# Neural Networks

## ACM

## November 8th, 2023

```
## Registered S3 method overwritten by 'printr':
## method from
## knit_print.data.frame rmarkdown
```

Our example data set is from the Wisconsin cancer study. We read in the data and remove any rows with missing data. The following code uses the package mlbench that contains this data set. We show the top few lines of the data.

```
library(mlbench)
data("BreastCancer")

#Clean off rows with missing data
BreastCancer = BreastCancer[which(complete.cases(BreastCancer)==TRUE),]
dim(BreastCancer)
```

```
## [1] 683 11
```

head(BreastCancer)

Id	Cl.t	hicknes@ell.size	Cel	l.shapeMarg.ac	dhes <b>i5p</b> ith	.c.sizeBare.nı	ıcleBl.cro	omati <b>N</b> ormal	l.nucle <b>Mi</b> tos	ses Class
1000025	55	1	1	1	2	1	3	1	1	benign
1002945	55	4	4	5	7	10	3	2	1	benign
1015425	63	1	1	1	2	2	3	1	1	benign
1016277	76	8	8	1	3	4	3	7	1	benign
1017023	34	1	1	3	2	1	3	1	1	benign
1017122	28	10	10	8	7	10	9	7	1	malignant

## ?BreastCancer

```
## Wisconsin Breast Cancer Database
##
## Description:
##
        The objective is to identify each of a number of benign or
##
##
        malignant classes. Samples arrive periodically as Dr. Wolberg
        reports his clinical cases. The database therefore reflects this
##
##
        chronological grouping of the data. This grouping information
##
        appears immediately below, having been removed from the data
        itself. Each variable except for the first was converted into 11
##
##
        primitive numerical attributes with values ranging from 0 through
##
        10. There are 16 missing attribute values. See cited below for
##
        more details.
##
## Format:
```

```
##
##
        A data frame with 699 observations on 11 variables, one being a
##
        character variable, 9 being ordered or nominal, and 1 target
##
        class.
##
          [,1]
                                   Sample code number
##
                 Τd
          [,2]
                 Cl.thickness
                                   Clump Thickness
##
          [,3]
                 Cell.size
##
                                   Uniformity of Cell Size
##
          [, 4]
                 Cell.shape
                                   Uniformity of Cell Shape
          [,5]
                 Marg.adhesion
##
                                   Marginal Adhesion
##
          [,6]
                 Epith.c.size
                                   Single Epithelial Cell Size
          [,7]
                 Bare.nuclei
                                   Bare Nuclei
##
                                   Bland Chromatin
##
          [8,]
                 Bl.cromatin
          [,9]
                 Normal.nucleoli Normal Nucleoli
##
##
          [,10] Mitoses
                                   Mitoses
##
          [,11] Class
                                   Class
str(BreastCancer)
## 'data.frame':
                    683 obs. of 11 variables:
## $ Id
                      : chr "1000025" "1002945" "1015425" "1016277" ...
                      : Ord.factor w/ 10 levels "1"<"2"<"3"<"4"<..: 5 5 3 6 4 8 1 2 2 4 ...
## $ Cl.thickness
                      : Ord.factor w/ 10 levels "1"<"2"<"3"<"4"<..: 1 4 1 8 1 10 1 1 1 2 ...
## $ Cell.size
## $ Cell.shape
                      : Ord.factor w/ 10 levels "1"<"2"<"3"<"4"<..: 1 4 1 8 1 10 1 2 1 1 ...
## $ Marg.adhesion : Ord.factor w/ 10 levels "1"<"2"<"3"<"4"<..: 1 5 1 1 3 8 1 1 1 1 ...
## $ Epith.c.size
                      : Ord.factor w/ 10 levels "1"<"2"<"3"<"4"<..: 2 7 2 3 2 7 2 2 2 2 ...
                      : Factor w/ 10 levels "1","2","3","4",..: 1 10 2 4 1 10 10 1 1 1 ...
## $ Bare.nuclei
                      : Factor w/ 10 levels "1", "2", "3", "4", ...: 3 3 3 3 3 9 3 3 1 2 ...
## $ Bl.cromatin
## $ Normal.nucleoli: Factor w/ 10 levels "1", "2", "3", "4", ..: 1 2 1 7 1 7 1 1 1 1 ...
## $ Mitoses
                      : Factor w/ 9 levels "1", "2", "3", "4", ...: 1 1 1 1 1 1 1 1 5 1 ...
##
    $ Class
                      : Factor w/ 2 levels "benign", "malignant": 1 1 1 1 1 2 1 1 1 1 ...
Since neuralnet only deals with quantitative variables, you can convert all the qualitative variables (factors)
to binary ("dummy"), with the model.matrix function.
y = as.matrix(BreastCancer[,11])
y[which(y=="benign")] = 0
y[which(y=="malignant")] = 1
y = as.numeric(y)
x = model.matrix(~0 + Cl.thickness + Cell.size + Cell.shape +
                          Marg.adhesion + Epith.c.size + Bare.nuclei + Bl.cromatin +
                          Normal.nucleoli + Mitoses, data = BreastCancer)
dim(x)
## [1] 683 81
df <- data.frame(y,x)</pre>
Let's split the data into training and validation:
set.seed(92739847)
ids <- sample(1:dim(df)[1],size=dim(df)[1])</pre>
df_jumbled <- df[ids,]</pre>
train <- df_jumbled[1:450,]</pre>
test <- df_jumbled[451:nrow(df_jumbled),]</pre>
```

# Fitting with neuralnet

In the first example, we will create a simple neural network with minimum effort using the neuralnet package. The neuralnet package is outdated, but it is still popular among the R community.

The neuralnet function is simple. It doesn't provide us the freedom to create fully customizable model architecture. In our case, we are providing it with a machine-learning formula and data, just like GLM. The formula consists of target variables and features.

```
library("neuralnet")
?neuralnet
```

Training of neural networks

#### Description:

Train neural networks using backpropagation, resilient backpropagation (RPROP) with (Riedmiller, 1994) or without weight backtracking (Riedmiller and Braun, 1993) or the modified globally convergent version (GRPROP) by Anastasiadis et al. (2005). The function allows flexible settings through custom-choice of error and activation function. Furthermore, the calculation of generalized weights (Intrator O. and Intrator N., 1993) is implemented.

#### Usage:

```
neuralnet(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)
```

## Arguments:

formula: a symbolic description of the model to be fitted.

data: a data frame containing the variables specified in 'formula'.

hidden: a vector of integers specifying the number of hidden neurons (vertices) in each layer.

threshold: a numeric value specifying the threshold for the partial derivatives of the error function as stopping criteria.

stepmax: the maximum steps for the training of the neural network.

Reaching this maximum leads to a stop of the neural network's training process.

rep: the number of repetitions for the neural network's training.

startweights: a vector containing starting values for the weights. Set to 'NULL' for random initialization.

- learningrate.limit: a vector or a list containing the lowest and highest limit for the learning rate. Used only for RPROP and GRPROP.
- learningrate.factor: a vector or a list containing the multiplication factors for the upper and lower learning rate. Used only for RPROP and GRPROP.
- learningrate: a numeric value specifying the learning rate used by traditional backpropagation. Used only for traditional backpropagation.
- lifesign: a string specifying how much the function will print during the calculation of the neural network. 'none', 'minimal' or 'full'.
- lifesign.step: an integer specifying the stepsize to print the minimal threshold in full lifesign mode.
- algorithm: a string containing the algorithm type to calculate the neural network. The following types are possible: 'backprop', 'rprop+', 'rprop-', 'sag', or 'slr'. 'backprop' refers to backpropagation, 'rprop+' and 'rprop-' refer to the resilient backpropagation with and without weight backtracking, while 'sag' and 'slr' induce the usage of the modified globally convergent algorithm (grprop). See Details for more information.
- err.fct: a differentiable function that is used for the calculation of the error. Alternatively, the strings 'sse' and 'ce' which stand for the sum of squared errors and the cross-entropy can be used.
- act.fct: a differentiable function that is used for smoothing the result of the cross product of the covariate or neurons and the weights. Additionally the strings, 'logistic' and 'tanh' are possible for the logistic function and tangent hyperbolicus.
- linear.output: logical. If act.fct should not be applied to the output neurons set linear output to TRUE, otherwise to FALSE.
- exclude: a vector or a matrix specifying the weights, that are excluded from the calculation. If given as a vector, the exact positions of the weights must be known. A matrix with n-rows and 3 columns will exclude n weights, where the first column stands for the layer, the second column for the input neuron and the third column for the output neuron of the weight.
- constant.weights: a vector specifying the values of the weights that are excluded from the training process and treated as fix.

```
likelihood: logical. If the error function is equal to the negative log-likelihood function, the information criteria AIC and BIC will be calculated. Furthermore the usage of confidence.interval is meaningfull.
```

#### Details:

The globally convergent algorithm is based on the resilient backpropagation without weight backtracking and additionally modifies one learning rate, either the learningrate associated with the smallest absolute gradient (sag) or the smallest learningrate (slr) itself. The learning rates in the grprop algorithm are limited to the boundaries defined in learningrate.limit.

Now we'll fit a neural network. How many layers?

- There's a lot of discussion on this. See http://www.faqs.org/faqs/ai-faq/neural-nets/part1/preamble. html for some.
- One thing that is agreed upon is that the situations in which performance improves with a second (or third, etc.) hidden layer are very small.
- One hidden layer is sufficient for the large majority of problems.

How about the size of the hidden layer(s):

## <environment: 0x111551ac8>

## attr(,"type")

- A common rule of thumb is that the optimal size of the hidden layer is usually between the size of the input and size of the output layers.
- One way to choose would be to use the mean.

In this example we'll use 81 input layers and 1 output layer, so we'll choose 40.

```
Breast_NN <- neuralnet(y ~ ., data = train,</pre>
                      hidden = 40, lifesign = "minimal", algorithm="backprop",
                      linear.output = FALSE, err.fct = 'ce',
                      learningrate=0.1)
                                                         2282 error: 0.04201 time: 9.63 secs
## hidden: 40
                 thresh: 0.01
                                  rep: 1/1
                                               steps:
# Look at the error and activation function
Breast_NN$err.fct
## function (x, y)
## {
##
       -(y * log(x) + (1 - y) * log(1 - x))
## }
## <bytecode: 0x111558fc0>
## <environment: 0x11155c060>
## attr(,"type")
## [1] "ce"
Breast_NN$act.fct
## function (x)
## {
##
       1/(1 + \exp(-x))
## }
## <bytecode: 0x11154e4b0>
```

```
## [1] "logistic"
```

# Here are the parameters:
dim(Breast\_NN\$result.matrix)

## [1] 3324 1

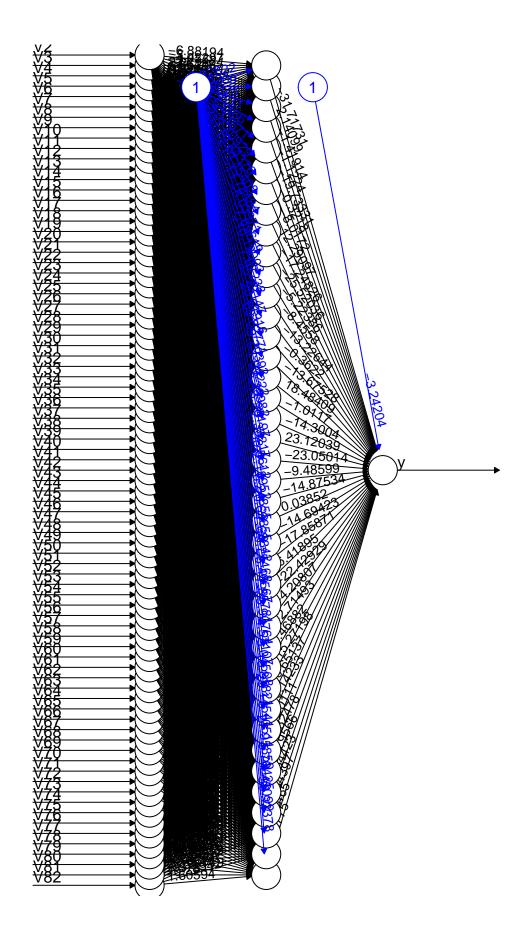
3321/81

## [1] 41

head(data.frame(Breast\_NN\$result.matrix))

	Breast_NN.result.matrix
error	0.0420063
reached.threshold	0.0099975
steps	2282.0000000
Intercept.to.1layhid1	-7.3351334
Cl.thickness1.to.1layhid1	1.9221154
Cl. thickness 2. to. 1 layhid 1	1.6221521

#plot(Breast\_NN, rep="best")



```
valid_pred <- predict(Breast_NN, newdata = test)
table(valid_pred>0.5, test$y)
```

/	0	1
FALSE	152	9
TRUE	1	71

```
# Accuracy
sum(diag(table(valid_pred>0.5, test$y)))/length(test$y)
```

## [1] 0.9570815

# Fitting with TensorFlow

TensorFlow is an open source deep neural net framework, based on a graphical model. It is more than just a neural net platform, and supports numerical computing based on data flow graphs. Data may be represented in n-dimensional structures like vectors and matrices, or higher-dimensional tensors. Because these mathematical objects are folded into a data flow graph for computation, the moniker for this software library is an obvious one.

The computations for deep learning nets involve tensor computations, which are known to be implemented more efficiently on GPUs than CPUs. Therefore like other deep learning libraries, TensorFlow may be implemented on CPUs and GPUs. The generality and speed of the TensorFlow software, ease of installation, its documentation and examples, and runnability on multiple platforms has made TensorFlow the most popular deep learning toolkit today. (Opinions on this may, of course, differ.) There is a wealth of tutorial material on TF of very high quality that you may refer to here: https://www.tensorflow.org/tutorials/.

Rather than run TensorFlow natively, it is often easier to use it through an easy to use interface program. One of the most popular high-level APIs is Keras See: https://keras.io/. The site contains several examples, which make it easy to get up and running. Though originally written in Python, Keras has been extended to R via the keras package.

Keras is a high-level neural networks API developed with a focus on enabling fast experimentation. Being able to go from idea to result with the least possible delay is key to doing good research. Keras has the following key features:

- Allows the same code to run on CPU or on GPU, seamlessly.
- User-friendly API which makes it easy to quickly prototype deep learning models.
- Built-in support for convolutional networks (for computer vision), recurrent networks (for sequence processing), and any combination of both.
- Supports arbitrary network architectures: multi-input or multi-output models, layer sharing, model sharing, etc. This means that Keras is appropriate for building essentially any deep learning model, from a memory network to a neural Turing machine.

```
library(tensorflow)
library(keras)
library(reticulate)
```

To use these functions were going to convert the outcome (benign, malignant) in the data set to "one-hot encoding" using the to\_categorial function. What is one-hot encoding replaces a single vector of 1s (malignant) and 0s (benign) to a bivariate dependent variable as a two-column matrix, where the first column contains a 1 if the cell is benign and the second column a 1 if the cell is malignant, for each row of the data set. This is because TensorFlow/Keras requires this format as input, to facilitate tensor calculations.

```
y_train = as.matrix(train[,1])
y_test = as.matrix(test[,1])
x_train = as.matrix(train[,-1])
x_test = as.matrix(test[,-1])

Y_train = to_categorical(y_train,2)
Y_test = to_categorical(y_test,2)
```

TensorFlow is structured in a manner where one describes the neural net first, layer by layer. There is not a single function that is called, which generates the deep learning net, and runs the model. Here, we first describe for each layer in the neural net, the number of nodes, the type of activation function, and any other hyperparameters needed in the model fitting stage, such as the extent of dropout for example.

In the output layer we also state the nature of the activation function, such as sigmoid or softmax. And then, we specify a compile function which describes the loss function that will be minimized, along with the minimization algorithm. At this point in the program specification, the model is not actually run. See below for the code block that builds up the deep learning network.

The core data structure of Keras is a model, a way to organize layers. The simplest type of model is the Sequential model, a linear stack of layers.

We begin by creating a sequential model and then adding layers using the pipe (%>%) operator:

```
?keras_model_sequential
```

```
Keras Model composed of a linear stack of layers
Description:
    Keras Model composed of a linear stack of layers
Usage:
     keras_model_sequential(layers = NULL, name = NULL, ...)
Arguments:
  layers: List of layers to add to the model
   name: Name of model
     ...: Arguments passed on to 'sequential_model_input_layer'
          'input_shape' an integer vector of dimensions (not including
              the batch axis), or a 'tf$TensorShape' instance (also not
              including the batch axis).
          'batch_size' Optional input batch size (integer or NULL).
          'dtype' Optional datatype of the input. When not provided,
              the Keras default float type will be used.
          'input_tensor' Optional tensor to use as layer input. If set,
              the layer will use the 'tf$TypeSpec' of this tensor
              rather than creating a new placeholder tensor.
```

```
'sparse' Boolean, whether the placeholder created is meant to be sparse. Default to 'FALSE'.
```

- 'ragged' Boolean, whether the placeholder created is meant to be ragged. In this case, values of 'NULL' in the 'shape' argument represent ragged dimensions. For more information about 'RaggedTensors', see this guide. Default to 'FALSE'.
- 'type\_spec' A 'tf\$TypeSpec' object to create Input from. This 'tf\$TypeSpec' represents the entire batch. When provided, all other args except name must be 'NULL'.
- 'input\_layer\_name,name' Optional name of the input layer (string).

```
model <- keras_model_sequential()
n <- nrow(x_train)
model %>%
  layer_dense(units = n/2, activation = 'relu', input_shape = c(ncol(x_train))) %>%
  # set rate: the fraction of the input units to drop.
  layer_dropout(rate = 0.25) %>%
  layer_dense(units = n/10, activation = 'relu') %>%
  layer_dropout(rate = 0.2) %>%
  layer_dense(units = 2, activation = 'softmax')
```

The input\_shape argument to the first layer specifies the shape of the input data (a length ncol(x\_train) numeric vector). The final layer outputs a length 2 numeric vector (probabilities for each class) using a softmax activation function.

#### summary(model)

```
## Model: "sequential"
## Layer (type) Output Shape
                                            Param #
## -----
## dense_2 (Dense)
                          (None, 225)
                                               18450
## dropout_1 (Dropout)
                          (None, 225)
                                               0
## dense_1 (Dense)
                          (None, 45)
                                               10170
## dropout (Dropout)
                          (None, 45)
## dense (Dense)
                          (None, 2)
                                               92
## Total params: 28712 (112.16 KB)
## Trainable params: 28712 (112.16 KB)
## Non-trainable params: 0 (0.00 Byte)
```

Next, compile the model with appropriate loss function, optimizer, and metrics:

```
? {\tt compile.keras.engine.training.Model}\\
```

Configure a Keras model for training

## Description:

Configure a Keras model for training

#### Usage:

```
## S3 method for class 'keras.engine.training.Model'
compile(
  object,
  optimizer = NULL,
  loss = NULL,
  metrics = NULL,
  loss_weights = NULL,
  weighted_metrics = NULL,
  run_eagerly = NULL,
  steps_per_execution = NULL,
  ...,
  target_tensors = NULL,
  sample_weight_mode = NULL
)
```

#### Arguments:

object: Model object to compile.

optimizer: String (name of optimizer) or optimizer instance. For most models, this defaults to '"rmsprop"'

loss: String (name of objective function), objective function or a 'keras\$losses\$Loss' subclass instance. An objective function is any callable with the signature 'loss = fn(y\_true, y\_pred)', where y\_true = ground truth values with shape = [batch\_size, d0, .. dN], except sparse loss functions such as sparse categorical crossentropy where shape = [batch\_size, d0, .. dN-1]. y\_pred = predicted values with shape = [batch\_size, d0, .. dN]. It returns a weighted loss float tensor. If a custom 'Loss' instance is used and reduction is set to 'NULL', return value has the shape [batch\_size, d0, ... dN-1] i.e. per-sample or per-timestep loss values; otherwise, it is a scalar. If the model has multiple outputs, you can use a different loss on each output by passing a dictionary or a list of losses. The loss value that will be minimized by the model will then be the sum of all individual losses, unless 'loss\_weights' is specified.

metrics: List of metrics to be evaluated by the model during training
 and testing. Each of this can be a string (name of a built-in
 function), function or a 'keras\$metrics\$Metric' class
 instance. See '?tf\$keras\$metrics'. Typically you will use
 'metrics=list('accuracy')'. A function is any callable with
 the signature 'result = fn(y\_true, y\_pred)'. To specify
 different metrics for different outputs of a multi-output
 model, you could also pass a dictionary, such as
 'metrics=list(output\_a = 'accuracy', output\_b = c('accuracy',
 'mse'))'. You can also pass a list to specify a metric or a
 list of metrics for each output, such as
 'metrics=list(list('accuracy'), list('accuracy', 'mse'))' or
 'metrics=list('accuracy', c('accuracy', 'mse'))'. When you

pass the strings ''accuracy'' or ''acc'', this is converted to one of 'tf.keras.metrics.BinaryAccuracy', 'tf.keras.metrics.CategoricalAccuracy', 'tf.keras.metrics.SparseCategoricalAccuracy' based on the loss function used and the model output shape. A similar conversion is done for the strings ''crossentropy'' and ''ce''.

- loss\_weights: Optional list, dictionary, or named vector specifying scalar numeric coefficients to weight the loss contributions of different model outputs. The loss value that will be minimized by the model will then be the \_weighted sum\_ of all individual losses, weighted by the 'loss\_weights' coefficients. If a list, it is expected to have a 1:1 mapping to the model's outputs. If a dict, it is expected to map output names (strings) to scalar coefficients.
- run\_eagerly: Bool. Defaults to 'FALSE'. If 'TRUE', this Model's logic
   will not be wrapped in a 'tf.function'. Recommended to leave
   this as 'NULL' unless your Model cannot be run inside a
   'tf.function'. 'run\_eagerly=True' is not supported when using
   'tf.distribute.experimental.ParameterServerStrategy'. If the
   model's logic uses tensors in R control flow expressions like
   'if' and 'for', the model is still traceable with
   'tf.function', but you will have to enter a
   'tfautograph::autograph({})' directly.
- steps\_per\_execution: Int. Defaults to 1. The number of batches to run during each 'tf.function' call. Running multiple batches inside a single 'tf.function' call can greatly improve performance on TPUs or small models with a large Python/R overhead. At most, one full epoch will be run each execution. If a number larger than the size of the epoch is passed, the execution will be truncated to the size of the epoch. Note that if 'steps\_per\_execution' is set to 'N', 'Callback.on\_batch\_begin' and 'Callback.on\_batch\_end' methods will only be called every 'N' batches (i.e. before/after each 'tf.function' execution).
  - ...: Arguments supported for backwards compatibility only.
- target\_tensors: By default, Keras will create a placeholder for the
   model's target, which will be fed with the target data during
   training. If instead you would like to use your own target
   tensor (in turn, Keras will not expect external data for
   these targets at training time), you can specify them via the
   'target\_tensors' argument. It should be a single tensor (for
   a single-output sequential model).

sample weight mode: If you need to do timestep-wise sample weighting

```
(2D weights), set this to "temporal". 'NULL' defaults to sample-wise weights (1D). If the model has multiple outputs, you can use a different 'sample_weight_mode' on each output by passing a list of modes.
```

```
model %>% compile(
  loss = 'categorical_crossentropy',
  optimizer = optimizer_rmsprop(),
  metrics = c('accuracy')
)
```

From this I got the following message:

WARNING:absl:At this time, the v2.11+ optimizer tf.keras.optimizers.RMSprop runs slowly on M1/M2 Macs, please use the legacy Keras optimizer instead, located at tf.keras.optimizers.legacy.RMSprop.

This error apparently happens when trying to use ADAM (on python or R). The following does work:

```
model %>% compile(
  loss = 'categorical_crossentropy',
  metrics = c('accuracy')
)
```

Training and Evaluation

Use the fit() function to train the model for 30 epochs using batches of 90 subjects:

```
?fit.keras.engine.training.Model
```

Train a Keras model

Description:

Trains the model for a fixed number of epochs (iterations on a dataset).

Usage:

```
## S3 method for class 'keras.engine.training.Model'
fit(
 object,
 x = NULL,
  y = NULL,
  batch_size = NULL,
  epochs = 10,
  verbose = getOption("keras.fit_verbose", default = "auto"),
  callbacks = NULL,
  view_metrics = getOption("keras.view_metrics", default = "auto"),
  validation_split = 0,
  validation_data = NULL,
  shuffle = TRUE,
  class_weight = NULL,
  sample_weight = NULL,
  initial_epoch = 0,
  steps_per_epoch = NULL,
  validation_steps = NULL,
)
```

#### Arguments:

object: Model to train.

- x: Vector, matrix, or array of training data (or list if the
  model has multiple inputs). If all inputs in the model are
  named, you can also pass a list mapping input names to data.
  'x' can be 'NULL' (default) if feeding from framework-native
  tensors (e.g. TensorFlow data tensors). You can also pass a
  'tfdataset' or a generator returning a list with (inputs,
  targets) or (inputs, targets, sample\_weights).
- y: Vector, matrix, or array of target (label) data (or list if the model has multiple outputs). If all outputs in the model are named, you can also pass a list mapping output names to data. 'y' can be 'NULL' (default) if feeding from framework-native tensors (e.g. TensorFlow data tensors).
- batch\_size: Integer or 'NULL'. Number of samples per gradient update.

  If unspecified, 'batch\_size' will default to 32.
  - epochs: Number of epochs to train the model. Note that in conjunction with 'initial\_epoch', 'epochs' is to be understood as "final epoch". The model is not trained for a number of iterations given by 'epochs', but merely until the epoch of index 'epochs' is reached.
- verbose: Verbosity mode (0 = silent, 1 = progress bar, 2 = one line
   per epoch). Defaults to 1 in most contexts, 2 if in knitr
   render or running on a distributed training server.
- callbacks: List of callbacks to be called during training.
- view\_metrics: View realtime plot of training metrics (by epoch). The
   default ('"auto"') will display the plot when running within
   RStudio, 'metrics' were specified during model 'compile()',
   'epochs > 1' and 'verbose > 0'. Use the global
   'keras.view\_metrics' option to establish a different default.
- validation\_split: Float between 0 and 1. Fraction of the training data to be used as validation data. The model will set apart this fraction of the training data, will not train on it, and will evaluate the loss and any model metrics on this data at the end of each epoch. The validation data is selected from the last samples in the 'x' and 'y' data provided, before shuffling.
- validation\_data: Data on which to evaluate the loss and any model
   metrics at the end of each epoch. The model will not be
   trained on this data. This could be a list (x\_val, y\_val) or
   a list (x\_val, y\_val, val\_sample\_weights). 'validation\_data'
   will override 'validation\_split'.

- shuffle: shuffle: Logical (whether to shuffle the training data before
   each epoch) or string (for "batch"). "batch" is a special
   option for dealing with the limitations of HDF5 data; it
   shuffles in batch-sized chunks. Has no effect when
   'steps\_per\_epoch' is not 'NULL'.
- class\_weight: Optional named list mapping indices (integers) to a
   weight (float) value, used for weighting the loss function
   (during training only). This can be useful to tell the model
   to "pay more attention" to samples from an under-represented
   class.
- sample\_weight: Optional array of the same length as x, containing
   weights to apply to the model's loss for each sample. In the
   case of temporal data, you can pass a 2D array with shape
   (samples, sequence\_length), to apply a different weight to
   every timestep of every sample. In this case you should make
   sure to specify 'sample\_weight\_mode="temporal"' in
   'compile()'.
- steps\_per\_epoch: Total number of steps (batches of samples) before declaring one epoch finished and starting the next epoch.

  When training with input tensors such as TensorFlow data tensors, the default 'NULL' is equal to the number of samples in your dataset divided by the batch size, or 1 if that cannot be determined.

#### ...: Unused

Epoch 7/30

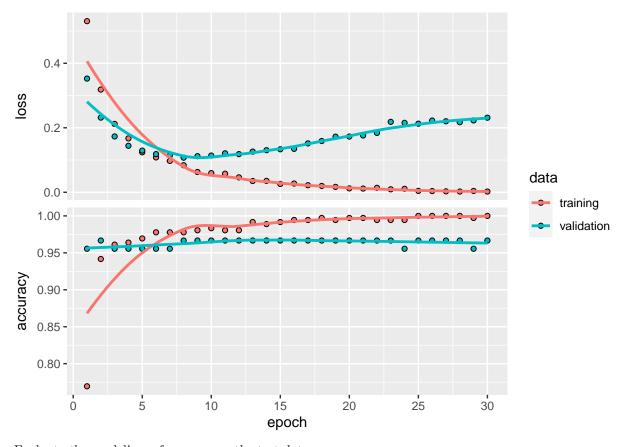
```
history <- model %>% fit(
  x_train, Y_train,
  epochs = 30, batch_size = 90,
  validation_split = 0.2
)
```

```
Epoch 1/30
4/4 - 1s - loss: 0.5306 - accuracy: 0.7694 - val_loss: 0.3525 - val_accuracy: 0.9556 - 715ms/epoch - 17
Epoch 2/30
4/4 - 0s - loss: 0.3185 - accuracy: 0.9417 - val_loss: 0.2315 - val_accuracy: 0.9667 - 71ms/epoch - 18m
Epoch 3/30
4/4 - 0s - loss: 0.2120 - accuracy: 0.9611 - val_loss: 0.1731 - val_accuracy: 0.9556 - 40ms/epoch - 10m
Epoch 4/30
4/4 - 0s - loss: 0.1671 - accuracy: 0.9639 - val_loss: 0.1442 - val_accuracy: 0.9556 - 45ms/epoch - 11m
Epoch 5/30
4/4 - 0s - loss: 0.1239 - accuracy: 0.9694 - val_loss: 0.1293 - val_accuracy: 0.9556 - 60ms/epoch - 15m
Epoch 6/30
4/4 - 0s - loss: 0.1081 - accuracy: 0.9778 - val_loss: 0.1183 - val_accuracy: 0.9556 - 48ms/epoch - 12m
```

```
4/4 - Os - loss: 0.0973 - accuracy: 0.9778 - val_loss: 0.1143 - val_accuracy: 0.9556 - 45ms/epoch - 11m
Epoch 8/30
4/4 - Os - loss: 0.0839 - accuracy: 0.9778 - val loss: 0.1073 - val accuracy: 0.9667 - 48ms/epoch - 12m
Epoch 9/30
4/4 - Os - loss: 0.0629 - accuracy: 0.9806 - val_loss: 0.1120 - val_accuracy: 0.9667 - 40ms/epoch - 10m
Epoch 10/30
4/4 - Os - loss: 0.0593 - accuracy: 0.9833 - val loss: 0.1139 - val accuracy: 0.9667 - 40ms/epoch - 10m
Epoch 11/30
4/4 - Os - loss: 0.0576 - accuracy: 0.9806 - val_loss: 0.1208 - val_accuracy: 0.9667 - 32ms/epoch - 8ms
Epoch 12/30
4/4 - Os - loss: 0.0463 - accuracy: 0.9806 - val_loss: 0.1184 - val_accuracy: 0.9667 - 36ms/epoch - 9ms
Epoch 13/30
4/4 - Os - loss: 0.0350 - accuracy: 0.9917 - val_loss: 0.1261 - val_accuracy: 0.9667 - 40ms/epoch - 10m
Epoch 14/30
4/4 - Os - loss: 0.0353 - accuracy: 0.9889 - val_loss: 0.1305 - val_accuracy: 0.9667 - 34ms/epoch - 8ms
Epoch 15/30
4/4 - Os - loss: 0.0259 - accuracy: 0.9917 - val_loss: 0.1333 - val_accuracy: 0.9667 - 25ms/epoch - 6ms
4/4 - Os - loss: 0.0271 - accuracy: 0.9944 - val_loss: 0.1347 - val_accuracy: 0.9667 - 39ms/epoch - 10m
Epoch 17/30
4/4 - Os - loss: 0.0219 - accuracy: 0.9944 - val_loss: 0.1516 - val_accuracy: 0.9667 - 39ms/epoch - 10m
Epoch 18/30
4/4 - Os - loss: 0.0197 - accuracy: 0.9972 - val_loss: 0.1589 - val_accuracy: 0.9667 - 30ms/epoch - 7ms
Epoch 19/30
4/4 - Os - loss: 0.0168 - accuracy: 0.9944 - val loss: 0.1724 - val accuracy: 0.9667 - 31ms/epoch - 8ms
Epoch 20/30
4/4 - Os - loss: 0.0120 - accuracy: 0.9972 - val_loss: 0.1728 - val_accuracy: 0.9667 - 31ms/epoch - 8ms
Epoch 21/30
4/4 - Os - loss: 0.0115 - accuracy: 0.9972 - val_loss: 0.1761 - val_accuracy: 0.9667 - 64ms/epoch - 16m
Epoch 22/30
4/4 - Os - loss: 0.0138 - accuracy: 0.9944 - val_loss: 0.1841 - val_accuracy: 0.9667 - 59ms/epoch - 15m
Epoch 23/30
4/4 - Os - loss: 0.0092 - accuracy: 0.9944 - val_loss: 0.2183 - val_accuracy: 0.9667 - 43ms/epoch - 11m
Epoch 24/30
4/4 - Os - loss: 0.0107 - accuracy: 0.9944 - val_loss: 0.2153 - val_accuracy: 0.9556 - 41ms/epoch - 10m
Epoch 25/30
4/4 - Os - loss: 0.0044 - accuracy: 1.0000 - val loss: 0.2127 - val accuracy: 0.9667 - 37ms/epoch - 9ms
Epoch 26/30
4/4 - Os - loss: 0.0038 - accuracy: 1.0000 - val_loss: 0.2225 - val_accuracy: 0.9667 - 44ms/epoch - 11m
Epoch 27/30
4/4 - Os - loss: 0.0029 - accuracy: 1.0000 - val loss: 0.2202 - val accuracy: 0.9667 - 35ms/epoch - 9ms
Epoch 28/30
4/4 - Os - loss: 0.0023 - accuracy: 1.0000 - val_loss: 0.2172 - val_accuracy: 0.9667 - 87ms/epoch - 22m
Epoch 29/30
4/4 - Os - loss: 0.0041 - accuracy: 0.9972 - val_loss: 0.2228 - val_accuracy: 0.9556 - 33ms/epoch - 8ms
Epoch 30/30
4/4 - Os - loss: 0.0023 - accuracy: 1.0000 - val_loss: 0.2313 - val_accuracy: 0.9667 - 25ms/epoch - 6ms
```

The history object returned by fit() includes loss and accuracy metrics which we can plot:

#### plot(history)



Evaluate the model's performance on the test data:

```
model %>% evaluate(x_test, Y_test)
## 8/8 - 0s - loss: 0.0582 - accuracy: 0.9785 - 108ms/epoch - 14ms/step
      accuracy
   loss
## 0.05818005 0.97854078
Generate predictions on new data:
model %>% predict(x_test) %>% k_argmax()
## 8/8 - 0s - 69ms/epoch - 9ms/step
## tf.Tensor(
 0 0 0 0 0 1 0 1 0 0 0], shape=(233), dtype=int64)
```

# Example with image data

Let's see an example with the minst image data:

```
mnist <- dataset_mnist()
x_train <- mnist$train$x</pre>
```

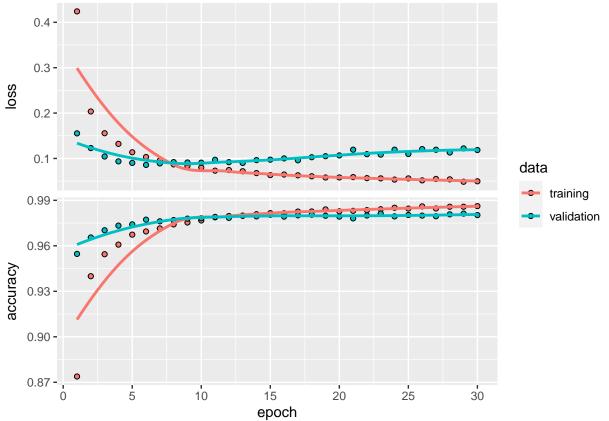
```
y_train <- mnist$train$y</pre>
x_test <- mnist$test$x</pre>
y_test <- mnist$test$y</pre>
dim(x_train)
## [1] 60000
               28
                    28
dim(x_test)
## [1] 10000
               28
                    28
# reshape
x_train <- array_reshape(x_train, c(nrow(x_train), 784))</pre>
x_test <- array_reshape(x_test, c(nrow(x_test), 784))</pre>
Now we normalize the values, which are pixel intensities ranging in (0.255) and create the outcome.
x_train <- x_train / 255</pre>
x_test <- x_test / 255
y_train <- to_categorical(y_train, 10)</pre>
y_test <- to_categorical(y_test, 10)</pre>
Now create the model in Keras.
model <- keras model sequential()</pre>
model %>%
layer_dense(units = 256, activation = 'relu', input_shape = c(784)) %>%
layer_dropout(rate = 0.4) %>%
layer_dense(units = 128, activation = 'relu') %>%
layer dropout(rate = 0.3) %>%
layer_dense(units = 10, activation = 'softmax')
summary(model)
## Model: "sequential_1"
## Layer (type)
                                    Output Shape
                                                                   Param #
## =========
                              _____
## dense_5 (Dense)
                                    (None, 256)
                                                                   200960
## dropout 3 (Dropout)
                                    (None, 256)
## dense_4 (Dense)
                                     (None, 128)
                                                                   32896
## dropout_2 (Dropout)
                                    (None, 128)
## dense 3 (Dense)
                                    (None, 10)
                                                                   1290
## -----
## Total params: 235146 (918.54 KB)
## Trainable params: 235146 (918.54 KB)
## Non-trainable params: 0 (0.00 Byte)
## ______
model %>% compile(
loss = 'categorical_crossentropy',
metrics = c('accuracy')
Now run the model to get a fitted deep learning network.
history <- model %>% fit(
x_train, y_train,
epochs = 30, batch_size = 128,
```

```
validation_split = 0.2
)
```

## Epoch 26/30

```
## Epoch 1/30
## 375/375 - 3s - loss: 0.4241 - accuracy: 0.8738 - val_loss: 0.1553 - val_accuracy: 0.9547 - 3s/epoch
## Epoch 2/30
## 375/375 - 2s - loss: 0.2035 - accuracy: 0.9400 - val_loss: 0.1229 - val_accuracy: 0.9655 - 2s/epoch
## Epoch 3/30
## 375/375 - 3s - loss: 0.1556 - accuracy: 0.9545 - val_loss: 0.1043 - val_accuracy: 0.9703 - 3s/epoch
## Epoch 4/30
## 375/375 - 3s - loss: 0.1321 - accuracy: 0.9608 - val_loss: 0.0936 - val_accuracy: 0.9733 - 3s/epoch
## Epoch 5/30
## 375/375 - 2s - loss: 0.1137 - accuracy: 0.9674 - val_loss: 0.0902 - val_accuracy: 0.9742 - 2s/epoch
## Epoch 6/30
## 375/375 - 2s - loss: 0.1032 - accuracy: 0.9695 - val_loss: 0.0857 - val_accuracy: 0.9772 - 2s/epoch
## Epoch 7/30
## 375/375 - 2s - loss: 0.0955 - accuracy: 0.9715 - val_loss: 0.0890 - val_accuracy: 0.9762 - 2s/epoch
## Epoch 8/30
## 375/375 - 2s - loss: 0.0869 - accuracy: 0.9741 - val_loss: 0.0920 - val_accuracy: 0.9770 - 2s/epoch
## Epoch 9/30
## 375/375 - 2s - loss: 0.0835 - accuracy: 0.9754 - val_loss: 0.0911 - val_accuracy: 0.9779 - 2s/epoch
## Epoch 10/30
## 375/375 - 2s - loss: 0.0801 - accuracy: 0.9767 - val_loss: 0.0907 - val_accuracy: 0.9782 - 2s/epoch
## Epoch 11/30
## 375/375 - 2s - loss: 0.0731 - accuracy: 0.9788 - val_loss: 0.0971 - val_accuracy: 0.9791 - 2s/epoch
## Epoch 12/30
## 375/375 - 2s - loss: 0.0745 - accuracy: 0.9796 - val_loss: 0.0918 - val_accuracy: 0.9784 - 2s/epoch
## Epoch 13/30
## 375/375 - 2s - loss: 0.0718 - accuracy: 0.9799 - val_loss: 0.0900 - val_accuracy: 0.9797 - 2s/epoch
## Epoch 14/30
## 375/375 - 2s - loss: 0.0677 - accuracy: 0.9809 - val_loss: 0.0963 - val_accuracy: 0.9794 - 2s/epoch
## Epoch 15/30
## 375/375 - 2s - loss: 0.0634 - accuracy: 0.9816 - val_loss: 0.0973 - val_accuracy: 0.9804 - 2s/epoch
## Epoch 16/30
## 375/375 - 2s - loss: 0.0646 - accuracy: 0.9814 - val_loss: 0.1001 - val_accuracy: 0.9793 - 2s/epoch
## Epoch 17/30
## 375/375 - 2s - loss: 0.0629 - accuracy: 0.9826 - val_loss: 0.0959 - val_accuracy: 0.9801 - 2s/epoch
## Epoch 18/30
## 375/375 - 2s - loss: 0.0607 - accuracy: 0.9826 - val_loss: 0.1027 - val_accuracy: 0.9805 - 2s/epoch
## Epoch 19/30
## 375/375 - 2s - loss: 0.0580 - accuracy: 0.9840 - val_loss: 0.1050 - val_accuracy: 0.9798 - 2s/epoch
## Epoch 20/30
## 375/375 - 2s - loss: 0.0582 - accuracy: 0.9827 - val_loss: 0.1067 - val_accuracy: 0.9793 - 2s/epoch
## Epoch 21/30
## 375/375 - 2s - loss: 0.0590 - accuracy: 0.9831 - val_loss: 0.1193 - val_accuracy: 0.9781 - 2s/epoch
## Epoch 22/30
## 375/375 - 2s - loss: 0.0566 - accuracy: 0.9835 - val_loss: 0.1095 - val_accuracy: 0.9800 - 2s/epoch
## Epoch 23/30
## 375/375 - 2s - loss: 0.0561 - accuracy: 0.9841 - val_loss: 0.1085 - val_accuracy: 0.9812 - 2s/epoch
## Epoch 24/30
## 375/375 - 2s - loss: 0.0534 - accuracy: 0.9851 - val_loss: 0.1194 - val_accuracy: 0.9794 - 2s/epoch
## Epoch 25/30
## 375/375 - 2s - loss: 0.0561 - accuracy: 0.9846 - val_loss: 0.1098 - val_accuracy: 0.9803 - 2s/epoch
```

```
## 375/375 - 2s - loss: 0.0517 - accuracy: 0.9860 - val_loss: 0.1206 - val_accuracy: 0.9799 - 2s/epoch
## Epoch 27/30
## 375/375 - 2s - loss: 0.0549 - accuracy: 0.9846 - val_loss: 0.1192 - val_accuracy: 0.9795 - 2s/epoch
## Epoch 28/30
## 375/375 - 2s - loss: 0.0540 - accuracy: 0.9858 - val_loss: 0.1131 - val_accuracy: 0.9808 - 2s/epoch
## Epoch 29/30
## 375/375 - 2s - loss: 0.0486 - accuracy: 0.9858 - val_loss: 0.1221 - val_accuracy: 0.9812 - 2s/epoch
## Epoch 30/30
## 375/375 - 2s - loss: 0.0497 - accuracy: 0.9862 - val_loss: 0.1185 - val_accuracy: 0.9803 - 2s/epoch
plot(history)
```



```
model %>% evaluate(x_test, y_test)

## 313/313 - 0s - loss: 0.1102 - accuracy: 0.9816 - 300ms/epoch - 958us/step

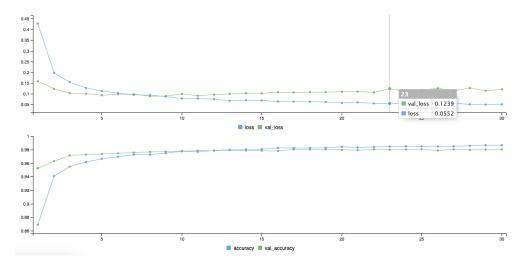
## loss accuracy
## 0.1101681 0.9816000

model %>% predict(x_test) %>% k_argmax()

## 313/313 - 0s - 378ms/epoch - 1ms/step

## tf.Tensor([7 2 1 ... 4 5 6], shape=(10000), dtype=int64)
```

The keras package also plots the progress of the model by showing the loss function evolution by epoch, as well as accuracy, for the training and validation samples.



Forest recommended using PyTouch. There is an R package torch that allows you to use PyTorch-like functionality natively from R. No Python installation is required: torch is built directly on top of libtorch, a C++ library that provides the tensor-computation and automatic-differentiation capabilities essential to building neural networks. See https://torch.mlverse.org/ for more information.

# Using nnet with some

Now were going to do a Neural Net on some simulated data. We're going to use the **nnet** package for the neural network:

```
library(clusterGeneration)

## Loading required package: MASS
library(nnet)
```

Now we'll simulate the data. Part of the difficulty in simulating multivariate normal data is getting a random positive definite matrix. The **clusterGeneration** package helps with this.

```
#define number of variables and observations
set.seed(2)
num.vars<-8
num.obs<-10000
#define correlation matrix for explanatory variables
#define actual parameter values
cov.mat<-genPositiveDefMat(num.vars,covMethod=c("unifcorrmat"))$Sigma</pre>
rand.vars<-mvrnorm(num.obs,rep(0,num.vars),Sigma=cov.mat)</pre>
parms1<-runif(num.vars,-10,10)
y1<-rand.vars <pre>%*% matrix(parms1) + rnorm(num.obs,sd=20)
parms2<-runif(num.vars,-10,10)</pre>
y2<-rand.vars ** matrix(parms2) + rnorm(num.obs,sd=20)
#prep data and create neural network
rand.vars<-data.frame(rand.vars)</pre>
resp<-apply(cbind(y1,y2),2, function(y) (y-min(y))/(max(y)-min(y)))
resp<-data.frame(resp)</pre>
names(resp)<-c('Y1','Y2')</pre>
```

This model has 8 variables with 2 outcomes and a total of 10,000 observations. We'll fit this model with 8

hidden levels with the **nnet** function.

Some info about the **nnet** function:

- it is used for single-hidden layer networks only.
- The call is:

```
nnet(x, y, weights, size, Wts, mask,linout = FALSE, entropy = FALSE, softmax = FALSE, censored = FALSE, skip = FALSE, rang = 0.7, decay = 0, maxit = 100, Hess = FALSE, trace = TRUE, MaxNWts = 1000, abstol = 1.0e-4, reltol = 1.0e-8, ...)
```

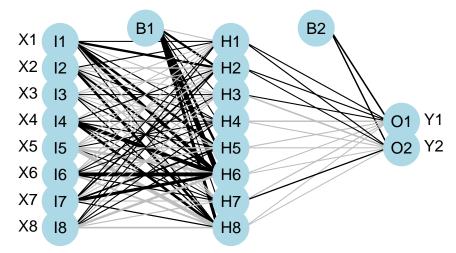
- Some of the options (from the help file):
  - formula-A formula of the form class  $\sim x1 + x2 + \dots$
  - x-matrix or data frame of x values for examples.
  - y-matrix or data frame of target values for examples.
  - weights-(case) weights for each example if missing defaults to 1.
  - size-number of units in the hidden layer. Can be zero if there are skip-layer units.
  - Wts-initial parameter vector. If missing chosen at random.
  - linout-switch for linear output units. Default logistic output units.
  - entropy-switch for entropy (= maximum conditional likelihood) fitting. Default by least-squares.
  - softmax-switch for softmax (log-linear model) and maximum conditional likelihood fitting. linout, entropy, softmax and censored are mutually exclusive. censored A variant on softmax, in which non-zero targets mean possible classes. Thus for softmax a row of (0, 1, 1) means one example each of classes 2 and 3, but for censored it means one example whose class is only known to be 2 or 3.
  - rang-Initial random weights on [-rang, rang]. Value about 0.5 unless the inputs are large, in which case it should be chosen so that rang \*  $\max(|x|)$  is about 1.
  - decay-parameter for weight decay. Default 0.
  - maxit-maximum number of iterations. Default 100.
  - abstol-Stop if the fit criterion falls below abstol, indicating an essentially perfect fit.
  - reltol-Stop if the optimizer is unable to reduce the fit criterion by a factor of at least 1 reltol.

#### mod1<-nnet(rand.vars,resp,size=8,linout=T)</pre>

```
## # weights: 90
## initial value 30066.949169
## iter 10 value 131.361932
## iter
        20 value 51.449404
## iter 30 value 44.110444
## iter 40 value 39.959512
## iter
        50 value 37.678074
## iter 60 value 35.715896
## iter
        70 value 34.182676
        80 value 33.162657
## iter
## iter 90 value 32.665243
## iter 100 value 32.413667
## final value 32.413667
## stopped after 100 iterations
```

To plot the network we're going to import a function from Github

```
library(devtools)
library(reshape)
source_url('https://gist.github.com/fawda123/7471137/raw/cd6e6a0b0bdb4e065c597e52165e5ac887f5fe95/nnet_
plot.nnet(mod1)
```



 $Full\ url\ is\ 'https://gist.github.com/fawda123/7471137/raw/cd6e6a0b0bdb4e065c597e52165e5ac887f5fe95/nn$ et plot update.r'

The shows all of the connections that fit. The black (gray) lines indicate a positive (negative) association. The thickness of the line indicates the strength of the association.

We can also visualize the effect that each variable has on the outcome using a method discribed in Gevrey et al. (2003) [1] (see below for reference). The hard thing about visualizing the effect one variable, say  $X_1$ , has on the outcome, say Y, is that all of the other variables, say  $X_2, X_3, \ldots, X_r$  interact with this relationship. As a result, we visualize the effect between  $X_1$  and Y for fixed values of  $X_2, X_3, \ldots, X_r$ . One way to do this is to:

- Set  $X_2, X_3, \ldots, X_r$  to a fixed quantile, for example  $Q_1$ , then feed all values of  $X_1$  into the network and calculate the expected value of Y for each value.
- Plot the expectation of Y by  $X_1$ .
- Set  $X_2, X_3, \ldots, X_r$  to a different fixed quantile, repeat as necessary.

This method will give you some idea of what is impacting the outcome, but it will not give any information on the interactions between the variables.

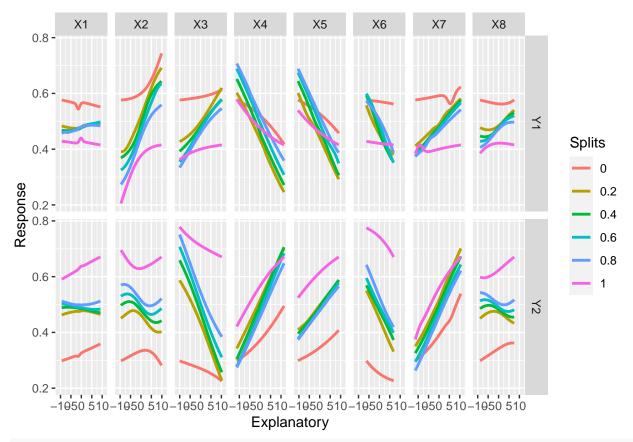
```
library(ggplot2)
source('https://gist.githubusercontent.com/fawda123/6860630/raw/b8bf4a6c88d6b392b1bfa6ef24759ae98f31877
lek.fun(mod1)
## Warning: Using `size` aesthetic for lines was deprecated in ggplot2 3.4.0.
```

## i Please use `linewidth` instead.

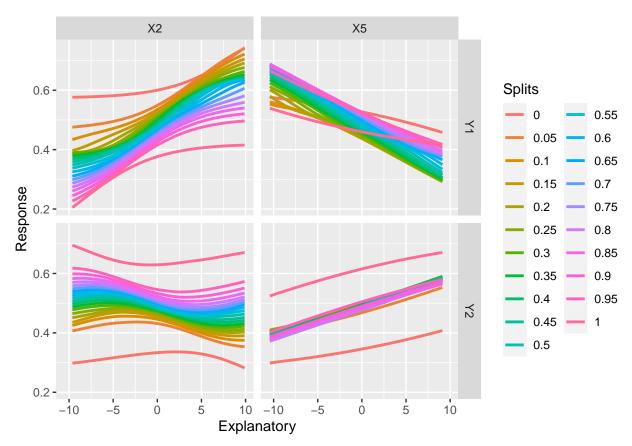
## This warning is displayed once every 8 hours.

## Call `lifecycle::last\_lifecycle\_warnings()` to see where this warning was

## generated.



lek.fun(mod1,var.sens=c('X2','X5'),split.vals=seq(0,1,by=0.05))



 $Full\ url\ is\ 'https://gist.githubusercontent.com/fawda123/6860630/raw/b8bf4a6c88d6b392b1bfa6ef24759ae98f31877c/lek\ fun.r'$ 

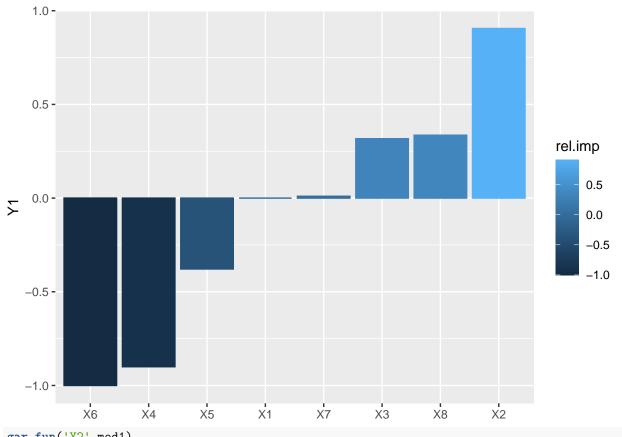
Next we're going to look at some measures of variable importance. The goal here is to measure the relative importance of explanatory variables for their relation to one or more response variables. The method we'll use here is described in Garson (1991) [2]. Here is the basic idea:

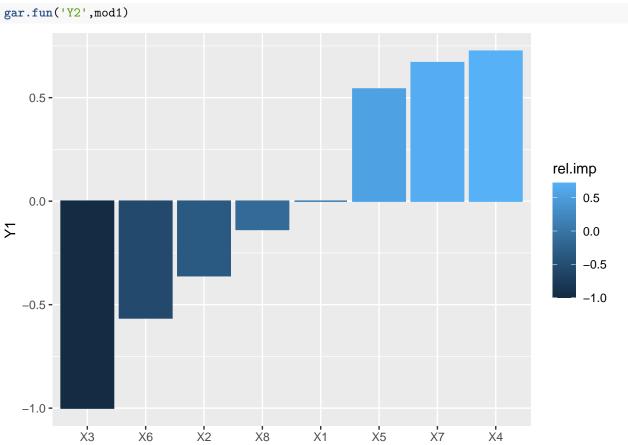
- Identify all weighted connections between a specific input node and a specific response variable.
- Do this for all other explanatory variables until we have a list of all weights for each input variable.
- The connections are "tallied"" for each input node and scaled relative to all other inputs.
- A single value is obtained for each explanatory variable that describes the relationship with response variable in the model (see the appendix in Goh 1995 [3] for a more detailed description).

To do this we will import 'gar.fun' from Github (this is not a package just a function).

gar.fun('Y1',mod1)

```
source_url('https://gist.githubusercontent.com/fawda123/6206737/raw/d6f365c283a8cae23fb20892dc223bc5764
#create a pretty color vector for the bar plot
cols<-colorRampPalette(c('lightgreen','lightblue'))(num.vars)
#use the function on the model created above
par(mar=c(3,4,1,1),family='serif')</pre>
```





- [1] Gevrey M, Dimopoulos I, Lek S. 2003. Review and comparison of methods to study the contribution of variables in artificial neural network models. Ecological Modelling. 160:249-264.
- [2] Garson, G.D. 1991. Interpreting neural network connection weights. Artificial Intelligence Expert. 6(4):46-51.
- [3] Goh, A.T.C. 1995. Back-propagation neural networks for modeling complex systems. Artificial Intelligence in Engineering. 9(3):143-151.