

# Package ‘NeuralSens’

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**Version** 0.2.1

**Title** Sensitivity Analysis of Neural Networks

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**Description** Analysis functions to quantify inputs importance in neural network models. Functions are available for calculating and plotting the inputs importance and obtaining the activation function of each neuron layer and its derivatives. The importance of a given input is defined as the distribution of the derivatives of the output with respect to that input in each training data point.

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**Imports** ggplot2, gridExtra, NeuralNetTools, reshape2, caret,  
fastDummies, stringr, Hmisc, ggforce, scales, ggnewscale

**Suggests** h2o, neural, RSNNS, nnet, neuralnet

**RoxygenNote** 7.1.0

**NeedsCompilation** no

**URL** <https://github.com/JaiPizGon/NeuralSens>

**BugReports** <https://github.com/JaiPizGon/NeuralSens/issues>

**License** GPL (>= 2)

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---

ActFunc                      *Activation function of neuron*

---

**Description**

Evaluate activation function of a neuron

**Usage**

ActFunc(type = "sigmoid", ...)

**Arguments**

type	character name of the activation function
...	extra arguments needed to calculate the functions

**Value**

numeric output of the neuron

**Examples**

```
# Return the sigmoid activation function of a neuron
ActivationFunction <- ActFunc("sigmoid")
# Return the tanh activation function of a neuron
ActivationFunction <- ActFunc("tanh")
# Return the activation function of several layers of neurons
actfuncs <- c("linear", "sigmoid", "linear")
ActivationFunctions <- sapply(actfuncs, ActFunc)
```

---

CombineSens

*Sensitivity analysis plot over time of the data*

---

**Description**

Plot of sensitivity of the neural network output respect to the inputs over the time variable from the data provided

**Usage**

```
CombineSens(object, comb_type = "mean")
```

**Arguments**

object	SensMLP object generated by <a href="#">SensAnalysisMLP</a> with several outputs (classification MLP)
comb_type	Function to combine the matrixes of the raw_sens component of object. It can be "mean", "median" or "sqmean". It can also be a function to combine the rows of the matrixes

**Value**

SensMLP object with the sensitivities combined

**Examples**

```
## Not run:
# mod should be a neural network classification model
sens <- SensAnalysisMLP(mod)
combinesens <- CombineSens(sens, "sqmean")

## End(Not run)
```

---

ComputeHessMeasures *Plot sensitivities of a neural network model*

---

## Description

Function to plot the sensitivities created by [SensAnalysisMLP](#).

## Usage

```
ComputeHessMeasures(sens)
```

## Arguments

sens                    [SensAnalysisMLP](#) object created by [SensAnalysisMLP](#).

## Value

[SensAnalysisMLP](#) object with the sensitivities calculated

## Examples

```
## Load data -----
data("DAILY_DEMAND_TR")
fdata <- DAILY_DEMAND_TR

## Parameters of the NNET -----
hidden_neurons <- 5
iters <- 250
decay <- 0.1

#####
##### REGRESSION NNET #####
#####

## Regression dataframe -----
# Scale the data
fdata.Reg.tr <- fdata[,2:ncol(fdata)]
fdata.Reg.tr[,3] <- fdata.Reg.tr[,3]/10
fdata.Reg.tr[,1] <- fdata.Reg.tr[,1]/1000

# Normalize the data for some models
preProc <- caret::preProcess(fdata.Reg.tr, method = c("center","scale"))
nnetData <- predict(preProc, fdata.Reg.tr)

#' ## TRAIN nnet NNET -----
# Create a formula to train NNET
form <- paste(names(fdata.Reg.tr)[2:ncol(fdata.Reg.tr)], collapse = " + ")
form <- formula(paste(names(fdata.Reg.tr)[1], form, sep = " ~ "))

set.seed(150)
nnetmod <- nnet::nnet(form,
```

```

                                data = nntrData,
                                linear.output = TRUE,
                                size = hidden_neurons,
                                decay = decay,
                                maxit = iters)
# Try SensAnalysisMLP
sens <- NeuralSens::SensAnalysisMLP(nnetmod, trData = nntrData, plot = FALSE)

```

---

ComputeSensMeasures     *Plot sensitivities of a neural network model*

---

## Description

Function to plot the sensitivities created by [SensAnalysisMLP](#).

## Usage

```
ComputeSensMeasures(sens)
```

## Arguments

sens                    SensAnalysisMLP object created by [SensAnalysisMLP](#).

## Value

SensAnalysisMLP object with the sensitivities calculated

## Examples

```

## Load data -----
data("DAILY_DEMAND_TR")
fdata <- DAILY_DEMAND_TR

## Parameters of the NNET -----
hidden_neurons <- 5
iters <- 250
decay <- 0.1

#####
##### REGRESSION NNET #####
#####

## Regression dataframe -----
# Scale the data
fdata.Reg.tr <- fdata[,2:ncol(fdata)]
fdata.Reg.tr[,3] <- fdata.Reg.tr[,3]/10
fdata.Reg.tr[,1] <- fdata.Reg.tr[,1]/1000

# Normalize the data for some models
preProc <- caret::preProcess(fdata.Reg.tr, method = c("center","scale"))
nntrData <- predict(preProc, fdata.Reg.tr)

```

```

#' ## TRAIN nnet NNET -----
# Create a formula to train NNET
form <- paste(names(fdata.Reg.tr)[2:ncol(fdata.Reg.tr)], collapse = " + ")
form <- formula(paste(names(fdata.Reg.tr)[1], form, sep = " ~ "))

set.seed(150)
nnetmod <- nnet::nnet(form,
                      data = nnrData,
                      linear.output = TRUE,
                      size = hidden_neurons,
                      decay = decay,
                      maxit = iters)

# Try SensAnalysisMLP
sens <- NeuralSens::SensAnalysisMLP(nnetmod, trData = nnrData, plot = FALSE)

```

---

DAILY\_DEMAND\_TR      *Data frame with 4 variables*

---

### Description

Training dataset with values of temperature and working day to predict electrical demand

### Format

A data frame with 1980 rows and 4 variables:

**DATE** date of the measure

**DEM** electrical demand

**WD** Working Day: index which express how much work is made that day

**TEMP** weather temperature

### Author(s)

Jose Portela Gonzalez

---

DAILY\_DEMAND\_TV      *Data frame with 3 variables*

---

### Description

Validation dataset with values of temperature and working day to predict electrical demand

**Format**

A data frame with 7 rows and 3 variables:

**DATE** date of the measure

**WD** Working Day: index which express how much work is made that day

**TEMP** weather temperature

**Author(s)**

Jose Portela Gonzalez

---

Der2ActFunc

*Second derivative of activation function of neuron*

---

**Description**

Evaluate derivative of activation function of a neuron

**Usage**

```
Der2ActFunc(type = "sigmoid", ...)
```

**Arguments**

`type` character name of the activation function  
`...` extra arguments needed to calculate the functions

**Value**

numeric output of the neuron

**Examples**

```
# Return derivative of the sigmoid activation function of a neuron
ActivationFunction <- Der2ActFunc("sigmoid")
# Return derivative of the tanh activation function of a neuron
ActivationFunction <- Der2ActFunc("tanh")
# Return derivative of the activation function of several layers of neurons
actfuncs <- c("linear", "sigmoid", "linear")
ActivationFunctions <- sapply(actfuncs, Der2ActFunc)
```

DerActFunc

*Derivative of activation function of neuron*

---

**Description**

Evaluate derivative of activation function of a neuron

**Usage**

```
DerActFunc(type = "sigmoid", ...)
```

**Arguments**

type	character name of the activation function
...	extra arguments needed to calculate the functions

**Value**

numeric output of the neuron

**Examples**

```
# Return derivative of the sigmoid activation function of a neuron
ActivationFunction <- DerActFunc("sigmoid")
# Return derivative of the tanh activation function of a neuron
ActivationFunction <- DerActFunc("tanh")
# Return derivative of the activation function of several layers of neurons
actfuncs <- c("linear", "sigmoid", "linear")
ActivationFunctions <- sapply(actfuncs, DerActFunc)
```

---

diag3Darray*Define function to create a 'diagonal' array or get the diagonal of an array*

---

**Description**

Define function to create a 'diagonal' array or get the diagonal of an array

**Usage**

```
diag3Darray(x = 1, dim = length(x), out = "vector")
```



**Arguments**

x	number or vector defining the value of the diagonal of 3D array
dim	integer defining the length of the diagonal. Default is length(x). If length(x) != 1, dim must be equal to length(x).
out	character specifying which type of diagonal to return ("vector" or "matrix"). See Details

**Details**

The diagonal of a 3D array has been defined as those elements in positions  $c(int,int,int)$ , i.e., the three digits are the same.

If the diagonal should be returned, out specifies if it should return a "vector" with the elements of position  $c(int,int,int)$ , or "matrix" with the elements of position  $c(int,dim,int)$ , i.e.,  $dim = 2 \rightarrow$  elements  $(1,1,1),(2,1,2),(3,1,3),(1,2,1),(2,2,2),(3,2,3),(3,1,3),(3,2,3),(3,3,3)$ .

**Value**

array with all elements zero except the diagonal, with dimensions  $c(dim,dim,dim)$

**Examples**

```
x <- diag3Darray(c(1,4,6), dim = 3)
x
# , , 1
#
# [,1] [,2] [,3]
# [1,] 1 0 0
# [2,] 0 0 0
# [3,] 0 0 0
#
# , , 2
#
# [,1] [,2] [,3]
# [1,] 0 0 0
# [2,] 0 4 0
# [3,] 0 0 0
#
# , , 3
#
# [,1] [,2] [,3]
# [1,] 0 0 0
# [2,] 0 0 0
# [3,] 0 0 6
diag3Darray(x)
# 1, 4, 6
```

---

```
diag3Darray<-          Define function to change the diagonal of array
```

---

**Description**

Define function to change the diagonal of array

**Usage**

```
diag3Darray(x) <- value
```

**Arguments**

x	3D array whose diagonal must be c hanged
value	vector defining the new values of diagonal.

**Details**

The diagonal of a 3D array has been defined as those elements in positions `c(int,int,int)`, i.e., the three digits are the same.

**Value**

array with all elements zero except the diagonal, with dimensions `c(dim,dim,dim)`

**Examples**

```
x <- array(1, dim = c(3,3,3))
diag3Darray(x) <- c(2,2,2)
x
# , , 1
#
# [,1] [,2] [,3]
# [1,]  2  1  1
# [2,]  1  1  1
# [3,]  1  1  1
#
# , , 2
#
# [,1] [,2] [,3]
# [1,]  1  1  1
# [2,]  1  2  1
# [3,]  1  1  1
#
# , , 3
#
# [,1] [,2] [,3]
# [1,]  1  1  1
# [2,]  1  1  1
# [3,]  1  1  2
```

**Description**

Function for evaluating the sensitivities of the inputs variables in a mlp model

**Usage**

```
HessianMLP(  
  MLP.fit,  
  .returnSens = TRUE,  
  plot = TRUE,  
  .rawSens = FALSE,  
  sens_origin_layer = 1,  
  sens_end_layer = "last",  
  sens_origin_input = TRUE,  
  sens_end_input = FALSE,  
  ...  
)  
  
## Default S3 method:  
HessianMLP(  
  MLP.fit,  
  .returnSens = TRUE,  
  plot = TRUE,  
  .rawSens = FALSE,  
  sens_origin_layer = 1,  
  sens_end_layer = "last",  
  sens_origin_input = TRUE,  
  sens_end_input = FALSE,  
  trData,  
  actfunc = NULL,  
  deractfunc = NULL,  
  der2actfunc = NULL,  
  preProc = NULL,  
  terms = NULL,  
  output_name = NULL,  
  ...  
)  
  
## S3 method for class 'train'  
HessianMLP(  
  MLP.fit,  
  .returnSens = TRUE,  
  plot = TRUE,  
  .rawSens = FALSE,
```

```
sens_origin_layer = 1,
sens_end_layer = "last",
sens_origin_input = TRUE,
sens_end_input = FALSE,
...
)

## S3 method for class 'H2OMultinomialModel'
HessianMLP(
  MLP.fit,
  .returnSens = TRUE,
  plot = TRUE,
  .rawSens = FALSE,
  sens_origin_layer = 1,
  sens_end_layer = "last",
  sens_origin_input = TRUE,
  sens_end_input = FALSE,
  ...
)

## S3 method for class 'H2ORegressionModel'
HessianMLP(
  MLP.fit,
  .returnSens = TRUE,
  plot = TRUE,
  .rawSens = FALSE,
  sens_origin_layer = 1,
  sens_end_layer = "last",
  sens_origin_input = TRUE,
  sens_end_input = FALSE,
  ...
)

## S3 method for class 'list'
HessianMLP(
  MLP.fit,
  .returnSens = TRUE,
  plot = TRUE,
  .rawSens = FALSE,
  sens_origin_layer = 1,
  sens_end_layer = "last",
  sens_origin_input = TRUE,
  sens_end_input = FALSE,
  trData,
  actfunc,
  ...
)
```

```
## S3 method for class 'mlp'  
HessianMLP(  
  MLP.fit,  
  .returnSens = TRUE,  
  plot = TRUE,  
  .rawSens = FALSE,  
  sens_origin_layer = 1,  
  sens_end_layer = "last",  
  sens_origin_input = TRUE,  
  sens_end_input = FALSE,  
  trData,  
  preProc = NULL,  
  terms = NULL,  
  ...  
)  
  
## S3 method for class 'nn'  
HessianMLP(  
  MLP.fit,  
  .returnSens = TRUE,  
  plot = TRUE,  
  .rawSens = FALSE,  
  sens_origin_layer = 1,  
  sens_end_layer = "last",  
  sens_origin_input = TRUE,  
  sens_end_input = FALSE,  
  preProc = NULL,  
  terms = NULL,  
  ...  
)  
  
## S3 method for class 'nnet'  
HessianMLP(  
  MLP.fit,  
  .returnSens = TRUE,  
  plot = TRUE,  
  .rawSens = FALSE,  
  sens_origin_layer = 1,  
  sens_end_layer = "last",  
  sens_origin_input = TRUE,  
  sens_end_input = FALSE,  
  trData,  
  preProc = NULL,  
  terms = NULL,  
  ...  
)  
  
## S3 method for class 'nnetar'
```

```

HessianMLP(
  MLP.fit,
  .returnSens = TRUE,
  plot = TRUE,
  .rawSens = FALSE,
  sens_origin_layer = 1,
  sens_end_layer = "last",
  sens_origin_input = TRUE,
  sens_end_input = FALSE,
  ...
)

## S3 method for class 'numeric'
HessianMLP(
  MLP.fit,
  .returnSens = TRUE,
  plot = TRUE,
  .rawSens = FALSE,
  sens_origin_layer = 1,
  sens_end_layer = "last",
  sens_origin_input = TRUE,
  sens_end_input = FALSE,
  trData,
  actfunc = NULL,
  preProc = NULL,
  terms = NULL,
  ...
)

```

### Arguments

MLP.fit	fitted neural network model
.returnSens	DEPRECATED
plot	logical whether or not to plot the analysis. By default is TRUE.
.rawSens	DEPRECATED
sens_origin_layer	numeric specifies the layer of neurons with respect to which the derivative must be calculated. The input layer is specified by 1 (default).
sens_end_layer	numeric specifies the layer of neurons of which the derivative is calculated. It may also be 'last' to specify the output layer (default).
sens_origin_input	logical specifies if the derivative must be calculated with respect to the inputs (TRUE) or output (FALSE) of the sens_origin_layer layer of the model. By default is TRUE.
sens_end_input	logical specifies if the derivative calculated is of the output (FALSE) or from the input (TRUE) of the sens_end_layer layer of the model. By default is FALSE.
...	additional arguments passed to or from other methods

trData	data.frame containing the data to evaluate the sensitivity of the model
actfunc	character vector indicating the activation function of each neurons layer.
deractfunc	character vector indicating the derivative of the activation function of each neurons layer.
der2actfunc	character vector indicating the second derivative of the activation function of each neurons layer.
preProc	preProcess structure applied to the training data. See also <a href="#">preProcess</a>
terms	function applied to the training data to create factors. See also <a href="#">train</a>
output_name	character name of the output variable in order to avoid changing the name of the output variable in trData to '.outcome'

### Details

In case of using an input of class factor and a package which need to enter the input data as matrix, the dummies must be created before training the neural network.

After that, the training data must be given to the function using the trData argument.

### Value

SensMLP object with the sensitivity metrics and sensitivities of the MLP model passed to the function.

### Plots

- Plot 1: colorful plot with the classification of the classes in a 2D map
- Plot 2: b/w plot with probability of the chosen class in a 2D map
- Plot 3: plot with the stats::predictions of the data provided

### References

[https://www.researchgate.net/publication/220577792\\_Use\\_of\\_some\\_sensitivity\\_criteria\\_for\\_choosing\\_networks\\_with\\_good\\_generalization\\_ability](https://www.researchgate.net/publication/220577792_Use_of_some_sensitivity_criteria_for_choosing_networks_with_good_generalization_ability)

### Examples

```
## Load data -----
data("DAILY_DEMAND_TR")
fdata <- DAILY_DEMAND_TR
## Parameters of the NNET -----
hidden_neurons <- 5
iters <- 100
decay <- 0.1

#####
##### REGRESSION NNET #####
#####
## Regression dataframe -----
# Scale the data
```

```

fdata.Reg.tr <- fdata[,2:ncol(fdata)]
fdata.Reg.tr[,3] <- fdata.Reg.tr[,3]/10
fdata.Reg.tr[,1] <- fdata.Reg.tr[,1]/1000

# Normalize the data for some models
preProc <- caret::preProcess(fdata.Reg.tr, method = c("center","scale"))
ntrData <- predict(preProc, fdata.Reg.tr)

#' ## TRAIN nnet NNET -----
# Create a formula to train NNET
form <- paste(names(fdata.Reg.tr)[2:ncol(fdata.Reg.tr)], collapse = " + ")
form <- formula(paste(names(fdata.Reg.tr)[1], form, sep = " ~ "))

set.seed(150)
nnetmod <- nnet::nnet(form,
                      data = ntrData,
                      linear.output = TRUE,
                      size = hidden_neurons,
                      decay = decay,
                      maxit = iters)

# Try HessianMLP
NeuralSens::HessianMLP(nnetmod, trData = ntrData, plot = FALSE)

# Try HessianMLP to calculate sensitivities with respect to output of hidden neurones
NeuralSens::HessianMLP(nnetmod, trData = ntrData,
                       sens_origin_layer = 2,
                       sens_end_layer = "last",
                       sens_origin_input = FALSE,
                       sens_end_input = FALSE)

## Train caret NNET -----
# Create trainControl
ctrl_tune <- caret::trainControl(method = "boot",
                                 savePredictions = FALSE,
                                 summaryFunction = caret::defaultSummary)

set.seed(150) #For replication
caretmod <- caret::train(form = DEM~,
                          data = fdata.Reg.tr,
                          method = "nnet",
                          linout = TRUE,
                          tuneGrid = data.frame(size = 3,
                                                  decay = decay),
                          maxit = iters,
                          preProcess = c("center","scale"),
                          trControl = ctrl_tune,
                          metric = "RMSE")

# Try HessianMLP
NeuralSens::HessianMLP(caretmod)

## Train h2o NNET -----
# Create a cluster with 4 available cores
h2o::h2o.init(ip = "localhost",
              nthreads = 4,

```



```

max_mem_size = "2g")

# Reset the cluster
h2o::h2o.removeAll()
fdata_h2o <- h2o::as.h2o(x = fdata.Reg.tr, destination_frame = "fdata_h2o")

set.seed(150)
h2omod <-h2o:: h2o.deeplearning(x = names(fdata.Reg.tr)[2:ncol(fdata.Reg.tr)],
                               y = names(fdata.Reg.tr)[1],
                               distribution = "AUTO",
                               training_frame = fdata_h2o,
                               standardize = TRUE,
                               activation = "Tanh",
                               hidden = c(hidden_neurons),
                               stopping_rounds = 0,
                               epochs = iters,
                               seed = 150,
                               model_id = "nnet_h2o",
                               adaptive_rate = FALSE,
                               rate_decay = decay,
                               export_weights_and_biases = TRUE)

# Try HessianMLP
NeuralSens::HessianMLP(h2omod)

# Turn off the cluster
h2o::h2o.shutdown(prompt = FALSE)
rm(fdata_h2o)

## Train neural NNET -----
set.seed(150)
neuralmod <- neural::mlptrain(as.matrix(nntrData[,2:ncol(nntrData)]),
                             hidden_neurons,
                             as.matrix(nntrData[1]),
                             it=iters,
                             visual=FALSE)

# Try HessianMLP
trData <- nntrData
NeuralSens::HessianMLP(neuralmod, trData = trData, output_name = "DEM")

## Train RSNNs NNET -----
# Normalize data using RSNNs algorithms
trData <- as.data.frame(RSNNs::normalizeData(fdata.Reg.tr))
names(trData) <- names(fdata.Reg.tr)
set.seed(150)
RSNNsmod <-RSNNs::mlp(x = trData[,2:ncol(trData)],
                     y = trData[,1],
                     size = hidden_neurons,
                     linOut = TRUE,
                     learnFuncParams=c(decay),
                     maxit=iters)

```

```

# Try HessianMLP
NeuralSens::HessianMLP(RSNNSmod, trData = trData, output_name = "DEM")

## TRAIN neuralnet NNET -----
# Create a formula to train NNET
form <- paste(names(fdata.Reg.tr)[2:ncol(fdata.Reg.tr)], collapse = " + ")
form <- formula(paste(names(fdata.Reg.tr)[1], form, sep = " ~ "))

set.seed(150)
nnmod <- neuralnet::neuralnet(form,
                               nntrData,
                               linear.output = TRUE,
                               rep = 1,
                               hidden = hidden_neurons,
                               lifesign = "minimal",
                               threshold = 7,
                               stepmax = iters,
                               learningrate = decay,
                               act.fct = "tanh")

# Try HessianMLP
NeuralSens::HessianMLP(nnmod)

## USE DEFAULT METHOD -----
NeuralSens::HessianMLP(caretmod$finalModel$wts,
                       trData = fdata.Reg.tv,
                       mlpstr = caretmod$finalModel$n,
                       coefnames = caretmod$coefnames,
                       actfun = c("linear", "sigmoid", "linear"),
                       output_name = "DEM")

#####
##### CLASSIFICATION NNET #####
#####
## Regression dataframe -----
# Scale the data
fdata.Reg.cl <- fdata[,2:ncol(fdata)]
fdata.Reg.cl[,2:3] <- fdata.Reg.cl[,2:3]/10
fdata.Reg.cl[,1] <- fdata.Reg.cl[,1]/1000

# Normalize the data for some models
preProc <- caret::preProcess(fdata.Reg.cl, method = c("center", "scale"))
nntrData <- predict(preProc, fdata.Reg.cl)

# Factorize the output
fdata.Reg.cl$DEM <- factor(round(fdata.Reg.cl$DEM, digits = 1))

# Normalize the data for some models
preProc <- caret::preProcess(fdata.Reg.cl, method = c("center", "scale"))
nntrData <- predict(preProc, fdata.Reg.cl)

## Train caret NNET -----

```

```

# Create trainControl
ctrl_tune <- caret::trainControl(method = "boot",
                                savePredictions = FALSE,
                                summaryFunction = caret::defaultSummary)

set.seed(150) #For replication
caretmod <- caret::train(form = DEM~,
                          data = fdata.Reg.c1,
                          method = "nnet",
                          linout = FALSE,
                          tuneGrid = data.frame(size = hidden_neurons,
                                                  decay = decay),

                          maxit = iters,
                          preProcess = c("center", "scale"),
                          trControl = ctrl_tune,
                          metric = "Accuracy")

# Try HessianMLP
NeuralSens::HessianMLP(caretmod)

## Train h2o NNET -----
# Create local cluster with 4 available cores
h2o::h2o.init(ip = "localhost",
             nthreads = 4,
             max_mem_size = "2g")

# Reset the cluster
h2o::h2o.removeAll()
fdata_h2o <- h2o::as.h2o(x = fdata.Reg.c1, destination_frame = "fdata_h2o")

set.seed(150)
h2omod <- h2o::h2o.deeplearning(x = names(fdata.Reg.c1)[2:ncol(fdata.Reg.c1)],
                               y = names(fdata.Reg.c1)[1],
                               distribution = "AUTO",
                               training_frame = fdata_h2o,
                               standardize = TRUE,
                               activation = "Tanh",
                               hidden = c(hidden_neurons),
                               stopping_rounds = 0,
                               epochs = iters,
                               seed = 150,
                               model_id = "nnet_h2o",
                               adaptive_rate = FALSE,
                               rate_decay = decay,
                               export_weights_and_biases = TRUE)

# Try HessianMLP
NeuralSens::HessianMLP(h2omod)

# Apaga el cluster
h2o::h2o.shutdown(prompt = FALSE)
rm(fdata_h2o)

## Train neural NNET -----

```

```

# set.seed(150)
# neuralmod <- mlptrain(as.matrix(nntrData[,2:ncol(nntrData)]),
#                       hidden_neurons,
#                       as.matrix(nntrData[1]),
#                       it=iters,
#                       visual=FALSE)
#
# # Try HessianMLP
# NeuralSens::HessianMLP(neuralmod, trData = trData)

### Train RSNNs NNET -----
# # Normalize data using RSNNs algorithms
# trData <- as.data.frame(RSNNs::normalizeData(fdata.Reg.cl))
# names(trData) <- names(fdata.Reg.tr)
# set.seed(150)
# RSNNsmod <- RSNNs::mlp(x = trData[,2:ncol(trData)],
#                        y = trData[,1],
#                        size = hidden_neurons,
#                        linOut = FALSE,
#                        learnFuncParams=c(decay),
#                        maxit=iters)
#
# # Try HessianMLP
# NeuralSens::HessianMLP(RSNNsmod, trData = trData, output_name = "DEM")

## TRAIN neuralnet NNET -----
# Create a formula to train NNET
# form <- paste(names(fdata.Reg.tr)[2:ncol(fdata.Reg.tr)], collapse = " + ")
# form <- formula(paste(names(fdata.Reg.tr)[1], form, sep = " ~ "))
#
# set.seed(150)
# nnmod <- neuralnet(form,
#                    nntrData,
#                    linear.output = FALSE,
#                    rep = 1,
#                    hidden = hidden_neurons,
#                    lifesign = "minimal",
#                    threshold = 4,
#                    stepmax = iters,
#                    learningrate = decay,
#                    act.fct = "tanh")
#
# # Try HessianMLP
# NeuralSens::HessianMLP(nnmod)

## TRAIN nnet NNET -----
# Create a formula to train NNET
form <- paste(names(fdata.Reg.tr)[2:ncol(fdata.Reg.tr)], collapse = " + ")
form <- formula(paste(names(fdata.Reg.tr)[1], form, sep = " ~ "))

set.seed(150)
nnetmod <- nnet::nnet(form,
                      data = nntrData,

```

```

        linear.output = TRUE,
        size = hidden_neurons,
        decay = decay,
        maxit = iters)
# Try HessianMLP
NeuralSens::HessianMLP(nnetmod, trData = nnetData)

```

---

HessMLP

*Constructor of the HessMLP Class*


---

## Description

Create an object of HessMLP class

## Usage

```

HessMLP(
  sens = list(),
  raw_sens = list(),
  mlp_struct = numeric(),
  trData = data.frame(),
  coefnames = character(),
  output_name = character()
)

```

## Arguments

<code>sens</code>	list of sensitivity measures, one list per output neuron
<code>raw_sens</code>	list of sensitivities, one array per output neuron
<code>mlp_struct</code>	numeric vector describing the structure of the MLP model
<code>trData</code>	data.frame with the data used to calculate the sensitivities
<code>coefnames</code>	character vector with the name of the predictor(s)
<code>output_name</code>	character vector with the name of the output(s)

## Value

HessMLP object

---

HessToSensMLP	<i>Convert a HessMLP to a SensMLP object</i>
---------------	--

---

**Description**

Auxiliary function to turn a HessMLP object to a SensMLP object in order to use the plot-related functions associated with SensMLP

**Usage**

```
HessToSensMLP(x)
```

**Arguments**

x	HessMLP object
---	----------------

**Value**

SensMLP object

---

is.HessMLP	<i>Check if object is of class HessMLP</i>
------------	--

---

**Description**

Check if object is of class HessMLP

**Usage**

```
is.HessMLP(object)
```

**Arguments**

object	HessMLP object
--------	----------------

**Value**

TRUE if object is a HessMLP object

---

is.SensMLP	<i>Check if object is of class SensMLP</i>
------------	--

---

**Description**

Check if object is of class SensMLP

**Usage**

```
is.SensMLP(object)
```

**Arguments**

object	SensMLP object
--------	----------------

**Value**

TRUE if object is a SensMLP object

---

NeuralSens	<i>NeuralSens: Sensitivity Analysis of Neural Networks</i>
------------	--

---

**Description**

Visualization and analysis tools to aid in the interpretation of neural network models.

---

plot.HessMLP	<i>Plot method for the HessMLP Class</i>
--------------	--

---

**Description**

Plot the sensitivities and sensitivity metrics of a HessMLP object.

**Usage**

```
## S3 method for class 'HessMLP'
plot(x, plotType = c("sensitivities", "time", "matrix", "interactions"), ...)
```

**Arguments**

x	HessMLP object created by <a href="#">HessianMLP</a>
plotType	character specifying which type of plot should be created. It can be: <ul style="list-style-type: none"> <li>"sensitivities" (default): use <a href="#">HessianMLP</a> function</li> <li>"time": use <a href="#">SensTimePlot</a> function</li> <li>"features": use <a href="#">SensFeaturePlot</a> function</li> </ul>
...	additional parameters passed to plot function of the NeuralSens package

**Value**

list of graphic objects created by `ggplot`

**Examples**

```

#' ## Load data -----
data("DAILY_DEMAND_TR")
fdata <- DAILY_DEMAND_TR

## Parameters of the NNET -----
hidden_neurons <- 5
iters <- 250
decay <- 0.1

#####
##### REGRESSION NNET #####
#####
## Regression dataframe -----
# Scale the data
fdata.Reg.tr <- fdata[,2:ncol(fdata)]
fdata.Reg.tr[,3] <- fdata.Reg.tr[,3]/10
fdata.Reg.tr[,1] <- fdata.Reg.tr[,1]/1000

# Normalize the data for some models
preProc <- caret::preProcess(fdata.Reg.tr, method = c("center","scale"))
nntrData <- predict(preProc, fdata.Reg.tr)

#' ## TRAIN nnet NNET -----
# Create a formula to train NNET
form <- paste(names(fdata.Reg.tr)[2:ncol(fdata.Reg.tr)], collapse = " + ")
form <- formula(paste(names(fdata.Reg.tr)[1], form, sep = " ~ "))

set.seed(150)
nnetmod <- nnet::nnet(form,
                      data = nntrData,
                      linear.output = TRUE,
                      size = hidden_neurons,
                      decay = decay,
                      maxit = iters)

# Try HessianMLP
sens <- NeuralSens::HessianMLP(nnetmod, trData = nntrData, plot = FALSE)
## Not run:
plot(sens)
plot(sens,"time")

## End(Not run)

```



**Description**

Plot the sensitivities and sensitivity metrics of a SensMLP object.

**Usage**

```
## S3 method for class 'SensMLP'
plot(x, plotType = c("sensitivities", "time", "features"), ...)
```

**Arguments**

x	SensMLP object created by <a href="#">SensAnalysisMLP</a>
plotType	character specifying which type of plot should be created. It can be: <ul style="list-style-type: none"> <li>• "sensitivities" (default): use <a href="#">SensAnalysisMLP</a> function</li> <li>• "time": use <a href="#">SensTimePlot</a> function</li> <li>• "features": use <a href="#">SensFeaturePlot</a> function</li> </ul>
...	additional parameters passed to plot function of the NeuralSens package

**Value**

list of graphic objects created by [ggplot](#)

**Examples**

```
' ## Load data -----
data("DAILY_DEMAND_TR")
fdata <- DAILY_DEMAND_TR

## Parameters of the NNET -----
hidden_neurons <- 5
iters <- 250
decay <- 0.1

#####
##### REGRESSION NNET #####
#####

## Regression dataframe -----
# Scale the data
fdata.Reg.tr <- fdata[,2:ncol(fdata)]
fdata.Reg.tr[,3] <- fdata.Reg.tr[,3]/10
fdata.Reg.tr[,1] <- fdata.Reg.tr[,1]/1000

# Normalize the data for some models
preProc <- caret::preProcess(fdata.Reg.tr, method = c("center","scale"))
nntrData <- predict(preProc, fdata.Reg.tr)

' ## TRAIN nnet NNET -----
# Create a formula to train NNET
form <- paste(names(fdata.Reg.tr)[2:ncol(fdata.Reg.tr)], collapse = " + ")
form <- formula(paste(names(fdata.Reg.tr)[1], form, sep = " ~ "))
```

```

set.seed(150)
nnetmod <- nnet::nnet(form,
                      data = nntrData,
                      linear.output = TRUE,
                      size = hidden_neurons,
                      decay = decay,
                      maxit = iters)

# Try SensAnalysisMLP
sens <- NeuralSens::SensAnalysisMLP(nnetmod, trData = nntrData, plot = FALSE)
## Not run:
plot(sens)
plot(sens,"time")
plot(sens,"features")

## End(Not run)

```

---

PlotSensMLP

*Neural network structure sensitivity plot*


---

## Description

Plot a neural interpretation diagram colored by sensitivities of the model

## Usage

```

PlotSensMLP(
  MLP.fit,
  metric = "mean",
  sens_neg_col = "red",
  sens_pos_col = "blue",
  ...
)

```

## Arguments

MLP.fit	fitted neural network model
metric	metric to plot in the NID. It can be "mean" (default), "median" or "sqmean". It can be any metric to combine the raw sensitivities
sens_neg_col	character string indicating color of negative sensitivity measure, default 'red'. The same is passed to argument neg_col of <a href="#">plotnet</a>
sens_pos_col	character string indicating color of positive sensitivity measure, default 'blue'. The same is passed to argument pos_col of <a href="#">plotnet</a>
...	additional arguments passed to <a href="#">plotnet</a> and/or <a href="#">SensAnalysisMLP</a>

## Value

A graphics object

**Examples**

```

## Load data -----
data("DAILY_DEMAND_TR")
fdata <- DAILY_DEMAND_TR
## Parameters of the NNET -----
hidden_neurons <- 5
iters <- 100
decay <- 0.1

#####
##### REGRESSION NNET #####
#####
## Regression dataframe -----
# Scale the data
fdata.Reg.tr <- fdata[,2:ncol(fdata)]
fdata.Reg.tr[,3] <- fdata.Reg.tr[,3]/10
fdata.Reg.tr[,1] <- fdata.Reg.tr[,1]/1000

# Normalize the data for some models
preProc <- caret::preProcess(fdata.Reg.tr, method = c("center","scale"))
nnetData <- predict(preProc, fdata.Reg.tr)

#' ## TRAIN nnet NNET -----
# Create a formula to train NNET
form <- paste(names(fdata.Reg.tr)[2:ncol(fdata.Reg.tr)], collapse = " + ")
form <- formula(paste(names(fdata.Reg.tr)[1], form, sep = " ~ "))

set.seed(150)
nnetmod <- nnet::nnet(form,
                      data = nnetData,
                      linear.output = TRUE,
                      size = hidden_neurons,
                      decay = decay,
                      maxit = iters)

# Try SensAnalysisMLP
NeuralSens::PlotSensMLP(nnetmod, trData = nnetData)

```

---

print.HessMLP

*Print method for the HessMLP Class*


---

**Description**

Print the sensitivities of a HessMLP object.

**Usage**

```

## S3 method for class 'HessMLP'
print(x, n = 5, ...)

```

**Arguments**

x HessMLP object created by [HessianMLP](#)  
 n integer specifying number of sensitivities to print per each output  
 ... additional parameters

**Examples**

```
## Load data -----
data("DAILY_DEMAND_TR")
fdata <- DAILY_DEMAND_TR

## Parameters of the NNET -----
hidden_neurons <- 5
iters <- 250
decay <- 0.1

#####
##### REGRESSION NNET #####
#####

## Regression dataframe -----
# Scale the data
fdata.Reg.tr <- fdata[,2:ncol(fdata)]
fdata.Reg.tr[,3] <- fdata.Reg.tr[,3]/10
fdata.Reg.tr[,1] <- fdata.Reg.tr[,1]/1000

# Normalize the data for some models
preProc <- caret::preProcess(fdata.Reg.tr, method = c("center","scale"))
nntrData <- predict(preProc, fdata.Reg.tr)

#' ## TRAIN nnet NNET -----
# Create a formula to train NNET
form <- paste(names(fdata.Reg.tr)[2:ncol(fdata.Reg.tr)], collapse = " + ")
form <- formula(paste(names(fdata.Reg.tr)[1], form, sep = " ~ "))

set.seed(150)
nnetmod <- nnet::nnet(form,
                      data = nntrData,
                      linear.output = TRUE,
                      size = hidden_neurons,
                      decay = decay,
                      maxit = iters)

# Try HessianMLP
sens <- NeuralSens::HessianMLP(nnetmod, trData = nntrData, plot = FALSE)
sens
```



```
sens <- NeuralSens::SensAnalysisMLP(nnetmod, trData = nnetData, plot = FALSE)
sens
```

---

```
print.summary.HessMLP Print method of the summary HessMLP Class
```

---

## Description

Print the sensitivity metrics of a HessMLP object. This metrics are the mean sensitivity, the standard deviation of sensitivities and the mean of sensitivities square

## Usage

```
## S3 method for class 'summary.HessMLP'
print(x, ...)
```

## Arguments

```
x          summary.HessMLP object created by summary method of HessMLP object
...        additional parameters
```

## Examples

```
## Load data -----
data("DAILY_DEMAND_TR")
fdata <- DAILY_DEMAND_TR

## Parameters of the NNET -----
hidden_neurons <- 5
iters <- 250
decay <- 0.1

#####
##### REGRESSION NNET #####
#####
## Regression dataframe -----
# Scale the data
fdata.Reg.tr <- fdata[,2:ncol(fdata)]
fdata.Reg.tr[,3] <- fdata.Reg.tr[,3]/10
fdata.Reg.tr[,1] <- fdata.Reg.tr[,1]/1000

# Normalize the data for some models
preProc <- caret::preProcess(fdata.Reg.tr, method = c("center","scale"))
nnetData <- predict(preProc, fdata.Reg.tr)

#' ## TRAIN nnet NNET -----
# Create a formula to train NNET
form <- paste(names(fdata.Reg.tr)[2:ncol(fdata.Reg.tr)], collapse = " + ")
form <- formula(paste(names(fdata.Reg.tr)[1], form, sep = " ~ "))
```

```

set.seed(150)
nnetmod <- nnet::nnet(form,
                      data = nntrData,
                      linear.output = TRUE,
                      size = hidden_neurons,
                      decay = decay,
                      maxit = iters)

# Try HessianMLP
sens <- NeuralSens::HessianMLP(nnetmod, trData = nntrData, plot = FALSE)
print(summary(sens))

```

---

print.summary.SensMLP *Print method of the summary SensMLP Class*

---

## Description

Print the sensitivity metrics of a SensMLP object. This metrics are the mean sensitivity, the standard deviation of sensitivities and the mean of sensitivities square

## Usage

```

## S3 method for class 'summary.SensMLP'
print(x, ...)

```

## Arguments

x	summary.SensMLP object created by summary method of SensMLP object
...	additional parameters

## Examples

```

## Load data -----
data("DAILY_DEMAND_TR")
fdata <- DAILY_DEMAND_TR

## Parameters of the NNET -----
hidden_neurons <- 5
iters <- 250
decay <- 0.1

#####
##### REGRESSION NNET #####
#####

## Regression dataframe -----
# Scale the data
fdata.Reg.tr <- fdata[,2:ncol(fdata)]
fdata.Reg.tr[,3] <- fdata.Reg.tr[,3]/10
fdata.Reg.tr[,1] <- fdata.Reg.tr[,1]/1000

```

```

# Normalize the data for some models
preProc <- caret::preProcess(fdata.Reg.tr, method = c("center","scale"))
nntrData <- predict(preProc, fdata.Reg.tr)

#' ## TRAIN nnet NNET -----
# Create a formula to train NNET
form <- paste(names(fdata.Reg.tr)[2:ncol(fdata.Reg.tr)], collapse = " + ")
form <- formula(paste(names(fdata.Reg.tr)[1], form, sep = " ~ "))

set.seed(150)
nnetmod <- nnet::nnet(form,
                      data = nntrData,
                      linear.output = TRUE,
                      size = hidden_neurons,
                      decay = decay,
                      maxit = iters)

# Try SensAnalysisMLP
sens <- NeuralSens::SensAnalysisMLP(nnetmod, trData = nntrData, plot = FALSE)
print(summary(sens))

```

---

SensAnalysisMLP

*Sensitivity of MLP models*


---

## Description

Function for evaluating the sensitivities of the inputs variables in a mlp model

## Usage

```

SensAnalysisMLP(
  MLP.fit,
  .returnSens = TRUE,
  plot = TRUE,
  .rawSens = FALSE,
  sens_origin_layer = 1,
  sens_end_layer = "last",
  sens_origin_input = TRUE,
  sens_end_input = FALSE,
  ...
)

```

## Default S3 method:

```

SensAnalysisMLP(
  MLP.fit,
  .returnSens = TRUE,
  plot = TRUE,
  .rawSens = FALSE,
  sens_origin_layer = 1,

```



```
    sens_end_layer = "last",
    sens_origin_input = TRUE,
    sens_end_input = FALSE,
    trData,
    actfunc = NULL,
    deractfunc = NULL,
    preProc = NULL,
    terms = NULL,
    output_name = NULL,
    ...
)

## S3 method for class 'train'
SensAnalysisMLP(
  MLP.fit,
  .returnSens = TRUE,
  plot = TRUE,
  .rawSens = FALSE,
  sens_origin_layer = 1,
  sens_end_layer = "last",
  sens_origin_input = TRUE,
  sens_end_input = FALSE,
  ...
)

## S3 method for class 'H2OMultinomialModel'
SensAnalysisMLP(
  MLP.fit,
  .returnSens = TRUE,
  plot = TRUE,
  .rawSens = FALSE,
  sens_origin_layer = 1,
  sens_end_layer = "last",
  sens_origin_input = TRUE,
  sens_end_input = FALSE,
  ...
)

## S3 method for class 'H2ORegressionModel'
SensAnalysisMLP(
  MLP.fit,
  .returnSens = TRUE,
  plot = TRUE,
  .rawSens = FALSE,
  sens_origin_layer = 1,
  sens_end_layer = "last",
  sens_origin_input = TRUE,
  sens_end_input = FALSE,
```

```
    ...
  )

## S3 method for class 'list'
SensAnalysisMLP(
  MLP.fit,
  .returnSens = TRUE,
  plot = TRUE,
  .rawSens = FALSE,
  sens_origin_layer = 1,
  sens_end_layer = "last",
  sens_origin_input = TRUE,
  sens_end_input = FALSE,
  trData,
  actfunc,
  ...
)

## S3 method for class 'mlp'
SensAnalysisMLP(
  MLP.fit,
  .returnSens = TRUE,
  plot = TRUE,
  .rawSens = FALSE,
  sens_origin_layer = 1,
  sens_end_layer = "last",
  sens_origin_input = TRUE,
  sens_end_input = FALSE,
  trData,
  preProc = NULL,
  terms = NULL,
  ...
)

## S3 method for class 'nn'
SensAnalysisMLP(
  MLP.fit,
  .returnSens = TRUE,
  plot = TRUE,
  .rawSens = FALSE,
  sens_origin_layer = 1,
  sens_end_layer = "last",
  sens_origin_input = TRUE,
  sens_end_input = FALSE,
  preProc = NULL,
  terms = NULL,
  ...
)
```

```
## S3 method for class 'nnet'  
SensAnalysisMLP(  
  MLP.fit,  
  .returnSens = TRUE,  
  plot = TRUE,  
  .rawSens = FALSE,  
  sens_origin_layer = 1,  
  sens_end_layer = "last",  
  sens_origin_input = TRUE,  
  sens_end_input = FALSE,  
  trData,  
  preProc = NULL,  
  terms = NULL,  
  ...  
)  
  
## S3 method for class 'nnetar'  
SensAnalysisMLP(  
  MLP.fit,  
  .returnSens = TRUE,  
  plot = TRUE,  
  .rawSens = FALSE,  
  sens_origin_layer = 1,  
  sens_end_layer = "last",  
  sens_origin_input = TRUE,  
  sens_end_input = FALSE,  
  ...  
)  
  
## S3 method for class 'numeric'  
SensAnalysisMLP(  
  MLP.fit,  
  .returnSens = TRUE,  
  plot = TRUE,  
  .rawSens = FALSE,  
  sens_origin_layer = 1,  
  sens_end_layer = "last",  
  sens_origin_input = TRUE,  
  sens_end_input = FALSE,  
  trData,  
  actfunc = NULL,  
  preProc = NULL,  
  terms = NULL,  
  ...  
)
```

**Arguments**

MLP.fit	fitted neural network model
.returnSens	DEPRECATED
plot	logical whether or not to plot the analysis. By default is TRUE.
.rawSens	DEPRECATED
sens_origin_layer	numeric specifies the layer of neurons with respect to which the derivative must be calculated. The input layer is specified by 1 (default).
sens_end_layer	numeric specifies the layer of neurons of which the derivative is calculated. It may also be 'last' to specify the output layer (default).
sens_origin_input	logical specifies if the derivative must be calculated with respect to the inputs (TRUE) or output (FALSE) of the sens_origin_layer layer of the model. By default is TRUE.
sens_end_input	logical specifies if the derivative calculated is of the output (FALSE) or from the input (TRUE) of the sens_end_layer layer of the model. By default is FALSE.
...	additional arguments passed to or from other methods
trData	data.frame containing the data to evaluate the sensitivity of the model
actfunc	character vector indicating the activation function of each neurons layer.
deractfunc	character vector indicating the derivative of the activation function of each neurons layer.
preProc	preProcess structure applied to the training data. See also <a href="#">preProcess</a>
terms	function applied to the training data to create factors. See also <a href="#">train</a>
output_name	character name of the output variable in order to avoid changing the name of the output variable in trData to '.outcome'

**Details**

In case of using an input of class factor and a package which need to enter the input data as matrix, the dummies must be created before training the neural network.

After that, the training data must be given to the function using the trData argument.

**Value**

SensMLP object with the sensitivity metrics and sensitivities of the MLP model passed to the function.

**Plots**

- Plot 1: colorful plot with the classification of the classes in a 2D map
- Plot 2: b/w plot with probability of the chosen class in a 2D map
- Plot 3: plot with the stats::predictions of the data provided



```

summaryFunction = caret::defaultSummary)
set.seed(150) #For replication
caretmod <- caret::train(form = DEM~,
  data = fdata.Reg.tr,
  method = "nnet",
  linout = TRUE,
  tuneGrid = data.frame(size = 3,
                        decay = decay),
  maxit = iters,
  preProcess = c("center", "scale"),
  trControl = ctrl_tune,
  metric = "RMSE")

# Try SensAnalysisMLP
NeuralSens::SensAnalysisMLP(caretmod)

## Train h2o NNET -----
# Create a cluster with 4 available cores
h2o::h2o.init(ip = "localhost",
  nthreads = 4,
  max_mem_size = "2g")

# Reset the cluster
h2o::h2o.removeAll()
fdata_h2o <- h2o::as.h2o(x = fdata.Reg.tr, destination_frame = "fdata_h2o")

set.seed(150)
h2omod <- h2o:: h2o.deeplearning(x = names(fdata.Reg.tr)[2:ncol(fdata.Reg.tr)],
  y = names(fdata.Reg.tr)[1],
  distribution = "AUTO",
  training_frame = fdata_h2o,
  standardize = TRUE,
  activation = "Tanh",
  hidden = c(hidden_neurons),
  stopping_rounds = 0,
  epochs = iters,
  seed = 150,
  model_id = "nnet_h2o",
  adaptive_rate = FALSE,
  rate_decay = decay,
  export_weights_and_biases = TRUE)

# Try SensAnalysisMLP
NeuralSens::SensAnalysisMLP(h2omod)

# Turn off the cluster
h2o::h2o.shutdown(prompt = FALSE)
rm(fdata_h2o)

## Train neural NNET -----
set.seed(150)
neuralmod <- neural::mlptrain(as.matrix(nntrData[,2:ncol(nntrData)]),
  hidden_neurons,

```



```
##### CLASSIFICATION NNET #####
#####
## Regression dataframe -----
# Scale the data
fdata.Reg.cl <- fdata[,2:ncol(fdata)]
fdata.Reg.cl[,2:3] <- fdata.Reg.cl[,2:3]/10
fdata.Reg.cl[,1] <- fdata.Reg.cl[,1]/1000

# Normalize the data for some models
preProc <- caret::preProcess(fdata.Reg.cl, method = c("center","scale"))
nntrData <- predict(preProc, fdata.Reg.cl)

# Factorize the output
fdata.Reg.cl$DEM <- factor(round(fdata.Reg.cl$DEM, digits = 1))

# Normalize the data for some models
preProc <- caret::preProcess(fdata.Reg.cl, method = c("center","scale"))
nntrData <- predict(preProc, fdata.Reg.cl)

## Train caret NNET -----
# Create trainControl
ctrl_tune <- caret::trainControl(method = "boot",
                                savePredictions = FALSE,
                                summaryFunction = caret::defaultSummary)

set.seed(150) #For replication
caretmod <- caret::train(form = DEM~.,
                        data = fdata.Reg.cl,
                        method = "nnet",
                        linout = FALSE,
                        tuneGrid = data.frame(size = hidden_neurons,
                                             decay = decay),
                        maxit = iters,
                        preProcess = c("center","scale"),
                        trControl = ctrl_tune,
                        metric = "Accuracy")

# Try SensAnalysisMLP
NeuralSens::SensAnalysisMLP(caretmod)

## Train h2o NNET -----
# Create local cluster with 4 available cores
h2o::h2o.init(ip = "localhost",
             nthreads = 4,
             max_mem_size = "2g")

# Reset the cluster
h2o::h2o.removeAll()
fdata_h2o <- h2o::as.h2o(x = fdata.Reg.cl, destination_frame = "fdata_h2o")

set.seed(150)
h2omod <- h2o::h2o.deeplearning(x = names(fdata.Reg.cl)[2:ncol(fdata.Reg.cl)],
                              y = names(fdata.Reg.cl)[1],
                              distribution = "AUTO",
```



```

        training_frame = fdata_h2o,
        standardize = TRUE,
        activation = "Tanh",
        hidden = c(hidden_neurons),
        stopping_rounds = 0,
        epochs = iters,
        seed = 150,
        model_id = "nnet_h2o",
        adaptive_rate = FALSE,
        rate_decay = decay,
        export_weights_and_biases = TRUE)

# Try SensAnalysisMLP
NeuralSens::SensAnalysisMLP(h2omod)

# Apaga el cluster
h2o::h2o.shutdown(prompt = FALSE)
rm(fdata_h2o)

## Train neural NNET -----
# set.seed(150)
# neuralmod <- mlptrain(as.matrix(nntrData[,2:ncol(nntrData)]),
#                       hidden_neurons,
#                       as.matrix(nntrData[1]),
#                       it=iters,
#                       visual=FALSE)
#
# # Try SensAnalysisMLP
# NeuralSens::SensAnalysisMLP(neuralmod, trData = trData)

# ## Train RSNNs NNET -----
# # Normalize data using RSNNs algorithms
# trData <- as.data.frame(RSNNs::normalizeData(fdata.Reg.cl))
# names(trData) <- names(fdata.Reg.tr)
# set.seed(150)
# RSNNsmod <- RSNNs::mlp(x = trData[,2:ncol(trData)],
#                        y = trData[,1],
#                        size = hidden_neurons,
#                        linOut = FALSE,
#                        learnFuncParams=c(decay),
#                        maxit=iters)
#
# # Try SensAnalysisMLP
# NeuralSens::SensAnalysisMLP(RSNNsmod, trData = trData, output_name = "DEM")

## TRAIN neuralnet NNET -----
# Create a formula to train NNET
# form <- paste(names(fdata.Reg.tr)[2:ncol(fdata.Reg.tr)], collapse = " + ")
# form <- formula(paste(names(fdata.Reg.tr)[1], form, sep = " ~ "))
#
# set.seed(150)
# nnmod <- neuralnet(form,
#                    nntrData,

```

```

#           linear.output = FALSE,
#           rep = 1,
#           hidden = hidden_neurons,
#           lifesign = "minimal",
#           threshold = 4,
#           stepmax = iters,
#           learningrate = decay,
#           act.fct = "tanh")
#
# # Try SensAnalysisMLP
# NeuralSens::SensAnalysisMLP(nnmod)

## TRAIN nnet NNET -----
# Create a formula to train NNET
form <- paste(names(fdata.Reg.tr)[2:ncol(fdata.Reg.tr)], collapse = " + ")
form <- formula(paste(names(fdata.Reg.tr)[1], form, sep = " ~ "))

set.seed(150)
nnetmod <- nnet::nnet(form,
                      data = nntrData,
                      linear.output = TRUE,
                      size = hidden_neurons,
                      decay = decay,
                      maxit = iters)
# Try SensAnalysisMLP
NeuralSens::SensAnalysisMLP(nnetmod, trData = nntrData)

```

---

SensFeaturePlot

*Feature sensitivity plot*


---

## Description

Show the distribution of the sensitivities of the output in `geom_sina()` plot which color depends on the input values

## Usage

```
SensFeaturePlot(object, fdata = NULL, ...)
```

## Arguments

object	fitted neural network model or array containing the raw sensitivities from the function <a href="#">SensAnalysisMLP</a>
fdata	data.frame containing the data to evaluate the sensitivity of the model. Not needed if the raw sensitivities has been passed as object
...	further arguments that should be passed to <a href="#">SensAnalysisMLP</a> function

**Value**

list of Feature sensitivity plot as described in <https://www.r-bloggers.com/a-gentle-introduction-to-shap-values>

**Examples**

```
## Load data -----
data("DAILY_DEMAND_TR")
fdata <- DAILY_DEMAND_TR

## Parameters of the NNET -----
hidden_neurons <- 5
iters <- 250
decay <- 0.1

#####
##### REGRESSION NNET #####
#####
## Regression dataframe -----
# Scale the data
fdata.Reg.tr <- fdata[,2:ncol(fdata)]
fdata.Reg.tr[,3] <- fdata.Reg.tr[,3]/10
fdata.Reg.tr[,1] <- fdata.Reg.tr[,1]/1000

# Normalize the data for some models
preProc <- caret::preProcess(fdata.Reg.tr, method = c("center","scale"))
nnetData <- predict(preProc, fdata.Reg.tr)

#' ## TRAIN nnet NNET -----
# Create a formula to train NNET
form <- paste(names(fdata.Reg.tr)[2:ncol(fdata.Reg.tr)], collapse = " + ")
form <- formula(paste(names(fdata.Reg.tr)[1], form, sep = " ~ "))

set.seed(150)
nnetmod <- nnet::nnet(form,
                      data = nnetData,
                      linear.output = TRUE,
                      size = hidden_neurons,
                      decay = decay,
                      maxit = iters)

# Try SensAnalysisMLP
sens <- NeuralSens::SensAnalysisMLP(nnetmod, trData = nnetData, plot = FALSE)
NeuralSens::SensFeaturePlot(sens)
```

---

SensitivityPlots

*Plot sensitivities of a neural network model*


---

**Description**

Function to plot the sensitivities created by [SensAnalysisMLP](#).

**Usage**

```
SensitivityPlots(
  sens = NULL,
  der = TRUE,
  zoom = TRUE,
  quit.legend = FALSE,
  output = 1
)
```

**Arguments**

sens	SensAnalysisMLP object created by <a href="#">SensAnalysisMLP</a> or HessMLP object created by <a href="#">HessianMLP</a> .
der	logical indicating if density plots should be created. By default is TRUE
zoom	logical indicating if the distributions should be zoomed when there is any of them which is too tiny to be appreciated in the third plot. <a href="#">facet_zoom</a> function from ggforce package is required.
quit.legend	logical indicating if legend of the third plot should be removed. By default is FALSE
output	numeric or character specifying the output neuron or output name to be plotted. By default is the first output (output = 1).

**Value**

List with the following plot for each output:

- Plot 1: colorful plot with the classification of the classes in a 2D map
- Plot 2: b/w plot with probability of the chosen class in a 2D map
- Plot 3: plot with the stats::predictions of the data provided if param der is FALSE

**Examples**

```
## Load data -----
data("DAILY_DEMAND_TR")
fdata <- DAILY_DEMAND_TR

## Parameters of the NNET -----
hidden_neurons <- 5
iters <- 250
decay <- 0.1

#####
##### REGRESSION NNET #####
#####

## Regression dataframe -----
# Scale the data
fdata.Reg.tr <- fdata[,2:ncol(fdata)]
fdata.Reg.tr[,3] <- fdata.Reg.tr[,3]/10
fdata.Reg.tr[,1] <- fdata.Reg.tr[,1]/1000
```

```

# Normalize the data for some models
preProc <- caret::preProcess(fdata.Reg.tr, method = c("center","scale"))
nntrData <- predict(preProc, fdata.Reg.tr)

#' ## TRAIN nnet NNET -----
# Create a formula to train NNET
form <- paste(names(fdata.Reg.tr)[2:ncol(fdata.Reg.tr)], collapse = " + ")
form <- formula(paste(names(fdata.Reg.tr)[1], form, sep = " ~ "))

set.seed(150)
nnetmod <- nnet::nnet(form,
                      data = nntrData,
                      linear.output = TRUE,
                      size = hidden_neurons,
                      decay = decay,
                      maxit = iters)

# Try SensAnalysisMLP
sens <- NeuralSens::SensAnalysisMLP(nnetmod, trData = nntrData, plot = FALSE)
NeuralSens::SensitivityPlots(sens)

```

---

SensMatPlot

*Plot sensitivities of a neural network model*


---

## Description

Function to plot the sensitivities created by [HessianMLP](#).

## Usage

```

SensMatPlot(
  hess,
  sens = NULL,
  output = 1,
  metric = c("mean", "std", "meanSensSQ"),
  senstype = c("matrix", "interactions"),
  ...
)

```

## Arguments

<code>hess</code>	HessMLP object created by <a href="#">HessianMLP</a> .
<code>sens</code>	SensMLP object created by <a href="#">SensAnalysisMLP</a> .
<code>output</code>	numeric or character specifying the output neuron or output name to be plotted. By default is the first output ( <code>output = 1</code> ).
<code>metric</code>	character specifying the metric to be plotted. It can be "mean", "std" or "meanSensSQ".



```
H <- NeuralSens::HessianMLP(nnetmod, trData = nntrData, plot = FALSE)
NeuralSens::SensMatPlot(H)
S <- NeuralSens::SensAnalysisMLP(nnetmod, trData = nntrData, plot = FALSE)
NeuralSens::SensMatPlot(H, S, senstype = "interactions")
```

---

SensMLP

*Constructor of the SensMLP Class*

---

## Description

Create an object of SensMLP class

## Usage

```
SensMLP(
  sens = list(),
  raw_sens = list(),
  mlp_struct = numeric(),
  trData = data.frame(),
  coefnames = character(),
  output_name = character()
)
```

## Arguments

<code>sens</code>	list of sensitivity measures, one data.frame per output neuron
<code>raw_sens</code>	list of sensitivities, one matrix per output neuron
<code>mlp_struct</code>	numeric vector describing the structure of the MLP model
<code>trData</code>	data.frame with the data used to calculate the sensitivities
<code>coefnames</code>	character vector with the name of the predictor(s)
<code>output_name</code>	character vector with the name of the output(s)

## Value

SensMLP object

---

SensTimePlot                      *Sensitivity analysis plot over time of the data*

---

### Description

Plot of sensitivity of the neural network output respect to the inputs over the time variable from the data provided

### Usage

```
SensTimePlot(
  object,
  fdata = NULL,
  date.var = NULL,
  facet = FALSE,
  smooth = FALSE,
  nspline = NULL,
  ...
)
```

### Arguments

object	fitted neural network model or array containing the raw sensitivities from the function <a href="#">SensAnalysisMLP</a>
fdata	data.frame containing the data to evaluate the sensitivity of the model. Not needed if the raw sensitivities has been passed as object
date.var	Posixct vector with the date of each sample of fdata If NULL, the first variable with Posixct format of fdata is used as dates
facet	logical if TRUE, function <code>facet_grid</code> from <code>ggplot2</code> is used
smooth	logical if TRUE, <code>geom_smooth</code> plots are added to each variable plot
nspline	integer if smooth is TRUE, this determine the degree of the spline used to perform <code>geom_smooth</code> . If nspline is NULL, the square root of the length of the timeseries is used as degrees of the spline.
...	further arguments that should be passed to <a href="#">SensAnalysisMLP</a> function

### Value

list of `geom_line` plots for the inputs variables representing the sensitivity of each output respect to the inputs over time

### Examples

```
## Load data -----
data("DAILY_DEMAND_TR")
fdata <- DAILY_DEMAND_TR
fdata[,3] <- ifelse(as.data.frame(fdata)[,3] %in% c("SUN","SAT"), 0, 1)
```



```

## Parameters of the NNET -----
hidden_neurons <- 5
iters <- 250
decay <- 0.1

#####
##### REGRESSION NNET #####
#####
## Regression dataframe -----
# Scale the data
fdata.Reg.tr <- fdata[,2:ncol(fdata)]
fdata.Reg.tr[,3] <- fdata.Reg.tr[,3]/10
fdata.Reg.tr[,1] <- fdata.Reg.tr[,1]/1000

# Normalize the data for some models
preProc <- caret::preProcess(fdata.Reg.tr, method = c("center","scale"))
nntrData <- predict(preProc, fdata.Reg.tr)

#' ## TRAIN nnet NNET -----
# Create a formula to train NNET
form <- paste(names(fdata.Reg.tr)[2:ncol(fdata.Reg.tr)], collapse = " + ")
form <- formula(paste(names(fdata.Reg.tr)[1], form, sep = " ~ "))

set.seed(150)
nnetmod <- nnet::nnet(form,
                      data = nntrData,
                      linear.output = TRUE,
                      size = hidden_neurons,
                      decay = decay,
                      maxit = iters)

# Try SensTimePlot
NeuralSens::SensTimePlot(nnetmod, fdata = nntrData, date.var = NULL)

```

---

simdata

*Simulated data to test the package functionalities*


---

## Description

data.frame with 2000 rows of 4 columns with 3 input variables X1, X2, X3 and one output variable Y. The data is already scaled, and has been generated using the following code:

```

set.seed(150)
simdata <- data.frame( "X1" = rnorm(2000,0,1), "X2" = rnorm(2000,0,1), "X3" = rnorm(2000,0,1)
)
simdata$Y <- simdata$X1^2 + 0.5*simdata$X2 + 0.1*rnorm(2000,0,1)

```

## Format

A data frame with 2000 rows and 4 variables:

**X1** Random input 1  
**X2** Random input 2  
**X3** Random input 3  
**Y** Output

**Author(s)**

Jaime Pizarroso Gonzalo

---

summary.HessMLP

*Summary Method for the HessMLP Class*

---

**Description**

Print the sensitivity metrics of a HessMLP object. This metrics are the mean sensitivity, the standard deviation of sensitivities and the mean of sensitivities square

**Usage**

```
## S3 method for class 'HessMLP'
summary(object, ...)
```

**Arguments**

object            HessMLP object created by [HessianMLP](#)  
...                additional parameters

**Value**

summary object of the HessMLP object passed

**Examples**

```
## Load data -----
data("DAILY_DEMAND_TR")
fdata <- DAILY_DEMAND_TR

## Parameters of the NNET -----
hidden_neurons <- 5
iters <- 250
decay <- 0.1

#####
##### REGRESSION NNET #####
#####
## Regression dataframe -----
# Scale the data
fdata.Reg.tr <- fdata[,2:ncol(fdata)]
```

```

fdata.Reg.tr[,3] <- fdata.Reg.tr[,3]/10
fdata.Reg.tr[,1] <- fdata.Reg.tr[,1]/1000

# Normalize the data for some models
preProc <- caret::preProcess(fdata.Reg.tr, method = c("center","scale"))
nntrData <- predict(preProc, fdata.Reg.tr)

#' ## TRAIN nnet NNET -----
# Create a formula to train NNET
form <- paste(names(fdata.Reg.tr)[2:ncol(fdata.Reg.tr)], collapse = " + ")
form <- formula(paste(names(fdata.Reg.tr)[1], form, sep = " ~ "))

set.seed(150)
nnetmod <- nnet::nnet(form,
                      data = nntrData,
                      linear.output = TRUE,
                      size = hidden_neurons,
                      decay = decay,
                      maxit = iters)

# Try HessianMLP
sens <- NeuralSens::HessianMLP(nnetmod, trData = nntrData, plot = FALSE)
summary(sens)

```

---

summary.SensMLP

*Summary Method for the SensMLP Class*


---

## Description

Print the sensitivity metrics of a SensMLP object. This metrics are the mean sensitivity, the standard deviation of sensitivities and the mean of sensitivities square

## Usage

```

## S3 method for class 'SensMLP'
summary(object, ...)

```

## Arguments

object	SensMLP object created by <a href="#">SensAnalysisMLP</a>
...	additional parameters

## Value

summary object of the SensMLP object passed

**Examples**

```

## Load data -----
data("DAILY_DEMAND_TR")
fdata <- DAILY_DEMAND_TR

## Parameters of the NNET -----
hidden_neurons <- 5
iters <- 250
decay <- 0.1

#####
##### REGRESSION NNET #####
#####

## Regression dataframe -----
# Scale the data
fdata.Reg.tr <- fdata[,2:ncol(fdata)]
fdata.Reg.tr[,3] <- fdata.Reg.tr[,3]/10
fdata.Reg.tr[,1] <- fdata.Reg.tr[,1]/1000

# Normalize the data for some models
preProc <- caret::preProcess(fdata.Reg.tr, method = c("center","scale"))
nntrData <- predict(preProc, fdata.Reg.tr)

#' ## TRAIN nnet NNET -----
# Create a formula to train NNET
form <- paste(names(fdata.Reg.tr)[2:ncol(fdata.Reg.tr)], collapse = " + ")
form <- formula(paste(names(fdata.Reg.tr)[1], form, sep = " ~ "))

set.seed(150)
nnetmod <- nnet::nnet(form,
                      data = nntrData,
                      linear.output = TRUE,
                      size = hidden_neurons,
                      decay = decay,
                      maxit = iters)

# Try SensAnalysisMLP
sens <- NeuralSens::SensAnalysisMLP(nnetmod, trData = nntrData, plot = FALSE)
summary(sens)

```

---

syntheticdata

---

*List of 4 dataframes to test the functions with different variables types*


---

**Description**

List of 4 dataframes to test the functions with different variables types (numeric and character output and inputs)

**Format**

list of 4 data.frames with 4 columns for 3 inputs and one output:

**RegOutNumInp** data.frame

- X1 Input 1 of the subset 1 (numeric)
- X2 Input 2 of the subset 1 (numeric)
- X3 Input 3 of the subset 1 (numeric)
- Y Output of the subset 1 (numeric)

**ClsOutNumInp** data.frame

- X1 Input 1 of the subset 2 (numeric)
- X2 Input 2 of the subset 2 (numeric)
- X3 Input 3 of the subset 2 (numeric)
- Y Output of the subset 2 (character)

**ClsOutClsInp** data.frame

- X1 Input 1 of the subset 3 (character)
- X2 Input 2 of the subset 3 (numeric)
- X3 Input 3 of the subset 3 (numeric)
- Y Output of the subset 3 (character)

**ClsOutClsInp** data.frame

- X1 Input 1 of the subset 4 (numeric)
- X2 Input 2 of the subset 4 (character)
- X3 Input 3 of the subset 4 (numeric)
- Y Output of the subset 4 (numeric)

**Author(s)**

Jose Portela Gonzalez

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