Neural Networks

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3 Preprocess the data: Normalize the data

```
new_data <- rbind(S0,Data)
maxs <- apply(new_data %>% dplyr::select(-c(idfile,RESPONSE)), 2, max)
mins <- apply(new_data %>% dplyr::select(-c(idfile,RESPONSE)), 2, min)

scaled_data <- as.data.frame(scale(new_data %>% dplyr::select(-c(idfile,RESPONSE)), center = mins, scal
#scaled_data$RESPONSE <- ifelse(new_data$RESPONSE =="GO",1,0)
scaled_data$RESPONSE <- as.factor(new_data$RESPONSE)
#scaled_data$RESPONSE <- as.factor(scaled_data$RESPONSE)
scaled_data$idfile <- new_data$idfile

#select random ind for train and test
set.seed(123)

## 75% of the sample size
smp_size <- floor(0.75 * nrow(scaled_data))

## set the seed to make your partition reproducible
set.seed(123)
train_ind <- sample(seq_len(nrow(scaled_data)), size = smp_size)
```

```
train <- scaled_data[train_ind,]
test <- scaled_data[-train_ind,]
```

4 Building Neural Network

```
library(h2o)
```

```
##
## ----------------------------------------------------------------------
##
## Your next step is to start H2O:
##     > h2o.init()
##
## For H2O package documentation, ask for help:
##     > ??h2o
##
## After starting H2O, you can use the Web UI at http://localhost:54321
## For more information visit http://docs.h2o.ai
##
## ----------------------------------------------------------------------
```

```
##
## Attaching package: 'h2o'
```

```
## The following objects are masked from 'package:stats':
##
##     cor, sd, var
```

```
## The following objects are masked from 'package:base':
##
##     %*%, %in%, &&, ||, apply, as.factor, as.numeric, colnames,
##     colnames<-, ifelse, is.character, is.factor, is.numeric, log,
##     log10, log1p, log2, round, signif, trunc
```

```
#generate same set of random numbers (for reproducibility)
set.seed(121)

#launch h2o cluster
localH2O <- h2o.init(nthreads = -1)


#import r objects to h2o cloud
train_h2o <- as.h2o(train)
test_h2o <- as.h2o(test)
```

```
#build the mlp(multi layer perceptron) deep learning model using h2o
set.seed(100)

dl_model <- h2o.deeplearning(
  model_id="dl_model_first",
  training_frame=train_h2o,
  validation_frame = test_h2o,
  x= colnames(train_h2o[,1:48]),
  y= "RESPONSE",
```

```
  activation="Tanh",
  hidden=c(5,4),
  stopping_metric="mean_per_class_error",
  stopping_tolerance=0.01,
  epochs=100,
  seed = 123, # give seed
  export_weights_and_biases = T, # export weights and biases defaults to false
  reproducible = T # Force reproducibility on small data (will be slow - only uses 1 thread). Defaults
)
```

```
summary(dl_model)
```

```
## Model Details:
## ==============
##
## H2OBinomialModel: deeplearning
## Model Key:  dl_model_first
## Status of Neuron Layers: predicting RESPONSE, 2-class classification, bernoulli distribution, CrossE
batch size 1
##   layer units    type dropout       l1       l2 mean_rate rate_rms
## 1     1    48   Input  0.00 %
## 2     2     5    Tanh  0.00 % 0.000000 0.000000  0.002543 0.002428
## 3     3     4    Tanh  0.00 % 0.000000 0.000000  0.003763 0.004709
## 4     4     2 Softmax         0.000000 0.000000  0.002780 0.000511
##   momentum mean_weight weight_rms mean_bias bias_rms
## 1
## 2 0.000000   -0.008720   0.196638 -0.038391 0.123508
## 3 0.000000   -0.032180   0.416094  0.235844 0.537879
## 4 0.000000   -0.194668   3.183959  0.000000 0.637211
##
## H2OBinomialMetrics: deeplearning
## ** Reported on training data. **
## ** Metrics reported on full training frame **
##
## MSE:  0.02160276
## RMSE:  0.1469788
## LogLoss:  0.07299448
## Mean Per-Class Error:  0.1421513
## AUC:  0.9892086
## Gini:  0.9784173
##
## Confusion Matrix (vertical: actual; across: predicted) for F1-optimal threshold:
##        GO NOGO    Error      Rate
## GO     60   23 0.277108    =23/83
## NOGO    7  966 0.007194    =7/973
## Totals 67  989 0.028409  =30/1056
##
## Maximum Metrics: Maximum metrics at their respective thresholds
##                         metric threshold    value idx
## 1                       max f1  0.336047 0.984709 332
## 2                       max f2  0.336047 0.989551 332
## 3                 max f0point5  0.800684 0.988976 280
## 4                 max accuracy  0.458565 0.971591 319
## 5                max precision  0.999996 1.000000   0
```

```
## 6                   max recall  0.088233 1.000000 386
## 7              max specificity  0.999996 1.000000   0
## 8             max absolute_mcc  0.641986 0.808694 303
## 9   max min_per_class_accuracy  0.800684 0.958890 280
## 10 max mean_per_class_accuracy  0.800684 0.961373 280
##
## Gains/Lift Table: Extract with `h2o.gainsLift(<model>, <data>)` or `h2o.gainsLift(<model>, valid=<T/
## H2OBinomialMetrics: deeplearning
## ** Reported on validation data. **
## ** Metrics reported on full validation frame **
##
## MSE:  0.02120419
## RMSE:  0.1456166
## LogLoss:  0.07595011
## Mean Per-Class Error:  0.06857903
## AUC:  0.9840426
## Gini:  0.9680851
##
## Confusion Matrix (vertical: actual; across: predicted) for F1-optimal threshold:
##        GO NOGO    Error    Rate
## GO     21    3 0.125000   =3/24
## NOGO    4  325 0.012158  =4/329
## Totals 25  328 0.019830  =7/353
##
## Maximum Metrics: Maximum metrics at their respective thresholds
##                         metric threshold    value idx
## 1                       max f1  0.449576 0.989346 326
## 2                       max f2  0.281052 0.989709 334
## 3                 max f0point5  0.449576 0.990250 326
## 4                 max accuracy  0.449576 0.980170 326
## 5                max precision  0.999999 1.000000   0
## 6                   max recall  0.051224 1.000000 350
## 7              max specificity  0.999999 1.000000   0
## 8             max absolute_mcc  0.449576 0.846697 326
## 9   max min_per_class_accuracy  0.925779 0.916667 302
## 10 max mean_per_class_accuracy  0.966708 0.946809 292
##
## Gains/Lift Table: Extract with `h2o.gainsLift(<model>, <data>)` or `h2o.gainsLift(<model>, valid=<T/
##
##
## Scoring History:
##              timestamp   duration training_speed   epochs iterations
## 1  2018-06-04 22:41:20  0.000 sec                 0.00000          0
## 2  2018-06-04 22:41:20  0.034 sec  75428 obs/sec  1.00000          1
## 3  2018-06-04 22:41:20  0.067 sec  66000 obs/sec  2.00000          2
## 4  2018-06-04 22:41:20  0.102 sec  64653 obs/sec  3.00000          3
## 5  2018-06-04 22:41:20  0.219 sec  33792 obs/sec  4.00000          4
## 6  2018-06-04 22:41:21  0.318 sec  25756 obs/sec  5.00000          5
## 7  2018-06-04 22:41:21  0.356 sec  27911 obs/sec  6.00000          6
## 8  2018-06-04 22:41:21  0.436 sec  28651 obs/sec  7.00000          7
## 9  2018-06-04 22:41:21  0.492 sec  28540 obs/sec  8.00000          8
## 10 2018-06-04 22:41:21  0.548 sec  28455 obs/sec  9.00000          9
## 11 2018-06-04 22:41:21  0.583 sec  30085 obs/sec 10.00000         10
## 12 2018-06-04 22:41:21  0.649 sec  30649 obs/sec 11.00000         11
```

```
## 13 2018-06-04 22:41:21  0.706 sec  30608 obs/sec 12.00000         12
## 14 2018-06-04 22:41:21  0.753 sec  31200 obs/sec 13.00000         13
## 15 2018-06-04 22:41:21  0.817 sec  31657 obs/sec 14.00000         14
## 16 2018-06-04 22:41:21  0.882 sec  32260 obs/sec 15.00000         15
## 17 2018-06-04 22:41:21  0.991 sec  29231 obs/sec 16.00000         16
## 18 2018-06-04 22:41:21  1.037 sec  29526 obs/sec 17.00000         17
## 19 2018-06-04 22:41:21  1.071 sec  30364 obs/sec 18.00000         18
## 20 2018-06-04 22:41:21  1.103 sec  31301 obs/sec 19.00000         19
##         samples training_rmse training_logloss training_auc training_lift
## 1      0.000000
## 2   1056.000000       0.34876          0.41973      0.74189       1.08530
## 3   2112.000000       0.26678          0.22887      0.86701       1.08530
## 4   3168.000000       0.23017          0.17621      0.91605       1.08530
## 5   4224.000000       0.21174          0.15128      0.93714       1.08530
## 6   5280.000000       0.20034          0.13640      0.95234       1.08530
## 7   6336.000000       0.19395          0.12663      0.95937       1.08530
## 8   7392.000000       0.18517          0.11657      0.96674       1.08530
## 9   8448.000000       0.18058          0.11007      0.97101       1.08530
## 10  9504.000000       0.17723          0.10600      0.97429       1.08530
## 11 10560.000000       0.17258          0.09953      0.97789       1.08530
## 12 11616.000000       0.16842          0.09492      0.98023       1.08530
## 13 12672.000000       0.16619          0.09167      0.98191       1.08530
## 14 13728.000000       0.16203          0.08787      0.98331       1.08530
## 15 14784.000000       0.15879          0.08458      0.98484       1.08530
## 16 15840.000000       0.15608          0.08191      0.98608       1.08530
## 17 16896.000000       0.15388          0.07925      0.98705       1.08530
## 18 17952.000000       0.15095          0.07675      0.98803       1.08530
## 19 19008.000000       0.14907          0.07468      0.98873       1.08530
## 20 20064.000000       0.14698          0.07299      0.98921       1.08530
##    training_classification_error validation_rmse validation_logloss
## 1
## 2                        0.07860         0.35161            0.41492
## 3                        0.07670         0.26557            0.21827
## 4                        0.06913         0.22815            0.16376
## 5                        0.05871         0.21085            0.14001
## 6                        0.05019         0.19750            0.12624
## 7                        0.04640         0.19071            0.11648
## 8                        0.04072         0.17763            0.10623
## 9                        0.03883         0.17297            0.10066
## 10                       0.03788         0.16468            0.09508
## 11                       0.03598         0.16398            0.09187
## 12                       0.03409         0.15909            0.08814
## 13                       0.03409         0.15822            0.08670
## 14                       0.03409         0.15207            0.08274
## 15                       0.03220         0.15053            0.08088
## 16                       0.03125         0.14833            0.07885
## 17                       0.03030         0.14991            0.07936
## 18                       0.02936         0.14661            0.07686
## 19                       0.02936         0.14730            0.07686
## 20                       0.02841         0.14562            0.07595
##    validation_auc validation_lift validation_classification_error
## 1
## 2         0.73252         1.07295                         0.06516
## 3         0.86955         1.07295                         0.06799
```

```
## 4         0.92705         1.07295                       0.06516
## 5         0.94871         1.07295                       0.05949
## 6         0.96137         1.07295                       0.04533
## 7         0.96682         1.07295                       0.03966
## 8         0.97264         1.07295                       0.02833
## 9         0.97619         1.07295                       0.02550
## 10        0.97809         1.07295                       0.02550
## 11        0.97910         1.07295                       0.02550
## 12        0.98050         1.07295                       0.02266
## 13        0.98100         1.07295                       0.02266
## 14        0.98265         1.07295                       0.02266
## 15        0.98341         1.07295                       0.01983
## 16        0.98417         1.07295                       0.01983
## 17        0.98366         1.07295                       0.02266
## 18        0.98379         1.07295                       0.02266
## 19        0.98417         1.07295                       0.02266
## 20        0.98404         1.07295                       0.01983
##
## Variable Importances: (Extract with `h2o.varimp`)
## =================================================
##
## Variable Importances:
##                  variable relative_importance scaled_importance percentage
## 1   MassAccu.SLHTLFGDELCK            1.000000          1.000000   0.034675
## 2 MassAccu.ECCHGDLLECADDR            0.925454          0.925454   0.032090
## 3          RT.HLVDEPQNLIK            0.890437          0.890437   0.030876
## 4   Charge.VPQVSTPTLVEVSR            0.872659          0.872659   0.030259
## 5  TotalArea.SLHTLFGDELCK            0.860369          0.860369   0.029833
##
## ---
##                variable relative_importance scaled_importance percentage
## 43         RT.NECFLSHK            0.384706          0.384706   0.013340
## 44 MassAccu.EACFAVEGPK            0.356352          0.356352   0.012356
## 45     FWHM.EACFAVEGPK            0.344777          0.344777   0.011955
## 46      MZ.HLVDEPQNLIK            0.331787          0.331787   0.011505
## 47 Charge.SLHTLFGDELCK            0.322294          0.322294   0.011175
## 48   MZ.VPQVSTPTLVEVSR            0.267940          0.267940   0.009291
```

The accuracy is 98.57% . The net could be optmizied further to improve the accuracy

5 build the mlp(multi layer perceptron) deep learning model2 using h2o

```
set.seed(100)

dl_model2 <- h2o.deeplearning(
  model_id="dl_model_first",
  training_frame=train_h2o,
  validation_frame = test_h2o,
  x= colnames(train_h2o[,1:48]),
  y= "RESPONSE",
  activation="Tanh",
```

```
  hidden=c(5,4),
  stopping_metric="mean_per_class_error",
  stopping_tolerance=0.01,
  epochs=100,
  seed = 123, # give seed
  export_weights_and_biases = T, # export weights and biases defaults to false
  reproducible = T # Force reproducibility on small data (will be slow - only uses 1 thread). Defaults
)
```

5.0.1 Tuning the ANN

The simplest hyperparameter search method is a brute-force scan of the full Cartesian product of all combinations specified by a grid search. There are a lot of paramters to tune and due to limited computational capabilities we shall try to tune only some of them.

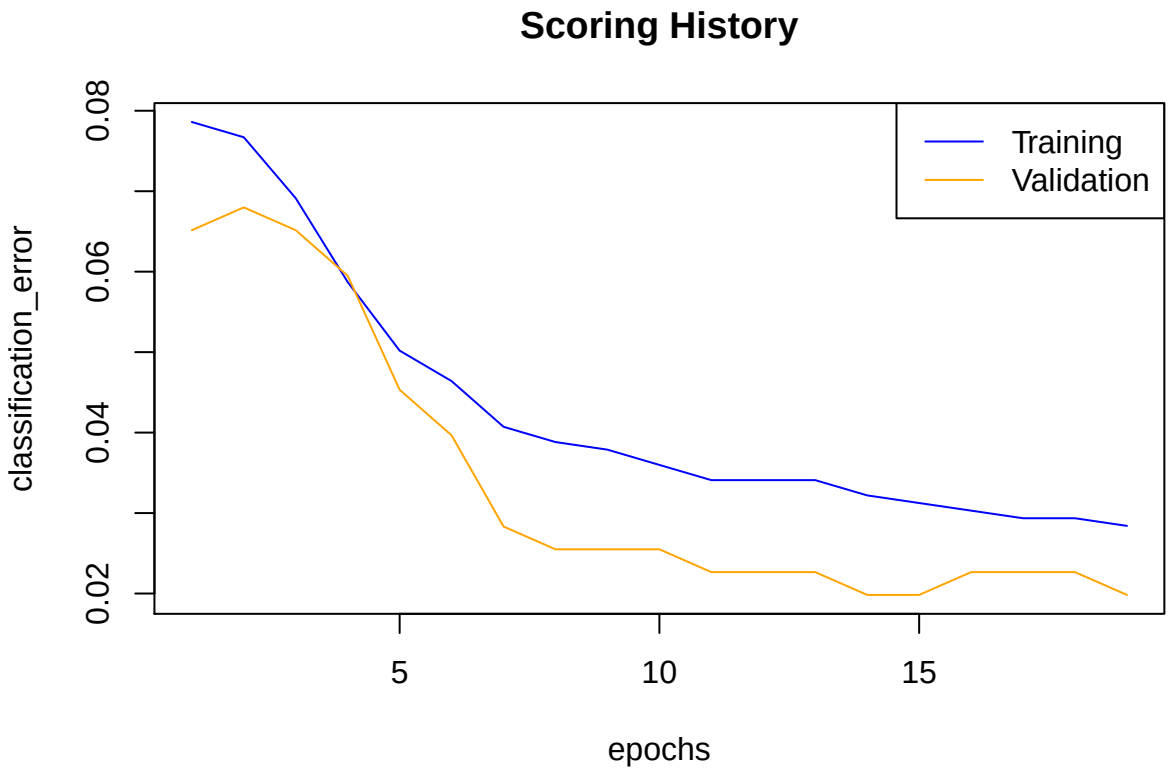
```
#hyperparamters to tune
hyper_params <- list(
  hidden=list(c(32,32,32),c(50,200,50)),  # different architectures of hidden layer
  input_dropout_ratio=c(0,0.05),      # values for drop out
  rate=c(0.01,0.02),                  # the learning rae
  activation = c("Rectifier")   # activation functions
)

#grid search

grid <- h2o.grid(
  algorithm="deeplearning",
  grid_id="dl_grid",
  model_id="dl_model_first",
  training_frame=train_h2o,
  x= colnames(train_h2o[,1:12]),
  y= "label",
  stopping_metric="mean_per_class_error",
  hyper_params = hyper_params,
  epochs=1000,
  stopping_tolerance=0.01,
  variable_importances=T
)
```

```
# sort the model in the grid in decreasing order of error
grid <- h2o.getGrid("dl_grid", sort_by = "err", decreasing = FALSE)
grid

# best model and its full set of parameters
grid@summary_table[1, ]
best_dl_model <- h2o.getModel(grid@model_ids[[1]])
best_dl_model

print(h2o.performance(best_dl_model))

# storing the confusion matrix
best_dl_confusion <- as.data.frame(h2o.confusionMatrix(best_dl_model))
```

5.0.2 Plotting the model

```
plot(dl_model,timesteps = "epochs",metric = "classification_error")
```

```
## Warning in plot.window(...): "timesteps" is not a graphical parameter

## Warning in plot.xy(xy, type, ...): "timesteps" is not a graphical parameter

## Warning in title(...): "timesteps" is not a graphical parameter

## Warning in plot.window(...): "timesteps" is not a graphical parameter

## Warning in plot.xy(xy, type, ...): "timesteps" is not a graphical parameter

## Warning in axis(side = side, at = at, labels = labels, ...): "timesteps" is
## not a graphical parameter

## Warning in axis(side = side, at = at, labels = labels, ...): "timesteps" is
## not a graphical parameter

## Warning in box(...): "timesteps" is not a graphical parameter

## Warning in title(...): "timesteps" is not a graphical parameter
```



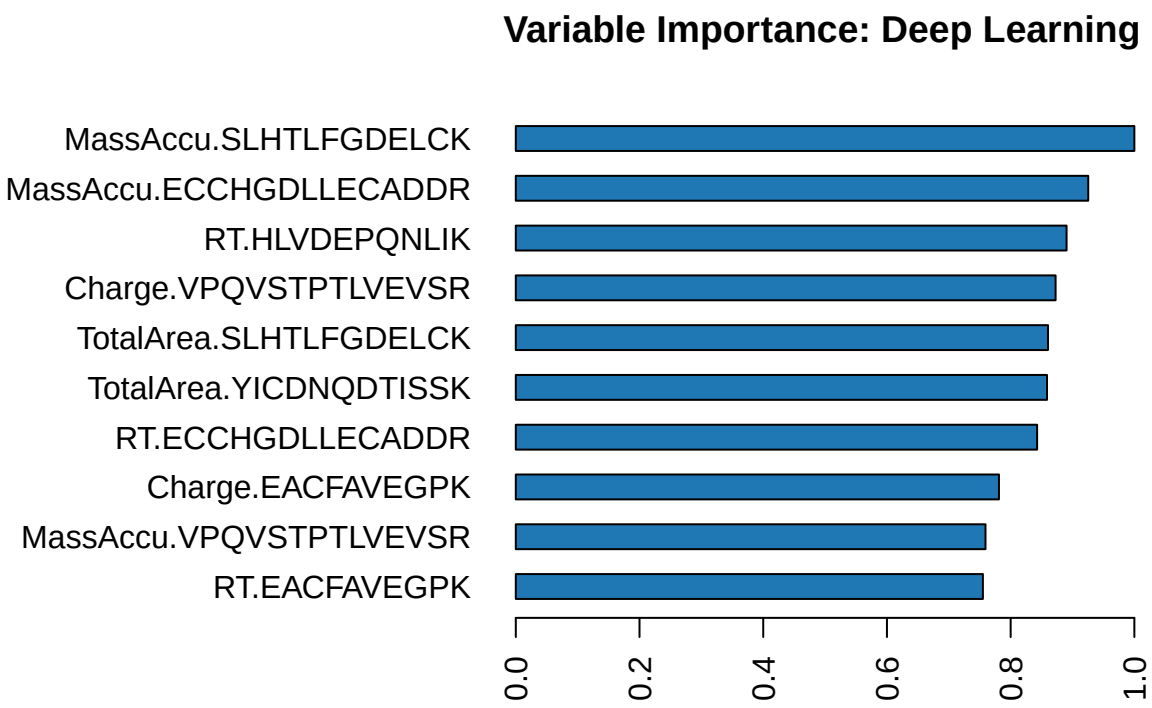
The training accuracy and testing accuracy decreases with increase in epochs.

5.0.3 Predictons on test data

```
dl_predict <- as.data.frame(h2o.predict(dl_model, test_h2o))
```

5.0.4 Variable importance

```
h2o.varimp_plot(dl_model)
```



5.0.5 Getting weights for neural network

```
weights1<- h2o.weights(dl_model,matrix_id = 1)
print(head(weights1))
```

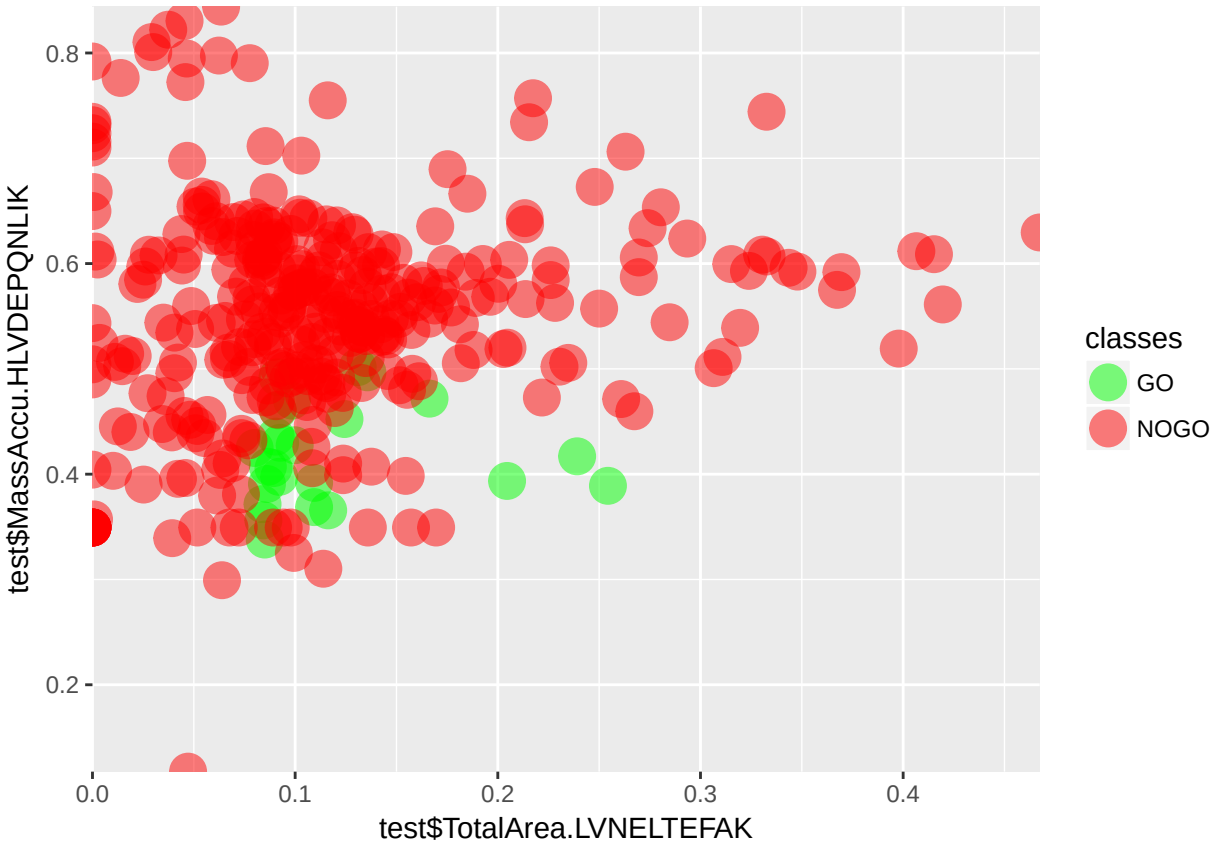
```
##   RT.EACFAVEGPK MZ.EACFAVEGPK Charge.EACFAVEGPK TotalArea.EACFAVEGPK
## 1   -0.23583737    -0.2797842       -0.30021629          -0.49712917
## 2   -0.31172439     0.1067308        0.20294011           0.09682767
## 3    0.15955730    -0.2717285        0.34951603          -0.13898845
## 4   -0.16535486    -0.1180188        0.14910677           0.02682342
## 5    0.04370809    -0.1684333       -0.05766352           0.04393569
##   MassAccu.EACFAVEGPK FWHM.EACFAVEGPK RT.ECCHGDLLECADDR MZ.ECCHGDLLECADDR
## 1         -0.11241128      0.03293785        -0.3784887       -0.20930095
## 2          0.16646102     -0.01113706         0.1443341        0.10131175
## 3         -0.09741532     -0.24260718        -0.1864207        0.26914412
```

```
## 4          0.03393902     -0.22448434        -0.1328639        0.10982639
## 5         -0.01928469     -0.10195930         0.2842945       -0.07123732
##   Charge.ECCHGDLLECADDR TotalArea.ECCHGDLLECADDR MassAccu.ECCHGDLLECADDR
## 1           -0.08028070               0.04380139               0.2390468
## 2            0.17654702               0.22064185               0.3332438
## 3            0.17712097               0.05794469               0.1121283
## 4           -0.09680744              -0.37012294               0.2191533
## 5           -0.25219941              -0.07897471              -0.2872470
##   FWHM.ECCHGDLLECADDR RT.HLVDEPQNLIK MZ.HLVDEPQNLIK Charge.HLVDEPQNLIK
## 1        -0.177995548      0.2089175   -0.007526016        -0.25721249
## 2        -0.053703718      0.2001829   -0.103207536         0.25190017
## 3         0.002204252      0.3230875   -0.080076307        -0.04167950
## 4         0.239626080     -0.3683851    0.216559514         0.01580123
## 5         0.021929504     -0.1893954    0.080183007         0.11831298
##   TotalArea.HLVDEPQNLIK MassAccu.HLVDEPQNLIK FWHM.HLVDEPQNLIK
## 1            0.20658407          -0.03116613      -0.01719454
## 2            0.05558940           0.18113561       0.15477853
## 3           -0.08160750          -0.11139227      -0.21041989
## 4           -0.07090132           0.13873971       0.19957870
## 5            0.17626619          -0.51180947       0.01717483
##   RT.LVNELTEFAK MZ.LVNELTEFAK Charge.LVNELTEFAK TotalArea.LVNELTEFAK
## 1    0.13477133   -0.10674237        0.09982824           0.11847905
## 2    0.25755301   -0.28599012        0.21880627          -0.07164115
## 3   -0.04675132   -0.14938121       -0.25736502           0.22915508
## 4   -0.18672875   -0.07407859        0.03334839          -0.13678196
## 5    0.32723492   -0.02658161        0.19788770           0.06873327
##   MassAccu.LVNELTEFAK FWHM.LVNELTEFAK RT.NECFLSHK  MZ.NECFLSHK
## 1         -0.09730984    -0.085679427  0.12883815  0.292881101
## 2          0.06985192    -0.299628794  0.01590926  0.146213681
## 3         -0.10182326    -0.224256024 -0.27157819 -0.231285438
## 4         -0.12174950    -0.109187134 -0.14838588 -0.178881302
## 5         -0.45769987    -0.001172399  0.05864862  0.005703649
##   Charge.NECFLSHK TotalArea.NECFLSHK MassAccu.NECFLSHK FWHM.NECFLSHK
## 1      0.01242616        0.292510897        -0.1439769    0.01307709
## 2      0.12708127        0.047977872        -0.1019750   -0.18202820
## 3      0.12362847        0.091072686        -0.2498159    0.08090138
## 4      0.20265849        0.009479483        -0.1671181   -0.21013930
## 5      0.20184378       -0.055024203         0.1134884    0.19007911
##   RT.SLHTLFGDELCK MZ.SLHTLFGDELCK Charge.SLHTLFGDELCK
## 1     -0.10318555    -0.134392232        -0.047550403
## 2     -0.23059729    -0.153181806         0.036417175
## 3      0.31246373    -0.005469696         0.003266339
## 4      0.22693875     0.192572594        -0.317640662
## 5     -0.04229377     0.291551530        -0.047417101
##   TotalArea.SLHTLFGDELCK MassAccu.SLHTLFGDELCK FWHM.SLHTLFGDELCK
## 1             -0.2143636            0.11644069        -0.1376150
## 2             -0.3995810           -0.37309504         0.2236235
## 3              0.0460235            0.09098575         0.1052235
## 4              0.2126222            0.46947935         0.2968217
## 5              0.1401082           -0.28656608         0.1849351
##   RT.VPQVSTPTLVEVSR MZ.VPQVSTPTLVEVSR Charge.VPQVSTPTLVEVSR
## 1       -0.35019854       -0.06006742            0.23780479
## 2       -0.21153511        0.08133842           -0.29036209
## 3        0.03918119        0.12063876           -0.35590869
```

```
## 4       -0.19612859        0.09823170           -0.05662033
## 5        0.04685416       -0.01915597            0.29162684
##   TotalArea.VPQVSTPTLVEVSR MassAccu.VPQVSTPTLVEVSR FWHM.VPQVSTPTLVEVSR
## 1               0.22272693             -0.21007168         -0.04567311
## 2               0.13274157             -0.31248918         -0.04669969
## 3               0.16547132             -0.26304877         -0.35921317
## 4              -0.06847159              0.14238121          0.15663911
## 5              -0.28570506             -0.04939715          0.12096434
##   RT.YICDNQDTISSK MZ.YICDNQDTISSK Charge.YICDNQDTISSK
## 1       0.1365843     -0.19785093          0.27808824
## 2      -0.2237834      0.32785612          0.16589519
## 3       0.2327577      0.01206885         -0.21181442
## 4       0.2032687     -0.11087516         -0.04950723
## 5       0.1047876      0.04063049          0.05824081
##   TotalArea.YICDNQDTISSK MassAccu.YICDNQDTISSK FWHM.YICDNQDTISSK
## 1            -0.28742716             0.1310544         0.1410810
## 2             0.24357809            -0.2643718        -0.2426255
## 3            -0.04995213            -0.1191344         0.3911833
## 4             0.24030717             0.2192163        -0.1944355
## 5            -0.26405954             0.1498870        -0.1128908
```

5.0.6 Plotting decision boundary for neural networks

```
Color <- c("GREEN","RED")
names(Color) <- c('GO','NOGO')
ggplot(data = test,aes(x = test$TotalArea.LVNELTEFAK, y = test$MassAccu.HLVDEPQNLIK)) +
  geom_point(aes(color = test$RESPONSE), size = 6, alpha = .5) +
  scale_colour_manual(name = 'classes', values = Color) +
  scale_x_continuous(expand = c(0,0)) +
  scale_y_continuous(expand = c(0,0))
```



6 build the mlp(multi layer perceptron) deep learning model using h2o

```
set.seed(100)

dl_model2 <- h2o.deeplearning(
  model_id="dl_model_first",
  training_frame=train_h2o,
  validation_frame = test_h2o,
  x= colnames(train_h2o[,1:48]),
  y= "RESPONSE",
  activation="Tanh",
  hidden=c(5,5),
  stopping_metric="mean_per_class_error",
  stopping_rounds = 5,
  stopping_tolerance=0.01,
  rate = 0.005, # Defaults to 0.005
  mini_batch_size = 1,# defaults to 1
  epochs=100,
  seed = 123, # give seed
  export_weights_and_biases = T, # export weights and biases defaults to false
  reproducible = T # Force reproducibility on small data (will be slow - only uses 1 thread). Defaults
)
```

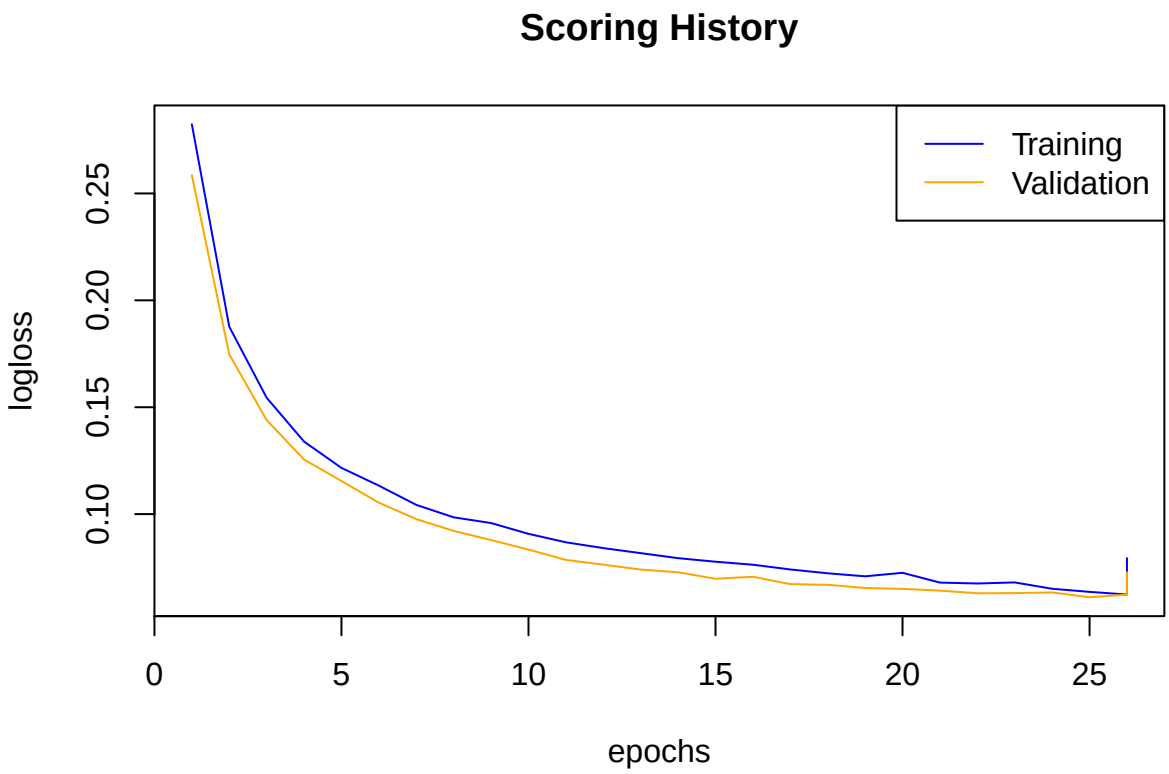
```
summary(dl_model2)
```

```
## Model Details:
## ==============
##
## H2OBinomialModel: deeplearning
## Model Key:  dl_model_first
## Status of Neuron Layers: predicting RESPONSE, 2-class classification, bernoulli distribution, CrossE
batch size 1
##   layer units    type dropout       l1       l2 mean_rate rate_rms
## 1     1    48   Input  0.00 %
## 2     2     5    Tanh  0.00 % 0.000000 0.000000  0.002646 0.002210
## 3     3     5    Tanh  0.00 % 0.000000 0.000000  0.001168 0.001267
## 4     4     2 Softmax         0.000000 0.000000  0.002892 0.000555
##   momentum mean_weight weight_rms mean_bias bias_rms
## 1
## 2 0.000000    0.014566   0.199495 -0.033308 0.046426
## 3 0.000000   -0.024504   0.494151  0.287324 0.076459
## 4 0.000000    0.140694   2.875058  0.000000 0.493199
##
## H2OBinomialMetrics: deeplearning
## ** Reported on training data. **
## ** Metrics reported on full training frame **
##
## MSE:  0.02220305
## RMSE:  0.1490069
## LogLoss:  0.07940421
## Mean Per-Class Error:  0.1235652
## AUC:  0.9843856
## Gini:  0.9687713
##
## Confusion Matrix (vertical: actual; across: predicted) for F1-optimal threshold:
##        GO NOGO    Error      Rate
## GO     63   20 0.240964    =20/83
## NOGO    6  967 0.006166    =6/973
## Totals 69  987 0.024621  =26/1056
##
## Maximum Metrics: Maximum metrics at their respective thresholds
##                         metric threshold    value idx
## 1                       max f1  0.450857 0.986735 330
## 2                       max f2  0.450857 0.990982 330
## 3                 max f0point5  0.771159 0.987241 295
## 4                 max accuracy  0.455604 0.975379 328
## 5                max precision  0.999989 1.000000   0
## 6                   max recall  0.138910 1.000000 376
## 7              max specificity  0.999989 1.000000   0
## 8             max absolute_mcc  0.455604 0.820879 328
## 9   max min_per_class_accuracy  0.888299 0.945529 267
## 10 max mean_per_class_accuracy  0.904772 0.951095 260
##
## Gains/Lift Table: Extract with `h2o.gainsLift(<model>, <data>)` or `h2o.gainsLift(<model>, valid=<T/
## H2OBinomialMetrics: deeplearning
## ** Reported on validation data. **
## ** Metrics reported on full validation frame **
```

```
##
## MSE:  0.02081881
## RMSE:  0.1442873
## LogLoss:  0.07279464
## Mean Per-Class Error:  0.06705927
## AUC:  0.9864488
## Gini:  0.9728977
##
## Confusion Matrix (vertical: actual; across: predicted) for F1-optimal threshold:
##        GO NOGO    Error    Rate
## GO     21    3 0.125000   =3/24
## NOGO    3  326 0.009119  =3/329
## Totals 24  329 0.016997  =6/353
##
## Maximum Metrics: Maximum metrics at their respective thresholds
##                         metric threshold    value idx
## 1                        max f1  0.510167 0.990881 327
## 2                        max f2  0.510167 0.990881 327
## 3                  max f0point5  0.510167 0.990881 327
## 4                  max accuracy  0.510167 0.983003 327
## 5                 max precision  0.999993 1.000000   0
## 6                    max recall  0.134955 1.000000 347
## 7               max specificity  0.999993 1.000000   0
## 8              max absolute_mcc  0.510167 0.865881 327
## 9   max min_per_class_accuracy  0.865585 0.951368 312
## 10 max mean_per_class_accuracy  0.865585 0.954851 312
##
## Gains/Lift Table: Extract with `h2o.gainsLift(<model>, <data>)` or `h2o.gainsLift(<model>, valid=<T/
##
##
## Scoring History:
##             timestamp   duration training_speed  epochs iterations
## 1 2018-06-04 22:41:28  0.000 sec                0.00000          0
## 2 2018-06-04 22:41:28  0.269 sec  75428 obs/sec 1.00000          1
## 3 2018-06-04 22:41:28  0.498 sec   9345 obs/sec 2.00000          2
## 4 2018-06-04 22:41:28  0.534 sec  12878 obs/sec 3.00000          3
## 5 2018-06-04 22:41:28  0.588 sec  15249 obs/sec 4.00000          4
##       samples training_rmse training_logloss training_auc training_lift
## 1    0.000000
## 2 1056.000000       0.28237          0.28231      0.82289       0.98664
## 3 2112.000000       0.23118          0.18770      0.91223       1.08530
## 4 3168.000000       0.20979          0.15442      0.93608       1.08530
## 5 4224.000000       0.19559          0.13393      0.94915       1.08530
##   training_classification_error validation_rmse validation_logloss
## 1
## 2                       0.07860         0.27834            0.25853
## 3                       0.07008         0.23571            0.17472
## 4                       0.05682         0.21349            0.14398
## 5                       0.04830         0.19823            0.12551
##   validation_auc validation_lift validation_classification_error
## 1
## 2        0.83169         1.07295                         0.06516
## 3        0.91958         1.07295                         0.06516
## 4        0.94453         1.07295                         0.05949
```

```
## 5        0.95517         1.07295                         0.05099
##
## ---
##              timestamp   duration training_speed   epochs iterations
## 23 2018-06-04 22:41:30  2.257 sec  18750 obs/sec 22.00000         22
## 24 2018-06-04 22:41:30  2.330 sec  18769 obs/sec 23.00000         23
## 25 2018-06-04 22:41:30  2.370 sec  19287 obs/sec 24.00000         24
## 26 2018-06-04 22:41:30  2.524 sec  18435 obs/sec 25.00000         25
## 27 2018-06-04 22:41:30  2.580 sec  18702 obs/sec 26.00000         26
## 28 2018-06-04 22:41:30  2.613 sec  18538 obs/sec 26.00000         26
##         samples training_rmse training_logloss training_auc training_lift
## 23 23232.000000       0.13724          0.06755      0.98882       1.08530
## 24 24288.000000       0.13779          0.06805      0.98912       1.08530
## 25 25344.000000       0.13530          0.06507      0.98995       1.08530
## 26 26400.000000       0.13294          0.06364      0.99016       1.08530
## 27 27456.000000       0.13219          0.06239      0.99060       1.08530
## 28 27456.000000       0.14901          0.07940      0.98439       1.08530
##    training_classification_error validation_rmse validation_logloss
## 23                       0.02178         0.13439            0.06297
## 24                       0.02178         0.13462            0.06304
## 25                       0.02083         0.13604            0.06335
## 26                       0.02083         0.13296            0.06112
## 27                       0.01894         0.13525            0.06236
## 28                       0.02462         0.14429            0.07279
##    validation_auc validation_lift validation_classification_error
## 23        0.99012         1.07295                         0.01983
## 24        0.99050         1.07295                         0.01983
## 25        0.98999         1.07295                         0.01983
## 26        0.99101         1.07295                         0.01983
## 27        0.99012         1.07295                         0.01983
## 28        0.98645         1.07295                         0.01700
##
## Variable Importances: (Extract with `h2o.varimp`)
## =================================================
##
## Variable Importances:
##                  variable relative_importance scaled_importance percentage
## 1   Charge.VPQVSTPTLVEVSR            1.000000          1.000000   0.034240
## 2    MassAccu.HLVDEPQNLIK            0.985779          0.985779   0.033753
## 3 MassAccu.ECCHGDLLECADDR            0.950572          0.950572   0.032548
## 4    TotalArea.EACFAVEGPK            0.910523          0.910523   0.031177
## 5          RT.HLVDEPQNLIK            0.906599          0.906599   0.031042
##
## ---
##                 variable relative_importance scaled_importance percentage
## 43   FWHM.VPQVSTPTLVEVSR            0.344528          0.344528   0.011797
## 44    TotalArea.NECFLSHK            0.340728          0.340728   0.011667
## 45   Charge.SLHTLFGDELCK            0.319727          0.319727   0.010948
## 46     MZ.VPQVSTPTLVEVSR            0.309764          0.309764   0.010606
## 47   FWHM.ECCHGDLLECADDR            0.267567          0.267567   0.009162
## 48 MassAccu.YICDNQDTISSK            0.236624          0.236624   0.008102
```

```
plot(dl_model2)
```



6.0.1 shutdown h2o

6.1 Simulating 3 effects

6.2 Main Data

```
head(Train)
```

```
##   idfile                                                                PepSeq
## 1  14811                                                EAC(Carbamidomethyl)FAVEGPK
## 2  14811 EC(Carbamidomethyl)C(Carbamidomethyl)HGDLLEC(Carbamidomethyl)ADDR
## 4  14811                                                          HLVDEPQNLIK
## 5  14811                                                           LVNELTEFAK
## 6  14811                                              NEC(Carbamidomethyl)FLSHK
## 7  14811                                           SLHTLFGDELC(Carbamidomethyl)K
##        RT      MZ Charge TotalArea   MassAccu    FWHM
## 1 734.913 554.261      2  2.36e+08 -0.0652368 2.04135
## 2 715.251 583.893      3  1.88e+08  0.2566130 1.90107
## 4 739.787 653.362      2  9.38e+08  0.1110990 1.97179
## 5 792.170 582.319      2  6.85e+08  0.0907428 1.67105
## 6 675.845 517.740      2  3.88e+08  0.0501789 1.95090
## 7 777.652 710.350      2  7.87e+07 -0.4440630 1.83461
```

```
nrow(Train)
```

```
## [1] 856
```

```
Train %>% group_by(PepSeq) %>% summarise(Count = n())
```

```
## # A tibble: 8 x 2
##   PepSeq                                                          Count
##   <fct>                                                           <int>
## 1 EAC(Carbamidomethyl)FAVEGPK                                       107
## 2 EC(Carbamidomethyl)C(Carbamidomethyl)HGDLLEC(Carbamidomethyl)ADDR  107
## 3 HLVDEPQNLIK                                                       107
## 4 LVNELTEFAK                                                        107
## 5 NEC(Carbamidomethyl)FLSHK                                         107
## 6 SLHTLFGDELC(Carbamidomethyl)K                                     107
## 7 VPQVSTPTLVEVSR                                                    107
## 8 YIC(Carbamidomethyl)DNQDTISSK                                     107
```

6.2.1 Simulation 1: Spike in mean X 10

```
spike_mean <- function(num_col,value){
  # Train Data
  #one peptide LVNELTEFAK

  #generate multivariate normal data
  #parameters from a training sample
  n<-100 #incontrol observations
  m<-100 #ooc observations

  # Simularing in Control data with n observations
  mean <-c(with(data=Train,tapply(RT,INDEX=PepSeq,FUN=mean))[5],
           with(data=Train,tapply(TotalArea,INDEX=PepSeq,FUN=mean)) [5],
           with(data=Train,tapply(MassAccu,INDEX=PepSeq,FUN=mean)) [5],
           with(data=Train,tapply(FWHM,INDEX=PepSeq,FUN=mean)) [5]
           )
  covar<- cov(Train[Train$PepSeq=="LVNELTEFAK",c(3,6,7,8)])


  Sim_ic_1 <-data.frame(idfile=1:n,PepSeq=rep("LVNELTEFAK",n),mvrnorm(n, mean, covar))
  colnames(Sim_ic_1)<-c("idfile","PepSeq","RT","TotalArea","MassAccu","FWHM")

  RESPONSE <- c("GO")
  Sim_ic_1 <- cbind(Sim_ic_1,RESPONSE) # simulation effect 1  incontrol observation



  # Simulating Out of Control data with m observations
  # Sim_oc_1 <-data.frame(idfile=(n+1):(n+m),PepSeq=rep("LVNELTEFAK",m),
  #                    mvrnorm(m, mean+(10*c(covar[1,1],1.0*covar[2,2],3.0*covar[3,3],1.0*covar[4,4])),
  #                   covar))
  if(num_col == 1)
    Sim_oc_1 <- data.frame(idfile=(n+1):(n+m),PepSeq=rep("LVNELTEFAK",m), # increase in mean FWHM X 10
                    mvrnorm(m, mean*c(value,1,1,1),
                   covar))
  else if(num_col == 2)
```

```
    Sim_oc_1 <- data.frame(idfile=(n+1):(n+m),PepSeq=rep("LVNELTEFAK",m), # increase in mean FWHM X 10
                    mvrnorm(m, mean*c(1,value,1,1),
                   covar))
  else if(num_col == 3)
    Sim_oc_1 <- data.frame(idfile=(n+1):(n+m),PepSeq=rep("LVNELTEFAK",m), # increase in mean FWHM X 10
                    mvrnorm(m, mean*c(1,1,value,1),
                   covar))
  else
    Sim_oc_1 <- data.frame(idfile=(n+1):(n+m),PepSeq=rep("LVNELTEFAK",m), # increase in mean FWHM X 10
                    mvrnorm(m, mean*c(1,1,1,value),
                   covar))

  colnames(Sim_oc_1) <- c("idfile","PepSeq","RT","TotalArea","MassAccu","FWHM")

  RESPONSE <- c("NOGO")
  Sim_oc_1 <- cbind(Sim_oc_1,RESPONSE)
  new_data <- rbind(Sim_ic_1,Sim_oc_1)
return(new_data)
}
```

```
new_data <- spike_mean(1,10)
maxs <- apply(new_data %>% dplyr::select(-c(idfile,PepSeq, RESPONSE)), 2, max)
mins <- apply(new_data %>% dplyr::select(-c(idfile,PepSeq, RESPONSE)), 2, min)

scaled_data <- as.data.frame(scale(new_data %>% dplyr::select(-c(idfile,PepSeq,RESPONSE)), center = mins
#scaled_data$RESPONSE <- ifelse(new_data$RESPONSE =="GO",1,0)
scaled_data$RESPONSE <- as.factor(new_data$RESPONSE)
#scaled_data$RESPONSE <- as.factor(scaled_data$RESPONSE)
scaled_data$idfile <- new_data$idfile

#select random ind for train and test
set.seed(123)

## 75% of the sample size
smp_size <- floor(0.75 * nrow(scaled_data))

## set the seed to make your partition reproducible
set.seed(123)
train_ind <- sample(seq_len(nrow(scaled_data)), size = smp_size)


train_sim1 <- scaled_data[train_ind,]
test_sim1 <- scaled_data[-train_ind,]

#Building Neural Network
library(h2o)
#generate same set of random numbers (for reproducibility)
set.seed(121)

#launch h2o cluster
localH2O <- h2o.init(nthreads = -1)
```

```
##  Connection successful!
##
```

```
## R is connected to the H2O cluster:
##     H2O cluster uptime:         32 minutes 41 seconds
##     H2O cluster timezone:       America/New_York
##     H2O data parsing timezone:  UTC
##     H2O cluster version:        3.18.0.8
##     H2O cluster version age:    1 month and 16 days
##     H2O cluster name:           H2O_started_from_R_Shantam_Gupta_kyo754
##     H2O cluster total nodes:    1
##     H2O cluster total memory:   2.33 GB
##     H2O cluster total cores:    4
##     H2O cluster allowed cores:  4
##     H2O cluster healthy:        TRUE
##     H2O Connection ip:          localhost
##     H2O Connection port:        54321
##     H2O Connection proxy:       NA
##     H2O Internal Security:      FALSE
##     H2O API Extensions:         Algos, AutoML, Core V3, Core V4
##     R Version:                  R version 3.3.3 (2017-03-06)
```

```
#import r objects to h2o cloud
train_h2o <- as.h2o(train_sim1)
test_h2o <- as.h2o(test_sim1)

set.seed(100)

dl_model_sim1 <- h2o.deeplearning(
  model_id="dl_model_first",
  training_frame=train_h2o,
  validation_frame = test_h2o,
  x= colnames(train_h2o[,1:4]),
  y= "RESPONSE",
  activatio="Tanh",
  hidden=c(2,2),
  stopping_metric="mean_per_class_error",
  stopping_rounds = 5,
  stopping_tolerance=0.001,
  rate = 0.005, # Defaults to 0.005
  mini_batch_size = 1,# defaults to 1
  epochs=100,
  seed = 123, # give seed
  export_weights_and_biases = T, # export weights and biases defaults to false
  reproducible = T # Force reproducibility on small data (will be slow - only uses 1 thread). Defaults
)
summary(dl_model_sim1)
```

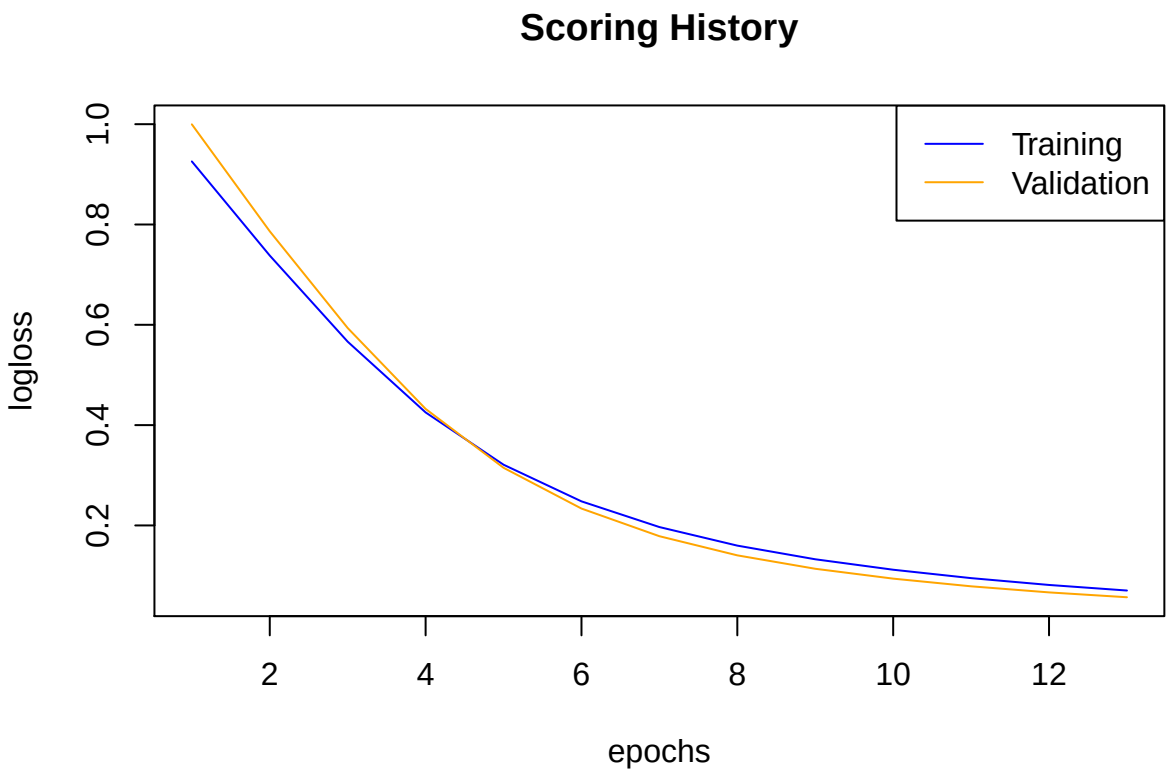
```
## Model Details:
## ==============
##
## H2OBinomialModel: deeplearning
## Model Key:  dl_model_first
## Status of Neuron Layers: predicting RESPONSE, 2-class classification, bernoulli distribution, CrossE
batch size 1
##   layer units    type dropout       l1       l2 mean_rate rate_rms
## 1     1     4   Input  0.00 %
## 2     2     2    Tanh  0.00 % 0.000000 0.000000  0.002463 0.001915
```

```
## 3     3     2    Tanh  0.00 % 0.000000 0.000000  0.101875 0.102434
## 4     4     2 Softmax         0.000000 0.000000  0.006101 0.004078
##   momentum mean_weight weight_rms mean_bias bias_rms
## 1
## 2 0.000000   -0.408571   0.598224 -0.009116 0.012083
## 3 0.000000    0.723658   1.104087  0.014922 0.024276
## 4 0.000000   -2.140051   3.418088  0.000000 0.010361
##
## H2OBinomialMetrics: deeplearning
## ** Reported on training data. **
## ** Metrics reported on full training frame **
##
## MSE:  0.01541795
## RMSE:  0.124169
## LogLoss:  0.07021577
## Mean Per-Class Error:  0
## AUC:  1
## Gini:  1
##
## Confusion Matrix (vertical: actual; across: predicted) for F1-optimal threshold:
##        GO NOGO    Error    Rate
## GO     74    0 0.000000   =0/74
## NOGO    0   76 0.000000   =0/76
## Totals 74   76 0.000000  =0/150
##
## Maximum Metrics: Maximum metrics at their respective thresholds
##                         metric threshold    value idx
## 1                       max f1  0.574902 1.000000  75
## 2                       max f2  0.574902 1.000000  75
## 3                 max f0point5  0.574902 1.000000  75
## 4                 max accuracy  0.574902 1.000000  75
## 5                max precision  0.995948 1.000000   0
## 6                   max recall  0.574902 1.000000  75
## 7              max specificity  0.995948 1.000000   0
## 8             max absolute_mcc  0.574902 1.000000  75
## 9   max min_per_class_accuracy  0.574902 1.000000  75
## 10 max mean_per_class_accuracy  0.574902 1.000000  75
##
## Gains/Lift Table: Extract with `h2o.gainsLift(<model>, <data>)` or `h2o.gainsLift(<model>, valid=<T/
## H2OBinomialMetrics: deeplearning
## ** Reported on validation data. **
## ** Metrics reported on full validation frame **
##
## MSE:  0.008488261
## RMSE:  0.09213176
## LogLoss:  0.05680938
## Mean Per-Class Error:  0
## AUC:  1
## Gini:  1
##
## Confusion Matrix (vertical: actual; across: predicted) for F1-optimal threshold:
##        GO NOGO    Error   Rate
## GO     26    0 0.000000  =0/26
## NOGO    0   24 0.000000  =0/24
```

```
## Totals 26   24 0.000000  =0/50
##
## Maximum Metrics: Maximum metrics at their respective thresholds
##                         metric threshold    value idx
## 1                       max f1  0.849627 1.000000  23
## 2                       max f2  0.849627 1.000000  23
## 3                 max f0point5  0.849627 1.000000  23
## 4                 max accuracy  0.849627 1.000000  23
## 5                max precision  0.996744 1.000000   0
## 6                   max recall  0.849627 1.000000  23
## 7              max specificity  0.996744 1.000000   0
## 8             max absolute_mcc  0.849627 1.000000  23
## 9   max min_per_class_accuracy  0.849627 1.000000  23
## 10 max mean_per_class_accuracy  0.849627 1.000000  23
##
## Gains/Lift Table: Extract with `h2o.gainsLift(<model>, <data>)` or `h2o.gainsLift(<model>, valid=<T/
##
##
## Scoring History:
##              timestamp   duration training_speed   epochs iterations
## 1  2018-06-04 22:41:33  0.000 sec                0.00000          0
## 2  2018-06-04 22:41:33  0.010 sec  75000 obs/sec  1.00000          1
## 3  2018-06-04 22:41:33  0.018 sec  60000 obs/sec  2.00000          2
## 4  2018-06-04 22:41:33  0.027 sec  45000 obs/sec  3.00000          3
## 5  2018-06-04 22:41:33  0.036 sec  42857 obs/sec  4.00000          4
## 6  2018-06-04 22:41:33  0.048 sec  35714 obs/sec  5.00000          5
## 7  2018-06-04 22:41:33  0.063 sec  34615 obs/sec  6.00000          6
## 8  2018-06-04 22:41:33  0.083 sec  30882 obs/sec  7.00000          7
## 9  2018-06-04 22:41:33  0.109 sec  26086 obs/sec  8.00000          8
## 10 2018-06-04 22:41:33  0.128 sec  24545 obs/sec  9.00000          9
## 11 2018-06-04 22:41:33  0.146 sec  23437 obs/sec 10.00000         10
## 12 2018-06-04 22:41:33  0.166 sec  21710 obs/sec 11.00000         11
## 13 2018-06-04 22:41:33  0.181 sec  21428 obs/sec 12.00000         12
## 14 2018-06-04 22:41:33  0.197 sec  21428 obs/sec 13.00000         13
##        samples training_rmse training_logloss training_auc training_lift
## 1     0.000000
## 2   150.000000       0.51282          0.92573      0.73471       1.97368
## 3   300.000000       0.47114          0.73804      0.78841       1.97368
## 4   450.000000       0.42235          0.56635      0.85188       1.97368
## 5   600.000000       0.37093          0.42528      0.90807       1.97368
## 6   750.000000       0.32329          0.32105      0.94488       1.97368
## 7   900.000000       0.28263          0.24797      0.96871       1.97368
## 8  1050.000000       0.24851          0.19671      0.98204       1.97368
## 9  1200.000000       0.21949          0.15974      0.98826       1.97368
## 10 1350.000000       0.19487          0.13251      0.99307       1.97368
## 11 1500.000000       0.17370          0.11167      0.99449       1.97368
## 12 1650.000000       0.15499          0.09491      0.99716       1.97368
## 13 1800.000000       0.13851          0.08131      0.99876       1.97368
## 14 1950.000000       0.12417          0.07022      1.00000       1.97368
##    training_classification_error validation_rmse validation_logloss
## 1
## 2                        0.33333         0.54310            0.99967
## 3                        0.28667         0.49791            0.78645
## 4                        0.22667         0.44524            0.59359
```

```
## 5                       0.17333         0.38546           0.43234
## 6                       0.13333         0.32573           0.31490
## 7                       0.11333         0.27222           0.23361
## 8                       0.08000         0.22776           0.17848
## 9                       0.06000         0.19166           0.14033
## 10                      0.03333         0.16306           0.11355
## 11                      0.03333         0.14021           0.09392
## 12                      0.02000         0.12113           0.07858
## 13                      0.01333         0.10527           0.06647
## 14                      0.00000         0.09213           0.05681
##    validation_auc validation_lift validation_classification_error
## 1
## 2         0.75641         2.08333                         0.32000
## 3         0.80449         2.08333                         0.28000
## 4         0.86218         2.08333                         0.24000
## 5         0.91987         2.08333                         0.16000
## 6         0.96955         2.08333                         0.08000
## 7         0.99359         2.08333                         0.04000
## 8         0.99840         2.08333                         0.02000
## 9         1.00000         2.08333                         0.00000
## 10        1.00000         2.08333                         0.00000
## 11        1.00000         2.08333                         0.00000
## 12        1.00000         2.08333                         0.00000
## 13        1.00000         2.08333                         0.00000
## 14        1.00000         2.08333                         0.00000
##
## Variable Importances: (Extract with `h2o.varimp`)
## =================================================
##
## Variable Importances:
##    variable relative_importance scaled_importance percentage
## 1        RT            1.000000          1.000000   0.401582
## 2  MassAccu            0.724706          0.724706   0.291029
## 3      FWHM            0.510556          0.510556   0.205031
## 4 TotalArea            0.254886          0.254886   0.102358
```

```
plot(dl_model_sim1)
```




```
new_data <- spike_mean(2,10)
maxs <- apply(new_data %>% dplyr::select(-c(idfile,PepSeq, RESPONSE)), 2, max)
mins <- apply(new_data %>% dplyr::select(-c(idfile,PepSeq, RESPONSE)), 2, min)

scaled_data <- as.data.frame(scale(new_data %>% dplyr::select(-c(idfile,PepSeq,RESPONSE)), center = mins
#scaled_data$RESPONSE <- ifelse(new_data$RESPONSE =="GO",1,0)
scaled_data$RESPONSE <- as.factor(new_data$RESPONSE)
#scaled_data$RESPONSE <- as.factor(scaled_data$RESPONSE)
scaled_data$idfile <- new_data$idfile

#select random ind for train and test
set.seed(123)

## 75% of the sample size
smp_size <- floor(0.75 * nrow(scaled_data))

## set the seed to make your partition reproducible
set.seed(123)
train_ind <- sample(seq_len(nrow(scaled_data)), size = smp_size)


train_sim1 <- scaled_data[train_ind,]
test_sim1 <- scaled_data[-train_ind,]

#Building Neural Network
library(h2o)
```

```r
#generate same set of random numbers (for reproducibility)
set.seed(121)

#launch h2o cluster
localH2O <- h2o.init(nthreads = -1)
```

```
##  Connection successful!
##
## R is connected to the H2O cluster:
##     H2O cluster uptime:         32 minutes 43 seconds
##     H2O cluster timezone:       America/New_York
##     H2O data parsing timezone:  UTC
##     H2O cluster version:        3.18.0.8
##     H2O cluster version age:    1 month and 16 days
##     H2O cluster name:           H2O_started_from_R_Shantam_Gupta_kyo754
##     H2O cluster total nodes:    1
##     H2O cluster total memory:   2.33 GB
##     H2O cluster total cores:    4
##     H2O cluster allowed cores:  4
##     H2O cluster healthy:        TRUE
##     H2O Connection ip:          localhost
##     H2O Connection port:        54321
##     H2O Connection proxy:       NA
##     H2O Internal Security:      FALSE
##     H2O API Extensions:         Algos, AutoML, Core V3, Core V4
##     R Version:                  R version 3.3.3 (2017-03-06)
```

```r
#import r objects to h2o cloud
train_h2o <- as.h2o(train_sim1)
test_h2o <- as.h2o(test_sim1)

set.seed(100)

dl_model_sim1 <- h2o.deeplearning(
  model_id="dl_model_first",
  training_frame=train_h2o,
  validation_frame = test_h2o,
  x= colnames(train_h2o[,1:4]),
  y= "RESPONSE",
  activatio="Tanh",
  hidden=c(2,2),
  stopping_metric="mean_per_class_error",
  stopping_rounds = 5,
  stopping_tolerance=0.001,
  rate = 0.005, # Defaults to 0.005
  mini_batch_size = 1,# defaults to 1
  epochs=100,
  seed = 123, # give seed
  export_weights_and_biases = T, # export weights and biases defaults to false
  reproducible = T # Force reproducibility on small data (will be slow - only uses 1 thread). Defaults
)
summary(dl_model_sim1)
```

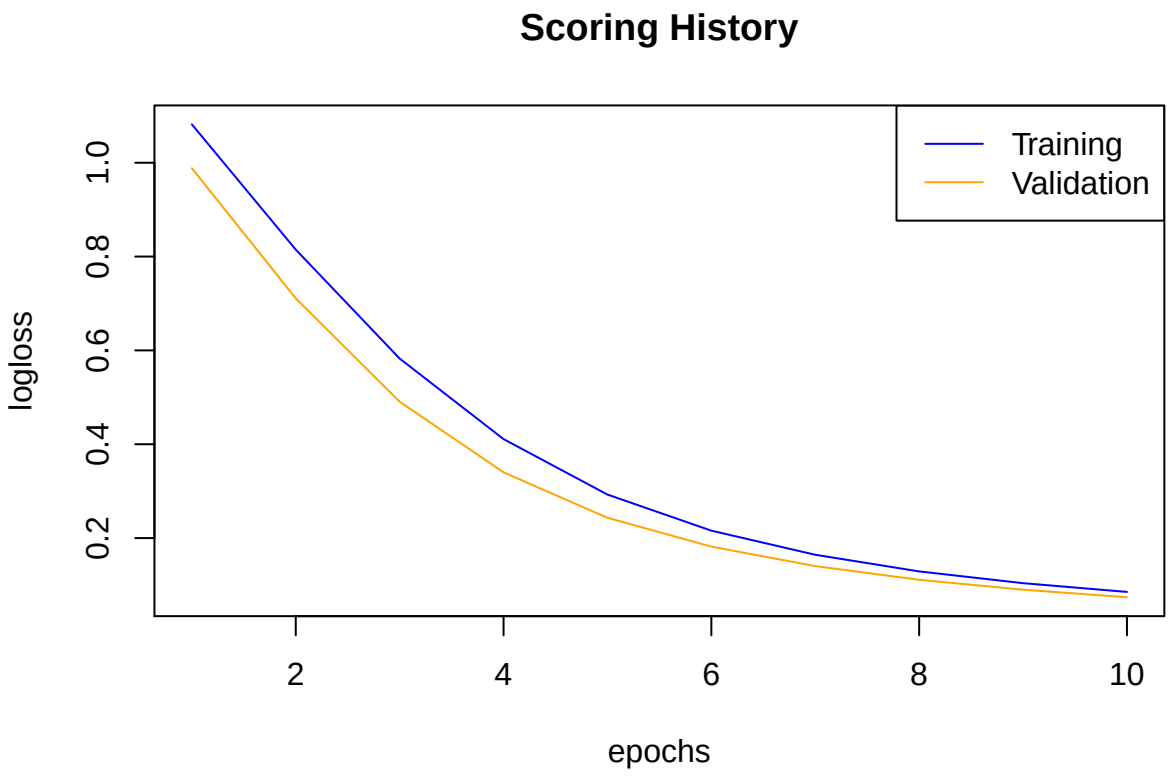
```
## Model Details:
## ==============
```

```
##
## H2OBinomialModel: deeplearning
## Model Key:  dl_model_first
## Status of Neuron Layers: predicting RESPONSE, 2-class classification, bernoulli distribution, CrossE
batch size 1
##   layer units    type dropout       l1       l2 mean_rate rate_rms
## 1     1     4   Input  0.00 %
## 2     2     2    Tanh  0.00 % 0.000000 0.000000  0.003115 0.003149
## 3     3     2    Tanh  0.00 % 0.000000 0.000000  0.103662 0.106827
## 4     4     2 Softmax         0.000000 0.000000  0.004898 0.003095
##   momentum mean_weight weight_rms mean_bias bias_rms
## 1
## 2 0.000000   -0.411499   0.646284 -0.026006 0.024857
## 3 0.000000    0.788713   1.074335  0.009208 0.023556
## 4 0.000000   -2.140051   3.415698 -0.000000 0.017427
##
## H2OBinomialMetrics: deeplearning
## ** Reported on training data. **
## ** Metrics reported on full training frame **
##
## MSE:  0.01960665
## RMSE:  0.1400237
## LogLoss:  0.08526118
## Mean Per-Class Error:  0
## AUC:  1
## Gini:  1
##
## Confusion Matrix (vertical: actual; across: predicted) for F1-optimal threshold:
##        GO NOGO    Error    Rate
## GO     74    0 0.000000   =0/74
## NOGO    0   76 0.000000   =0/76
## Totals 74   76 0.000000  =0/150
##
## Maximum Metrics: Maximum metrics at their respective thresholds
##                         metric threshold    value idx
## 1                        max f1  0.607347 1.000000  75
## 2                        max f2  0.607347 1.000000  75
## 3                  max f0point5  0.607347 1.000000  75
## 4                  max accuracy  0.607347 1.000000  75
## 5                 max precision  0.996383 1.000000   0
## 6                    max recall  0.607347 1.000000  75
## 7               max specificity  0.996383 1.000000   0
## 8              max absolute_mcc  0.607347 1.000000  75
## 9   max min_per_class_accuracy  0.607347 1.000000  75
## 10 max mean_per_class_accuracy  0.607347 1.000000  75
##
## Gains/Lift Table: Extract with `h2o.gainsLift(<model>, <data>)` or `h2o.gainsLift(<model>, valid=<T/
## H2OBinomialMetrics: deeplearning
## ** Reported on validation data. **
## ** Metrics reported on full validation frame **
##
## MSE:  0.01650105
## RMSE:  0.1284564
## LogLoss:  0.07390136
```

```
## Mean Per-Class Error:  0
## AUC:  1
## Gini:  1
##
## Confusion Matrix (vertical: actual; across: predicted) for F1-optimal threshold:
##        GO NOGO    Error   Rate
## GO     26    0 0.000000  =0/26
## NOGO    0   24 0.000000  =0/24
## Totals 26   24 0.000000  =0/50
##
## Maximum Metrics: Maximum metrics at their respective thresholds
##                         metric threshold    value idx
## 1                       max f1  0.900900 1.000000  23
## 2                       max f2  0.900900 1.000000  23
## 3                 max f0point5  0.900900 1.000000  23
## 4                 max accuracy  0.900900 1.000000  23
## 5                max precision  0.996023 1.000000   0
## 6                   max recall  0.900900 1.000000  23
## 7              max specificity  0.996023 1.000000   0
## 8             max absolute_mcc  0.900900 1.000000  23
## 9   max min_per_class_accuracy  0.900900 1.000000  23
## 10 max mean_per_class_accuracy  0.900900 1.000000  23
##
## Gains/Lift Table: Extract with `h2o.gainsLift(<model>, <data>)` or `h2o.gainsLift(<model>, valid=<T/
##
##
## Scoring History:
##              timestamp   duration training_speed   epochs iterations
## 1  2018-06-04 22:41:36  0.000 sec                 0.00000          0
## 2  2018-06-04 22:41:36  0.140 sec  50000 obs/sec  1.00000          1
## 3  2018-06-04 22:41:36  0.174 sec  12500 obs/sec  2.00000          2
## 4  2018-06-04 22:41:36  0.348 sec   7377 obs/sec  3.00000          3
## 5  2018-06-04 22:41:37  0.360 sec   8823 obs/sec  4.00000          4
## 6  2018-06-04 22:41:37  0.373 sec   9868 obs/sec  5.00000          5
## 7  2018-06-04 22:41:37  0.383 sec  11111 obs/sec  6.00000          6
## 8  2018-06-04 22:41:37  0.394 sec  12209 obs/sec  7.00000          7
## 9  2018-06-04 22:41:37  0.407 sec  13043 obs/sec  8.00000          8
## 10 2018-06-04 22:41:37  0.419 sec  13636 obs/sec  9.00000          9
## 11 2018-06-04 22:41:37  0.438 sec  14423 obs/sec 10.00000         10
##        samples training_rmse training_logloss training_auc training_lift
## 1     0.000000
## 2   150.000000       0.55022          1.08180      0.67710       1.97368
## 3   300.000000       0.49915          0.81487      0.76618       1.97368
## 4   450.000000       0.43912          0.58269      0.84780       1.97368
## 5   600.000000       0.37585          0.41091      0.91430       1.97368
## 6   750.000000       0.31580          0.29276      0.95110       1.97368
## 7   900.000000       0.26485          0.21578      0.97173       1.97368
## 8  1050.000000       0.22307          0.16440      0.98506       1.97368
## 9  1200.000000       0.18920          0.12895      0.99413       1.97368
## 10 1350.000000       0.16215          0.10391      0.99680       1.97368
## 11 1500.000000       0.14002          0.08526      1.00000       1.97368
##    training_classification_error validation_rmse validation_logloss
## 1
## 2                       0.42667         0.54451            0.98841
```

```
## 3                       0.34000         0.47942            0.71093
## 4                       0.27333         0.40275            0.49068
## 5                       0.18667         0.33205            0.34009
## 6                       0.12000         0.27604            0.24326
## 7                       0.08667         0.23371            0.18177
## 8                       0.06000         0.19973            0.14025
## 9                       0.02667         0.17167            0.11110
## 10                      0.02000         0.14833            0.08998
## 11                      0.00000         0.12846            0.07390
##    validation_auc validation_lift validation_classification_error
## 1
## 2         0.73718         2.08333                          0.38000
## 3         0.82372         2.08333                          0.30000
## 4         0.89744         2.08333                          0.24000
## 5         0.95513         2.08333                          0.12000
## 6         0.97756         2.08333                          0.08000
## 7         0.99679         2.08333                          0.02000
## 8         1.00000         2.08333                          0.00000
## 9         1.00000         2.08333                          0.00000
## 10        1.00000         2.08333                          0.00000
## 11        1.00000         2.08333                          0.00000
##
## Variable Importances: (Extract with `h2o.varimp`)
## =================================================
##
## Variable Importances:
##    variable relative_importance scaled_importance percentage
## 1 TotalArea            1.000000          1.000000   0.406007
## 2  MassAccu            0.690363          0.690363   0.280292
## 3      FWHM            0.517246          0.517246   0.210006
## 4        RT            0.255402          0.255402   0.103695
```

```
plot(dl_model_sim1)
```




```
new_data <- spike_mean(3,10)
maxs <- apply(new_data %>% dplyr::select(-c(idfile,PepSeq, RESPONSE)), 2, max)
mins <- apply(new_data %>% dplyr::select(-c(idfile,PepSeq, RESPONSE)), 2, min)

scaled_data <- as.data.frame(scale(new_data %>% dplyr::select(-c(idfile,PepSeq,RESPONSE)), center = mins
#scaled_data$RESPONSE <- ifelse(new_data$RESPONSE =="GO",1,0)
scaled_data$RESPONSE <- as.factor(new_data$RESPONSE)
#scaled_data$RESPONSE <- as.factor(scaled_data$RESPONSE)
scaled_data$idfile <- new_data$idfile

#select random ind for train and test
set.seed(123)

## 75% of the sample size
smp_size <- floor(0.75 * nrow(scaled_data))

## set the seed to make your partition reproducible
set.seed(123)
train_ind <- sample(seq_len(nrow(scaled_data)), size = smp_size)


train_sim1 <- scaled_data[train_ind,]
test_sim1 <- scaled_data[-train_ind,]

#Building Neural Network
library(h2o)
```

```r
#generate same set of random numbers (for reproducibility)
set.seed(121)

#launch h2o cluster
localH2O <- h2o.init(nthreads = -1)
```

```
##  Connection successful!
##
## R is connected to the H2O cluster:
##     H2O cluster uptime:         32 minutes 46 seconds
##     H2O cluster timezone:       America/New_York
##     H2O data parsing timezone:  UTC
##     H2O cluster version:        3.18.0.8
##     H2O cluster version age:    1 month and 16 days
##     H2O cluster name:           H2O_started_from_R_Shantam_Gupta_kyo754
##     H2O cluster total nodes:    1
##     H2O cluster total memory:   2.34 GB
##     H2O cluster total cores:    4
##     H2O cluster allowed cores:  4
##     H2O cluster healthy:        TRUE
##     H2O Connection ip:          localhost
##     H2O Connection port:        54321
##     H2O Connection proxy:       NA
##     H2O Internal Security:      FALSE
##     H2O API Extensions:         Algos, AutoML, Core V3, Core V4
##     R Version:                  R version 3.3.3 (2017-03-06)
```

```r
#import r objects to h2o cloud
train_h2o <- as.h2o(train_sim1)
test_h2o <- as.h2o(test_sim1)

set.seed(100)

dl_model_sim1 <- h2o.deeplearning(
  model_id="dl_model_first",
  training_frame=train_h2o,
  validation_frame = test_h2o,
  x= colnames(train_h2o[,1:4]),
  y= "RESPONSE",
  activatio="Tanh",
  hidden=c(2,2),
  stopping_metric="mean_per_class_error",
  stopping_rounds = 5,
  stopping_tolerance=0.001,
  rate = 0.005, # Defaults to 0.005
  mini_batch_size = 1,# defaults to 1
  epochs=100,
  seed = 123, # give seed
  export_weights_and_biases = T, # export weights and biases defaults to false
  reproducible = T # Force reproducibility on small data (will be slow - only uses 1 thread). Defaults
)
summary(dl_model_sim1)
```

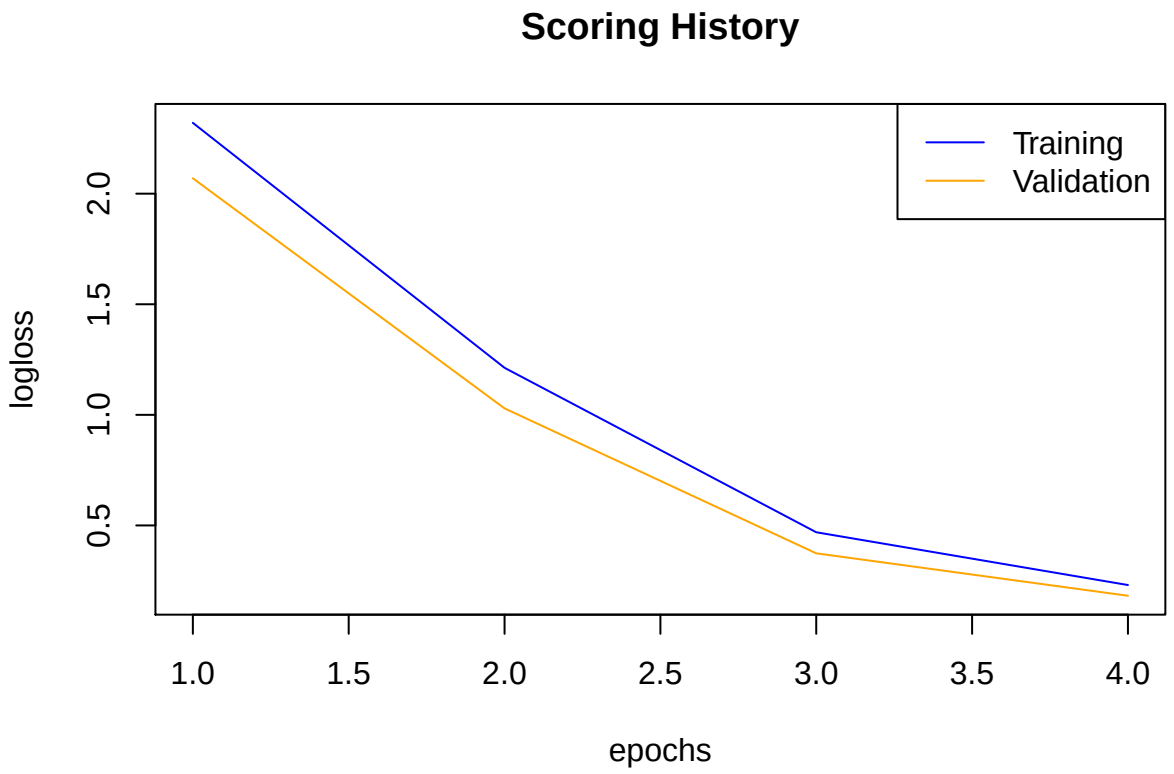
```
## Model Details:
## ==============
```

```
##
## H2OBinomialModel: deeplearning
## Model Key:  dl_model_first
## Status of Neuron Layers: predicting RESPONSE, 2-class classification, bernoulli distribution, CrossE
batch size 1
##   layer units    type dropout       l1       l2 mean_rate rate_rms
## 1     1     4   Input  0.00 %
## 2     2     2    Tanh  0.00 % 0.000000 0.000000  0.006331 0.005909
## 3     3     2    Tanh  0.00 % 0.000000 0.000000  0.096842 0.098050
## 4     4     2 Softmax         0.000000 0.000000  0.001924 0.000296
##   momentum mean_weight weight_rms mean_bias bias_rms
## 1
## 2 0.000000   -0.327752   0.676920 -0.023756 0.015411
## 3 0.000000    0.980989   1.081806 -0.057519 0.053647
## 4 0.000000   -2.140051   3.382374 -0.000000 0.004583
##
## H2OBinomialMetrics: deeplearning
## ** Reported on training data. **
## ** Metrics reported on full training frame **
##
## MSE:  0.0557924
## RMSE:  0.2362042
## LogLoss:  0.230534
## Mean Per-Class Error:  0
## AUC:  1
## Gini:  1
##
## Confusion Matrix (vertical: actual; across: predicted) for F1-optimal threshold:
##        GO NOGO    Error    Rate
## GO     74    0 0.000000   =0/74
## NOGO    0   76 0.000000   =0/76
## Totals 74   76 0.000000  =0/150
##
## Maximum Metrics: Maximum metrics at their respective thresholds
##                         metric threshold    value idx
## 1                       max f1  0.560585 1.000000  75
## 2                       max f2  0.560585 1.000000  75
## 3                 max f0point5  0.560585 1.000000  75
## 4                 max accuracy  0.560585 1.000000  75
## 5                max precision  0.979840 1.000000   0
## 6                   max recall  0.560585 1.000000  75
## 7              max specificity  0.979840 1.000000   0
## 8             max absolute_mcc  0.560585 1.000000  75
## 9   max min_per_class_accuracy  0.560585 1.000000  75
## 10 max mean_per_class_accuracy  0.560585 1.000000  75
##
## Gains/Lift Table: Extract with `h2o.gainsLift(<model>, <data>)` or `h2o.gainsLift(<model>, valid=<T/
## H2OBinomialMetrics: deeplearning
## ** Reported on validation data. **
## ** Metrics reported on full validation frame **
##
## MSE:  0.03796815
## RMSE:  0.1948542
## LogLoss:  0.1820889
```

```
## Mean Per-Class Error:  0
## AUC:  1
## Gini:  1
##
## Confusion Matrix (vertical: actual; across: predicted) for F1-optimal threshold:
##        GO NOGO    Error   Rate
## GO     26    0 0.000000  =0/26
## NOGO    0   24 0.000000  =0/24
## Totals 26   24 0.000000  =0/50
##
## Maximum Metrics: Maximum metrics at their respective thresholds
##                         metric threshold    value idx
## 1                       max f1  0.618661 1.000000  23
## 2                       max f2  0.618661 1.000000  23
## 3                 max f0point5  0.618661 1.000000  23
## 4                 max accuracy  0.618661 1.000000  23
## 5                max precision  0.980413 1.000000   0
## 6                   max recall  0.618661 1.000000  23
## 7              max specificity  0.980413 1.000000   0
## 8             max absolute_mcc  0.618661 1.000000  23
## 9   max min_per_class_accuracy  0.618661 1.000000  23
## 10 max mean_per_class_accuracy  0.618661 1.000000  23
##
## Gains/Lift Table: Extract with `h2o.gainsLift(<model>, <data>)` or `h2o.gainsLift(<model>, valid=<T/
##
##
## Scoring History:
##             timestamp   duration training_speed  epochs iterations
## 1 2018-06-04 22:41:39  0.000 sec                0.00000          0
## 2 2018-06-04 22:41:39  0.018 sec  75000 obs/sec 1.00000          1
## 3 2018-06-04 22:41:39  0.038 sec  27272 obs/sec 2.00000          2
## 4 2018-06-04 22:41:39  0.053 sec  23684 obs/sec 3.00000          3
## 5 2018-06-04 22:41:39  0.077 sec  17142 obs/sec 4.00000          4
##      samples training_rmse training_logloss training_auc training_lift
## 1   0.000000
## 2 150.000000       0.83951          2.32023      0.07913       0.00000
## 3 300.000000       0.66654          1.21269      0.31294       0.98684
## 4 450.000000       0.39809          0.46915      0.84495       1.97368
## 5 600.000000       0.23620          0.23053      1.00000       1.97368
##   training_classification_error validation_rmse validation_logloss
## 1
## 2                       0.49333         0.80521            2.06955
## 3                       0.46000         0.62335            1.02920
## 4                       0.21333         0.34090            0.37388
## 5                       0.00000         0.19485            0.18209
##   validation_auc validation_lift validation_classification_error
## 1
## 2        0.21474         0.00000                         0.52000
## 3        0.41346         2.08333                         0.48000
## 4        0.94551         2.08333                         0.16000
## 5        1.00000         2.08333                         0.00000
##
## Variable Importances: (Extract with `h2o.varimp`)
## =================================================
```

```
##
## Variable Importances:
##    variable relative_importance scaled_importance percentage
## 1  MassAccu            1.000000          1.000000   0.461504
## 2      FWHM            0.516957          0.516957   0.238578
## 3        RT            0.388668          0.388668   0.179372
## 4 TotalArea            0.261205          0.261205   0.120547
```

```
plot(dl_model_sim1)
```




```
new_data <- spike_mean(4,10)
maxs <- apply(new_data %>% dplyr::select(-c(idfile,PepSeq, RESPONSE)), 2, max)
mins <- apply(new_data %>% dplyr::select(-c(idfile,PepSeq, RESPONSE)), 2, min)

scaled_data <- as.data.frame(scale(new_data %>% dplyr::select(-c(idfile,PepSeq,RESPONSE)), center = mins
#scaled_data$RESPONSE <- ifelse(new_data$RESPONSE =="GO",1,0)
scaled_data$RESPONSE <- as.factor(new_data$RESPONSE)
#scaled_data$RESPONSE <- as.factor(scaled_data$RESPONSE)
scaled_data$idfile <- new_data$idfile

#select random ind for train and test
set.seed(123)

## 75% of the sample size
smp_size <- floor(0.75 * nrow(scaled_data))

## set the seed to make your partition reproducible
```

```r
set.seed(123)
train_ind <- sample(seq_len(nrow(scaled_data)), size = smp_size)


train_sim1 <- scaled_data[train_ind,]
test_sim1 <- scaled_data[-train_ind,]

#Building Neural Network
library(h2o)
#generate same set of random numbers (for reproducibility)
set.seed(121)

#launch h2o cluster
localH2O <- h2o.init(nthreads = -1)
```

```
##  Connection successful!
##
## R is connected to the H2O cluster:
##     H2O cluster uptime:         32 minutes 48 seconds
##     H2O cluster timezone:       America/New_York
##     H2O data parsing timezone:  UTC
##     H2O cluster version:        3.18.0.8
##     H2O cluster version age:    1 month and 16 days
##     H2O cluster name:           H2O_started_from_R_Shantam_Gupta_kyo754
##     H2O cluster total nodes:    1
##     H2O cluster total memory:   2.34 GB
##     H2O cluster total cores:    4
##     H2O cluster allowed cores:  4
##     H2O cluster healthy:        TRUE
##     H2O Connection ip:          localhost
##     H2O Connection port:        54321
##     H2O Connection proxy:       NA
##     H2O Internal Security:      FALSE
##     H2O API Extensions:         Algos, AutoML, Core V3, Core V4
##     R Version:                  R version 3.3.3 (2017-03-06)
```

```r
#import r objects to h2o cloud
train_h2o <- as.h2o(train_sim1)
test_h2o <- as.h2o(test_sim1)

set.seed(100)

dl_model_sim1 <- h2o.deeplearning(
  model_id="dl_model_first",
  training_frame=train_h2o,
  validation_frame = test_h2o,
  x= colnames(train_h2o[,1:4]),
  y= "RESPONSE",
  activatio="Tanh",
  hidden=c(2,2),
  stopping_metric="mean_per_class_error",
  stopping_rounds = 5,
  stopping_tolerance=0.001,
  rate = 0.005, # Defaults to 0.005
```

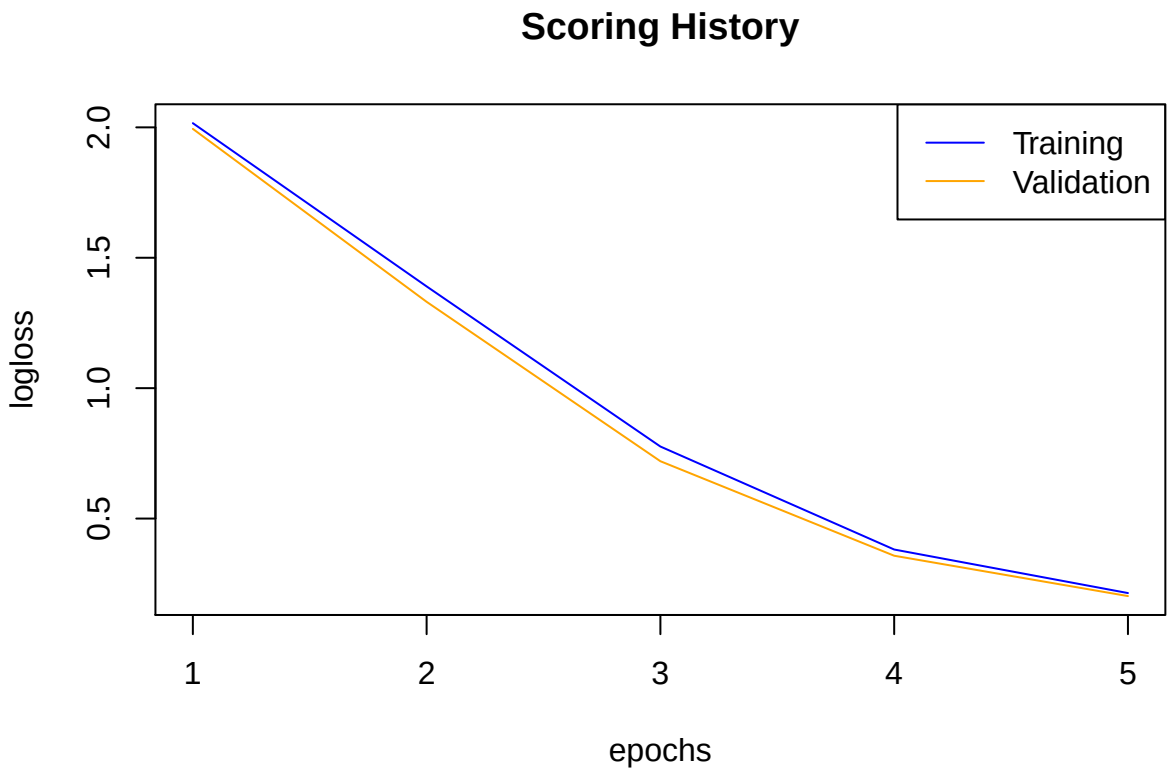
```
  mini_batch_size = 1,# defaults to 1
  epochs=100,
  seed = 123, # give seed
  export_weights_and_biases = T, # export weights and biases defaults to false
  reproducible = T # Force reproducibility on small data (will be slow - only uses 1 thread). Defaults
)
summary(dl_model_sim1)
```

```
## Model Details:
## ==============
##
## H2OBinomialModel: deeplearning
## Model Key:  dl_model_first
## Status of Neuron Layers: predicting RESPONSE, 2-class classification, bernoulli distribution, CrossE
batch size 1
##   layer units    type dropout       l1       l2 mean_rate rate_rms
## 1     1     4   Input  0.00 %
## 2     2     2    Tanh  0.00 % 0.000000 0.000000  0.005736 0.005790
## 3     3     2    Tanh  0.00 % 0.000000 0.000000  0.089002 0.092362
## 4     4     2 Softmax         0.000000 0.000000  0.002051 0.000427
##   momentum mean_weight weight_rms mean_bias bias_rms
## 1
## 2 0.000000   -0.355588   0.640451 -0.017582 0.007727
## 3 0.000000    0.929416   0.993226 -0.020121 0.016930
## 4 0.000000   -2.140049   3.382085  0.000000 0.003513
##
## H2OBinomialMetrics: deeplearning
## ** Reported on training data. **
## ** Metrics reported on full training frame **
##
## MSE:  0.05340267
## RMSE:  0.2310902
## LogLoss:  0.2143473
## Mean Per-Class Error:  0
## AUC:  1
## Gini:  1
##
## Confusion Matrix (vertical: actual; across: predicted) for F1-optimal threshold:
##        GO NOGO    Error    Rate
## GO     74    0 0.000000   =0/74
## NOGO    0   76 0.000000   =0/76
## Totals 74   76 0.000000  =0/150
##
## Maximum Metrics: Maximum metrics at their respective thresholds
##                         metric threshold    value idx
## 1                       max f1  0.555791 1.000000  75
## 2                       max f2  0.555791 1.000000  75
## 3                 max f0point5  0.555791 1.000000  75
## 4                 max accuracy  0.555791 1.000000  75
## 5                max precision  0.982771 1.000000   0
## 6                   max recall  0.555791 1.000000  75
## 7              max specificity  0.982771 1.000000   0
## 8             max absolute_mcc  0.555791 1.000000  75
## 9   max min_per_class_accuracy  0.555791 1.000000  75
```

```
## 10 max mean_per_class_accuracy  0.555791 1.000000  75
##
## Gains/Lift Table: Extract with `h2o.gainsLift(<model>, <data>)` or `h2o.gainsLift(<model>, valid=<T/
## H2OBinomialMetrics: deeplearning
## ** Reported on validation data. **
## ** Metrics reported on full validation frame **
##
## MSE:  0.04908478
## RMSE:  0.2215508
## LogLoss:  0.2028255
## Mean Per-Class Error:  0
## AUC:  1
## Gini:  1
##
## Confusion Matrix (vertical: actual; across: predicted) for F1-optimal threshold:
##        GO NOGO    Error   Rate
## GO     26    0 0.000000  =0/26
## NOGO    0   24 0.000000  =0/24
## Totals 26   24 0.000000  =0/50
##
## Maximum Metrics: Maximum metrics at their respective thresholds
##                         metric threshold    value idx
## 1                       max f1  0.613594 1.000000  23
## 2                       max f2  0.613594 1.000000  23
## 3                 max f0point5  0.613594 1.000000  23
## 4                 max accuracy  0.613594 1.000000  23
## 5                max precision  0.982706 1.000000   0
## 6                   max recall  0.613594 1.000000  23
## 7              max specificity  0.982706 1.000000   0
## 8             max absolute_mcc  0.613594 1.000000  23
## 9   max min_per_class_accuracy  0.613594 1.000000  23
## 10 max mean_per_class_accuracy  0.613594 1.000000  23
##
## Gains/Lift Table: Extract with `h2o.gainsLift(<model>, <data>)` or `h2o.gainsLift(<model>, valid=<T/
##
##
## Scoring History:
##             timestamp   duration training_speed  epochs iterations
## 1 2018-06-04 22:41:41  0.000 sec                0.00000          0
## 2 2018-06-04 22:41:41  0.082 sec   5172 obs/sec 1.00000          1
## 3 2018-06-04 22:41:41  0.114 sec   7692 obs/sec 2.00000          2
## 4 2018-06-04 22:41:41  0.245 sec   9375 obs/sec 3.00000          3
## 5 2018-06-04 22:41:41  0.281 sec   8108 obs/sec 4.00000          4
## 6 2018-06-04 22:41:41  0.300 sec   9036 obs/sec 5.00000          5
##      samples training_rmse training_logloss training_auc training_lift
## 1   0.000000
## 2 150.000000       0.75348          2.01605      0.28432       0.98684
## 3 300.000000       0.68028          1.39024      0.41234       0.98684
## 4 450.000000       0.53602          0.77622      0.64047       1.97368
## 5 600.000000       0.35511          0.38134      0.88549       1.97368
## 6 750.000000       0.23109          0.21435      1.00000       1.97368
##   training_classification_error validation_rmse validation_logloss
## 1
## 2                       0.49333         0.75249            1.99424
```

```
## 3                       0.46667         0.67211           1.33114
## 4                       0.33333         0.51869           0.71984
## 5                       0.18000         0.34038           0.35748
## 6                       0.00000         0.22155           0.20283
##   validation_auc validation_lift validation_classification_error
## 1
## 2        0.27564         2.08333                         0.52000
## 3        0.39103         2.08333                         0.48000
## 4        0.70994         2.08333                         0.40000
## 5        0.93910         2.08333                         0.08000
## 6        1.00000         2.08333                         0.00000
##
## Variable Importances: (Extract with `h2o.varimp`)
## =================================================
##
## Variable Importances:
##    variable relative_importance scaled_importance percentage
## 1      FWHM            1.000000          1.000000   0.386589
## 2  MassAccu            0.927834          0.927834   0.358690
## 3        RT            0.418689          0.418689   0.161861
## 4 TotalArea            0.240203          0.240203   0.092860
```

```
plot(dl_model_sim1)
```



6.2.1.1 Model with 12 Effects

- Increase in Mean (Logarathmic Drift) per feature
- Increase in 3 X Covariance per feature
- Increase in 1.5 X sigma mean shift per feature

```
#Simulation 1
#generate multivariate normal data
#parameters from a training sample
n<-1000 #incontrol observations
Data<-c()
Data0<-c()
Data1<-c()
Data2<-c()
Data3<-c()
Data4<-c()
S0<-c()

#one peptide LVNELTEFAK
mean <-c(with(data=Train,tapply(RT,INDEX=PepSeq,FUN=mean))[5],
         with(data=Train,tapply(TotalArea,INDEX=PepSeq,FUN=mean)) [5],
         with(data=Train,tapply(MassAccu,INDEX=PepSeq,FUN=mean)) [5],
         with(data=Train,tapply(FWHM,INDEX=PepSeq,FUN=mean)) [5]
)
covar<-cov(Train[Train$PepSeq=="LVNELTEFAK",c(3,6,7,8)])
#generate in-control observations

S0<-data.frame(idfile=12*n+1:(20*n),PepSeq=rep("LVNELTEFAK",n),mvrnorm(n, mean, covar))
colnames(S0)<-c("idfile","PepSeq","RT","TotalArea","MassAccu","FWHM")
#S0<- reshape(S0, idvar = "idfile", timevar = "PepSeq", direction = "wide")
RESPONSE<-c("GO")
S0 <- cbind(S0,RESPONSE)

#generate out-of-control observations
#Logarithmic drift
Data11 <-data.frame(idfile=((1):(n)),PepSeq=rep("LVNELTEFAK",n),
                  mvrnorm(n, mean+c(3.0*sqrt(covar[1,1]),1.0*sqrt(covar[2,2]),1.0*sqrt(covar[3,3]),1.0*
                          covar))
Data12 <-data.frame(idfile=((n+1):(2*n)),PepSeq=rep("LVNELTEFAK",n),
                  mvrnorm(n, mean+c(1.0*sqrt(covar[1,1]),3.0*sqrt(covar[2,2]),1.0*sqrt(covar[3,3]),1.0*
                          covar))

Data13 <-data.frame(idfile=((2*n+1):(3*n)),PepSeq=rep("LVNELTEFAK",n),
                  mvrnorm(n, mean+c(1.0*sqrt(covar[1,1]),1.0*sqrt(covar[2,2]),3.0*sqrt(covar[3,3]),1.0*
                          covar))

Data14 <-data.frame(idfile=((3*n + 1):(4*n)),PepSeq=rep("LVNELTEFAK",n),
                  mvrnorm(n, mean+c(1.0*sqrt(covar[1,1]),1.0*sqrt(covar[2,2]),1.0*sqrt(covar[3,3]),3.0*
                          covar))

#generate out-of-control observations for a 3 sigma fluctuation in all features large shift
covar21<- covar
covar21[1,1]<-3*covar[1,1]

Data21<-data.frame(idfile=((4*n+1):(5*n)),PepSeq=rep("LVNELTEFAK",n),
                  mvrnorm(n, mean,
```

```
                          covar21))
covar22<- covar
covar22[2,2]<-3*covar[2,2]

Data22<-data.frame(idfile=((5*n+1):(6*n)),PepSeq=rep("LVNELTEFAK",n),
                   mvrnorm(n, mean,
                           covar22))


covar23<-covar
covar23[3,3]<-3*covar[3,3]

Data23<-data.frame(idfile=((6*n+1):(7*n)),PepSeq=rep("LVNELTEFAK",n),
                   mvrnorm(n, mean,
                           covar23))

covar24<-covar
covar24[4,4]<-3*covar[4,4]

Data24<-data.frame(idfile=((7*n+1):(8*n)),PepSeq=rep("LVNELTEFAK",n),
                   mvrnorm(n, mean,
                           covar24))


#generate out-of-control observations for a 1.5 sigma step shift
Data31 <-data.frame(idfile=(8*n+1):(9*n),PepSeq=rep("LVNELTEFAK",n),
                   mvrnorm(n, mean+c(1.5*sqrt(covar[1,1]),1.0*sqrt(covar[2,2]),1.0*sqrt(covar[3,3]),1.0*
                           covar))

Data32 <-data.frame(idfile=(9*n+1):(10*n),PepSeq=rep("LVNELTEFAK",n),
                   mvrnorm(n, mean+c(1.0*sqrt(covar[1,1]),1.5*sqrt(covar[2,2]),1.0*sqrt(covar[3,3]),1.0*
                           covar))

Data33 <-data.frame(idfile=(10*n+1):(11*n),PepSeq=rep("LVNELTEFAK",n),
                   mvrnorm(n, mean+c(1.0*sqrt(covar[1,1]),1.0*sqrt(covar[2,2]),1.5*sqrt(covar[3,3]),1.0*
                           covar))

Data34 <-data.frame(idfile=(11*n+1):(12*n),PepSeq=rep("LVNELTEFAK",n),
                   mvrnorm(n, mean+c(1.0*sqrt(covar[1,1]),1.0*sqrt(covar[2,2]),1.0*sqrt(covar[3,3]),1.5*
                           covar))


#Merge all four type of disturbances + in-control observations
Data0<-rbind(Data11,Data12, Data13, Data14, Data21, Data22, Data23, Data24, Data31, Data32, Data33, Data
RESPONSE<-c("NOGO")
colnames(Data0) <- c("idfile","PepSeq","RT","TotalArea","MassAccu","FWHM")
Data0 <- cbind(Data0,RESPONSE)
Data0 <-rbind(S0,Data0)
```

```
#select random ind for train and test
set.seed(123)

## 75% of the sample size
smp_size <- floor(0.8 * nrow(Data0))
```

```
## set the seed to make your partition reproducible
set.seed(123)
train_ind <- sample(seq_len(nrow(Data0)), size = smp_size)

train_sim_all <- Data0[train_ind,]
test_sim_all <- Data0[-train_ind,]

#min max scaling & centering the train data 0-1
train_maxs <- apply(train_sim_all %>% dplyr::select(-c(idfile, PepSeq, RESPONSE)), 2, max)
train_mins <- apply(train_sim_all %>% dplyr::select(-c(idfile, PepSeq, RESPONSE)), 2, min)
train_sim_all_scaled_data <- as.data.frame(scale(train_sim_all %>% dplyr::select(-c(idfile,PepSeq,RESPO

#min max scaling & centering the test data 0-1
test_maxs <- apply(test_sim_all %>% dplyr::select(-c(idfile,PepSeq, RESPONSE)), 2, max)
test_mins <- apply(test_sim_all %>% dplyr::select(-c(idfile, PepSeq, RESPONSE)), 2, min)
test_sim_all_scaled_data <- as.data.frame(scale(test_sim_all %>% dplyr::select(-c(idfile,PepSeq, RESPONS



train_sim_all_scaled_data$RESPONSE <- as.factor(train_sim_all$RESPONSE)
train_sim_all_scaled_data$idfile <- train_sim_all$idfile

test_sim_all_scaled_data$RESPONSE <- as.factor(test_sim_all$RESPONSE)
test_sim_all_scaled_data$idfile <- test_sim_all$idfile
```

```
#Building Neural Network
library(h2o)
#generate same set of random numbers (for reproducibility)
set.seed(121)

#launch h2o cluster
localH2O <- h2o.init(nthreads = -1)
```

```
##  Connection successful!
##
## R is connected to the H2O cluster:
##     H2O cluster uptime:         32 minutes 52 seconds
##     H2O cluster timezone:       America/New_York
##     H2O data parsing timezone:  UTC
##     H2O cluster version:        3.18.0.8
##     H2O cluster version age:    1 month and 16 days
##     H2O cluster name:           H2O_started_from_R_Shantam_Gupta_kyo754
##     H2O cluster total nodes:    1
##     H2O cluster total memory:   2.34 GB
##     H2O cluster total cores:    4
##     H2O cluster allowed cores:  4
##     H2O cluster healthy:        TRUE
##     H2O Connection ip:          localhost
##     H2O Connection port:        54321
##     H2O Connection proxy:       NA
##     H2O Internal Security:      FALSE
##     H2O API Extensions:         Algos, AutoML, Core V3, Core V4
##     R Version:                  R version 3.3.3 (2017-03-06)
```

```r
#import r objects to h2o cloud
train_h2o <- as.h2o(train_sim_all)
test_h2o <- as.h2o(test_sim_all)

set.seed(100)

dl_model_sim1 <- h2o.deeplearning(
  model_id="dl_model_first",
  training_frame=train_h2o,
  validation_frame = test_h2o,
  x= colnames(train_h2o[,3:6]),
  y= "RESPONSE",
  activatio="Tanh",
  hidden=c(20,20),
  standardize = TRUE, #standardizes the data
  loss= "CrossEntropy",
  stopping_metric="logloss",
  stopping_rounds = 10,
  stopping_tolerance=0.00001,
  adaptive_rate = TRUE,
  shuffle_training_data = TRUE,
  rate = 0.005, # Defaults to 0.005 adaptive enabled so cannot specify the learning rare
  mini_batch_size = 1,# defaults to 1
  epochs=200,
  seed = 123, # give seed
  export_weights_and_biases = T, # export weights and biases defaults to false
  reproducible = T # Force reproducibility on small data (will be slow - only uses 1 thread). Defaults
)
summary(dl_model_sim1)
```

```
## Model Details:
## ==============
##
## H2OBinomialModel: deeplearning
## Model Key:  dl_model_first
## Status of Neuron Layers: predicting RESPONSE, 2-class classification, bernoulli distribution, CrossE
batch size 1
##   layer units    type dropout       l1       l2 mean_rate rate_rms
## 1     1     4   Input  0.00 %
## 2     2    20    Tanh  0.00 % 0.000000 0.000000  0.001635 0.001284
## 3     3    20    Tanh  0.00 % 0.000000 0.000000  0.104984 0.104947
## 4     4     2 Softmax         0.000000 0.000000  0.004494 0.001813
##   momentum mean_weight weight_rms mean_bias bias_rms
## 1
## 2 0.000000    0.008561   0.537289 -0.170672 0.505694
## 3 0.000000    0.002239   0.563893 -0.194312 0.880953
## 4 0.000000    0.037249   0.973738 -0.000000 2.371749
##
## H2OBinomialMetrics: deeplearning
## ** Reported on training data. **
## ** Metrics reported on temporary training frame with 10003 samples **
##
## MSE:  0.1200252
## RMSE:  0.3464466
```

```
## LogLoss:  0.3870544
## Mean Per-Class Error:  0.1837601
## AUC:  0.863129
## Gini:  0.7262579
##
## Confusion Matrix (vertical: actual; across: predicted) for F1-optimal threshold:
##          GO NOGO    Error         Rate
## GO     5780  476 0.076087    =476/6256
## NOGO   1092 2655 0.291433   =1092/3747
## Totals 6872 3131 0.156753  =1568/10003
##
## Maximum Metrics: Maximum metrics at their respective thresholds
##                         metric threshold    value idx
## 1                       max f1  0.336488 0.772027 214
## 2                       max f2  0.150029 0.775119 320
## 3                 max f0point5  0.632382 0.848559 141
## 4                 max accuracy  0.507659 0.849145 168
## 5                max precision  0.998129 1.000000   0
## 6                   max recall  0.067311 1.000000 399
## 7              max specificity  0.998129 1.000000   0
## 8             max absolute_mcc  0.507659 0.678064 168
## 9   max min_per_class_accuracy  0.214707 0.785962 268
## 10 max mean_per_class_accuracy  0.336488 0.816240 214
##
## Gains/Lift Table: Extract with `h2o.gainsLift(<model>, <data>)` or `h2o.gainsLift(<model>, valid=<T/
## H2OBinomialMetrics: deeplearning
## ** Reported on validation data. **
## ** Metrics reported on full validation frame **
##
## MSE:  0.1210775
## RMSE:  0.3479619
## LogLoss:  0.3900262
## Mean Per-Class Error:  0.1817058
## AUC:  0.8617871
## Gini:  0.7235742
##
## Confusion Matrix (vertical: actual; across: predicted) for F1-optimal threshold:
##          GO NOGO    Error       Rate
## GO     3785  205 0.051378  =205/3990
## NOGO    752 1658 0.312033  =752/2410
## Totals 4537 1863 0.149531  =957/6400
##
## Maximum Metrics: Maximum metrics at their respective thresholds
##                         metric threshold    value idx
## 1                       max f1  0.403103 0.776036 188
## 2                       max f2  0.150023 0.774529 323
## 3                 max f0point5  0.610394 0.846334 140
## 4                 max accuracy  0.414126 0.850625 186
## 5                max precision  0.998243 1.000000   0
## 6                   max recall  0.069866 1.000000 398
## 7              max specificity  0.998243 1.000000   0
## 8             max absolute_mcc  0.414126 0.679527 186
## 9   max min_per_class_accuracy  0.216114 0.785062 270
## 10 max mean_per_class_accuracy  0.403103 0.818294 188
```

```
##
## Gains/Lift Table: Extract with `h2o.gainsLift(<model>, <data>)` or `h2o.gainsLift(<model>, valid=<T/
##
##
## Scoring History:
##             timestamp   duration training_speed  epochs iterations
## 1 2018-06-04 22:41:45  0.000 sec               0.00000          0
## 2 2018-06-04 22:41:46  0.778 sec  42244 obs/sec 1.00000          1
## 3 2018-06-04 22:41:47  1.515 sec  43097 obs/sec 2.00000          2
## 4 2018-06-04 22:41:47  2.313 sec  42267 obs/sec 3.00000          3
## 5 2018-06-04 22:41:48  3.071 sec  43463 obs/sec 4.00000          4
##         samples training_rmse training_logloss training_auc training_lift
## 1      0.000000
## 2  25600.000000       0.36975          0.43144      0.84593       2.66960
## 3  51200.000000       0.35592          0.40547      0.85339       2.66960
## 4  76800.000000       0.35602          0.40475      0.85625       2.66960
## 5 102400.000000       0.35727          0.40764      0.85561       2.66960
##   training_classification_error validation_rmse validation_logloss
## 1
## 2                       0.16465         0.37272            0.43810
## 3                       0.16645         0.35816            0.41039
## 4                       0.16355         0.35821            0.41112
## 5                       0.16085         0.35890            0.41150
##   validation_auc validation_lift validation_classification_error
## 1
## 2        0.84254         2.65560                         0.16672
## 3        0.85139         2.65560                         0.16531
## 4        0.85166         2.65560                         0.16391
## 5        0.85475         2.65560                         0.16078
##
## ---
##              timestamp   duration training_speed   epochs iterations
## 60 2018-06-04 22:42:27 41.579 sec  47110 obs/sec 59.00000         59
## 61 2018-06-04 22:42:27 42.208 sec  47200 obs/sec 60.00000         60
## 62 2018-06-04 22:42:28 42.833 sec  47295 obs/sec 61.00000         61
## 63 2018-06-04 22:42:29 43.514 sec  47316 obs/sec 62.00000         62
## 64 2018-06-04 22:42:29 44.279 sec  47229 obs/sec 63.00000         63
## 65 2018-06-04 22:42:30 44.475 sec  47203 obs/sec 63.00000         63
##           samples training_rmse training_logloss training_auc
## 60 1510400.000000       0.35224          0.40197      0.86271
## 61 1536000.000000       0.34926          0.39379      0.86059
## 62 1561600.000000       0.34745          0.38957      0.86076
## 63 1587200.000000       0.34645          0.38705      0.86313
## 64 1612800.000000       0.34909          0.39267      0.86366
## 65 1612800.000000       0.34645          0.38705      0.86313
##    training_lift training_classification_error validation_rmse
## 60       2.66960                       0.15255         0.35452
## 61       2.66960                       0.15555         0.35167
## 62       2.66960                       0.14956         0.34926
## 63       2.66960                       0.15675         0.34796
## 64       2.66960                       0.15075         0.35193
## 65       2.66960                       0.15675         0.34796
##    validation_logloss validation_auc validation_lift
## 60            0.40690        0.86043         2.65560
```

```
## 61            0.39828        0.85978         2.65560
## 62            0.39369        0.85832         2.65560
## 63            0.39003        0.86179         2.65560
## 64            0.39799        0.85894         2.65560
## 65            0.39003        0.86179         2.65560
##    validation_classification_error
## 60                         0.15375
## 61                         0.15438
## 62                         0.15156
## 63                         0.14953
## 64                         0.15047
## 65                         0.14953
##
## Variable Importances: (Extract with `h2o.varimp`)
## =================================================
##
## Variable Importances:
##    variable relative_importance scaled_importance percentage
## 1        RT            1.000000          1.000000   0.277106
## 2 TotalArea            0.933698          0.933698   0.258734
## 3      FWHM            0.906112          0.906112   0.251089
## 4  MassAccu            0.768915          0.768915   0.213071
```

```
plot(dl_model_sim1)
```