predict(pruned_tree, newdata = testData)
```

```
mse_train_tree <- mean((trainData$LC50 - train_predictions_tree)^2)
mse_test_tree <- mean((testData$LC50 - test_predictions_tree)^2)
```

```
printcp(pruned_tree)
```

```
##
## Regression tree:
## rpart(formula = LC50 ~ ., data = trainData, method = "anova")
##
## Variables actually used in tree construction:
## [1] GATS1p MLOGP RDCHI SAacc TPSA
##
## Root node error: 949.5/364 = 2.6085
##
## n= 364
##
##      CP nsplit rel error  xerror   xstd
## 1 0.202576      0  1.00000 1.00521 0.081444
## 2 0.120003      1  0.79742 0.89217 0.074688
## 3 0.055504      2  0.67742 0.71621 0.060411
## 4 0.029750      4  0.56641 0.68528 0.057679
## 5 0.024807      5  0.53666 0.69253 0.060911
## 6 0.019644      6  0.51186 0.69168 0.061473
```

```
## 7 0.018758      7    0.49221 0.68003 0.061525
```

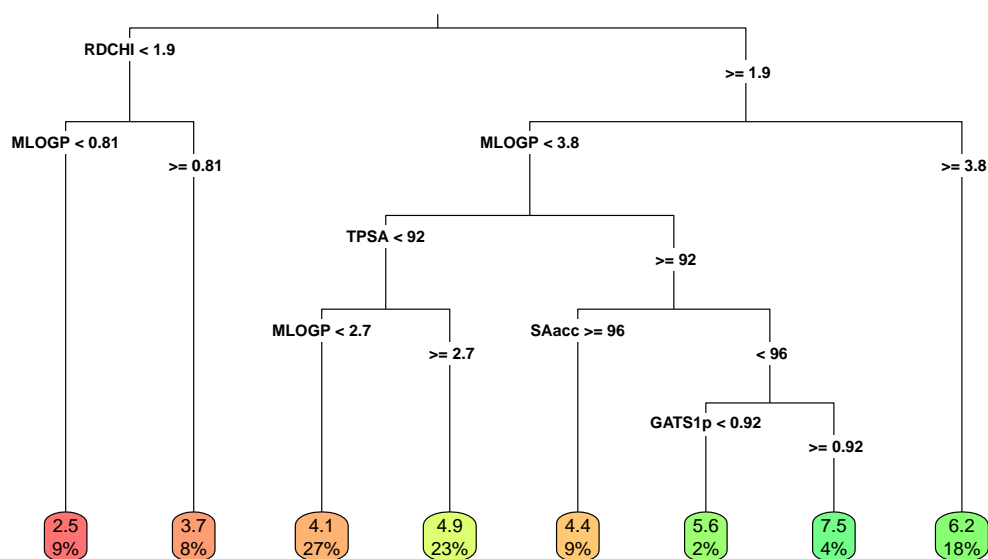
```
cat("Training Error (Tree):", mse_train_tree, "\n")
```

```
## Training Error (Tree): 1.283949
```

```
cat("Test Error (Tree):", mse_test_tree, "\n")
```

```
## Test Error (Tree): 2.016152
```

Pruned Regression Tree for LC50



Comparative Analysis of Regression Models

Training and Test Error Assessment for Various Models



Classification Model Comparison for Diabetes Prediction

k-NN Classification and Cross-Validation Comparison

```
library(mlbench)
data(PimaIndiansDiabetes2)
df <- PimaIndiansDiabetes2
head(df)

##   pregnant glucose pressure triceps insulin mass pedigree age diabetes
## 1         6      148       72      35      NA  33.6   0.627  50      pos
## 2         1       85       66      29      NA  26.6   0.351  31      neg
## 3         8      183       64      NA      NA  23.3   0.672  32      pos
## 4         1       89       66      23     94  28.1   0.167  21      neg
## 5         0      137       40      35    168  43.1   2.288  33      pos
## 6         5      116       74      NA      NA  25.6   0.201  30      neg

na_count <- sapply(df, function(x) sum(is.na(x)))
print(na_count)

## pregnant glucose pressure triceps insulin mass pedigree age
##         0         5        35       227      374        11         0         0
## diabetes
##         0

# KNN imputation

library(mlbench)
library(VIM)

df_imp <- kNN(df, k = 5)
df_imp <- df_imp[, 1:9]
df_imp$diabetes <- as.factor(df_imp$diabetes)
head(df_imp)

##   pregnant glucose pressure triceps insulin mass pedigree age diabetes
## 1         6      148       72      35     175  33.6   0.627  50      pos
## 2         1       85       66      29      55  26.6   0.351  31      neg
## 3         8      183       64      28     325  23.3   0.672  32      pos
## 4         1       89       66      23     94  28.1   0.167  21      neg
## 5         0      137       40      35    168  43.1   2.288  33      pos
## 6         5      116       74      27     112  25.6   0.201  30      neg

na_count_df_imp <- sapply(df_imp, function(x) sum(is.na(x)))
print(na_count_df_imp)

## pregnant glucose pressure triceps insulin mass pedigree age
##         0         0         0         0         0         0         0         0
## diabetes
##         0

library(caret)
set.seed(2024)
trainIndex <- createDataPartition(df_imp$diabetes,
                                   p = 2/3,
                                   list = FALSE,
                                   times = 1)
```

```

trainData <- df_imp[trainIndex, ]
testData <- df_imp[-trainIndex, ]

trainData$diabetes <- ifelse(trainData$diabetes == "pos", 1, 0)
testData$diabetes <- ifelse(testData$diabetes == "pos", 1, 0)
trainData$diabetes <- as.factor(trainData$diabetes)
testData$diabetes <- as.factor(testData$diabetes)

head(trainData)

##      pregnant glucose pressure triceps insulin mass pedigree age diabetes
## 1           6      148       72      35      175 33.6    0.627  50         1
## 2           1       85       66      29       55 26.6    0.351  31         0
## 3           8      183       64      28      325 23.3    0.672  32         1
## 5           0      137       40      35      168 43.1    2.288  33         1
## 9           2      197       70      45      543 30.5    0.158  53         1
## 12          10      168       74      32      171 38.0    0.537  34         1

library(class)
library(mlbench)
# Function: cross-validated k-NN errors
cv_knn_errors <- function(data, k_values, cv_type) {
  errors <- numeric(length(k_values))
  for (i in seq_along(k_values)) {
    k <- k_values[i]
    if (cv_type == "LOOCV") {
      control <- trainControl(method = "LOOCV")
    } else if (cv_type == "10-fold") {
      control <- trainControl(method = "cv", number = 10)
    }

    model <- train(diabetes ~ ., data = data, method = "knn",
                  trControl = control, tuneGrid = data.frame(k = k))
    errors[i] <- min(model$results$Accuracy)
  }
  return(1 - errors)
}

# k values (tested that >25 is too much)
k_values <- 1:25

# 5 fold
errors_10fold <- cv_knn_errors(df_imp, k_values, "10-fold")

# LOOCV
errors_loocv <- cv_knn_errors(df_imp, k_values, "LOOCV")

trainIndex <- createDataPartition(df_imp$diabetes, p = .67, list = FALSE)
trainData <- df_imp[trainIndex, ]
testData <- df_imp[-trainIndex, ]

# Loop for each k
test_errors <- numeric(length(k_values))
for (i in seq_along(k_values)) {

```

```

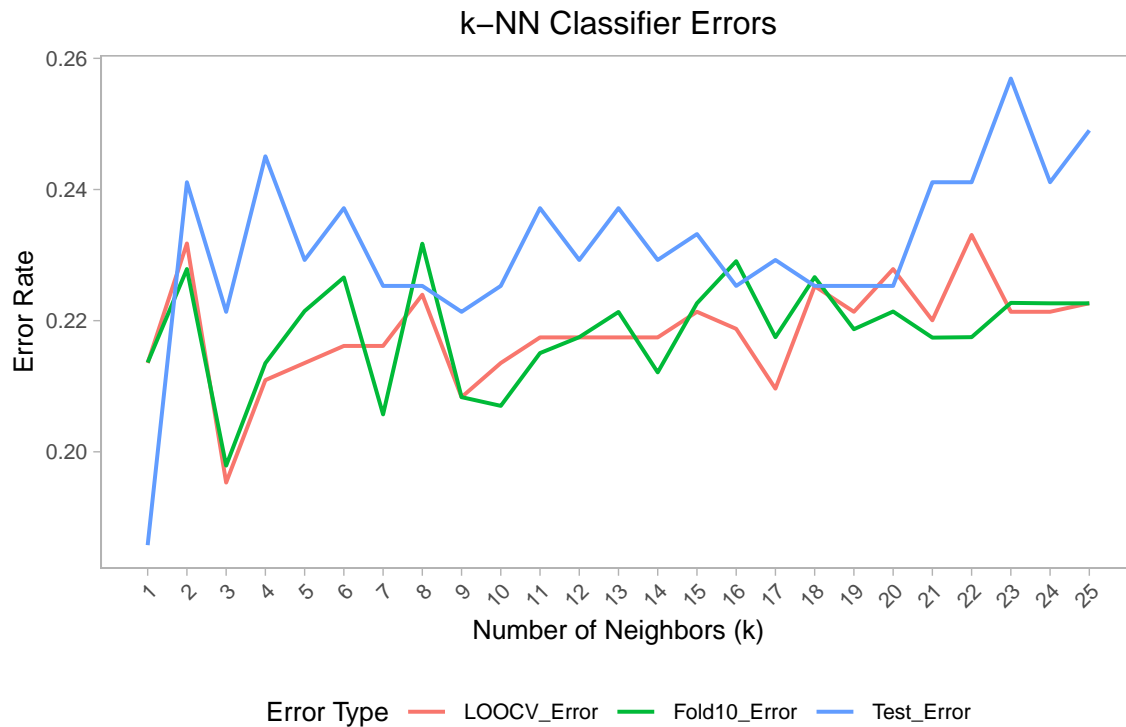
k <- k_values[i]
predictions <- knn(train = trainData[,-ncol(trainData)],
                    test = testData[,-ncol(testData)],
                    cl = trainData$diabetes, k = k)
test_errors[i] <- mean(predictions != testData$diabetes)
}

# Create a data frame for plotting
error_data <- data.frame(
  k = k_values,
  LOOCV_Error = errors_loocv,
  Fold10_Error = errors_10fold,
  Test_Error = test_errors
)

error_data_long <- reshape2::melt(error_data, id.vars = "k")

# Plotting
ggplot(error_data_long, aes(x = k, y = value, color = variable)) +
  geom_line(size = 0.7) +
  # geom_point(size = 1.3) +
  labs(title = "k-NN Classifier Errors",
       x = "Number of Neighbors (k)",
       y = "Error Rate",
       color = "Error Type") +
  scale_x_continuous(breaks = k_values) +
  theme_light() +
  theme(axis.text.x = element_text(angle = 45, hjust = 1),
        legend.position = "bottom",
        panel.grid = element_blank(),
        plot.title = element_text(hjust = 0.5),
        text = element_text(size = 10))

```



Generalized Additive Model for Diabetes Prediction

```
library(caret)
library(mgcv)
library(dplyr)
library(broom)

# model
gam_model <- gam(diabetes ~ s(pregnant) + s(glucose) + s(pressure) +
                 s(triceps) + s(insulin) + s(mass) +
                 s(pedigree) + s(age), data = trainData, family = binomial)
summary(gam_model)

##
## Family: binomial
## Link function: logit
##
## Formula:
## diabetes ~ s(pregnant) + s(glucose) + s(pressure) + s(triceps) +
##           s(insulin) + s(mass) + s(pedigree) + s(age)
##
## Parametric coefficients:
##              Estimate Std. Error z value Pr(>|z|)
## (Intercept) -1.3043      0.1805  -7.225   5e-13 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Approximate significance of smooth terms:
##              edf Ref.df Chi.sq  p-value
```

```
## s(pregnant) 1.000 1.001 8.278 0.004022 **
## s(glucose) 4.196 5.166 21.735 0.000627 ***
## s(pressure) 1.000 1.000 1.014 0.314007
## s(triceps) 1.107 1.206 2.598 0.112210
## s(insulin) 8.411 8.889 33.158 8.95e-05 ***
## s(mass) 3.916 4.866 16.355 0.005263 **
## s(pedigree) 1.000 1.000 0.001 0.971580
## s(age) 2.222 2.806 5.477 0.131900
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## R-sq.(adj) = 0.435 Deviance explained = 41.3%
## UBRE = -0.14736 Scale est. = 1 n = 515

# library(MASS)
# # full model
# full_model <- gam(diabetes ~ s(pregnant) + s(glucose) + s(pressure) +
#                   s(triceps) + s(insulin) + s(mass) +
#                   s(pedigree) + s(age),
#                   data = trainData, family = binomial)
# # stepwise AIC
# selected_model <- step(full_model, direction = "backward")
# summary(selected_model)
```

Tree-Based Methods for Diabetes Classification

```
library(rpart)
library(ipred)
library(randomForest)
library(caret)

classification_tree <- rpart(diabetes ~ ., data = trainData, method = "class")

tree_train_pred <- predict(classification_tree, trainData, type = "class")
tree_test_pred <- predict(classification_tree, testData, type = "class")

# error
tree_train_error <- mean(tree_train_pred != trainData$diabetes)
tree_test_error <- mean(tree_test_pred != testData$diabetes)

cat("Classification Tree Training Error:", tree_train_error, "\n")

## Classification Tree Training Error: 0.1359223
cat("Classification Tree Test Error:", tree_test_error, "\n")

## Classification Tree Test Error: 0.201581

bagged_trees <- bagging(diabetes ~ ., data = trainData)

bagged_train_pred <- predict(bagged_trees, trainData)
bagged_test_pred <- predict(bagged_trees, testData)

# error
bagged_train_error <- mean(bagged_train_pred != trainData$diabetes)
```

```

bagged_test_error <- mean(bagged_test_pred != testData$diabetes)

cat("Bagged Trees Training Error:", bagged_train_error, "\n")

## Bagged Trees Training Error: 0.001941748
cat("Bagged Trees Test Error:", bagged_test_error, "\n")

## Bagged Trees Test Error: 0.1936759
# Fit the random forest
random_forest <- randomForest(diabetes ~ ., data = trainData)

# Predict on training and test data
rf_train_pred <- predict(random_forest, trainData)
rf_test_pred <- predict(random_forest, testData)

# Calculate training and test error
rf_train_error <- mean(rf_train_pred != trainData$diabetes)
rf_test_error <- mean(rf_test_pred != testData$diabetes)

cat("Random Forest Training Error:", rf_train_error, "\n")

## Random Forest Training Error: 0
cat("Random Forest Test Error:", rf_test_error, "\n")

## Random Forest Test Error: 0.1818182
# Store the errors in a data frame
results <- data.frame(
  Model = c("Classification Tree", "Bagged Trees", "Random Forest"),
  Training_Error = c(tree_train_error, bagged_train_error, rf_train_error),
  Test_Error = c(tree_test_error, bagged_test_error, rf_test_error)
)

# Reshape the data for ggplot
results_long <- reshape2::melt(results, id.vars = "Model", variable.name = "Error_Type", value.name = "Error_Rate")

ggplot(results_long, aes(x = Model, y = Error_Rate, fill = Error_Type)) +
  geom_bar(stat = "identity", position = position_dodge(width = 0.9),
    width = 0.7) +
  geom_text(aes(label = round(Error_Rate, 3)),
    position = position_dodge(width = 0.9),
    vjust = -0.5, size = 2) + # Data labels
  theme_light() +
  labs(title = "Comparison of Training and Test Errors",
    x = "Model",
    y = "Error Rate",
    fill = "Error Type") +
  theme(legend.position = "bottom",
    panel.grid = element_blank(),
    plot.title = element_text(hjust = 0.5),
    axis.title = element_text(),
    text = element_text(size = 10))

```



Neural Network Modeling for Diabetes Prediction

```
library(nnet)
library(caret)

neurons <- seq(1, 100, by = 5)

# Initializing
train_errors <- c()
test_errors <- c()

# Loop
for (n in neurons) {
  # Fit NN
  nn_model <- nnet(diabetes ~ ., data = trainData,
                   size = n, linout = FALSE, maxit = 500, trace = FALSE)

  # Train
  train_pred <- predict(nn_model, trainData)
  train_pred_class <- ifelse(train_pred > 0.5, 1, 0) # Convert to binary
  train_error <- mean(train_pred_class != trainData$diabetes)
  train_errors <- c(train_errors, train_error)

  # Test
  test_pred <- predict(nn_model, testData)
  test_pred_class <- ifelse(test_pred > 0.5, 1, 0) # Convert to binary
  test_error <- mean(test_pred_class != testData$diabetes)
  test_errors <- c(test_errors, test_error)
}
```

```

}

# Results
error_results <- data.frame(
  Neurons = neurons,
  Training_Error = train_errors,
  Test_Error = test_errors
)
print(error_results)

##      Neurons Training_Error Test_Error
## 1          1              1          1
## 2          6              1          1
## 3         11              1          1
## 4         16              1          1
## 5         21              1          1
## 6         26              1          1
## 7         31              1          1
## 8         36              1          1
## 9         41              1          1
## 10        46              1          1
## 11        51              1          1
## 12        56              1          1
## 13        61              1          1
## 14        66              1          1
## 15        71              1          1
## 16        76              1          1
## 17        81              1          1
## 18        86              1          1
## 19        91              1          1
## 20        96              1          1

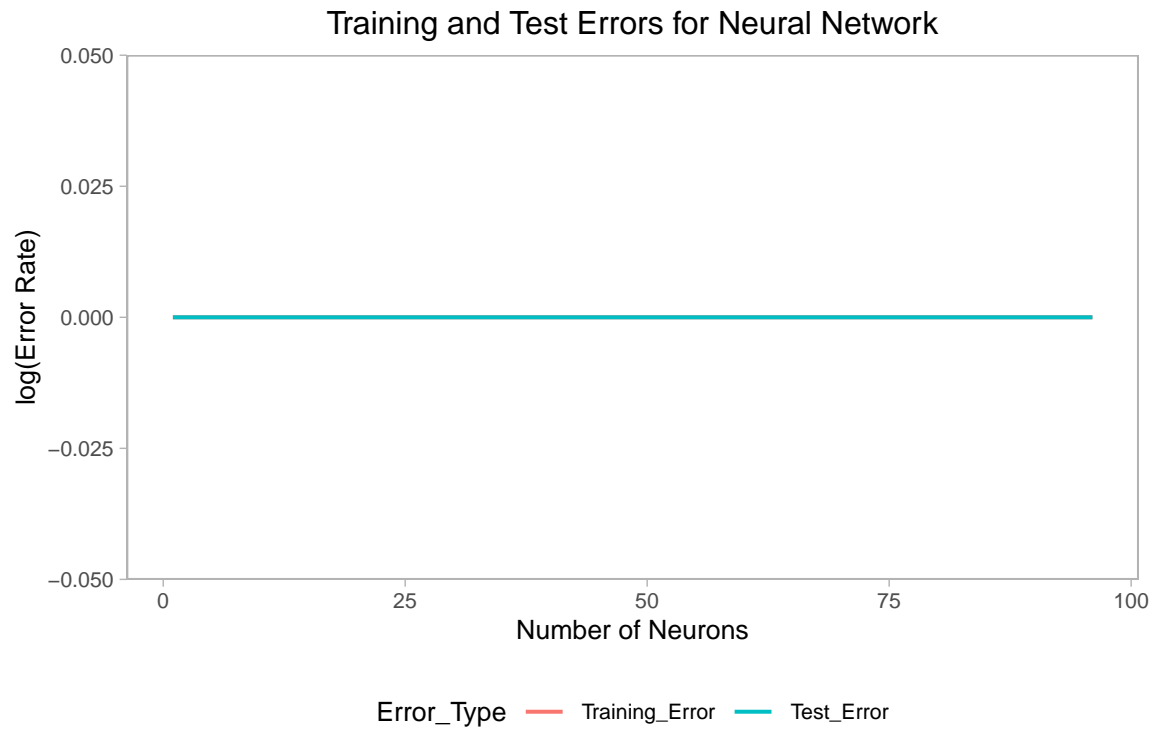
# Choose the optimal number of neurons based on test error
optimal_neurons <- neurons[which.min(test_errors)]
cat("Optimal number of neurons:", optimal_neurons, "\n")

## Optimal number of neurons: 1

library(ggplot2)
error_results_long <- reshape2::melt(error_results,
                                     id.vars = "Neurons",
                                     variable.name = "Error_Type",
                                     value.name = "Error")

ggplot(error_results_long, aes(x = Neurons, y = log10(Error),
                              color = Error_Type)) +
  geom_line(size = 0.7) +
  labs(title = "Training and Test Errors for Neural Network",
       x = "Number of Neurons",
       y = "log(Error Rate)") +
  theme_light() +
  theme(legend.position = "bottom",
        panel.grid = element_blank(),
        plot.title = element_text(hjust = 0.5),
        text = element_text(size = 10))

```

Comparing Classification Methods for Diabetes Analysis