Logistic Regression For Binary Classification

Introduction

For individuals who have studied cell biology or biochemistry, logistic regression may be familiar as dose-response curves, enzyme kinetic curves, sigmoidal curves, median lethal dose curve (LD-50) or even an exponential growth curve given limited resources.

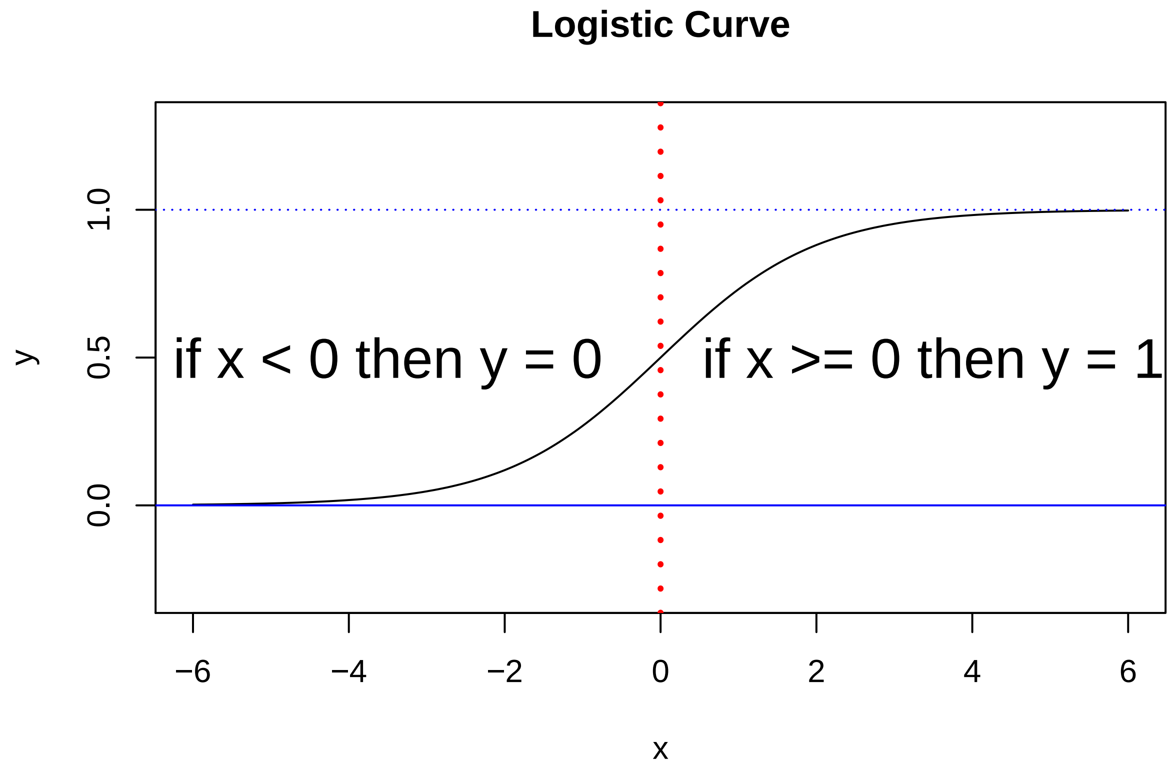
However, in the context of predictive modeling logistic regression is used as a binary classifier that can toggle between logical values of zero or one.

Logistic regression derives its name from its similarity to linear regression, as we shall see below. In logistic regression, the dependent variable (y) is NOT calculated as is found with linear regression. Instead, logistic regression is used for classification between two states. Instead the term logistic should be a reminder that the functions output are logical values, therefore 0's and 1's.

$$f(x) = \begin{cases} 0 & for \quad x < 0 \\ 1 & for \quad x \geq 0 \end{cases}$$

Using logistic regression we may now calculate the presence or absence of a product or quality that we wish to model.

As we can see in the figure below the functions domain (x) is ($-\infty$ to ∞), whereby its range is largely zero or one. In our simple case, the **decision boundary** at $x\ = 0$ our system changes from *zero*, absence, to *one*, the presence of a quality or item. In the Logistic/Sigmoidal Curve figure below, the **decision boundary** is denoted by the *red dotted line*.



The logistic growth curve is commonly denoted by:

$$f(x) \;=\; \frac{M}{1 + Ae^{-r(x-x_0)}}$$

where M is the curve's maximum value, r is the maximum growth rate (also called the Malthusian parameter[1]), x_0 is the midpoint of the curve, A is the number of times that the initial population must double to reach M.[2]

In the specific case of *Logistic Regression for Binary Classification* where we have a probability between 0 and 1, M and A take on the value one.

Since the logistic equation is exponential it is easier to work with the formula in terms of its odds or **log odds**. Odds are the probabilities of success over failure denoted as $\frac{p}{1-p}$ or more precisely log-odds as $ln\left(\frac{p}{1-p}\right)$.

Simply by using log-odds, logistic regression may be more easily expressed as a set of linear equations in x.[3] Hence we can now go from linear regression to logistic regression.

$$ln\;\left(\frac{Pr(y_i \;=\; 1|x_i)}{Pr(y_i \;=\; 0|x_i)}\right) \;=\; \beta_0 + \beta_1 x_1 + \;...\; + \beta_n x_n$$

Substitute (p for $Pr(y_i \;=\; 1|x_i)$) and ($1-p$ for $Pr(y_i \;=\; 0|x_i)$) and change notation to summation on the right hand side:

$$ln\left(\frac{p}{1-p}\right) \;=\; \sum_i^k \beta_i x_i$$

Eliminate the natural log by taking the exponent on both sides:

$$\frac{p}{1-p} \;=\; exp\left(\sum_i^k \beta_i x_i\right)$$

Substitute $u = \sum_i^k \beta_i x_i$:

$$\frac{p}{1-p} \;=\; e^u$$

Rearrange to solve for p:

$$p(u) \;=\; \frac{e^u}{1+e^u}$$

Take the derivative of both sides using quotient rule:

$$p'(u) \;=\; \frac{(e^u)(1+e^u) - (e^u)(e^u)}{(1+e^u)^2}$$

[1]https://en.wikipedia.org/wiki/Malthusian_growth_model
[2]https://en.wikipedia.org/wiki/Logistic_function
[3]http://juangabrielgomila.com/en/logistic-regression-derivation/

Simplify:

$$p'(u) \;=\; \frac{e^u}{(1+e^u)^2}$$

Separate out to produce two fractions:

$$p'(u) \;=\; \left(\frac{e^u}{1+e^u}\right) \cdot \left(\frac{1}{1+e^u}\right)$$

Substitute our previous success and failure variables back into place:

$$p'(u) \;=\; p(u) \cdot (1 - p(u))$$

Now we can calculate the probabilities as well as the values for any given x value.

Load libraries and protein dataset

```r
# Load Libraries
Libraries <- c("doMC", "knitr", "readr", "tidyverse", "caret")

for (p in Libraries) {  # Install Library if not present
    if (!require(p, character.only = TRUE)) { install.packages(p) }
    library(p, character.only = TRUE)
}
```

```r
# Import relevant data
c_m_TRANSFORMED <- read_csv("../00-data/02-aac_dpc_values/c_m_TRANSFORMED.csv",
                            col_types = cols(Class = col_factor(levels = c("0", "1")),
                                             PID = col_skip(),
                                             TotalAA = col_skip()))
```

```r
# Partition data into training and testing sets
set.seed(1000)
index <- createDataPartition(c_m_TRANSFORMED$Class, p = 0.8, list = FALSE)

training_set.1 <- c_m_TRANSFORMED[index, ]
```

The `test.set.1` and `Class.test` data sets are not produced since that the Logit run with 20 features was not deemed useful. The reason for its dismissal was that is contained extraneous features.

Logit Training #1 using 20 Features

- The first training (**test**) is to determine if all 20 features (amino acids) are necessary for our logistic regression model.

```r
set.seed(1000)
registerDoMC(cores = 3)  # Start multi-processor mode
start_time <- Sys.time() # Start timer

# Create model, 10X fold CV repeated 5X
tcontrol <- trainControl(method = "repeatedcv",
                         number = 10,
                         repeats = 5)

model_obj.1 <- train(Class ~ .,
                     data = training_set.1,
                     trControl = tcontrol,
                     method = "glm",
                     family = "binomial")

end_time <- Sys.time()  # End timer
end_time - start_time   # Display time
```

```
## Time difference of 1.594321 secs
```

```
registerDoSEQ()         # Stop multi-processor mode
```

Logit Results #1

```
summary(model_obj.1)
```

```
##
## Call:
## NULL
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -5.9372  -0.2835  -0.0194   0.0516   3.6884
##
## Coefficients:
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept)   8.0525     9.2156   0.874 0.382234
## A             5.0438     9.6899   0.521 0.602699
## C           -14.2228     2.6949  -5.278 1.31e-07 ***
## D           -36.2676     8.0845  -4.486 7.25e-06 ***
## E            27.6016    11.1292   2.480 0.013135 *
## F             5.6174     5.2654   1.067 0.286034
## G           -22.1970    10.3043  -2.154 0.031229 *
## H            90.1101    12.1105   7.441 1.00e-13 ***
## I            -5.9795     4.3945  -1.361 0.173610
## K            -2.8961     9.8468  -0.294 0.768669
## L            -3.7417     9.2217  -0.406 0.684926
## M            -0.1427    12.0747  -0.012 0.990570
## N             3.3478     9.6749   0.346 0.729319
## P           -39.7466    11.1010  -3.580 0.000343 ***
## Q            -5.6804    11.2516  -0.505 0.613664
## R           -83.6045    11.8104  -7.079 1.45e-12 ***
## S            -9.9745    10.0872  -0.989 0.322750
## T           -36.5980     9.2791  -3.944 8.01e-05 ***
## V            16.3411     9.7859   1.670 0.094946 .
## W             9.0169    13.8870   0.649 0.516141
## Y           -31.9282    11.1167  -2.872 0.004078 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 2593.68  on 1872  degrees of freedom
## Residual deviance:  657.72  on 1852  degrees of freedom
## AIC: 699.72
##
## Number of Fisher Scoring iterations: 8
```

The Akaike information criterion (AIC)[4] for model #1 is 699.72. This will be used later to compare the models generated to rate their ability to best utilize the features. - The list of probabilities for the estimates leaves us with only **9 important features** to try re-modeling, R, H, P, C, E, Y, T, D, G.

Logit Training #2 using 9 Features

- This test uses **ONLY** 9 features: (R, H, P, C, E, Y, T, D, G)

```r
# Data import & handling
c_m_9aa <- read_csv("../00-data/02-aac_dpc_values/c_m_TRANSFORMED.csv",
                     col_types = cols(Class = col_factor(levels = c("0", "1")),
                                      A = col_skip(),
                                      F = col_skip(),
                                      I = col_skip(),
                                      K = col_skip(),
                                      L = col_skip(),
                                      M = col_skip(),
                                      N = col_skip(),
                                      PID = col_skip(),
                                      Q = col_skip(),
                                      V = col_skip(),
                                      S = col_skip(),
                                      TotalAA = col_skip(),
                                      W = col_skip()))
```

```r
# Partition data into training and testing sets
set.seed(1000)
index <- createDataPartition(c_m_9aa$Class, p = 0.8, list = FALSE)

training_set.2 <- c_m_9aa[ index, ]
test_set.2     <- c_m_9aa[-index, ]

Class_test.2 <- as.factor(test_set.2$Class)
```

Logit Training #2 with 9 Features

```r
set.seed(1000)
registerDoMC(cores = 3)  # Start multi-core
start_time <- Sys.time() # Start timer

# Create model, 10X fold CV repeated 5X
fitControl <- trainControl(method = "repeatedcv",
```

[4]https://en.wikipedia.org/wiki/Akaike_information_criterion

```
                           number = 10,
                           repeats = 5,
                           savePredictions = "final") # IMPORTANT: Saves predictions

model_obj.2 <- train(Class ~ .,
                     data = training_set.2,
                     trControl = fitControl,
                     method = "glm",
                     family = "binomial")
end_time <- Sys.time()   # End timer
end_time - start_time    # Display time
```

```
## Time difference of 1.39758 secs
```

```
registerDoSEQ()          # Stop multi-core
```

Logit Summary #2

```
summary(model_obj.2)
```

```
##
## Call:
## NULL
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -6.2083  -0.2984  -0.0204   0.0601   3.5666
##
## Coefficients:
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept)    8.306      1.007   8.245  < 2e-16 ***
## C            -14.755      1.908  -7.733 1.05e-14 ***
## D            -31.411      4.949  -6.347 2.20e-10 ***
## E             21.932      5.092   4.307 1.66e-05 ***
## G            -23.259      5.071  -4.587 4.49e-06 ***
## H             94.580      8.431  11.218  < 2e-16 ***
## P            -29.394      6.264  -4.692 2.70e-06 ***
## R            -82.809      6.363 -13.015  < 2e-16 ***
## T            -40.915      5.624  -7.275 3.45e-13 ***
## Y            -37.860      6.291  -6.018 1.77e-09 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 2593.68  on 1872  degrees of freedom
## Residual deviance:  688.96  on 1863  degrees of freedom
## AIC: 708.96
##
## Number of Fisher Scoring iterations: 8
```

Logit Confusion Matrix #2

```r
Predicted_test_vals <- predict(model_obj.2, test_set.2[, -1])

confusionMatrix(Predicted_test_vals, Class_test.2, positive = "1")
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction   0   1
##          0 235  18
##          1   8 206
##
##                Accuracy : 0.9443
##                  95% CI : (0.9195, 0.9633)
##     No Information Rate : 0.5203
##     P-Value [Acc > NIR] : < 2e-16
##
##                   Kappa : 0.8883
##
##  Mcnemar's Test P-Value : 0.07756
##
##             Sensitivity : 0.9196
##             Specificity : 0.9671
##          Pos Pred Value : 0.9626
##          Neg Pred Value : 0.9289
##              Prevalence : 0.4797
##          Detection Rate : 0.4411
##    Detection Prevalence : 0.4582
##       Balanced Accuracy : 0.9434
##
##        'Positive' Class : 1
##
```

- The Akaike information criterion (AIC) for model #2 is 708.96. This will be used later to compare the models generated to rate their ability to best utilize the features.
- The number of unique false-positives and false-negatives is 26.

Obtain List of False Positives & False Negatives

```r
fp_fn_logit <- model_obj.2 %>% pluck("pred") %>% dplyr::filter(obs != pred)

# Write CSV in R
write.table(fp_fn_logit,
            file = "../00-data/03-ml_results/fp_fn_logit.csv",
            row.names = FALSE,
            na = "",
            col.names = TRUE,
            sep = ",")

nrow(fp_fn_logit) ## NOTE: NOT UNIQUE NOR SORTED
```

```
## [1] 536
```

- The logistic regression second test produced 536 protein samples which are either false-positives or false-negatives. The list of 536 proteins may have duplicates, therefore they are NOT UNIQUE NOR SORTED.

Conclusion

Logit is easy to implement and understand and can be used for parameter importance measurements.

Considering the Table Logit Models, below, it is clear that model #2 with 9 features best describes the better of the two models.

Akaike Information Criterion:[5]

$$AIC \; = \; 2K \; - \; ln(\widehat{L})$$

Where $ln(\widehat{L})$ is the log-likelihood, K is the number of parameters.

Model #	Features	AIC
1	20	699.72
2	9	708.96

Logit is a common machine learning method. It is easy to understand and explain. This supervised binary classification method is very useful for determining the importance of the features which can be applied. As we saw in Model#1 there were 11 features that had probabilities of the estimates used above the 5% threshold cut-off. In Model#2 only 9 features were used to describe the model and the AIC increased by 9.24.

The nine features which best described the logistic regression model were R, H, P, C, E, Y, T, D, G. If we compare this to the Boruta test carried out in the EDA we find the overlap interesting.

Test Model / Order of Importance (From Left To Right)

Test Model																				
Order	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
Boruta	R	H	P	K	C	E	Y	T	S	A	V	U	I	F	D	G	N	L	M	Q
Logit	R	H	P	.	C	E	Y	T	.	.	.	.	.	.	D	G	.	.	.	.

The first 7 out of 8 amino acid features are seen in the proper order as described by the Boruta Random Forest model. This is confirmation that Logit can pick up the importance of features similar to Boruta.

Logit produced 536 proteins which are false-negatives or false-positives. It should be noted that the 536 are NOT UNIQUE NOR SORTED. The number of FN/FP from the confusion matrix is 26. These proteins will be investigated further in the Outliers section which compares these FN/FP proteins to the PCA outliers.

[5]https://en.wikipedia.org/wiki/Akaike_information_criterion