Binary and Multiclass Classification using Neural Networks

by

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ABSTRACT

This analytical study was executed using the R programming language. The dataset used is the famous MNIST dataset [1]. The dataset is a multiclass data from which the training and testing data were sampled. Neural Network with backpropagation, which is an advanced Machine Learning algorithm was implemented as a binary and multiclass classifier. Then, a decision tree algorithm was executed. Last, the accuracy and confusion matrix of each model was reported.

Keyword: Neural Network, Algorithm, Machine Learning

INTRODUCTION

Machine Learning (ML) is a branch of data science that requires minimal amount of human intervention to find subtle patterns in large databases and make analytical decisions. It can also be considered as a branch of artificial intelligence based on the idea that machines can learn from data beyond the normal capability of human.

There are several algorithms used in ML, depending on the specific task to be accomplished. In this project, Neural Network (NN) with backpropagation, the decision tree, and the polynomial kernel perceptron were implemented using the MNIST dataset.

A NN is an algorithm, modeled loosely after the human brain, which is designed to recognize patterns in a dataset. Backpropagation in NN is the essence of neural net training. It is a method of improving the weights of a NN based on the error rate (i.e. loss) obtained in the previous epoch or iteration.

Vanilla decision trees are built using a recursive partitioning, which is commonly referred to as split and conquer because the algorithm splits the data into subsets, which are further split until the algorithm deduce that the data within the subsets are sufficiently homogenous, or until the specified stopping criterion is satisfied [2].

PURPOSE OF STUDY & SCOPE

The aim of this study is to implement binary and multiclass classification using NN and the decision tree. The resulting models are evaluated using the confusion matrix. The programming language used is R.

DATA DESCRIPTION

The raw MNIST dataset comprises of images of handwritten digits, and our labels are a single digit that indicate the number written in the image. Each image contains 780 features that were already processed into their numerical equivalent. Since the features are numbers between 0 and 255, the features were scaled by dividing by 255. Hence, the value of the features ranges from 0 to 1. The label comprises of 10 digits from 0 to 9. The dataset was stored in sparse format, which requires pre-processing before they could be deployed in ML algorithms. The preprocessing was done in R and the code used can be found in appendix A.

DATA ANALYSIS

Activation Function

The RELU requires some extensive technical manipulation in R, which is outside the scope of this project. To overcome that challenge, a custom activation function called "softplus" was written to approximate the standard RELU. Figure 1 shows how softplus compares with the RELU. The code can be found in appendix B.

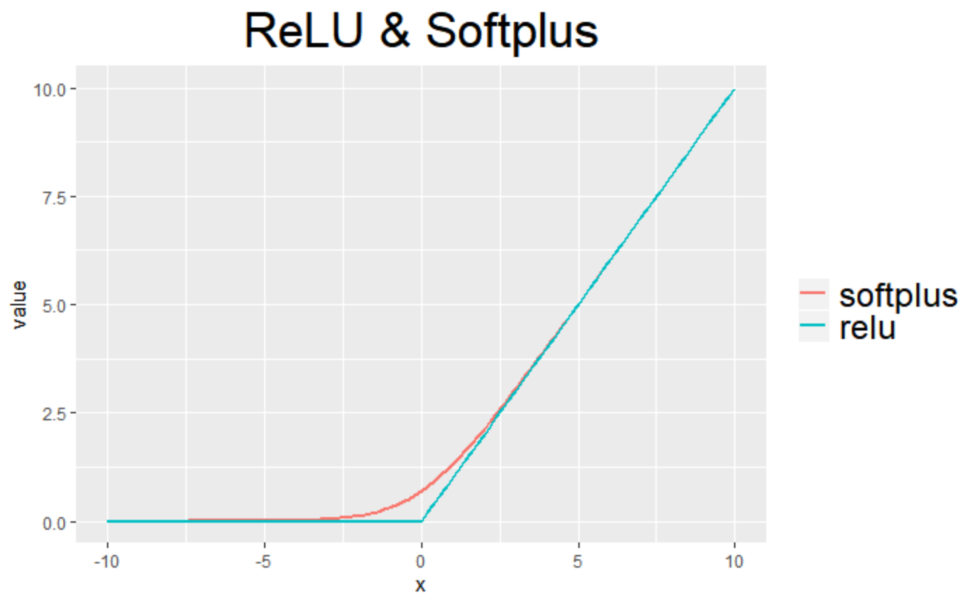


Figure 1. Comparison between Softplus and RELU

Binary Classification (Neural Network)

The processed MNIST dataset was split into training and testing data by ratio 70:30. Due to the ridiculous training time, the training data was sub-sampled. A two-layer NN for binary classification with a hidden layer comprising of 100 neurons and a singly output, as illustrated in Figure 2, was implemented. The binary classification was achieved by using the one-versus-the-rest rule. Simply put, a single label (i.e., 9) was arbitrarily selected from the 10 unique labels in the dataset. The Neural Network source code can be found in appendix B

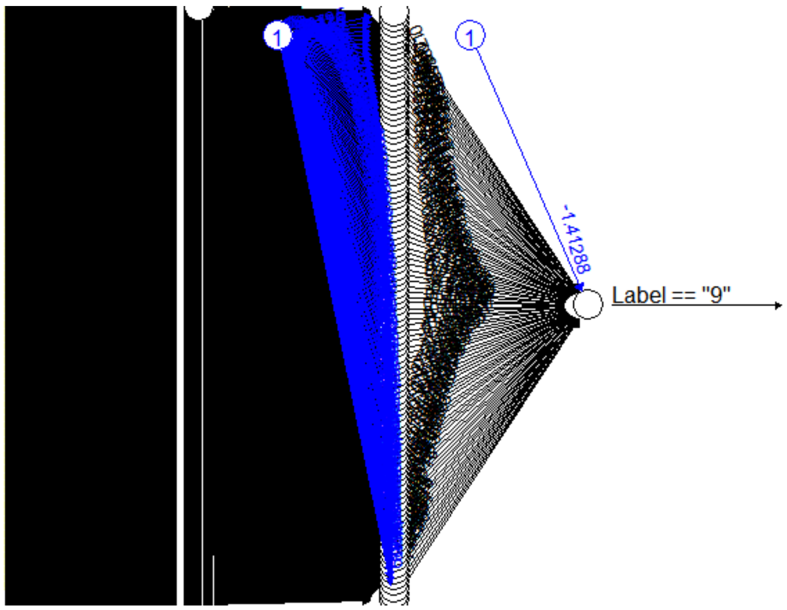


Figure 2. Binary Classification using Neural Network

The model was evaluated by fitting the model on the test data. The accuracy of the model is 86.3% and the confusion matrix is as summarized in Table 1.

Table 1. Confusion Matrix of the Binary Classifier

	FALSE	**TRUE**
FALSE	15255	1005
TRUE	1455	285

Multiclass Classification (Neural Network)

The same training and test data were used to implement the multiclass classifier, as shown in Figure 3. The accuracy of the model is 92.83% and the confusion matrix is as summarized in Table 2.

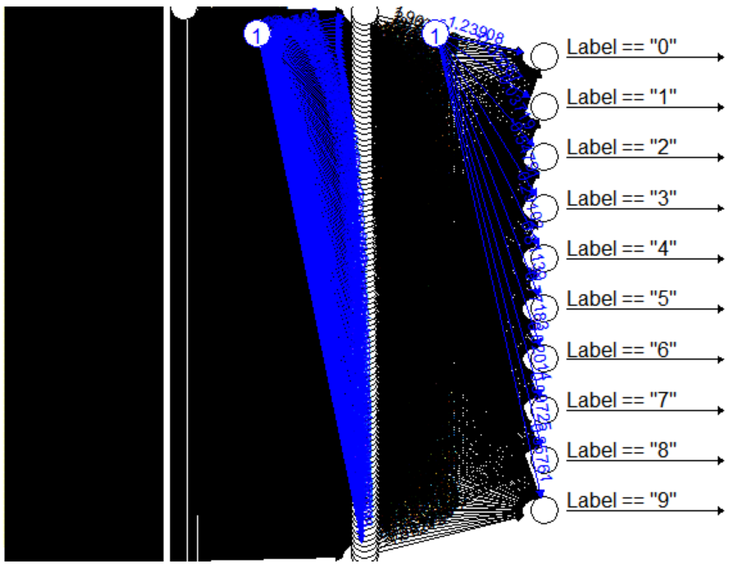


Figure 3. Multiclass Classification using Neural Network

Table 2. Confusion Matrix of the Multiclass Classifier

(Actual/Predicted)	0	1	2	3	4	5	6	7	8	9
0	1805	1	12	2	7	12	14	5	6	4
1	0	1946	25	9	8	11	3	9	17	5
2	9	7	1671	41	33	4	8	31	21	3
3	8	5	44	1600	6	40	6	29	46	15
4	6	8	8	2	1684	7	14	15	9	33
5	11	3	7	57	19	1430	29	6	30	11
6	17	6	14	0	8	30	1635	4	8	1
7	2	10	17	15	31	4	1	1729	6	36
8	9	23	18	25	18	42	14	11	1596	13
9	6	6	4	22	66	19	2	52	15	1548

Direct Multiclass classification (Decision Tree)

The decision tree algorithm implemented in the binary classification task is the C5.0 algorithm, which was developed by the famous computer scientist, J. Ross Quinlan as an improved version of C4.5 and the early Iterative Dichotomizer 3 (ID3).

Choosing the best splitting candidate is a major challenge that determines the efficiency of a decision tree. C5.0 uses the entropy concept to split the trees. High entropy indicates a diverse subset that provides little information on which class the subset belongs to. Entropy can be mathematically expressed as shown in equation (1).

$$Entropy\ (S) = \sum_{i=1}^{c} -p_i log_2(pi) \qquad (1)$$

Where "S" represents the segment of data, "c" refers to the number of class levels, and "p_i" is proportion of values falling into the ith class level. A quick illustration of the concept of entropy is shown in Figure 4. To determine the optimal feature to split upon, the algorithm computes the difference in homogeneity from splitting on each feature, which is a measure of "information gain." The higher the information gain, the better a feature is in producing homogenous subsets after splitting.

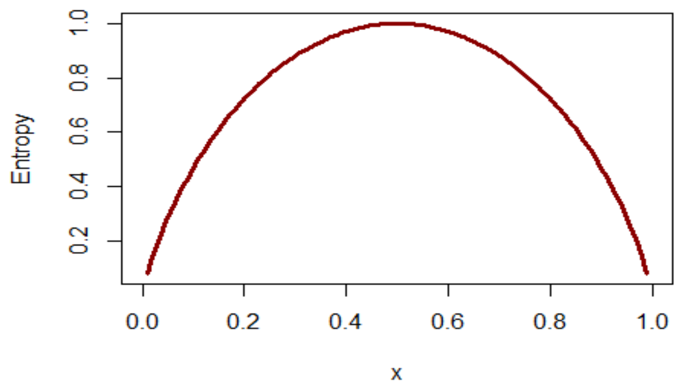
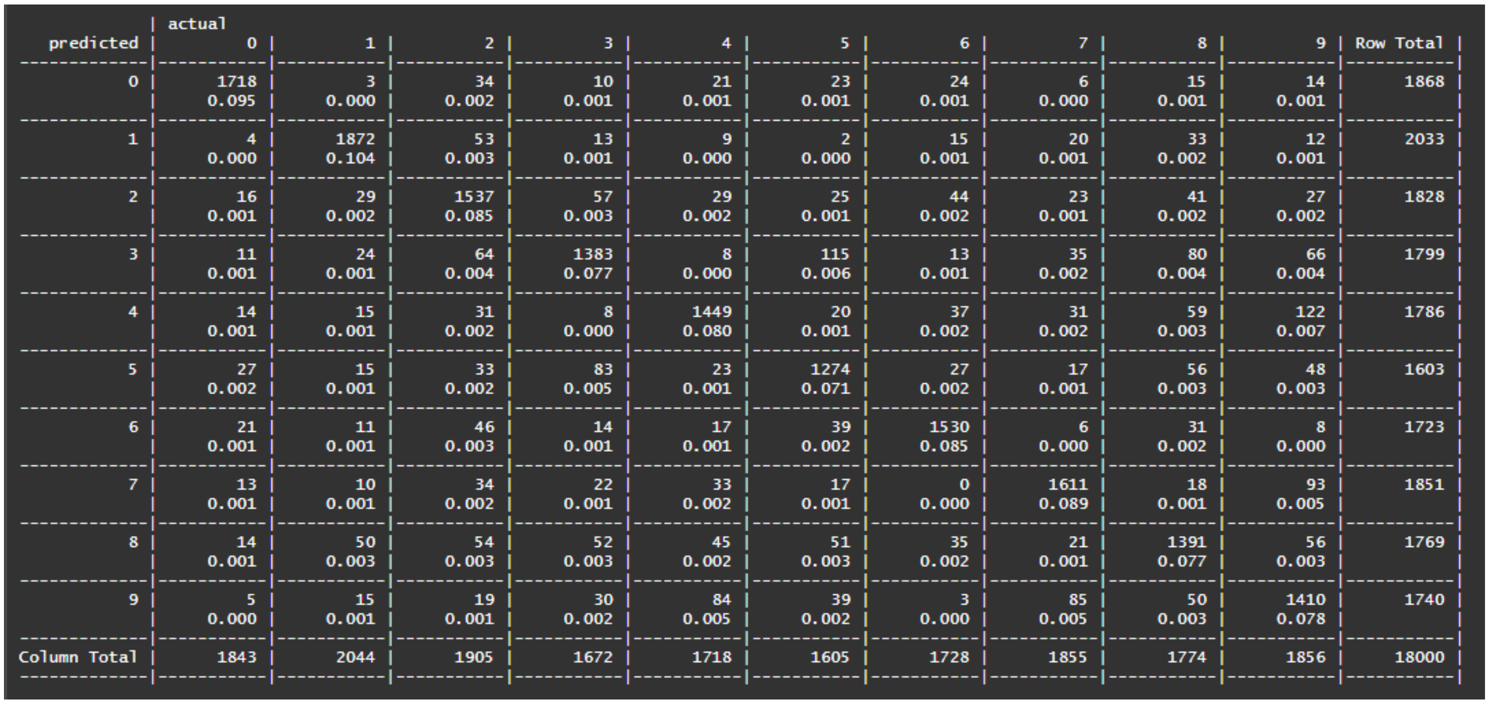


Figure 4. Illustration of Entropy

The confusion matrix of the decision tree implementation is shown in Figure 5. The resulting classification accuracy is approximately 84.3%.



```
             | actual 
   predicted |         0 |         1 |         2 |         3 |         4 |         5 |         6 |         7 |         8 |         9 | Row Total | 
-------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
           0 |      1718 |         3 |        34 |        10 |        21 |        23 |        24 |         6 |        15 |        14 |      1868 | 
             |     0.095 |     0.000 |     0.002 |     0.001 |     0.001 |     0.001 |     0.001 |     0.000 |     0.001 |     0.001 |           | 
-------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
           1 |         4 |      1872 |        53 |        13 |         9 |         2 |        15 |        20 |        33 |        12 |      2033 | 
             |     0.000 |     0.104 |     0.003 |     0.001 |     0.000 |     0.000 |     0.001 |     0.001 |     0.002 |     0.001 |           | 
-------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
           2 |        16 |        29 |      1537 |        57 |        29 |        25 |        44 |        23 |        41 |        27 |      1828 | 
             |     0.001 |     0.002 |     0.085 |     0.003 |     0.002 |     0.001 |     0.002 |     0.001 |     0.002 |     0.002 |           | 
-------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
           3 |        11 |        24 |        64 |      1383 |         8 |       115 |        13 |        35 |        80 |        66 |      1799 | 
             |     0.001 |     0.001 |     0.004 |     0.077 |     0.000 |     0.006 |     0.001 |     0.002 |     0.004 |     0.004 |           | 
-------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
           4 |        14 |        15 |        31 |         8 |      1449 |        20 |        37 |        31 |        59 |       122 |      1786 | 
             |     0.001 |     0.001 |     0.002 |     0.000 |     0.080 |     0.001 |     0.002 |     0.002 |     0.003 |     0.007 |           | 
-------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
           5 |        27 |        15 |        33 |        83 |        23 |      1274 |        27 |        17 |        56 |        48 |      1603 | 
             |     0.002 |     0.001 |     0.002 |     0.005 |     0.001 |     0.071 |     0.002 |     0.001 |     0.003 |     0.003 |           | 
-------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
           6 |        21 |        11 |        46 |        14 |        17 |        39 |      1530 |         6 |        31 |         8 |      1723 | 
             |     0.001 |     0.001 |     0.003 |     0.001 |     0.001 |     0.002 |     0.085 |     0.000 |     0.002 |     0.000 |           | 
-------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
           7 |        13 |        10 |        34 |        22 |        33 |        17 |         0 |      1611 |        18 |        93 |      1851 | 
             |     0.001 |     0.001 |     0.002 |     0.001 |     0.002 |     0.001 |     0.000 |     0.089 |     0.001 |     0.005 |           | 
-------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
           8 |        14 |        50 |        54 |        52 |        45 |        51 |        35 |        21 |      1391 |        56 |      1769 | 
             |     0.001 |     0.003 |     0.003 |     0.003 |     0.002 |     0.003 |     0.002 |     0.001 |     0.077 |     0.003 |           | 
-------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
           9 |         5 |        15 |        19 |        30 |        84 |        39 |         3 |        85 |        50 |      1410 |      1740 | 
             |     0.000 |     0.001 |     0.001 |     0.002 |     0.005 |     0.002 |     0.000 |     0.005 |     0.003 |     0.078 |           | 
-------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
Column Total |      1843 |      2044 |      1905 |      1672 |      1718 |      1605 |      1728 |      1855 |      1774 |      1856 |     18000 | 
-------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
```

Figure 5. Confusion Matrix of the Multiclass Classification Decision Tree

CONCLUSION

The analysis results showed that neural networks are powerful classifiers. However, comparing the classification accuracies, the vanilla decision tree algorithm is preferred because the interpretability is still within human comprehension, as compared to complete black-box models like neural networks.

REFERENCES

[1] Brett Lantz. (2015). Machine Learning with R. ISBN 978-1-78439-390-8

[2] https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/multiclass.html#mnist

APPENDIX: A

Pre-Processing

```r
read.libsvm = function( filename, dimensionality ) {

  content = readLines(filename )
  num_lines = length( content )
  yx = matrix( 0, num_lines, dimensionality + 1 )

  # loop over lines
  for ( i in 1:num_lines ) {

    # split by spaces
    line = as.vector( strsplit( content[i], ' ' )[[1]])

    # save label
    yx[i,1] = as.numeric( line[[1]] )

    # loop over values
    for ( j in 2:length( line )) {

      # split by colon
      index_value = strsplit( line[j], ':' )[[1]]

      index = as.numeric( index_value[1] ) + 1 # +1 because label goes first


      value = as.numeric( index_value[2] )

      yx[i, index] = value
    }
  }

  return( yx )
}
```

APPENDIX: C

```
neuralnet <-

  function (formula, data, hidden = 1, threshold = 0.01, stepmax = 1e+05,

            rep = 1, startweights = NULL, learningrate.limit = NULL,

            learningrate.factor = list(minus = 0.5, plus = 1.2), learningrate
= NULL,

            lifesign = "none", lifesign.step = 1000, algorithm = "rprop+",

            err.fct = "sse", act.fct = "logistic", linear.output = TRUE,

            exclude = NULL, constant.weights = NULL, likelihood = FALSE) {

    # Save call

    call <- match.call()


    # Check arguments

    if (is.null(data)) {

      stop("Missing 'data' argument.", call. = FALSE)

    }

    data <- as.data.frame(data)

    if (is.null(formula)) {

      stop("Missing 'formula' argument.", call. = FALSE)

    }

    formula <- stats::as.formula(formula)

    # Learning rate limit

    if (!is.null(learningrate.limit)) {
      if (length(learningrate.limit) != 2) {
        stop("Argument 'learningrate.factor' must consist of two components.",
             call. = FALSE)
      }
      learningrate.limit <- as.list(learningrate.limit)
      names(learningrate.limit) <- c("min", "max")

      if (is.na(learningrate.limit$min) || is.na(learningrate.limit$max)) {
        stop("'learningrate.limit' must be a numeric vector",
             call. = FALSE)
      }
    } else {
      learningrate.limit <- list(min = 1e-10, max = 0.1)
    }
    # Learning rate factor
    if (!is.null(learningrate.factor)) {
      if (length(learningrate.factor) != 2) {
        stop("Argument 'learningrate.factor' must consist of two components.",
             call. = FALSE)
      }
      learningrate.factor <- as.list(learningrate.factor)
      names(learningrate.factor) <- c("minus", "plus")
      if (is.na(learningrate.factor$minus) || is.na(learningrate.factor$plus))
{
        stop("'learningrate.factor' must be a numeric vector",
             call. = FALSE)
      }
    } else {
      learningrate.factor <- list(minus = 0.5, plus = 1.2)
    }


    # Learning rate (backprop)
    if (algorithm == "backprop") {
      if (is.null(learningrate) || !is.numeric(learningrate)) {
        stop("Argument  'learningrate'  must  be  a  numeric  value,  if  the
backpropagation algorithm is used.",
             call. = FALSE)
      }
    }
    # TODO: Rename?
    # Lifesign
    if (!(lifesign %in% c("none", "minimal", "full"))) {
      stop("Argument 'lifesign' must be one of 'none', 'minimal', 'full'.",
call. = FALSE)
    }


    # Algorithm
    if (!(algorithm %in% c("rprop+", "rprop-", "slr", "sag", "backprop"))) {

      stop("Unknown algorithm.", call. = FALSE)

    }


    # Threshold

    if (is.na(threshold)) {

      stop("Argument 'threshold' must be a numeric value.", call. = FALSE)

    }


    # Hidden units

    if (any(is.na(hidden))) {

      stop("Argument 'hidden' must be an integer vector or a single integer.",

           call. = FALSE)

    }

    if (length(hidden) > 1 && any(hidden == 0)) {

      stop("Argument 'hidden' contains at least one 0.", call. = FALSE)

    }

    # Replications

    if (is.na(rep)) {

      stop("Argument 'rep' must be an integer", call. = FALSE)

    }


    # Max steps

    if (is.na(stepmax)) {
      stop("Argument 'stepmax' must be an integer", call. = FALSE)
    }
    # Activation function
    if (!(is.function(act.fct) || act.fct %in% c("logistic", "tanh"))) {
      stop("Unknown activation function.", call. = FALSE)
    }

    # Error function
    if (!(is.function(err.fct) || err.fct %in% c("sse", "ce"))) {
      stop("Unknown error function.", call. = FALSE)
    }

    # Formula interface
    model.list <- list(response = attr(terms(as.formula(call("~",
formula[[2]]))), "term.labels"),
                       variables = attr(terms(formula, data = data),
"term.labels"))
    response <- as.matrix(model.frame(as.formula(call("~", formula[[2]])),
data))
    covariate <- cbind(intercept = 1, as.matrix(data[, model.list$variables]))

    # Multiclass response
    if (is.character(response)) {
      class.names <- unique(response[, 1])
      response <- model.matrix( ~ response[,1]-1) == 1
      colnames(response) <- class.names

      model.list$response <- class.names

    }

    # Activation function

    if (is.function(act.fct)) {

      act.deriv.fct <- Deriv::Deriv(act.fct)

      attr(act.fct, "type") <- "function"

    } else {

      converted.fct <- convert.activation.function(act.fct)

      act.fct <- converted.fct$fct

      act.deriv.fct <- converted.fct$deriv.fct

    }

    # Error function

    if (is.function(err.fct)) {

      attr(err.fct, "type") <- "function"

      err.deriv.fct <- Deriv::Deriv(err.fct)

    } else {

      converted.fct <- convert.error.function(err.fct)

      err.fct <- converted.fct$fct

      err.deriv.fct <- converted.fct$deriv.fct

    }

    if (attr(err.fct, "type") == "ce" && !all(response %in% 0:1)) {

      stop("Error function 'ce' only implemented for binary response.", call.
= FALSE)
```

```
    }


    # Fit network for each replication
    list.result <- lapply(1:rep, function(i) {
      # Show progress
      if (lifesign != "none") {
        lifesign <- display(hidden, threshold, rep, i, lifesign)
      }


      # Fit network
      calculate.neuralnet(learningrate.limit = learningrate.limit,
                          learningrate.factor = learningrate.factor, covariate
= covariate,
                          response = response, data = data, model.list =
model.list,
                          threshold = threshold, lifesign.step =
lifesign.step,
                          stepmax = stepmax, hidden = hidden, lifesign =
lifesign,
                          startweights = startweights, algorithm = algorithm,
                          err.fct = err.fct, err.deriv.fct = err.deriv.fct,
                          act.fct = act.fct, act.deriv.fct = act.deriv.fct,
                          rep = i, linear.output = linear.output, exclude =
exclude,
                          constant.weights = constant.weights, likelihood =
likelihood,
                          learningrate.bp = learningrate)
    })
    matrix <- sapply(list.result, function(x) {x$output.vector})
    if (all(sapply(matrix, is.null))) {
      list.result <- NULL
      matrix <- NULL
      ncol.matrix <- 0
    } else {
      ncol.matrix <- ncol(matrix)
    }

    # Warning if some replications did not converge
    if (ncol.matrix < rep) {
      warning(sprintf("Algorithm did not converge in %s of %s repetition(s)
within the stepmax.",
                      (rep - ncol.matrix), rep), call. = FALSE)
    }

    # Return output
    generate.output(covariate, call, rep, threshold, matrix,
                    startweights, model.list, response, err.fct, act.fct,
                    data, list.result, linear.output, exclude)
  }
```

```
# Display output of replication
display <- function (hidden, threshold, rep, i.rep, lifesign) {
  message("hidden: ", paste(hidden, collapse = ", "), "    thresh: ",
          threshold, "    rep: ", strrep(" ", nchar(rep) - nchar(i.rep)),
          i.rep, "/", rep, "    steps: ", appendLF = FALSE)
  utils::flush.console()

  if (lifesign == "full") {
    lifesign <- sum(nchar(hidden)) + 2 * length(hidden) -
      2 + max(nchar(threshold)) + 2 * nchar(rep) + 41
  }
  return(lifesign)
}

# Generate output object
generate.output   <-   function(covariate,   call,   rep,   threshold,   matrix,
startweights,
                            model.list,  response,  err.fct,  act.fct,  data,
list.result,
                            linear.output, exclude) {


  nn <- list(call = call, response = response, covariate = covariate[, -1, drop
= FALSE],
             model.list = model.list, err.fct = err.fct, act.fct = act.fct,
             linear.output = linear.output, data = data, exclude = exclude)
  if (!is.null(matrix)) {

    nn$net.result <- lapply(list.result, function(x) {x$net.result})

    nn$weights <- lapply(list.result, function(x) {x$weights})

    nn$generalized.weights      <-      lapply(list.result,      function(x)
{x$generalized.weights})

    nn$startweights <- lapply(list.result, function(x) {x$startweights})

    nn$result.matrix <- matrix

    rownames(nn$result.matrix) <- c(rownames(matrix)[rownames(matrix) != ""],

                                    get_weight_names(nn$weights[[1]],
model.list))

  }


  class(nn) <- c("nn")

  return(nn)

}


# Get names of all weights in network

get_weight_names <- function(weights, model.list) {

  # All hidden unit names

  if (length(weights) > 1) {

    hidden_units <- lapply(1:(length(weights) - 1), function(i) {

      paste0(i, "layhid", 1:ncol(weights[[i]]))

    })
  } else {
    hidden_units <- list()
  }

  # All unit names including input and output
  units <- c(list(model.list$variables),
             hidden_units,
             list(model.list$response))

  # Combine each layer with the next, add intercept
  weight_names <- do.call(c, lapply(1:(length(units) - 1), function(i) {
    as.vector(outer(c("Intercept", units[[i]]), units[[i + 1]], paste, sep =
".to."))
  }))
  return(weight_names)
```