

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](https://doi.org/10.18637/jss.v102.i07)>.

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magrittr, ggrepel, ggbreak, dplyr

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

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

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

License GPL (>= 2)

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ActFunc	<i>Activation function of neuron</i>
---------	--------------------------------------

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	<i>Sensitivity alpha-curve associated to MLP function</i>
-------------------	---

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_{α} 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 <code>plot_type='raw'</code> 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	<i>Sensitivity alpha-curve associated to MLP function of an input variable</i>
----------------	--

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	<i>Change significance of boot SensMLP Class</i>
-----------------	--

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"))
nnetData <- predict(preProc, fdata.Reg.tr)

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

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

```

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

```

ComputeSensMeasures *Plot sensitivities of a neural network model*

Description

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

Usage

```
ComputeSensMeasures(sens)
```

Arguments

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

Value

SensAnalysisMLP object with the sensitivities calculated

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	<i>Data frame with 3 variables</i>
-----------------	------------------------------------

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	<i>Second derivative of activation function of neuron</i>
-------------	---

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	<i>Derivative of activation function of neuron</i>
------------	--

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	<i>Define function to create a 'diagonal' array or get the diagonal of an array</i>
-------------	---

Description

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

Usage

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

Arguments

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

Details

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

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

Value

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

Examples

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

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

Description

Define function to change the diagonal of array

Usage

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

Arguments

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

Details

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

Value

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

Examples

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

diag4Darray	<i>Define function to create a 'diagonal' array or get the diagonal of an array</i>
-------------	---

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 changed
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 $P(X \leq x) \geq 1 - \alpha$.

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"))
nnetData <- predict(preProc, fdata.Reg.tr)

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

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

# Try HessDotPlot
NeuralSens::HessDotPlot(nnetmod, fdata = nnetData, 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-shap>

Examples

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

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

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

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

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

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

# Try SensAnalysisMLP
hess <- NeuralSens::HessianMLP(nnetmod, trData = nnetData, plot = FALSE)
NeuralSens::HessFeaturePlot(hess)
```

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"))
nnetData <- predict(preProc, fdata.Reg.tr)

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

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

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

# Try HessianMLP to calculate sensitivities with respect to output of hidden neurones
NeuralSens::HessianMLP(nnetmod, trData = nnetData,
                       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 structure 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	<i>Convert a HessMLP to a SensMLP object</i>
---------------	--

Description

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

Usage

HessToSensMLP(x)

Arguments

x HessMLP object

Value

SensMLP object

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

Description

Check if object is of class HessMLP

Usage

is.HessMLP(object)

Arguments

object HessMLP object

Value

TRUE if object is a HessMLP object

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

Description

Check if object is of class SensMLP

Usage

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

Arguments

object SensMLP object

Value

TRUE if object is a SensMLP object

References

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

kStepMAlgorithm	<i>k-StepM Algorithm for Hypothesis Testing</i>
-----------------	---

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]

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- 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: <ul style="list-style-type: none"> "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: <ul style="list-style-type: none"> • "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")
```

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"))
ntrData <- predict(preProc, fdata.Reg.tr)

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

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

```

```
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

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

```

nnetData <- predict(preProc, fdata.Reg.tr)

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

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

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

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"))
nnetData <- predict(preProc, fdata.Reg.tr)

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

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

```

                                data = nntrData,
                                linear.output = TRUE,
                                size = hidden_neurons,
                                decay = decay,
                                maxit = iters)

# Try SensAnalysisMLP
sens <- NeuralSens::SensAnalysisMLP(nnnetmod, 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

<code>sens</code>	SensAnalysisMLP object created by SensAnalysisMLP or HessMLP object created by HessianMLP .
<code>der</code>	logical indicating if density plots should be created. By default is TRUE
<code>zoom</code>	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.
<code>quit.legend</code>	logical indicating if legend of the third plot should be removed. By default is FALSE
<code>output</code>	numeric or character specifying the output neuron or output name to be plotted. By default is the first output (<code>output = 1</code>).
<code>plot_type</code>	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"))
nnetData <- predict(preProc, fdata.Reg.tr)

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

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

```

                                data = nntrData,
                                linear.output = TRUE,
                                size = hidden_neurons,
                                decay = decay,
                                maxit = iters)

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

```

SensMatPlot

Plot sensitivities of a neural network model

Description

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

Usage

```

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

```

Arguments

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

Details

Most of the code of this function is based on `ggcorrplot()` function from package `ggcorrplot`. However, due to the inability 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"))
nnetData <- predict(preProc, fdata.Reg.tr)

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

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

# Try HessianMLP
H <- NeuralSens::HessianMLP(nnetmod, trData = nnetData, plot = FALSE)
NeuralSens::SensMatPlot(H)
S <- NeuralSens::SensAnalysisMLP(nnetmod, trData = nnetData, 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

<code>sens</code>	list of sensitivity measures, one data.frame per output neuron
<code>raw_sens</code>	list of sensitivities, one matrix per output neuron
<code>mlp_struct</code>	numeric vector describing the structure of the MLP model
<code>trData</code>	data.frame with the data used to calculate the sensitivities
<code>coefnames</code>	character vector with the name of the predictor(s)
<code>output_name</code>	character vector with the name of the output(s)
<code>cv</code>	list list with critical values of significance for std and mean square.
<code>boot</code>	array bootstrapped sensitivity measures.
<code>boot.alpha</code>	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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