Package ‘NeuralSens’

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Version 1.1.3

Title Sensitivity Analysis of Neural Networks

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 <doi:10.18637/jss.v102.i07>.

Author José Portela González [aut],
Antonio Muñoz San Roque [aut],
Jaime Pizarroso Gonzalo [aut, ctb, cre]

Maintainer Jaime Pizarroso Gonzalo <jpizarroso@comillas.edu>

Imports ggplot2, gridExtra, NeuralNetTools, reshape2, caret, fastDummies, stringr, Hmisc, ggforce, scales, ggnewscale, magrittr, ggrepel, ggbreak, dplyr

Suggests h2o, RSNNS, nnet, neuralnet, plotly, e1071

RoxygenNote 7.3.1

NeedsCompilation no

URL https://github.com/JaiPizGon/NeuralSens

BugReports https://github.com/JaiPizGon/NeuralSens/issues

Encoding UTF-8

LazyData true

Repository CRAN

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R topics documented:

`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

References

Pizarroso J, Portela J, Muñoz A (2022). NeuralSens: Sensitivity Analysis of Neural Networks. Journal of Statistical Software, 102(7), 1-36.

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)
```

`AlphaSensAnalysis` *Sensitivity alpha-curve associated to MLP function*

Description

Obtain sensitivity alpha-curves associated to MLP function obtained from the sensitivities returned by `SensAnalysisMLP`.

Usage

```
AlphaSensAnalysis(
  sens,
  tol = NULL,
  max_alpha = 15,
  curve_equal_origin = FALSE,
  inp_var = NULL,
  line_width = 1,
  title = "Alpha curve of Lp norm values",
  alpha_bar = 1,
  kind = "line"
)
```

Arguments

sens	sensitivity object returned by SensAnalysisMLP
tol	difference between M_alpha and maximum sensitivity of the sensitivity of each input variable
max_alpha	maximum alpha value to analyze
curve_equal_origin	make all the curves begin at (1,0)
inp_var	character indicating which input variable to show in density plot. Only useful when choosing plot_type='raw' to show the density plot of one input variable. If NULL, all variables are plotted in density plot. By default is NULL.
line_width	int width of the line in the plot.
title	char title of the alpha-curves plot
alpha_bar	int alpha value to show as column plot.
kind	char select the type of plot: "line" or "bar"

Value

alpha-curves of the MLP function

Examples

```
mod <- RSNNS::mlp(simdata[, c("X1", "X2", "X3")], simdata[, "Y"],
                 maxit = 1000, size = 15, linOut = TRUE)

sens <- SensAnalysisMLP(mod, trData = simdata,
                        output_name = "Y", plot = FALSE)

AlphaSensAnalysis(sens)
```

AlphaSensCurve	*Sensitivity alpha-curve associated to MLP function of an input variable*

Description

Obtain sensitivity alpha-curve associated to MLP function obtained from the sensitivities returned by SensAnalysisMLP of an input variable.

Usage

```
AlphaSensCurve(sens, tol = NULL, max_alpha = 100)
```

Arguments

sens	raw sensitivities of the MLP output with respect to input variable.
tol	difference between M_alpha and maximum sensitivity of the sensitivity of each input variable
max_alpha	maximum alpha value to analyze

Value

alpha-curve of the MLP function

Examples

```
mod <- RSNNS::mlp(simdata[, c("X1", "X2", "X3")], simdata[, "Y"],
                  maxit = 1000, size = 15, linOut = TRUE)

sens <- SensAnalysisMLP(mod, trData = simdata,
                        output_name = "Y", plot = FALSE)

AlphaSensCurve(sens$raw_sens[[1]][,1])
```

ChangeBootAlpha	*Change significance of boot SensMLP Class*

Description

For a SensMLP Class object, change the significance level of the statistical tests

Usage

```
ChangeBootAlpha(x, boot.alpha)
```

Arguments

x	SensMLP object created by SensAnalysisMLP
boot.alpha	float significance level

Value

SensMLP object with changed significance level. All boot related metrics are changed

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


## TRAIN nnet NNET --------------------------------------------------------

set.seed(150)
nnetmod <- caret::train(DEM ~ .,
                 data = fdata.Reg.tr,
                 method = "nnet",
                 tuneGrid = expand.grid(size = c(1), decay = c(0.01)),
                 trControl = caret::trainControl(method="none"),
                 preProcess = c('center', 'scale'),
                 linout = FALSE,
                 trace = FALSE,
                 maxit = 300)
# Try SensAnalysisMLP
sens <- NeuralSens::SensAnalysisMLP(nnetmod, trData = fdata.Reg.tr,
                                    plot = FALSE, boot.R=2, output_name='DEM')
NeuralSens::ChangeBootAlpha(sens, boot.alpha=0.1)
```

`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 `SensAnalysisMLP` 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

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

#' ## TRAIN nnet NNET --------------------------------------------------------
# Create a formula to train NNET
form <- paste(names(fdata)[1:ncol(fdata)-1], collapse = " + ")
form <- formula(paste(names(fdata)[5], form, sep = " ~ "))

set.seed(150)
mod <- nnet::nnet(form,
                  data = fdata,
                  linear.output = TRUE,
                  size = hidden_neurons,
                  decay = decay,
                  maxit = iters)
# mod should be a neural network classification model
sens <- SensAnalysisMLP(mod, trData = fdata, output_name = 'Species')
combinesens <- CombineSens(sens, "sqmean")
```

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"))
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)
```

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

References

Pizarroso J, Portela J, Muñoz A (2022). NeuralSens: Sensitivity Analysis of Neural Networks. Journal of Statistical Software, 102(7), 1-36.

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)
```

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

References

Pizarroso J, Portela J, Muñoz A (2022). NeuralSens: Sensitivity Analysis of Neural Networks. Journal of Statistical Software, 102(7), 1-36.

`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

References

Pizarroso J, Portela J, Muñoz A (2022). NeuralSens: Sensitivity Analysis of Neural Networks. Journal of Statistical Software, 102(7), 1-36.

`Der2ActFunc` *Second derivative of activation function of neuron*

Description

Evaluate second 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)
```

`Der3ActFunc` *Third derivative of activation function of neuron*

Description

Evaluate third derivative of activation function of a neuron

Usage

```
Der3ActFunc(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 <- Der3ActFunc("sigmoid")
# Return derivative of the tanh activation function of a neuron
ActivationFunction <- Der3ActFunc("tanh")
# Return derivative of the activation function of several layers of neurons
actfuncs <- c("linear","sigmoid","linear")
ActivationFunctions <- sapply(actfuncs, Der3ActFunc)
```

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

References

Pizarroso J, Portela J, Muñoz A (2022). NeuralSens: Sensitivity Analysis of Neural Networks. Journal of Statistical Software, 102(7), 1-36.

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` -> 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
```

diag4Darray *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

```
diag4Darray(x = 1, dim = length(x))
```

Arguments

x	`number` or `vector` defining the value of the diagonal of `4D` `array`
dim	`integer` defining the length of the diagonal. Default is `length(x)`. If `length(x)` `!=` `1`, `dim` must be equal to `length(x)`.

Details

The diagonal of a 4D array has been defined as those elements in positions c(int,int,int,int), i.e., the four digits are the same.

Value

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

Examples

```
x <- diag4Darray(c(1,3,6,2), dim = 4)
x
# , , 1, 1
#
#      [,1] [,2] [,3] [,4]
# [1,]    1    0    0    0
# [2,]    0    0    0    0
# [3,]    0    0    0    0
# [4,]    0    0    0    0
#
# , , 2, 1
#
#      [,1] [,2] [,3] [,4]
# [1,]    0    0    0    0
# [2,]    0    0    0    0
# [3,]    0    0    0    0
# [4,]    0    0    0    0
#
# , , 3, 1
#
```

```
#      [,1] [,2] [,3] [,4]
# [1,]    0    0    0    0
# [2,]    0    0    0    0
# [3,]    0    0    0    0
# [4,]    0    0    0    0
#
# , , 4, 1
#
#      [,1] [,2] [,3] [,4]
# [1,]    0    0    0    0
# [2,]    0    0    0    0
# [3,]    0    0    0    0
# [4,]    0    0    0    0
#
# , , 1, 2
#
#      [,1] [,2] [,3] [,4]
# [1,]    0    0    0    0
# [2,]    0    0    0    0
# [3,]    0    0    0    0
# [4,]    0    0    0    0
#
# , , 2, 2
#
#      [,1] [,2] [,3] [,4]
# [1,]    0    0    0    0
# [2,]    0    3    0    0
# [3,]    0    0    0    0
# [4,]    0    0    0    0
#
# , , 3, 2
#
#      [,1] [,2] [,3] [,4]
# [1,]    0    0    0    0
# [2,]    0    0    0    0
# [3,]    0    0    0    0
# [4,]    0    0    0    0
#
# , , 4, 2
#
#      [,1] [,2] [,3] [,4]
# [1,]    0    0    0    0
# [2,]    0    0    0    0
# [3,]    0    0    0    0
# [4,]    0    0    0    0
#
# , , 1, 3
#
#      [,1] [,2] [,3] [,4]
# [1,]    0    0    0    0
# [2,]    0    0    0    0
# [3,]    0    0    0    0
# [4,]    0    0    0    0
```

```
#
# , , 2, 3
#
#      [,1] [,2] [,3] [,4]
# [1,]    0    0    0    0
# [2,]    0    0    0    0
# [3,]    0    0    0    0
# [4,]    0    0    0    0
#
# , , 3, 3
#
#      [,1] [,2] [,3] [,4]
# [1,]    0    0    0    0
# [2,]    0    0    0    0
# [3,]    0    0    6    0
# [4,]    0    0    0    0
#
# , , 4, 3
#
#      [,1] [,2] [,3] [,4]
# [1,]    0    0    0    0
# [2,]    0    0    0    0
# [3,]    0    0    0    0
# [4,]    0    0    0    0
#
# , , 1, 4
#
#      [,1] [,2] [,3] [,4]
# [1,]    0    0    0    0
# [2,]    0    0    0    0
# [3,]    0    0    0    0
# [4,]    0    0    0    0
#
# , , 2, 4
#
#      [,1] [,2] [,3] [,4]
# [1,]    0    0    0    0
# [2,]    0    0    0    0
# [3,]    0    0    0    0
# [4,]    0    0    0    0
#
# , , 3, 4
#
#      [,1] [,2] [,3] [,4]
# [1,]    0    0    0    0
# [2,]    0    0    0    0
# [3,]    0    0    0    0
# [4,]    0    0    0    0
#
# , , 4, 4
#
#      [,1] [,2] [,3] [,4]
# [1,]    0    0    0    0
```

```
# [2,]    0    0    0    0
# [3,]    0    0    0    0
# [4,]    0    0    0    2
diag4Darray(x)
# 1, 3, 6, 2
```

diag4Darray<- *Define function to change the diagonal of array*

Description

Define function to change the diagonal of array

Usage

```
diag4Darray(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(4,4,4,4))
diag4Darray(x) <- c(2,2,2,2)
x
# , , 1, 1
#
#      [,1] [,2] [,3] [,4]
# [1,]    2    1    1    1
# [2,]    1    1    1    1
# [3,]    1    1    1    1
# [4,]    1    1    1    1
#
# , , 2, 1
#
#      [,1] [,2] [,3] [,4]
# [1,]    1    1    1    1
# [2,]    1    1    1    1
```

```
# [3,]    1    1    1    1
# [4,]    1    1    1    1
#
# , , 3, 1
#
#      [,1] [,2] [,3] [,4]
# [1,]    1    1    1    1
# [2,]    1    1    1    1
# [3,]    1    1    1    1
# [4,]    1    1    1    1
#
# , , 4, 1
#
#      [,1] [,2] [,3] [,4]
# [1,]    1    1    1    1
# [2,]    1    1    1    1
# [3,]    1    1    1    1
# [4,]    1    1    1    1
#
# , , 1, 2
#
#      [,1] [,2] [,3] [,4]
# [1,]    1    1    1    1
# [2,]    1    1    1    1
# [3,]    1    1    1    1
# [4,]    1    1    1    1
#
# , , 2, 2
#
#      [,1] [,2] [,3] [,4]
# [1,]    1    1    1    1
# [2,]    1    2    1    1
# [3,]    1    1    1    1
# [4,]    1    1    1    1
#
# , , 3, 2
#
#      [,1] [,2] [,3] [,4]
# [1,]    1    1    1    1
# [2,]    1    1    1    1
# [3,]    1    1    1    1
# [4,]    1    1    1    1
#
# , , 4, 2
#
#      [,1] [,2] [,3] [,4]
# [1,]    1    1    1    1
# [2,]    1    1    1    1
# [3,]    1    1    1    1
# [4,]    1    1    1    1
#
# , , 1, 3
#
```

```
#      [,1] [,2] [,3] [,4]
# [1,]    1    1    1    1
# [2,]    1    1    1    1
# [3,]    1    1    1    1
# [4,]    1    1    1    1
#
# , , 2, 3
#
#      [,1] [,2] [,3] [,4]
# [1,]    1    1    1    1
# [2,]    1    1    1    1
# [3,]    1    1    1    1
# [4,]    1    1    1    1
#
# , , 3, 3
#
#      [,1] [,2] [,3] [,4]
# [1,]    1    1    1    1
# [2,]    1    1    1    1
# [3,]    1    1    2    1
# [4,]    1    1    1    1
#
# , , 4, 3
#
#      [,1] [,2] [,3] [,4]
# [1,]    1    1    1    1
# [2,]    1    1    1    1
# [3,]    1    1    1    1
# [4,]    1    1    1    1
#
# , , 1, 4
#
#      [,1] [,2] [,3] [,4]
# [1,]    1    1    1    1
# [2,]    1    1    1    1
# [3,]    1    1    1    1
# [4,]    1    1    1    1
#
# , , 2, 4
#
#      [,1] [,2] [,3] [,4]
# [1,]    1    1    1    1
# [2,]    1    1    1    1
# [3,]    1    1    1    1
# [4,]    1    1    1    1
#
# , , 3, 4
#
#      [,1] [,2] [,3] [,4]
# [1,]    1    1    1    1
# [2,]    1    1    1    1
# [3,]    1    1    1    1
# [4,]    1    1    1    1
```

```
#
# , , 4, 4
#
#      [,1] [,2] [,3] [,4]
# [1,]    1    1    1    1
# [2,]    1    1    1    1
# [3,]    1    1    1    1
# [4,]    1    1    1    2
```

`find_critical_value` *Find Critical Value*

Description

This function finds the smallest x such that the probability of a random variable being less than or equal to x is greater than or equal to 1 - alpha. It uses the uniroot function to find where the empirical cumulative distribution function (ECDF) crosses 1 - alpha.

Usage

```
find_critical_value(ecdf_func, alpha)
```

Arguments

`ecdf_func`	An ECDF function representing the distribution of a random variable.
`alpha`	A numeric value specifying the significance level.

Value

The smallest x such that P(X <= x) >= 1 - alpha.

Examples

```
data <- rnorm(100)
ecdf_data <- ecdf(data)
critical_val <- find_critical_value(ecdf_data, 0.05)
```

HessDotPlot *Second derivatives 3D scatter or surface plot against input values*

Description

3D Plot of second derivatives of the neural network output respect to the inputs. This function use `plotly` instead of `ggplot2` to achieve better visualization

Usage

```
HessDotPlot(
  object,
  fdata = NULL,
  input_vars = "all",
  input_vars2 = "all",
  output_vars = "all",
  surface = FALSE,
  grid = FALSE,
  color = NULL,
  ...
)
```

Arguments

`object`	fitted neural network model or `array` containing the raw second derivatives from the function `HessianMLP`
`fdata`	`data.frame` containing the data to evaluate the second derivatives of the model.
`input_vars`	`character vector` with the variables to create the scatter plot in x-axis. If `"all"`, then scatter plots are created for all the input variables in `fdata`.
`input_vars2`	`character vector` with the variables to create the scatter plot in y-axis. If `"all"`, then scatter plots are created for all the input variables in `fdata`.
`output_vars`	`character vector` with the variables to create the scatter plot. If `"all"`, then scatter plots are created for all the output variables in `fdata`.
`surface`	`logical` if `TRUE`, a 3D surface is created instead of 3D scatter plot (only for combinations of different inputs)
`grid`	`logical`. If `TRUE`, plots created are show together using `arrangeGrob`. It does not work on Windows platforms due to bugs in `plotly` library.
`color`	`character` specifying the name of a `numeric` variable of `fdata` to color the 3D scatter plot.
`...`	further arguments that should be passed to `HessianMLP` function

Value

list of 3D `geom_point` plots for the inputs variables representing the sensitivity of each output respect to the inputs

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 HessDotPlot
NeuralSens::HessDotPlot(nnetmod, fdata = nntrData, surface = TRUE, color = "WD")
```

`HessFeaturePlot` *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

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

Arguments

object — fitted neural network model or `array` containing the raw sensitivities from the function `SensAnalysisMLP`

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 `SensAnalysisMLP` function

Value

list of Feature sensitivity plot as described in https://www.r-bloggers.com/2019/03/a-gentle-introduction-to-sha

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
hess <- NeuralSens::HessianMLP(nnetmod, trData = nntrData, plot = FALSE)
NeuralSens::HessFeaturePlot(hess)
```

HessianMLP *Sensitivity of MLP models*

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 preProcess
terms	function applied to the training data to create factors. See also train
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

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"))
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
NeuralSens::HessianMLP(nnetmod, trData = nntrData, plot = FALSE)

# Try HessianMLP to calculate sensitivities with respect to output of hidden neurones
NeuralSens::HessianMLP(nnetmod, trData = nntrData,
                             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)

# 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 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")

## USE DEFAULT METHOD ----------------------------------------------------------
NeuralSens::HessianMLP(caretmod$finalModel$wts,
                            trData = fdata.Reg.tr,
                            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.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 HessianMLP
NeuralSens::HessianMLP(caretmod)

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

# 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 HessianMLP
NeuralSens::HessianMLP(h2omod)

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

## 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 = nntrData)
```

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

sens	`list` of sensitivity measures, one `list` per output neuron

`raw_sens`	`list` of sensitivities, one `array` per output neuron
`mlp_struct`	`numeric` vector describing the structur of the MLP model
`trData`	`data.frame` with the data used to calculate the sensitivities
`coefnames`	`character` vector with the name of the predictor(s)
`output_name`	`character` vector with the name of the output(s)

Value

`HessMLP` object

`HessToSensMLP` *Convert a HessMLP to a SensMLP object*

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` *Check if object is of class* `HessMLP`

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 — *Check if object is of class* SensMLP

Description

Check if object is of class `SensMLP`

Usage

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

Arguments

`object`	`SensMLP` object

Value

`TRUE` if `object` is a `SensMLP` object

References

Pizarroso J, Portela J, Muñoz A (2022). NeuralSens: Sensitivity Analysis of Neural Networks. Journal of Statistical Software, 102(7), 1-36.

kStepMAlgorithm — *k-StepM Algorithm for Hypothesis Testing*

Description

This function implements the k-stepM algorithm for multiple hypothesis testing. It tests each hypothesis using the critical value calculated from the ECDF of the k-max differences, updating the critical value, and iterating until all hypotheses are tested.

Usage

```
kStepMAlgorithm(original_stats, bootstrap_stats, num_hypotheses, alpha, k)
```

Arguments

`original_stats`	A numeric vector of original test statistics for each hypothesis.
`bootstrap_stats`	A numeric matrix of bootstrap test statistics, with rows representing bootstrap samples and columns representing hypotheses.
`num_hypotheses`	An integer specifying the total number of hypotheses.
`alpha`	A numeric value specifying the significance level.
`k`	An integer specifying the threshold number for controlling the k-familywise error rate.

Value

A list containing two elements: 'signif', a logical vector indicating which hypotheses are rejected, and 'cv', a numeric vector of critical values used for each hypothesis.

References

Romano, Joseph P., Azeem M. Shaikh, and Michael Wolf. "Formalized data snooping based on generalized error rates." Econometric Theory 24.2 (2008): 404-447.

Examples

```
original_stats <- rnorm(10)
bootstrap_stats <- matrix(rnorm(1000), ncol = 10)
result <- kStepMAlgorithm(original_stats, bootstrap_stats, 10, 0.05, 1)
```

`NeuralSens` *NeuralSens: Sensitivity Analysis of Neural Networks*

Description

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

Author(s)

Maintainer: Jaime Pizarroso Gonzalo <jpizarroso@comillas.edu> [contributor]

Authors:

- José Portela González <Jose.Portela@iit.comillas.edu>
- Antonio Muñoz San Roque <antonio.munoz@iit.comillas.edu>

See Also

Useful links:

- https://github.com/JaiPizGon/NeuralSens
- Report bugs at https://github.com/JaiPizGon/NeuralSens/issues

plot.HessMLP *Plot method for the HessMLP Class*

Description

Plot the sensitivities and sensitivity metrics of a HessMLP object.

Usage

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

Arguments

x	HessMLP object created by HessianMLP
plotType	character specifying which type of plot should be created. It can be: • "sensitivities" (default): use HessianMLP function • "time": use SensTimePlot function • "features": use HessFeaturePlot function • "matrix": use SensMatPlot function to show the values of second partial derivatives • "interactions": use SensMatPlot function to show the values of second partial derivatives and the first partial derivatives in the diagonal
...	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)

plot(sens)
plot(sens,"time")
```

`plot.SensMLP` *Plot method for the SensMLP Class*

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 `SensAnalysisMLP`
`plotType`	`character` specifying which type of plot should be created. It can be: • "sensitivities" (default): use `SensAnalysisMLP` function • "time": use `SensTimePlot` function • "features": use `SensFeaturePlot` function
`...`	additional parameters passed to plot function of the `NeuralSens` package

Value

list of graphic objects created by ggplot

References

Pizarroso J, Portela J, Muñoz A (2022). NeuralSens: Sensitivity Analysis of Neural Networks. Journal of Statistical Software, 102(7), 1-36.

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)

plot(sens)
plot(sens,"time")
plot(sens,"features")
```

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 plotnet
sens_pos_col	`character` string indicating color of positive sensitivity measure, default 'blue'. The same is passed to argument `pos_col` of plotnet
...	additional arguments passed to plotnet and/or SensAnalysisMLP

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"))
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
NeuralSens::PlotSensMLP(nnetmod, trData = nntrData)
```

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, round_digits = NULL, ...)
```

Arguments

x	HessMLP object created by HessianMLP
n	integer specifying number of sensitivities to print per each output
round_digits	integer number of decimal places, default NULL
...	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
```

print.SensMLP — *Print method for the SensMLP Class*

Description

Print the sensitivities of a SensMLP object.

Usage

```
## S3 method for class 'SensMLP'
print(x, n = 5, round_digits = NULL, ...)
```

Arguments

x	SensMLP object created by SensAnalysisMLP
n	integer specifying number of sensitivities to print per each output
round_digits	integer number of decimal places, default NULL
...	additional parameters

References

Pizarroso J, Portela J, Muñoz A (2022). NeuralSens: Sensitivity Analysis of Neural Networks. Journal of Statistical Software, 102(7), 1-36.

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)
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, round_digits = NULL, ...)
```

Arguments

`x`	`summary.HessMLP` object created by summary method of `HessMLP` object
`round_digits`	`integer` number of decimal places, default `NULL`
`...`	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)
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, round_digits = NULL, boot.alpha = NULL, ...)
```

Arguments

`x`	`summary.SensMLP` object created by summary method of `SensMLP` object
`round_digits`	`integer` number of decimal places, default `NULL`
`boot.alpha`	`float` significance level to show statistical metrics. If `NULL`, boot.alpha inherits from `x` is used. Defaults to `NULL`.
`...`	additional parameters

References

Pizarroso J, Portela J, Muñoz A (2022). NeuralSens: Sensitivity Analysis of Neural Networks. Journal of Statistical Software, 102(7), 1-36.

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,
  boot.R = NULL,
  boot.seed = 1,
  boot.alpha = 0.05,
  ...
)

## 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 `preProcess`
`terms`	function applied to the training data to create factors. See also `train`
`output_name`	`character` name of the output variable in order to avoid changing the name of the output variable in `trData` to '.outcome'
`boot.R`	`int` Number of bootstrap samples to calculate. Used to detect significant inputs and significant non-linearities. Only available for `train` objects. Defaults to `NULL`.
`boot.seed`	`int` Seed of bootstrap evaluations.
`boot.alpha`	`float` Significance level of statistical test.

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

Pizarroso J, Portela J, Muñoz A (2022). NeuralSens: Sensitivity Analysis of Neural Networks. Journal of Statistical Software, 102(7), 1-36.

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"))
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
NeuralSens::SensAnalysisMLP(nnetmod, trData = nntrData)

# Try SensAnalysisMLP to calculate sensitivities with respect to output of hidden neurones
NeuralSens::SensAnalysisMLP(nnetmod, trData = nntrData,
                             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 SensAnalysisMLP
NeuralSens::SensAnalysisMLP(caretmod)

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

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

## USE DEFAULT METHOD ----------------------------------------------------------
NeuralSens::SensAnalysisMLP(caretmod$finalModel$wts,
                            trData = fdata.Reg.tr,
                            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.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)

# 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 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)
```

SensDotPlot *Sensitivity scatter plot against input values*

Description

Plot of sensitivities of the neural network output respect to the inputs

Usage

```
SensDotPlot(
  object,
  fdata = NULL,
  input_vars = "all",
  output_vars = "all",
  smooth = FALSE,
  nspline = NULL,
  color = NULL,
  grid = FALSE,
  ...
)
```

Arguments

`object`	fitted neural network model or `array` containing the raw sensitivities from the function `SensAnalysisMLP`
`fdata`	`data.frame` containing the data to evaluate the sensitivity of the model.
`input_vars`	`character` `vector` with the variables to create the scatter plot. If `"all"`, then scatter plots are created for all the input variables in `fdata`.
`output_vars`	`character` `vector` with the variables to create the scatter plot. If `"all"`, then scatter plots are created for all the output variables in `fdata`.
`smooth`	`logical` if `TRUE`, `geom_smooth` plots are added to each variable plot
`nspline`	`integer` if `smooth` is TRUE, this determine the degree of the spline used to perform `geom_smooth`. If `nspline` is NULL, the square root of the length of the data is used as degrees of the spline.
`color`	`character` specifying the name of a `numeric` variable of `fdata` to color the scatter plot.
`grid`	`logical`. If `TRUE`, plots created are show together using `arrangeGrob`
`...`	further arguments that should be passed to `SensAnalysisMLP` function

Value

list of geom_point plots for the inputs variables representing the sensitivity of each output respect to the inputs

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 SensDotPlot
NeuralSens::SensDotPlot(nnetmod, fdata = 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 `SensAnalysisMLP`
`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 `SensAnalysisMLP` function

Value

list of Feature sensitivity plot as described in https://www.r-bloggers.com/2019/03/a-gentle-introduction-to-sha

References

Pizarroso J, Portela J, Muñoz A (2022). NeuralSens: Sensitivity Analysis of Neural Networks. Journal of Statistical Software, 102(7), 1-36.

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::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,
  plot_type = NULL,
  inp_var = NULL,
  title = "Sensitivity Plots",
  dodge_var = FALSE
)
```

Arguments

sens	`SensAnalysisMLP` object created by `SensAnalysisMLP` or `HessMLP` object created by `HessianMLP`.
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. `facet_zoom` 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`).
plot_type	`character` indicating which of the 3 plots to show. Useful when several variables are analyzed. Acceptable values are 'mean_sd', 'square', 'raw' corresponding to first, second and third plot respectively. If `NULL`, all plots are shown at the same time. By default is `NULL`.

inp_var — character indicating which input variable to show in density plot. Only useful when choosing plot_type='raw' to show the density plot of one input variable. If NULL, all variables are plotted in density plot. By default is NULL.

title — character title of the sensitivity plots

dodge_var — bool Flag to indicate that x ticks in meanSensSQ plot must dodge between them. Useful with too long input names.

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

References

Pizarroso J, Portela J, Muñoz A (2022). NeuralSens: Sensitivity Analysis of Neural Networks. Journal of Statistical Software, 102(7), 1-36.

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

`hess`	`HessMLP` object created by `HessianMLP`.
`sens`	`SensMLP` object created by `SensAnalysisMLP`.
`output`	`numeric` or `character` specifying the output neuron or output name to be plotted. By default is the first output (`output = 1`).
`metric`	`character` specifying the metric to be plotted. It can be "mean", "std" or "meanSensSQ".
`senstype`	`character` specifying the type of plot to be plotted. It can be "matrix" or "interactions". If type = "matrix", only the second derivatives are plotted. If type = "interactions" the main diagonal are the first derivatives respect each input variable.
`...`	further argument passed similar to `ggcorrplot` arguments.

Details

Most of the code of this function is based on `ggcorrplot()` function from package `ggcorrplot`. However, due to the inhability of changing the limits of the color scale, it keeps giving a warning if that function is used and the color scale overwritten.

Value

a list of ggplots, one for each output neuron.

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"))
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
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(),
  cv = NULL,
  boot = NULL,
  boot.alpha = NULL
)
```

Arguments

`sens`	`list` of sensitivity measures, one `data.frame` per output neuron
`raw_sens`	`list` of sensitivities, one `matrix` per output neuron
`mlp_struct`	`numeric` vector describing the structur of the MLP model
`trData`	`data.frame` with the data used to calculate the sensitivities
`coefnames`	`character` vector with the name of the predictor(s)
`output_name`	`character` vector with the name of the output(s)
`cv`	`list` list with critical values of significance for std and mean square.
`boot`	`array` bootstrapped sensitivity measures.
`boot.alpha`	`array` significance level. Defaults to `NULL`. Only available for analyzed `caret::train` models.

Value

`SensMLP` object

References

Pizarroso J, Portela J, Muñoz A (2022). NeuralSens: Sensitivity Analysis of Neural Networks. Journal of Statistical Software, 102(7), 1-36.

`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 SensAnalysisMLP
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 facet_grid from ggplot2 is used
smooth	logical if TRUE, geom_smooth plots are added to each variable plot
nspline	integer if smooth is TRUE, this determine the degree of the spline used to perform geom_smooth. 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 SensAnalysisMLP function

Value

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

References

Pizarroso J, Portela J, Muñoz A (2022). NeuralSens: Sensitivity Analysis of Neural Networks. Journal of Statistical Software, 102(7), 1-36.

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

References

Pizarroso J, Portela J, Muñoz A (2022). NeuralSens: Sensitivity Analysis of Neural Networks. Journal of Statistical Software, 102(7), 1-36.

`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 `SensAnalysisMLP`
`...`	additional parameters

Value

summary object of the `SensMLP` object passed

References

Pizarroso J, Portela J, Muñoz A (2022). NeuralSens: Sensitivity Analysis of Neural Networks. Journal of Statistical Software, 102(7), 1-36.

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)
```

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