# Package 'NeuralNetTools'

July 21, 2025

Type Package Title Visualization and Analysis Tools for Neural Networks Version 1.5.3 Date 2022-01-06 Author Marcus W. Beck [aut, cre] Maintainer Marcus W. Beck <mbafs2012@gmail.com> Description Visualization and analysis tools to aid in the interpretation of neural network models. Functions are available for plotting, quantifying variable importance, conducting a sensitivity analysis, and obtaining a simple list of model weights. BugReports https://github.com/fawda123/NeuralNetTools/issues License CC0 LazyData true **Imports** ggplot2 (>= 2.0.0), nnet, reshape2, scales, tidyr Suggests caret, neuralnet, RSNNS, knitr, rmarkdown **Depends** R (>= 3.1.1) RoxygenNote 7.1.1 VignetteBuilder knitr

NeedsCompilation no

**Repository** CRAN

Date/Publication 2022-01-06 15:30:02 UTC

# Contents

| bias_lines   | 2 |
|--------------|---|
| bias_points  | 3 |
| garson       | 4 |
| get_ys       | 7 |
| layer_lines  | 8 |
| layer_points | 9 |

|               | 29     |
|---------------|--------|
| pred_sens     | <br>   |
| plotnet       | <br>   |
| olden         | <br>   |
| neuralweights | <br>   |
| neuralskips   | <br>   |
| neuraldat     | <br>   |
| lekprofile    | <br>11 |
| lekgrps       | <br>10 |

## Index

bias\_lines

Plot connection weights for bias lines

#### Description

Plot connection weights for bias lines in plotnet

# Usage

```
bias_lines(
  bias_x,
  bias_y,
  mod_in,
  nid,
  rel_rsc,
  all_out,
  pos_col,
  neg_col,
  struct,
  y_names,
  x_range,
  y_range,
  layer_x,
  line_stag,
  max_sp
)
```

| bias_x  | numeric vector x axis locations for bias lines   |
|---------|--|
| bias_y  | numeric vector y axis locations for bias lines   |
| mod_in  | neural network model object  |
| nid     | logical value indicating if neural interpretation diagram is plotted, default $TRUE$   |
| rel_rsc | numeric indicating the scaling range for the width of connection weights in a neural interpretation diagram. Default is NULL for no rescaling. |

#### bias\_points

| all_out   | chr string indicating names of response variables for which connections are plot-<br>ted, default all |
|-----------|---|
| pos_col   | chr string indicating color of positive connection weights, default 'black'                           |
| neg_col   | chr string indicating color of negative connection weights, default 'grey'                            |
| struct    | numeric vector for network structure  |
| y_names   | chr string for names of output variables  |
| x_range   | numeric of x axis range for base plot   |
| y_range   | numeric of x axis range for base plot   |
| layer_x   | numeric indicating locations of layers on x axis  |
| line_stag | numeric value that specifies distance of connection weights from nodes                                |
| max_sp    | logical indicating if space is maximized in plot  |

bias\_points

Plot bias points

# Description

Plot bias points in plotnet

# Usage

```
bias_points(
    bias_x,
    bias_y,
    layer_name,
    node_labs,
    x_range,
    y_range,
    circle_cex,
    cex_val,
    bord_col,
    circle_col
)
```

| bias_x     | numeric vector of values for x locations          |
|------------|---|
| bias_y     | numeric vector for y location                     |
| layer_name | string indicating text to put in node             |
| node_labs  | logical indicating of node labels are included    |
| x_range    | numeric of x axis range for base plot             |
| y_range    | numeric of y axis range for base plot             |
| circle_cex | numeric value indicating size of nodes, default 5 |

garson

| cex_val    | numeric value indicating size of text labels, default 1              |
|------------|--|
| bord_col   | chr string indicating border color around nodes, default 'lightblue' |
| circle_col | chr string indicating color of nodes                                 |

| garsc | n |
|-------|---|
|-------|---|

#### Variable importance using Garson's algorithm

#### Description

Relative importance of input variables in neural networks using Garson's algorithm

#### Usage

```
garson(mod_in, ...)
## Default S3 method:
garson(
  mod_in,
  x_names,
  y_names,
  bar_plot = TRUE,
  x_{lab} = NULL,
  y_{lab} = NULL,
  . . .
)
## S3 method for class 'numeric'
garson(mod_in, struct, ...)
## S3 method for class 'nnet'
garson(mod_in, ...)
## S3 method for class 'mlp'
garson(mod_in, ...)
## S3 method for class 'nn'
garson(mod_in, ...)
## S3 method for class 'train'
garson(mod_in, ...)
```

| mod_in | input model object or a list of model weights as returned from neuralweights if using the default method |
|--------|--|
|        | arguments passed to other methods  |

#### garson

| x_names  | chr string of input variable names, obtained from the model object   |
|----------|--|
| y_names  | chr string of response variable names, obtained from the model object  |
| bar_plot | logical indicating if a ggplot object is returned (default T), otherwise numeric values are returned   |
| x_lab    | chr string of alternative names to be used for explanatory variables in the figure, default is taken from mod_in   |
| y_lab    | chr string of alternative name to be used for the y-axis in the figure   |
| struct   | numeric vector equal in length to the number of layers in the network. Each number indicates the number of nodes in each layer starting with the input and ending with the output. An arbitrary number of hidden layers can be included. |

#### Details

The weights that connect variables in a neural network are partially analogous to parameter coefficients in a standard regression model and can be used to describe relationships between variables. The weights dictate the relative influence of information that is processed in the network such that input variables that are not relevant in their correlation with a response variable are suppressed by the weights. The opposite effect is seen for weights assigned to explanatory variables that have strong positive or negative associations with a response variable. An obvious difference between a neural network and a regression model is that the number of weights is excessive in the former case. This characteristic is advantageous in that it makes neural networks very flexible for modeling non-linear functions with multiple interactions, although interpretation of the effects of specific variables is of course challenging.

A method described in Garson 1991 (also see Goh 1995) identifies the relative importance of explanatory variables for a single response variables in a supervised neural network by deconstructing the model weights. The relative importance (or strength of association) of a specific explanatory variable for the response variable can be determined by identifying all weighted connections between the nodes of interest. That is, all weights connecting the specific input node that pass through the hidden layer to the response variable are identified. This is repeated for all other explanatory variables until a list of all weights that are specific to each input variable is obtained. The connections are tallied for each input node and scaled relative to all other inputs. A single value is obtained for each explanatory variable that describes the relationship with the response variable in the model (see the appendix in Goh 1995 for a more detailed description). The original algorithm indicates relative importance as the absolute magnitude from zero to one such the direction of the response cannot be determined.

Misleading results may be produced if the neural network was created with a skip-layer using skip = TRUE with the nnet or train functions. Garson's algorithm does not describe the effects of skip layer connections on estimates of variable importance. As such, these values are removed prior to estimating variable importance.

The algorithm currently only works for neural networks with one hidden layer and one response variable.

#### Value

A ggplot object for plotting if bar\_plot = FALSE, otherwise a data.frame of relative importance values for each input variable. The default aesthetics for ggplot can be further modified, as shown with the examples.

#### References

Beck, M.W. 2018. NeuralNetTools: Visualization and Analysis Tools for Neural Networks. Journal of Statistical Software. 85(11):1-20.

Garson, G.D. 1991. Interpreting neural network connection weights. Artificial Intelligence Expert. 6(4):46-51.

Goh, A.T.C. 1995. Back-propagation neural networks for modeling complex systems. Artificial Intelligence in Engineering. 9(3):143-151.

Olden, J.D., Jackson, D.A. 2002. Illuminating the 'black-box': a randomization approach for understanding variable contributions in artificial neural networks. Ecological Modelling. 154:135-150.

Olden, J.D., Joy, M.K., Death, R.G. 2004. An accurate comparison of methods for quantifying variable importance in artificial neural networks using simulated data. Ecological Modelling. 178:389-397.

#### See Also

olden for a more flexible approach for variable importance

#### Examples

## using numeric input

```
wts_in <- c(13.12, 1.49, 0.16, -0.11, -0.19, -0.16, 0.56, -0.52, 0.81)
struct <- c(2, 2, 1) #two inputs, two hidden, one output
```

garson(wts\_in, struct)

## using nnet

library(nnet)

data(neuraldat)
set.seed(123)

 $mod <- nnet(Y1 \sim X1 + X2 + X3, data = neuraldat, size = 5)$ 

garson(mod)

## Not run:
## using RSNNS, no bias layers

library(RSNNS)

x <- neuraldat[, c('X1', 'X2', 'X3')]
y <- neuraldat[, 'Y1']
mod <- mlp(x, y, size = 5)</pre>

garson(mod)

## using neuralnet

#### get\_ys

```
library(neuralnet)
mod <- neuralnet(Y1 ~ X1 + X2 + X3, data = neuraldat, hidden = 5)</pre>
garson(mod)
## using caret
library(caret)
mod <- train(Y1 ~ X1 + X2 + X3, method = 'nnet', data = neuraldat, linout = TRUE)</pre>
garson(mod)
## modify the plot using ggplot2 syntax
library(ggplot2)
mod <- nnet(Y1 ~ X1 + X2 + X3, data = neuraldat, size = 5)</pre>
cols <- heat.colors(10)</pre>
garson(mod) +
  scale_y_continuous('Rel. Importance', limits = c(-1, 1)) +
  scale_fill_gradientn(colours = cols) +
  scale_colour_gradientn(colours = cols)
## End(Not run)
```

get\_ys

#### Get y locations for layers in plotnet

#### Description

Get y locations for input, hidden, output layers in plotnet

#### Usage

```
get_ys(lyr, max_sp, struct, y_range)
```

| lyr     | numeric indicating layer for getting y locations |
|---------|--|
| max_sp  | logical indicating if space is maximized in plot |
| struct  | numeric vector for network structure             |
| y_range | numeric vector indicating limits of y axis       |

layer\_lines

#### Description

Plot connection weights in plotnet

#### Usage

```
layer_lines(
 mod_in,
 h_layer,
 layer1 = 1,
  layer2 = 2,
 out_layer = FALSE,
  nid,
  rel_rsc,
 all_in,
 pos_col,
 neg_col,
 x_range,
 y_range,
 line_stag,
  x_names,
  layer_x,
  struct,
 max_sp,
 prune_col = NULL,
 prune_lty = "dashed",
  skip
)
```

| mod_in    | neural network model object  |
|-----------|--|
| h_layer   | numeric indicating which connections to plot for the layer   |
| layer1    | numeric indicating order of first layer (for multiple hiden layers)  |
| layer2    | numeric indicating order of second layer (for multiple hiden layers)   |
| out_layer | logical indicating if the lines are for the output layer   |
| nid       | logical value indicating if neural interpretation diagram is plotted, default $\ensuremath{TRUE}$  |
| rel_rsc   | numeric indicating the scaling range for the width of connection weights in a neural interpretation diagram. Default is NULL for no rescaling. |
| all_in    | chr string indicating names of input variables for which connections are plotted, default all  |
| pos_col   | chr string indicating color of positive connection weights, default 'black'  |

#### layer\_points

| neg_col   | chr string indicating color of negative connection weights, default 'grey' |
|-----------|--|
| x_range   | numeric of x axis range for base plot                                      |
| y_range   | numeric of y axis range for base plot                                      |
| line_stag | numeric value that specifies distance of connection weights from nodes     |
| x_names   | chr string for names of input variables                                    |
| layer_x   | numeric indicating locations of layers on x axis                           |
| struct    | numeric vector for network structure                                       |
| max_sp    | logical indicating if space is maximized in plot                           |
| prune_col | chr string indicating color of pruned connections, otherwise not shown     |
| prune_lty | line type for pruned connections, passed to segments                       |
| skip      | logical to plot connections for skip layer                                 |

layer\_points

Plot neural network nodes

# Description

Plot neural network nodes in plotnet

## Usage

```
layer_points(
  layer,
 x_loc,
 x_range,
 layer_name,
 cex_val,
 circle_cex,
 bord_col,
  in_col,
 node_labs,
 line_stag,
 var_labs,
 x_names,
 y_names,
  . . .
)
```

| layer   | specifies which layer, integer from struct                          |
|---------|---|
| x_loc   | indicates $x$ location for layer, integer from <code>layer_x</code> |
| x_range | numeric for total range of x-axis                                   |

| layer_name | string indicating text to put in node                              |
|------------|--|
| cex_val    | numeric indicating size of point text                              |
| circle_cex | numeric indicating size of circles                                 |
| bord_col   | chr string indicating border color around nodes, default lightblue |
| in_col     | chr string indicating interior color of nodes                      |
| node_labs  | logical indicating if node labels are to be plotted                |
| line_stag  | numeric indicating distance between of text from nodes             |
| var_labs   | chr string for variable labels                                     |
| x_names    | chr string for alternative names of input nodes                    |
| y_names    | chr string for alternative names of output nodes                   |
|            | values passed to get_ys  |

lekgrps

*Create optional barplot for* **lekprofile** *groups* 

#### Description

Create optional barplot of constant values of each variable for each group used with lekprofile

#### Usage

lekgrps(grps, position = "dodge", grp\_nms = NULL)

#### Arguments

| grps     | <pre>data.frame of values for each variable in each group used to create groups in<br/>lekprofile</pre> |
|----------|---|
| position | chr string indicating bar position (e.g., 'dodge', 'fill', 'stack'), passed to geom_bar                 |
| grp_nms  | optional chr string of alternative names for groups in legend   |

#### Value

A ggplot object

#### Examples

```
## enters used with kmeans clustering
x <- neuraldat[, c('X1', 'X2', 'X3')]
grps <- kmeans(x, 6)$center</pre>
```

lekgrps(grps)

lekprofile

#### Description

Conduct a sensitivity analysis of model responses in a neural network to input variables using Lek's profile method

#### Usage

```
lekprofile(mod_in, ...)
## Default S3 method:
lekprofile(
 mod_in,
 xvars,
 ysel = NULL,
 xsel = NULL,
 steps = 100,
 group_vals = seq(0, 1, by = 0.2),
 val_out = FALSE,
 group_show = FALSE,
 grp_nms = NULL,
 position = "dodge",
)
## S3 method for class 'nnet'
lekprofile(mod_in, xsel = NULL, ysel = NULL, ...)
## S3 method for class 'mlp'
lekprofile(mod_in, xvars, yvars, xsel = NULL, ysel = NULL, ...)
## S3 method for class 'train'
lekprofile(mod_in, xsel = NULL, ysel = NULL, ...)
## S3 method for class 'nn'
```

# lekprofile(mod\_in, xsel = NULL, ysel = NULL, ...)

| mod_in | input object for which an organized model list is desired. The input can be an object of class nnet or $mlp$ |
|--------|--|
|        | arguments passed to other methods  |
| xvars  | data.frame of explanatory variables used to create the input model, only needed for mlp objects              |

| ysel       | chr string indicating which response variables to plot if more than one, defaults to all  |
|------------|---|
| xsel       | chr string of names of explanatory variables to plot, defaults to all   |
| steps      | numeric value indicating number of observations to evaluate for each explana-<br>tory variable from minimum to maximum value, default 100   |
| group_vals | numeric vector with values from 0-1 indicating quantile values at which to hold<br>other explanatory variables constant or a single value indicating number of clus-<br>ters to define grouping scheme, see details |
| val_out    | logical value indicating if actual sensitivity values are returned rather than a plot, default FALSE  |
| group_show | logical if a barplot is returned that shows the values at which explanatory vari-<br>ables were held constant while not being evaluated   |
| grp_nms    | optional chr string of alternative names for groups in legend   |
| position   | chr string indicating bar position (e.g., 'dodge', 'fill', 'stack'), passed to geom_bar<br>used if group_show = TRUE  |
| yvars      | data.frame of explanatory variables used to create the input model, only needed for mlp objects   |

#### Details

The Lek profile method is described briefly in Lek et al. 1996 and in more detail in Gevrey et al. 2003. The profile method is fairly generic and can be extended to any statistical model in R with a predict method. However, it is one of few methods used to evaluate sensitivity in neural networks.

The profile method can be used to evaluate the effect of explanatory variables by returning a plot of the predicted response across the range of values for each separate variable. The original profile method evaluated the effects of each variable while holding the remaining explanatory variables at different quantiles (e.g., minimum, 20th percentile, maximum). This is implemented in in the function by creating a matrix of values for explanatory variables where the number of rows is the number of observations and the number of columns is the number of explanatory variables. All explanatory variables are held at their mean (or other constant value) while the variable of interest is sequenced from its minimum to maximum value across the range of observations. This matrix (or data frame) is then used to predict values of the response variable from a fitted model object. This is repeated for each explanatory variable to obtain all response curves. Values passed to group\_vals must range from zero to one to define the quantiles for holding unevaluated explanatory variables.

An alternative implementation of the profile method is to group the unevaluated explanatory variables using groupings defined by the statistical properties of the data. Covariance among predictors may present unlikely scenarios if holding all unevaluated variables at the same level. To address this issue, the function provides an option to hold unevaluated variable at mean values defined by natural clusters in the data. kmeans clustering is used on the input data.frame of explanatory variables if the argument passed to group\_vals is an integer value greater than one. The centers of the clusters are then used as constant values for the unevaluated variables. An arbitrary grouping scheme can also be passed to group\_vals as a data.frame where the user can specify exact values for holding each value constant (see the examples).

For all plots, the legend with the 'Groups' label indicates the colors that correspond to each group. The groups describe the values at which unevaluated explanatory variables were held constant,

#### lekprofile

either as specific quantiles, group assignments based on clustering, or in the arbitrary grouping defined by the user. The constant values of each explanatory variable for each group can be viewed as a barplot by using group\_show = TRUE.

Note that there is no predict method for neuralnet objects from the nn package. The lekprofile method for nn objects uses the nnet package to recreate the input model, which is then used for the sensitivity predictions. This approach only works for networks with one hidden layer.

#### Value

A ggplot object for plotting if val\_out = FALSE, otherwise a two-element list is returned with a data.frame in long form showing the predicted responses at different values of the explanatory variables and the grouping scheme that was used to hold unevaluated variables constant.

#### References

Beck, M.W. 2018. NeuralNetTools: Visualization and Analysis Tools for Neural Networks. Journal of Statistical Software. 85(11):1-20.

Lek, S., Delacoste, M., Baran, P., Dimopoulos, I., Lauga, J., Aulagnier, S. 1996. Application of neural networks to modelling nonlinear relationships in Ecology. Ecological Modelling. 90:39-52.

Gevrey, M., Dimopoulos, I., Lek, S. 2003. Review and comparison of methods to study the contribution of variables in artificial neural network models. Ecological Modelling. 160:249-264.

Olden, J.D., Joy, M.K., Death, R.G. 2004. An accurate comparison of methods for quantifying variable importance in artificial neural networks using simulated data. Ecological Modelling. 178:389-397.

#### Examples

| ## using nnet   |
|---|
| library(nnet)   |
| set.seed(123)   |
| mod <- nnet(Y1 ~ X1 + X2 + X3, data = neuraldat, size = 5)                    |
| <pre>lekprofile(mod)</pre>  |
| ## Not run:<br>## using RSNNS, no bias layers                                 |
| library(RSNNS)  |
| x <- neuraldat[, c('X1', 'X2', 'X3')]<br>y <- neuraldat[, 'Y1', drop = FALSE] |
| mod <- mlp(x, y, size = 5)  |
| <pre>lekprofile(mod, xvars = x)</pre>   |
| ## using neuralnet  |

#### neuraldat

```
library(neuralnet)
mod <- neuralnet(Y1 ~ X1 + X2 + X3, data = neuraldat, hidden = 5)</pre>
lekprofile(mod)
## back to nnet, not using formula to create model
## y variable must have a name attribute
mod <- nnet(x, y, size = 5)
lekprofile(mod)
## using caret
library(caret)
mod <- train(Y1 ~ X1 + X2 + X3, method = 'nnet', data = neuraldat, linout = TRUE)</pre>
lekprofile(mod)
## group by clusters instead of sequencing by quantiles
mod <- nnet(Y1 ~ X1 + X2 + X3, data = neuraldat, size = 5)</pre>
lekprofile(mod, group_vals = 6) # six clusters
## enter an arbitrary grouping scheme for the group values
## i.e. hold all values at 0.5
group_vals <- rbind(rep(0.5, length = ncol(x)))</pre>
group_vals <- data.frame(group_vals)</pre>
names(group_vals) <- names(group_vals)</pre>
lekprofile(mod, group_vals = group_vals, xsel = 'X3')
## End(Not run)
```

neuraldat

Simulated dataset for function examples

#### Description

A simulated dataset of 2000 observations containing two response variables and three explanatory variables. Explanatory variables were sampled from a standard normal distribution. Response variables were linear combinations of the explanatory variables. The response variables Y1 and Y2 are standardized from 0 to 1.

#### Usage

neuraldat

#### neuralskips

#### Format

A data frame with 2000 rows and 5 variables:

- Y1 numeric
- Y2 numeric
- X1 numeric
- X2 numeric
- X3 numeric ...

neuralskips

#### Get weights for the skip layer in a neural network

#### Description

Get weights for the skip layer in a neural network, only valid for networks created using skip = TRUE with the nnet function.

#### Usage

```
neuralskips(mod_in, ...)
## S3 method for class 'nnet'
neuralskips(mod_in, rel_rsc = NULL, ...)
```

#### Arguments

| mod_in  | input object for which an organized model list is desired.  |
|---------|---|
|         | arguments passed to other methods   |
| rel_rsc | numeric indicating the scaling range for the width of connection weights in a neural interpretation diagram. Default is NULL for no rescaling. Scaling is relative to all weights, not just those in the primary network. |

#### Details

This function is similar to neuralweights except only the skip layer weights are returned.

#### Value

Returns a list of connections for each output node, where each element of the list is the connection for each input node in sequential order to the respective output node. The first weight in each element is not the bias connection, unlike the results for neuralweights.

#### Examples

```
data(neuraldat)
set.seed(123)
## using nnet
library(nnet)
mod <- nnet(Y1 ~ X1 + X2 + X3, data = neuraldat, size = 5, linout = TRUE,
    skip = TRUE)
neuralskips(mod)</pre>
```

neuralweights Get weights for a neural network

#### Description

Get weights for a neural network in an organized list by extracting values from a neural network object. This function is generally not called by itself.

#### Usage

```
neuralweights(mod_in, ...)
## S3 method for class 'numeric'
neuralweights(mod_in, rel_rsc = NULL, struct, ...)
## S3 method for class 'nnet'
neuralweights(mod_in, rel_rsc = NULL, ...)
## S3 method for class 'mlp'
neuralweights(mod_in, rel_rsc = NULL, ...)
## S3 method for class 'nn'
neuralweights(mod_in, rel_rsc = NULL, ...)
```

#### Arguments

| mod_in  | input object for which an organized model list is desired. The input can be an object of class numeric, nnet, mlp, or nn   |
|---------|--|
|         | arguments passed to other methods  |
| rel_rsc | numeric indicating the scaling range for the width of connection weights in a neural interpretation diagram. Default is NULL for no rescaling.   |
| struct  | numeric vector equal in length to the number of layers in the network. Each<br>number indicates the number of nodes in each layer starting with the input and<br>ending with the output. An arbitrary number of hidden layers can be included. |

16

#### neuralweights

#### Details

Each element of the returned list is named using the construct 'layer node', e.g. 'out 1' is the first node of the output layer. Hidden layers are named using three values for instances with more than one hidden layer, e.g., 'hidden 1 1' is the first node in the first hidden layer, 'hidden 1 2' is the second node in the first hidden layer, 'hidden 2 1' is the first node in the second hidden layer, etc. The values in each element of the list represent the weights entering the specific node from the preceding layer in sequential order, starting with the bias layer if applicable. For example, the elements in a list item for 'hidden 1 1' of a neural network with a 3 5 1 structure (3 inputs, 5 hidden nodes, 1 output) would have four values indicating the weights in sequence from the bias layer, first input layer, second input layer, and third input layer going to the first hidden node.

The function will remove direct weight connections between input and output layers if the neural network was created with a skip-layer using skip = TRUE with the nnet or train functions. This may produce misleading results when evaluating variable performance with the garson function.

#### Value

Returns a two-element list with the first element being a vector indicating the number of nodes in each layer of the neural network and the second element being a named list of weight values for the input model.

#### Examples

```
data(neuraldat)
set.seed(123)
## using numeric input
wts_in <- c(13.12, 1.49, 0.16, -0.11, -0.19, -0.16, 0.56, -0.52, 0.81)
struct <- c(2, 2, 1) #two inputs, two hidden, one output</pre>
neuralweights(wts_in, struct = struct)
## using nnet
library(nnet)
mod <- nnet(Y1 \sim X1 + X2 + X3, data = neuraldat, size = 5, linout = TRUE)
neuralweights(mod)
## Not run:
## using RSNNS, no bias layers
library(RSNNS)
x <- neuraldat[, c('X1', 'X2', 'X3')]</pre>
y <- neuraldat[, 'Y1']</pre>
mod <- mlp(x, y, size = 5, linOut = TRUE)</pre>
neuralweights(mod)
```

```
# pruned model using code from RSSNS pruning demo
pruneFuncParams <- list(max_pr_error_increase = 10.0, pr_accepted_error = 1.0,
    no_of_pr_retrain_cycles = 1000, min_error_to_stop = 0.01, init_matrix_value = 1e-6,
    input_pruning = TRUE, hidden_pruning = TRUE)
mod <- mlp(x, y, size = 5, pruneFunc = "OptimalBrainSurgeon",
    pruneFuncParams = pruneFuncParams)
neuralweights(mod)
## using neuralnet
library(neuralnet)
mod <- neuralnet(Y1 ~ X1 + X2 + X3, data = neuraldat, hidden = 5)
neuralweights(mod)
## End(Not run)
```

```
olden
```

*Variable importance using connection weights* 

#### Description

Relative importance of input variables in neural networks as the sum of the product of raw inputhidden, hidden-output connection weights, proposed by Olden et al. 2004.

#### Usage

```
olden(mod_in, ...)
## Default S3 method:
olden(
   mod_in,
   x_names,
   y_names,
   out_var = NULL,
   bar_plot = TRUE,
   x_lab = NULL,
   y_lab = NULL,
   skip_wts = NULL,
   ...
)
## S3 method for class 'numeric'
olden(mod_in, struct, ...)
```

#### olden

```
## S3 method for class 'nnet'
olden(mod_in, ...)
## S3 method for class 'mlp'
olden(mod_in, ...)
## S3 method for class 'nn'
olden(mod_in, ...)
## S3 method for class 'train'
olden(mod_in, ...)
```

#### Arguments

| mod_in   | input model object or a list of model weights as returned from neuralweights if using the default method   |
|----------|--|
|          | arguments passed to or from other methods  |
| x_names  | chr string of input variable names, obtained from the model object   |
| y_names  | chr string of response variable names, obtained from the model object  |
| out_var  | chr string indicating the response variable in the neural network object to be<br>evaluated. Only one input is allowed for models with more than one response.<br>Names must be of the form 'Y1', 'Y2', etc. if using numeric values as weight<br>inputs for mod_in. |
| bar_plot | logical indicating if a ggplot object is returned (default T), otherwise numeric values are returned   |
| x_lab    | chr string of alternative names to be used for explanatory variables in the figure, default is taken from mod_in   |
| y_lab    | chr string of alternative names to be used for response variable in the figure, default is taken from out_var  |
| skip_wts | vector from neuralskips for nnet models with skip-layer connections  |
| struct   | numeric vector equal in length to the number of layers in the network. Each<br>number indicates the number of nodes in each layer starting with the input and<br>ending with the output. An arbitrary number of hidden layers can be included.                       |

#### Details

This method is similar to Garson's algorithm (Garson 1991, modified by Goh 1995) in that the connection weights between layers of a neural network form the basis for determining variable importance. However, Olden et al. 2004 describe a connection weights algorithm that consistently out-performed Garson's algorithm in representing the true variable importance in simulated datasets. This 'Olden' method calculates variable importance as the product of the raw input-hidden and hidden-output connection weights between each input and output neuron and sums the product across all hidden neurons. An advantage of this approach is the relative contributions of each connection weight are maintained in terms of both magnitude and sign as compared to Garson's algorithm which only considers the absolute magnitude. For example, connection weights that change sign (e.g., positive to negative) between the input-hidden to hidden-output layers would

have a cancelling effect whereas Garson's algorithm may provide misleading results based on the absolute magnitude. An additional advantage is that Olden's algorithm is capable of evaluating neural networks with multiple hidden layers wheras Garson's was developed for networks with a single hidden layer.

The importance values assigned to each variable are in units that are based directly on the summed product of the connection weights. The actual values should only be interpreted based on relative sign and magnitude between explanatory variables. Comparisons between different models should not be made.

The Olden function also works with networks that have skip layers by adding the input-output connection weights to the final summed product of all input-hidden and hidden-output connections. This was not described in the original method so interpret with caution.

By default, the results are shown only for the first response variable for networks with multiple output nodes. The plotted response variable can be changed with out\_var.

#### Value

A ggplot object for plotting if bar\_plot = FALSE, otherwise a data.frame of relative importance values for each input variable.

#### References

Beck, M.W. 2018. NeuralNetTools: Visualization and Analysis Tools for Neural Networks. Journal of Statistical Software. 85(11):1-20.

Garson, G.D. 1991. Interpreting neural network connection weights. Artificial Intelligence Expert. 6(4):46-51.

Goh, A.T.C. 1995. Back-propagation neural networks for modeling complex systems. Artificial Intelligence in Engineering. 9(3):143-151.

Olden, J.D., Jackson, D.A. 2002. Illuminating the 'black-box': a randomization approach for understanding variable contributions in artificial neural networks. Ecological Modelling. 154:135-150.

Olden, J.D., Joy, M.K., Death, R.G. 2004. An accurate comparison of methods for quantifying variable importance in artificial neural networks using simulated data. Ecological Modelling. 178:389-397.

#### Examples

## using numeric input

wts\_in <- c(13.12, 1.49, 0.16, -0.11, -0.19, -0.16, 0.56, -0.52, 0.81)
struct <- c(2, 2, 1) #two inputs, two hidden, one output</pre>

```
olden(wts_in, struct)
```

## using nnet

library(nnet)

data(neuraldat)
set.seed(123)

```
mod <- nnet(Y1 ~ X1 + X2 + X3, data = neuraldat, size = 5)</pre>
olden(mod)
## Not run:
## View the difference for a model w/ skip layers
set.seed(123)
mod <- nnet(Y1 ~ X1 + X2 + X3, data = neuraldat, size = 5, skip = TRUE)</pre>
olden(mod)
## using RSNNS, no bias layers
library(RSNNS)
x <- neuraldat[, c('X1', 'X2', 'X3')]</pre>
y <- neuraldat[, 'Y1']</pre>
mod <- mlp(x, y, size = 5)
olden(mod)
## using neuralnet
library(neuralnet)
mod <- neuralnet(Y1 ~ X1 + X2 + X3, data = neuraldat, hidden = 5)</pre>
olden(mod)
## using caret
library(caret)
mod <- train(Y1 ~ X1 + X2 + X3, method = 'nnet', data = neuraldat, linout = TRUE)</pre>
olden(mod)
## multiple hidden layers
x <- neuraldat[, c('X1', 'X2', 'X3')]</pre>
y <- neuraldat[, 'Y1']
mod <- mlp(x, y, size = c(5, 7, 6), linOut = TRUE)
olden(mod)
## End(Not run)
```

plotnet

Plot a neural network model

#### Description

Plot a neural interpretation diagram for a neural network object

#### Usage

```
plotnet(mod_in, ...)
## Default S3 method:
plotnet(
 mod_in,
  x_names,
  y_names,
  struct = NULL,
 nid = TRUE,
  all_out = TRUE,
  all_in = TRUE,
  bias = TRUE,
 bias_y = 0.95,
  rel_rsc = c(1, 7),
  circle_cex = 5,
  node_labs = TRUE,
  var_labs = TRUE,
  line_stag = NULL,
  cex_val = 1,
  alpha_val = 1,
  circle_col = "lightblue",
  pos_col = "black",
  neg_col = "grey",
  bord_col = "lightblue",
 max_sp = FALSE,
  pad_x = 1,
  prune_col = NULL,
  prune_lty = "dashed",
  skip = NULL,
  . . .
)
## S3 method for class 'nnet'
plotnet(mod_in, x_names = NULL, y_names = NULL, skip = FALSE, ...)
## S3 method for class 'numeric'
plotnet(mod_in, struct, x_names = NULL, y_names = NULL, ...)
## S3 method for class 'mlp'
plotnet(
 mod_in,
 x_names = NULL,
 y_names = NULL,
```

22

```
prune_col = NULL,
prune_lty = "dashed",
...
)
## S3 method for class 'nn'
plotnet(mod_in, x_names = NULL, y_names = NULL, ...)
## S3 method for class 'train'
plotnet(mod_in, x_names = NULL, y_names = NULL, skip = FALSE, ...)
```

| mod_in     | neural network object or numeric vector of weights   |
|------------|--|
|            | additional arguments passed to or from other methods   |
| x_names    | chr string indicating names for input variables, default from model object   |
| y_names    | chr string indicating names for output variables, default from model object  |
| struct     | numeric vector equal in length to the number of layers in the network. Each<br>number indicates the number of nodes in each layer starting with the input and<br>ending with the output. An arbitrary number of hidden layers can be included. |
| nid        | logical value indicating if neural interpretation diagram is plotted, default TRUE   |
| all_out    | chr string indicating names of response variables for which connections are plot-<br>ted, default all  |
| all_in     | chr string indicating names of input variables for which connections are plotted, default all  |
| bias       | logical value indicating if bias nodes and connections are plotted, default TRUE   |
| bias_y     | value from 0 to 1 for locattion of bias nodes on y-axis  |
| rel_rsc    | numeric indicating the scaling range for the width of connection weights   |
| circle_cex | numeric value indicating size of nodes, default 5  |
| node_labs  | logical value indicating if labels are plotted directly on nodes, default TRUE   |
| var_labs   | logical value indicating if variable names are plotted next to nodes, default TRUE   |
| line_stag  | numeric value that specifies distance of connection weights from nodes   |
| cex_val    | numeric value indicating size of text labels, default 1  |
| alpha_val  | numeric value (0-1) indicating transparency of connections, default 1  |
| circle_col | chr string indicating color of nodes, default 'lightblue', or two element list<br>with first element indicating color of input nodes and second indicating color of<br>remaining nodes   |
| pos_col    | chr string indicating color of positive connection weights, default 'black'  |
| neg_col    | chr string indicating color of negative connection weights, default 'grey'   |
| bord_col   | chr string indicating border color around nodes, default 'lightblue'   |
| max_sp     | logical value indicating if space between nodes in each layer is maximized, de-<br>fault FALSE   |

| pad_x     | numeric for increasing or decreasing padding on the x-axis, values less than one will increase padding and values greater than one will decrease padding |
|-----------|--|
| prune_col | chr string indicating color of pruned connections, otherwise not shown   |
| prune_lty | line type for pruned connections, passed to segments   |
| skip      | logical if skip layer connections are plotted instead of the primary network   |

#### Details

This function plots a neural network as a neural interpretation diagram as in Ozesmi and Ozesmi (1999). Options to plot without color-coding or shading of weights are also provided. The default settings plot positive weights between layers as black lines and negative weights as grey lines. Line thickness is in proportion to relative magnitude of each weight. The first layer includes only input variables with nodes labelled arbitrarily as 11 through In for n input variables. One through many hidden layers are plotted with each node in each layer labelled as H1 through Hn. The output layer is plotted last with nodes labeled as O1 through On. Bias nodes connected to the hidden and output layers are also shown. Neural networks created using mlp do not show bias layers.

A primary network and a skip layer network can be plotted for nnet models with a skip layer connection. The default is to plot the primary network, whereas the skip layer network can be viewed with skip = TRUE. If nid = TRUE, the line widths for both the primary and skip layer plots are relative to all weights. Viewing both plots is recommended to see which network has larger relative weights. Plotting a network with only a skip layer (i.e., no hidden layer, size = 0) will include bias connections to the output layer, whereas these are not included in the plot of the skip layer if size is greater than zero.

The numeric method for plotting requires the input weights to be in a specific order given the structure of the network. An additional argument struct (from neuralweights is also required that lists the number of nodes in the input, hidden, and output layers. The example below for the numeric input shows the correct weight vector for a simple neural network model with two input variables, one output variable, and one hidden layer with two nodes. Bias nodes are also connected to the hidden and output layer. Using the plot syntax of I, H, O, and B for input, hidden, output, and bias to indicate weighted connections between layers, the correct weight order for the mod\_in vector is B1-H1, I1-H1, I2-H1, B1-H2, I1-H2, I2-H2, B2-O1, H1-O1, H2-O1. For a generic network (three layers) with n input nodes, j hidden nodes, and k output nodes, the weights are ordered as the connections from B1, I1,...,In to H1,...,Hj, then B2, H1,...,Hj to O1,...,Ok.

#### Value

A graphics object unless wts\_only = TRUE, then neural network weights from neuralweights.

#### References

Beck, M.W. 2018. NeuralNetTools: Visualization and Analysis Tools for Neural Networks. Journal of Statistical Software. 85(11):1-20.

Ozesmi, S.L., Ozesmi, U. 1999. An artificial neural network approach to spatial habitat modeling with interspecific interaction. Ecological Modelling. 116:15-31.

#### Examples

```
## using numeric input
# B1-H1, I1-H1, I2-H1, B1-H2, I1-H2, I2-H2, B2-O1, H1-O1, H2-O1.
wts_in <- c(13.12, 1.49, 0.16, -0.11, -0.19, -0.16, 0.56, -0.52, 0.81)
struct <- c(2, 2, 1) #two inputs, two hidden, one output</pre>
plotnet(wts_in, struct = struct)
# numeric input, two hidden layers
# B1-H11, I1-H11, I2-H11, B1-H12, I1-H12, I2-H12, B2-H21, H11-H21, H12-H21,
# B2-H22, H11-H22, H12-H22, B3-01, H21-01, H22-01
wts_in <- c(1.12, 1.49, 0.16, -0.11, -0.19, -0.16, 0.5, 0.2, -0.12, -0.1,
0.89, 0.9, 0.56, -0.52, 0.81)
struct <- c(2, 2, 2, 1) # two inputs, two (two nodes each), one output</pre>
plotnet(wts_in, struct = struct)
## using nnet
library(nnet)
data(neuraldat)
set.seed(123)
mod <- nnet(Y1 \sim X1 + X2 + X3, data = neuraldat, size = 5)
plotnet(mod)
## plot the skip layer from nnet model
mod <- nnet(Y1 ~ X1 + X2 + X3, data = neuraldat, size = 5, skip = TRUE)</pre>
plotnet(mod, skip = TRUE)
## Not run:
## using RSNNS, no bias layers
library(RSNNS)
x <- neuraldat[, c('X1', 'X2', 'X3')]</pre>
y <- neuraldat[, 'Y1']</pre>
mod <- mlp(x, y, size = 5)
plotnet(mod)
# pruned model using code from RSSNS pruning demo
pruneFuncParams <- list(max_pr_error_increase = 10.0, pr_accepted_error = 1.0,</pre>
no_of_pr_retrain_cycles = 1000, min_error_to_stop = 0.01, init_matrix_value = 1e-6,
 input_pruning = TRUE, hidden_pruning = TRUE)
mod <- mlp(x, y, size = 5, pruneFunc = "OptimalBrainSurgeon",</pre>
```

```
plotnet
```

```
pruneFuncParams = pruneFuncParams)
plotnet(mod)
plotnet(mod, prune_col = 'lightblue')
## using neuralnet
library(neuralnet)
mod <- neuralnet(Y1 ~ X1 + X2 + X3, data = neuraldat, hidden = 5)</pre>
plotnet(mod)
## using caret
library(caret)
mod <- train(Y1 ~ X1 + X2 + X3, method = 'nnet', data = neuraldat, linout = TRUE)</pre>
plotnet(mod)
## a more complicated network with categorical response
AND <- c(rep(0, 7), 1)
OR <- c(0, rep(1, 7))
binary_data <- data.frame(expand.grid(c(0, 1), c(0, 1), c(0, 1)), AND, OR)</pre>
mod <- neuralnet(AND + OR ~ Var1 + Var2 + Var3, binary_data,</pre>
hidden = c(6, 12, 8), rep = 10, err.fct = 'ce', linear.output = FALSE)
plotnet(mod)
## recreate the previous example with numeric inputs
# get the weights and structure in the right format
wts <- neuralweights(mod)</pre>
struct <- wts$struct</pre>
wts <- unlist(wts$wts)</pre>
# plot
plotnet(wts, struct = struct)
## color input nodes by relative importance
mod <- nnet(Y1 ~ X1 + X2 + X3, data = neuraldat, size = 5)</pre>
rel_imp <- garson(mod, bar_plot = FALSE)$rel_imp</pre>
cols <- colorRampPalette(c('lightgreen', 'darkgreen'))(3)[rank(rel_imp)]</pre>
plotnet(mod, circle_col = list(cols, 'lightblue'))
## End(Not run)
```

26

pred\_sens

#### Description

Get predicted values for Lek Profile method, used iteratively in lekprofile

#### Usage

pred\_sens(mat\_in, mod\_in, var\_sel, step\_val, grps, ysel)

#### Arguments

| mat_in   | data.frame of only the explanatory variables used to create model                                       |
|----------|---|
| mod_in   | any model object with a predict method  |
| var_sel  | chr string of explanatory variable to select  |
| step_val | number of values to sequence range of selected explanatory variable                                     |
| grps     | matrix of values for holding explanatory values constant, one column per variable and one row per group |
| ysel     | chr string of response variable names for correct labelling   |

#### Details

Gets predicted output for a model's response variable based on matrix of explanatory variables that are restricted following Lek's profile method. The selected explanatory variable is sequenced across a range of values. All other explanatory variables are held constant at the values in grps.

#### Value

A list of predictions where each element is a data.frame with the predicted value of the response and the values of the explanatory variable defined by var\_sel. Each element of the list corresponds to a group defined by the rows in grps at which the other explanatory variables were held constant.

#### See Also

lekprofile

#### Examples

```
## using nnet
```

library(nnet)

data(neuraldat)
set.seed(123)

mod <- nnet(Y1 ~ X1 + X2 + X3, data = neuraldat, size = 5)</pre>

mat\_in <- neuraldat[, c('X1', 'X2', 'X3')]
grps <- apply(mat\_in, 2, quantile, seq(0, 1, by = 0.2))</pre>

pred\_sens(mat\_in, mod, 'X1', 100, grps, 'Y1')

# Index

\* datasets neuraldat, 14 bias\_lines, 2  $bias_points, 3$ data.frame, *10–12*, *27* garson, 4, 17 geom\_bar, *10*, *12* get\_ys, 7, 10 ggplot, 5, 10, 13, 20 kmeans, 12 layer\_lines, 8 layer\_points, 9 lekgrps, 10 lekprofile, *10*, *11*, *27* list, 27 mlp, 24 neuraldat, 14 neuralskips, 15, 19 neuralweights, 4, 15, 16, 19, 24 nnet, 5, 15, 17, 19, 24 olden, 6, 18 plotnet, 2, 3, 7-9, 21 pred\_sens, 27

segments, 9, 24

train, 5, 17