Package 'NeuralSens'

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Version 1.0.1

Title Sensitivity Analysis of Neural Networks

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Description Analysis functions to quantify inputs importance in neural network models. Functions are available for calculating and plotting the inputs importance and obtaining the activation function of each neuron layer and its derivatives. The importance of a given input is defined as the distribution of the derivatives of the output with respect to that input in each training data point <doi:10.18637/jss.v102.i07>.

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

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

RoxygenNote 7.2.0

NeedsCompilation no

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

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

License GPL (>= 2)

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 = 100,
  interpolate_alpha = FALSE,
  curve_equal_length = FALSE,
  curve_equal_origin = FALSE,
  curve_divided_max = FALSE
)
```

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
- `interpolate_alpha` interpolate alpha mean if difference of maximum sensitivity and last alpha evaluated is less than `tol`
- `curve_equal_length` make all the curves of the same length
- `curve_equal_origin` make all the curves begin at (1,0)
- `curve_divided_max` create second plot of curves divided by maximum alpha

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])
```

`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
```

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.

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

Description

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

`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, ...)
```

Arguments

x	summary.SensMLP object created by summary method of SensMLP object
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)
print(summary(sens))
```

SensAnalysisMLP *Sensitivity of MLP models*

Description

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

Usage

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

## Default S3 method:
SensAnalysisMLP(
  MLP.fit,
  .returnSens = TRUE,
  plot = TRUE,
  .rawSens = FALSE,
  sens_origin_layer = 1,
  sens_end_layer = "last",
  sens_origin_input = TRUE,
  sens_end_input = FALSE,
  trData,
  actfunc = NULL,
  deractfunc = NULL,
  preProc = NULL,
  terms = NULL,
  output_name = NULL,
  ...
)

## S3 method for class 'train'
SensAnalysisMLP(
  MLP.fit,
  .returnSens = TRUE,
  plot = TRUE,
  .rawSens = FALSE,
  sens_origin_layer = 1,
```

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

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

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

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

## S3 method for class 'mlp'
```

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

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

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

## S3 method for class 'nnetar'
SensAnalysisMLP(
```

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

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

Arguments

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

actfunc	character vector indicating the activation function of each neurons layer.
deractfunc	character vector indicating the derivative of the activation function of each neurons layer.
preProc	preProcess structure applied to the training data. See also 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

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
)
```

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).

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()
)
```

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)

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)
```

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

Description

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

Format

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

RegOutNumInp data.frame

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

ClsOutNumInp data.frame

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

ClsOutClsInp data.frame

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

ClsOutClsInp data.frame

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

Author(s)

Jose Portela Gonzalez

References

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

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