

logistic_regression

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```
wine_df <- read.csv("data/wine-quality-white-and-red (1).csv")
head(wine_df)
```

```
##      type fixed.acidity volatile.acidity citric.acid residual.sugar chlorides
## 1 white          7.0           0.27         0.36          20.7        0.045
## 2 white          6.3           0.30         0.34           1.6        0.049
## 3 white          8.1           0.28         0.40           6.9        0.050
## 4 white          7.2           0.23         0.32           8.5        0.058
## 5 white          7.2           0.23         0.32           8.5        0.058
## 6 white          8.1           0.28         0.40           6.9        0.050
##  free.sulfur.dioxide total.sulfur.dioxide density    pH sulphates alcohol
## 1              45              170  1.0010 3.00        0.45      8.8
## 2              14              132  0.9940 3.30        0.49      9.5
## 3              30              97   0.9951 3.26        0.44     10.1
## 4              47              186  0.9956 3.19        0.40      9.9
## 5              47              186  0.9956 3.19        0.40      9.9
## 6              30              97   0.9951 3.26        0.44     10.1
##      quality
## 1          6
## 2          6
## 3          6
## 4          6
## 5          6
## 6          6
```

```
quality_counts <- table(wine_df$quality)
print(quality_counts)
```

```
##
##      3      4      5      6      7      8      9
##    30   216  2138  2836  1079   193     5
```

Multinomial Logistic Regression

```
wine_df$quality <- as.factor(wine_df$quality)

set.seed(1)
```

```

index <- sample(1:nrow(wine_df), 0.7 * nrow(wine_df))
train <- wine_df[index, ]
test <- wine_df[-index, ]

multi_model <- multinom(quality ~ ., data = train)

```

```

## # weights: 98 (78 variable)
## initial value 8848.053448
## iter 10 value 6112.967244
## iter 20 value 5795.162701
## iter 30 value 5483.743022
## iter 40 value 4942.177481
## iter 50 value 4848.170190
## iter 60 value 4825.676791
## iter 70 value 4814.244712
## iter 80 value 4812.501302
## iter 90 value 4811.705139
## iter 100 value 4810.173610
## final value 4810.173610
## stopped after 100 iterations

```

```

predictions <- predict(multi_model, test)

confusionMatrix(predictions, test$quality)

```

```
## Confusion Matrix and Statistics
```

```
##
##           Reference
## Prediction  3   4   5   6   7   8   9
##           3   1   0   3   0   0   0   0
##           4   0   5   4   0   0   0   0
##           5   2  39 393 190  24   6   0
##           6   4  22 232 599 228  35   1
##           7   0   1   3  71  65  18   2
##           8   0   0   0   1   0   0   0
##           9   1   0   0   0   0   0   0
##

```

```
## Overall Statistics
```

```
##
##           Accuracy : 0.5451
##           95% CI : (0.5227, 0.5674)
##           No Information Rate : 0.4415
##           P-Value [Acc > NIR] : < 2.2e-16
##

```

```
##           Kappa : 0.2704
```

```
##
## McNemar's Test P-Value : NA
##

```

```
## Statistics by Class:
```

```
##
##           Class: 3 Class: 4 Class: 5 Class: 6 Class: 7 Class: 8
## Sensitivity 0.1250000 0.074627 0.6189 0.6957 0.20505 0.0000000

```

```
## Specificity      0.9984552 0.997876  0.8015  0.5207  0.94182 0.9994712
## Pos Pred Value   0.2500000 0.555556  0.6009  0.5343  0.40625 0.0000000
## Neg Pred Value   0.9964029 0.968058  0.8133  0.6840  0.85922 0.9697281
## Prevalence       0.0041026 0.034359  0.3256  0.4415  0.16256 0.0302564
## Detection Rate   0.0005128 0.002564  0.2015  0.3072  0.03333 0.0000000
## Detection Prevalence 0.0020513 0.004615  0.3354  0.5749  0.08205 0.0005128
## Balanced Accuracy 0.5617276 0.536251  0.7102  0.6082  0.57344 0.4997356
##               Class: 9
## Sensitivity      0.0000000
## Specificity      0.9994864
## Pos Pred Value   0.0000000
## Neg Pred Value   0.9984607
## Prevalence       0.0015385
## Detection Rate   0.0000000
## Detection Prevalence 0.0005128
## Balanced Accuracy 0.4997432
```

ROC Curve

```
predicted_probs_multi <- predict(multi_model, test, type = "probs")

true_labels <- test$quality

roc_list <- lapply(levels(true_labels), function(class_label) {
  binary_labels <- ifelse(true_labels == class_label, 1, 0)

  roc(binary_labels, predicted_probs_multi[, class_label])
})
```

```
## Setting levels: control = 0, case = 1

## Setting direction: controls < cases

## Setting levels: control = 0, case = 1

## Setting direction: controls < cases

## Setting levels: control = 0, case = 1

## Setting direction: controls < cases

## Setting levels: control = 0, case = 1

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## Setting direction: controls < cases
```

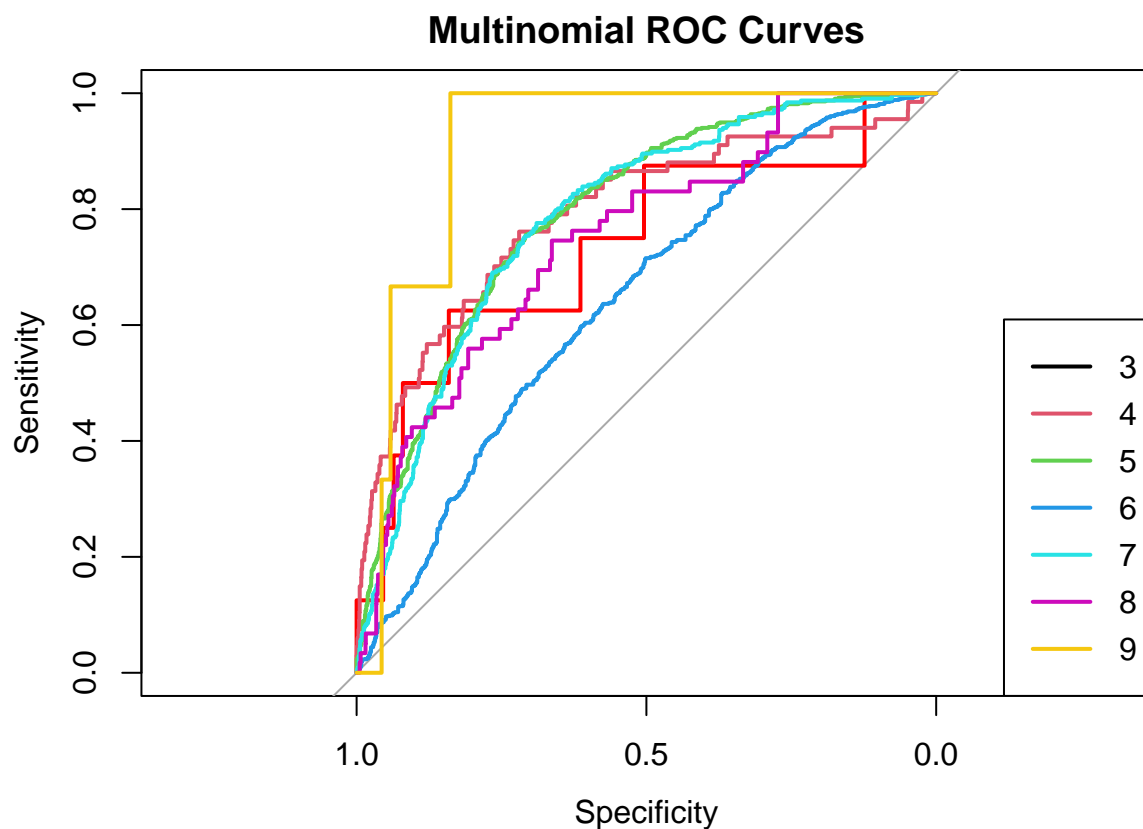
```
## Setting direction: controls < cases

## Setting levels: control = 0, case = 1

## Setting direction: controls < cases
```

```
plot(roc_list[[1]], col = "red", main = "Multinomial ROC Curves", lwd = 2)
for (i in 2:length(roc_list)) {
  lines(roc_list[[i]], col = i, lwd = 2)
}

legend("bottomright", legend = levels(true_labels), col = 1:length(roc_list), lwd = 2)
```



```
sapply(roc_list, auc)
```

```
## [1] 0.7366117 0.7912033 0.7940301 0.6434688 0.7860067 0.7477525 0.9121726
```

```
##Cross Validation
```

```
# wine_df$quality <- as.factor(wine_df$quality)
#
# control <- trainControl(method = "cv", number = 10)
#
```

```
# set.seed(1)
# multi_model_cv <- train(quality ~ ., data = wine_df, method = "multinom", trControl = control)
#
# print(multi_model_cv)
#
# predictions <- predict(multi_model_cv, newdata = test)
#
# confusionMatrix(predictions, test$quality)
```

Accuracy= 0.5477

RMSE

#Logistic Regression

Since logistic regression only has 2 output variables: 0 or 1 or “Yes” or “No”. I decided to split the data in a way where wines that have a quality ≥ 7 , are 0 and wines that have a quality < 7 , are 1.

(<https://vineroutes.com/wine-rating-system>) shows the scale for wine quality.

```
wine_df <- wine_df %>%
  mutate(quality = as.numeric(as.character(quality))) %>%
  mutate(quality_binary = ifelse(quality >= 7, 1, 0)) %>%
  mutate(quality_binary = as.factor(quality_binary))

set.seed(1)
index2 <- sample(1:nrow(wine_df), 0.7 * nrow(wine_df))
train2 <- wine_df[index2, ]
test2 <- wine_df[-index2, ]

log_model <- glm(quality_binary ~ . - quality, data = train2, family = binomial)
summary(log_model)
```

```
##
## Call:
## glm(formula = quality_binary ~ . - quality, family = binomial,
##      data = train2)
##
## Deviance Residuals:
##      Min       1Q   Median       3Q      Max
## -2.7802  -0.6248  -0.3639  -0.1678   3.0108
##
## Coefficients:
##              Estimate Std. Error z value Pr(>|z|)
## (Intercept)    3.291e+02  8.006e+01   4.111 3.94e-05 ***
## typewhite      -4.512e-01  3.089e-01  -1.460 0.144182
## fixed.acidity   4.660e-01  8.131e-02   5.731 9.98e-09 ***
## volatile.acidity -3.415e+00  4.702e-01  -7.263 3.78e-13 ***
## citric.acid     -2.504e-01  4.129e-01  -0.606 0.544203
## residual.sugar   1.931e-01  3.183e-02   6.068 1.29e-09 ***
## chlorides       -1.057e+01  3.441e+00  -3.071 0.002132 **
## free.sulfur.dioxide 1.305e-02  3.633e-03   3.592 0.000328 ***
## total.sulfur.dioxide -4.831e-03  1.647e-03  -2.933 0.003352 **
```

```
## density          -3.502e+02  8.113e+01  -4.316  1.59e-05 ***
## pH               2.576e+00  4.279e-01   6.020  1.74e-09 ***
## sulphates        2.193e+00  3.480e-01   6.301  2.97e-10 ***
## alcohol          5.474e-01  9.714e-02   5.636  1.75e-08 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
## Null deviance: 4518.9 on 4546 degrees of freedom
## Residual deviance: 3537.4 on 4534 degrees of freedom
## AIC: 3563.4
##
## Number of Fisher Scoring iterations: 6
```

```
predictions2 <- predict(log_model, test2, type = "response")
predicted_classes2 <- ifelse(predictions2 > 0.5, "1", "0")

confusionMatrix(as.factor(predicted_classes2), test2$quality_binary)
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction    0    1
##           0 1482  272
##           1   89  107
##
##           Accuracy : 0.8149
##           95% CI : (0.7969, 0.8319)
##       No Information Rate : 0.8056
##       P-Value [Acc > NIR] : 0.1583
##
##           Kappa : 0.2763
##
##  Mcnemar's Test P-Value : <2e-16
##
##           Sensitivity : 0.9433
##           Specificity : 0.2823
##           Pos Pred Value : 0.8449
##           Neg Pred Value : 0.5459
##           Prevalence : 0.8056
##           Detection Rate : 0.7600
##       Detection Prevalence : 0.8995
##           Balanced Accuracy : 0.6128
##
##           'Positive' Class : 0
##
```

```
log2_index <- sample(1:nrow(wine_df), 0.7 * nrow(wine_df))
log2_train <- wine_df[log2_index, ]
log2_test  <- wine_df[-log2_index, ]

log_model2 <- glm(quality_binary ~ . - quality - type - citric.acid, data = log2_train, family = binomial)
```

```
log_predictions2 <- predict(log_model2, log2_test, type = "response")
log_predicted_classes2 <- ifelse(log_predictions2 > 0.5, "1", "0")
```

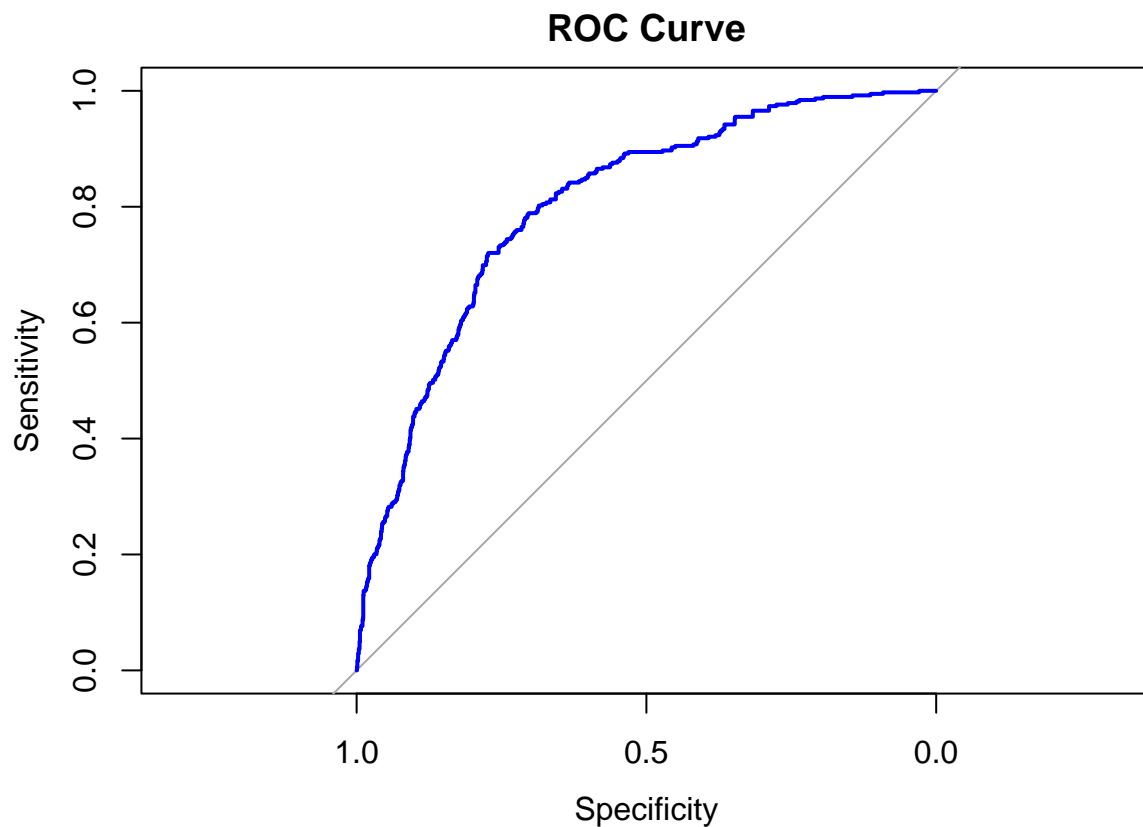
ROC Curve

```
predictions_prob <- predict(log_model, test2, type = "response")
roc_curve <- roc(test2$quality_binary, predictions_prob)
```

```
## Setting levels: control = 0, case = 1
```

```
## Setting direction: controls < cases
```

```
plot(roc_curve, col = "blue", main = "ROC Curve")
```



```
auc(roc_curve)
```

```
## Area under the curve: 0.8028
```

AUC = 0.8028. That means the model does an okay job in predicting it and is not completely due to random chance.

Cross Validation

```
control2 <- trainControl(method = "cv", number = 10)

set.seed(1)
cv_model <- train(quality_binary ~ . - quality, data = wine_df, method = "glm", family = binomial, trCon
print(cv_model)
```

```
## Generalized Linear Model
##
## 6497 samples
## 13 predictor
## 2 classes: '0', '1'
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 5847, 5847, 5847, 5847, 5848, 5847, ...
## Resampling results:
##
## Accuracy Kappa
## 0.8174517 0.2741793
```

```
predictions <- predict(cv_model, newdata = test2)

confusionMatrix(predictions, test2$quality_binary)
```

```
## Confusion Matrix and Statistics
##
##              Reference
## Prediction    0    1
##           0 1490  275
##           1   81  104
##
##              Accuracy : 0.8174
##              95% CI : (0.7996, 0.8344)
##      No Information Rate : 0.8056
##      P-Value [Acc > NIR] : 0.09824
##
##              Kappa : 0.2766
##
##  McNemar's Test P-Value : < 2e-16
##
##              Sensitivity : 0.9484
##              Specificity : 0.2744
##              Pos Pred Value : 0.8442
##              Neg Pred Value : 0.5622
##              Prevalence : 0.8056
##              Detection Rate : 0.7641
##      Detection Prevalence : 0.9051
##              Balanced Accuracy : 0.6114
##
```



```
##          'Positive' Class : 0
##
```

Since the data is a little skewed with a lot more samples landing in the 0 category than the 1 category, which might affect the accuracy of the model, I'm going to try adding weights to the regression to try to make it more accurate

Weighted Logistic Regression

```
wine_df <- wine_df %>%
  mutate(quality = as.numeric(as.character(quality))) %>%
  mutate(quality_binary = ifelse(quality >= 7, 1, 0))

set.seed(1)
index3 <- sample(1:nrow(wine_df), 0.7 * nrow(wine_df))
train3 <- wine_df[index3, ]
test3 <- wine_df[-index3, ]

weights <- ifelse(train3$quality_binary == 1, 0.8, 0.2)

log_model_weighted <- glm(quality_binary ~ . - quality, data = train3, family = binomial, weights = weights)
```

```
## Warning in eval(family$initialize): non-integer #successes in a binomial glm!
```

```
predictions_weighted <- predict(log_model_weighted, test3, type = "response")
predicted_classes_weighted <- ifelse(predictions_weighted > 0.5, "1", "0")

confusionMatrix(as.factor(predicted_classes_weighted), as.factor(test3$quality_binary))
```

```
## Confusion Matrix and Statistics
##
##              Reference
## Prediction    0    1
##           0 1124   91
##           1  447  288
##
##              Accuracy : 0.7241
##              95% CI : (0.7037, 0.7438)
##       No Information Rate : 0.8056
##       P-Value [Acc > NIR] : 1
##
##              Kappa : 0.3505
##
##  Mcnemar's Test P-Value : <2e-16
##
##              Sensitivity : 0.7155
##              Specificity : 0.7599
##              Pos Pred Value : 0.9251
##              Neg Pred Value : 0.3918
##              Prevalence : 0.8056
##              Detection Rate : 0.5764
```

```
##      Detection Prevalence : 0.6231
##      Balanced Accuracy : 0.7377
##
##      'Positive' Class : 0
##
```

```
predictions_prob2 <- predict(log_model_weighted, test3, type = "response")
```

```
# For normal logistic regression
roc_normal <- roc(test2$quality_binary, predictions_prob)
```

```
## Setting levels: control = 0, case = 1
```

```
## Setting direction: controls < cases
```

```
plot(roc_normal, col = "red", main = "ROC Curve Comparison")
auc(roc_normal)
```

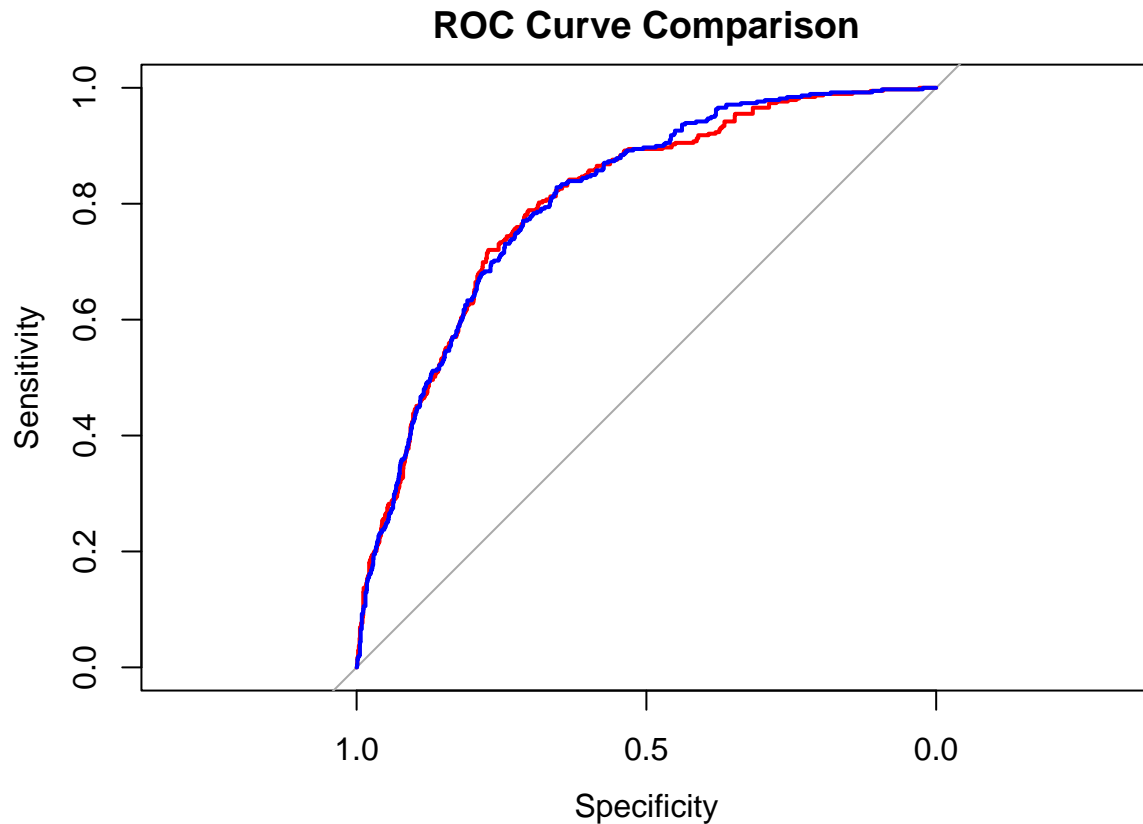
```
## Area under the curve: 0.8028
```

```
# For weighted logistic regression
roc_weighted <- roc(test3$quality_binary, predictions_prob2)
```

```
## Setting levels: control = 0, case = 1
```

```
## Setting direction: controls < cases
```

```
plot(roc_weighted, col = "blue", add = TRUE)
```



```
auc(roc_weighted)
```

```
## Area under the curve: 0.8053
```

The ROC curves for weighted/normal are basically the same. So the model's discriminatory power did not really improve.

Balances Logistic Regression

```
minority_class <- wine_df %>% filter(quality_binary == 1)
majority_class <- wine_df %>% filter(quality_binary == 0)

set.seed(1)
majority_class_undersampled <- majority_class %>%
  sample_n(nrow(minority_class))

balanced_df <- bind_rows(minority_class, majority_class_undersampled)

set.seed(1)
index_balanced <- sample(1:nrow(balanced_df), 0.7 * nrow(balanced_df))
train_balanced <- balanced_df[index_balanced, ]
test_balanced <- balanced_df[-index_balanced, ]
```

```
log_model_balanced <- glm(quality_binary ~ . - quality, data = train_balanced, family = binomial)

predictions_balanced <- predict(log_model_balanced, test_balanced, type = "response")
predicted_classes_balanced <- ifelse(predictions_balanced > 0.5, "1", "0")

confusionMatrix(as.factor(predicted_classes_balanced), as.factor(test_balanced$quality_binary))
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  0    1
##           0 301  72
##           1 104 290
##
##           Accuracy : 0.7705
##           95% CI : (0.7391, 0.7999)
##       No Information Rate : 0.528
##       P-Value [Acc > NIR] : < 2e-16
##
##           Kappa : 0.5418
##
##  Mcnemar's Test P-Value : 0.01945
##
##           Sensitivity : 0.7432
##           Specificity : 0.8011
##       Pos Pred Value : 0.8070
##       Neg Pred Value : 0.7360
##           Prevalence : 0.5280
##       Detection Rate : 0.3924
##       Detection Prevalence : 0.4863
##       Balanced Accuracy : 0.7722
##
##       'Positive' Class : 0
##
```

```
# For normal logistic regression
roc_normal <- roc(test2$quality_binary, predictions_prob)
```

```
## Setting levels: control = 0, case = 1
```

```
## Setting direction: controls < cases
```

```
plot(roc_normal, col = "red", main = "ROC Curve Comparison", lwd = 2)

auc_normal <- auc(roc_normal)
cat("AUC for Normal Logistic Regression:", auc_normal, "\n")
```

```
## AUC for Normal Logistic Regression: 0.8028011
```

```
# For weighted logistic regression
roc_weighted <- roc(test3$quality_binary, predictions_prob2)
```

```
## Setting levels: control = 0, case = 1
## Setting direction: controls < cases
```

```
lines(roc_weighted, col = "blue", lwd = 2)
```

```
auc_weighted <- auc(roc_weighted)
cat("AUC for Weighted Logistic Regression:", auc_weighted, "\n")
```

```
## AUC for Weighted Logistic Regression: 0.8052633
```

```
# For balanced logistic regression
roc_balanced <- roc(test_balanced$quality_binary, predictions_balanced)
```

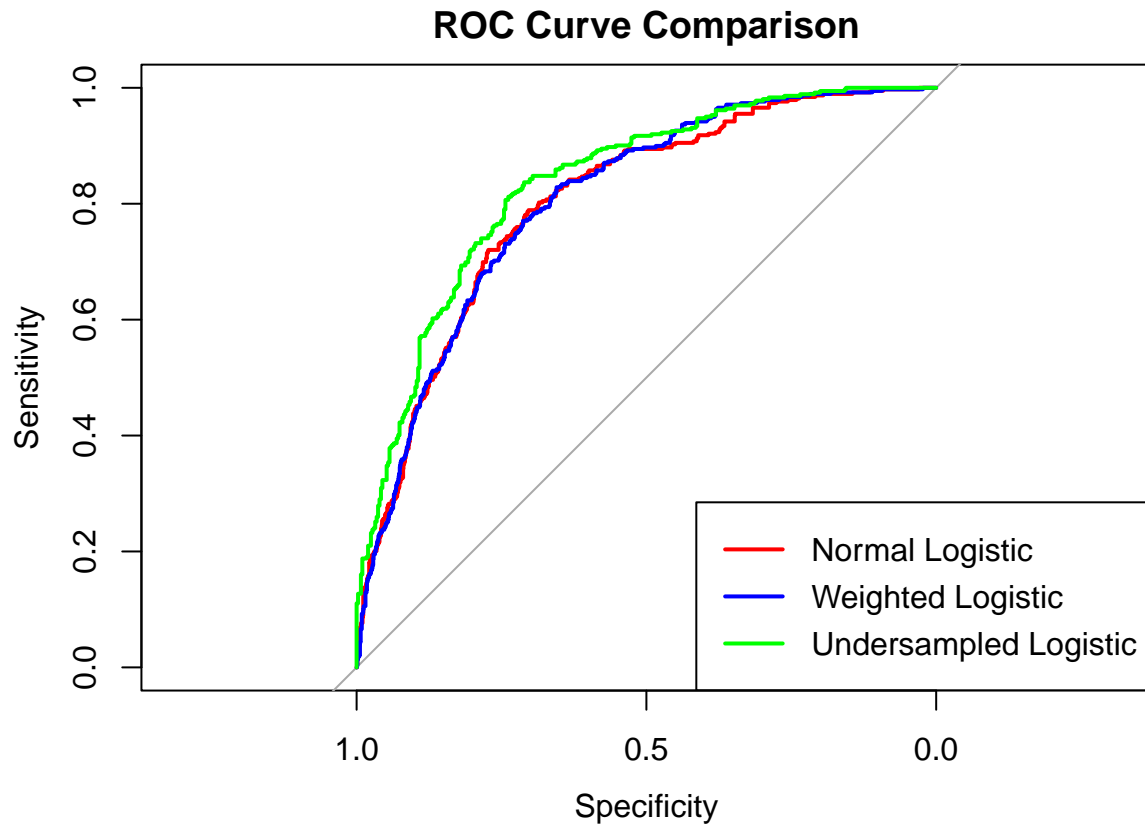
```
## Setting levels: control = 0, case = 1
## Setting direction: controls < cases
```

```
lines(roc_balanced, col = "green", lwd = 2)
```

```
auc_balanced <- auc(roc_balanced)
cat("AUC for Undersampled Logistic Regression:", auc_balanced, "\n")
```

```
## AUC for Undersampled Logistic Regression: 0.8355296
```

```
# Add Legend to the Plot
legend("bottomright",
      legend = c("Normal Logistic", "Weighted Logistic", "Undersampled Logistic"),
      col = c("red", "blue", "green"),
      lwd = 2)
```



RMSE

```
actual_normal <- as.numeric(as.character(test2$quality_binary))

rmse_normal <- sqrt(mean((predictions_prob - actual_normal)^2))
cat("RMSE for Normal Logistic Regression:", rmse_normal, "\n")
```

RMSE for Normal Logistic Regression: 0.3557835

```
actual_weighted <- as.numeric(as.character(test3$quality_binary))

rmse_weighted <- sqrt(mean((predictions_prob2 - actual_weighted)^2))
cat("RMSE for Weighted Logistic Regression:", rmse_weighted, "\n")
```

RMSE for Weighted Logistic Regression: 0.427233

```
actual_balanced <- as.numeric(as.character(test_balanced$quality_binary))

rmse_balanced <- sqrt(mean((predictions_balanced - actual_balanced)^2))
cat("RMSE for Undersampled Logistic Regression:", rmse_balanced, "\n")
```

RMSE for Undersampled Logistic Regression: 0.4077837

```
actual_normal2 <- as.numeric(as.character(log2_test$quality_binary))
rmse_log2 <- sqrt(mean((log_predictions2 - actual_normal2)^2))
cat("RMSE for Specific Predictors Logistic Regression:", rmse_log2, "\n")
```

```
## RMSE for Specific Predictors Logistic Regression: 0.3555901
```

```
AIC(log_model, log_model_weighted, log_model_balanced, log_model2)
```

```
## Warning in AIC.default(log_model, log_model_weighted, log_model_balanced, :
## models are not all fitted to the same number of observations
```

```
##           df      AIC
## log_model      13 3563.4361
## log_model_weighted 13  951.6473
## log_model_balanced 13 1953.6609
## log_model2      11 3573.4232
```