Package 'quarrint'

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Type Package

Title Interaction Prediction Between Groundwater and Quarry Extension Using Discrete Choice Models and Artificial Neural Networks

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Description An implementation of two interaction indices between extractive activity and groundwater resources based on hazard and vulnerability parameters used in the assessment of natural hazards. One index is based on a discrete choice model and the other is relying on an artificial neural network.

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quarrint-package .	•																•								2
as.data.frame.quarry																•	•								4
compute.ann						•	•	•		•		•	•	•	•	•	•	•		•	•		•		5
compute.dc		•								•				•		•	•	•							7

quarrint-package

compute.interaction	8
int.in.range	10
quarries	11
quarry	
train.ann	17
	20

Index

quarrint-package	Interaction Prediction Between Groundwater and Quarry Extension
	Using Discrete Choice Models and Artificial Neural Networks

Description

An implementation of two interaction indices between extractive activity and groundwater resources based on hazard and vulnerability parameters used in the assessment of natural hazards. One index is based on a discrete choice model and the other is relying on an artificial neural network.

Details

Package:	quarrint
Type:	Package
Version:	1.0.0
Date:	2016-11-23
Depends:	R(>= 2.10.0), neuralnet
License:	GPL-2

This package provides two interactions indices between quarries (extractive activity) and groundwater ressources using two different methodologies, namely the discrete choice models and artificial neural networks. The design of those indices is fully detailed in Barthelemy et al. (2016).

The quarries and the groudwater ressources are described by 6 parameters, each classified into 4 modalities. These parameters are grouped into 2 distinct categories:

- the geological, hydrogeological and piezometric contexts defining the hazard that a quarry represents;
- the relative position of the quarry and the water catchments, the production of the catchments and the potential quality of the groundwater characterising the vulnerability of the groundwater resources.

Each of the resulting 3327 physically feasible combinations of these parameters (out of a theoretical number of 4.6 = 4096 possible combinations) determines one particular quarry site type. These feasible combination are provided in the data frame quarries.

Depending on the values of the parameters, the interaction index can then be low, medium, high or very high. The interaction level can then be used to inform a quarry operator on the required level of investigation before considering any extension of the quarry.

quarrint-package

The method compute.interaction provides an interface to compute the 2 interaction indices. It takes as an input an object of type quarry that can be constructed with the method quarry.

The discrete choice-based and the neural network-based indices can be respectively be computed with the functions compute.dc and compute.ann also taking as an input an object of type quarry.

The package also includes the function train.ann to allow the training of custom artificial neural network that can be used with the functions compute.ann and compute.interaction.

Finally an auxillary function int.in.range is also provided to determine if a given integer is within a specified range.

Author(s)

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References

Barthelemy, J., Carletti, T., Collier L., Hallet, V., Moriame, M., Sartenaer, A. (2016) Interaction prediction between groundwater and quarry extension using discrete choice models and artificial neural networks *Environmental Earth Sciences* (in press)

Collier, L., Barthelemy, J., Carletti, T., Moriame, M., Sartenaer, A., Hallet, H. (2015) Calculation of an Interaction Index between the Extractive Activity and Groundwater Resources *Energy Procedia* 76, 412-420

See Also

neuralnet for training and using artifical neural network and BIOGEME to estimate discrete choice models (http://biogeme.epfl.ch/home.html).

Examples

as.data.frame.quarry Coerce a Quarry to a Data Frame

Description

Coerce an object of type quarry to a data.frame. The attributes to be stored in the data frame can be specified (default: keeping every attributes).

Usage

Arguments

х	An object of type quarry.
row.names	Not used.
optional	Not used.
attr	A vector listing the dummy variables to be retained in the data frame.
	Further arguments passed to or from other methods.

Value

A data frame with the columns listed in attr.

Note

The data frame will only stores the dummy variables of the quarry.

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See Also

as.data.frame for the generic method.

Examples

coercing to a data frame

compute.ann

```
q.df <- as.data.frame(q)
# coercing to a data frame, keeping only "H1", "Z1" and "C2"
q.df.subset <- as.data.frame(q, attr = c("H1","Z1","C2"))</pre>
```

compute.ann

Neural Network-based Interaction Index for a Quarry

Description

Given an object of type quarry, a neural network computes the interaction index (low, medium, high or very high).

Usage

S3 method for class 'quarry'
compute.ann(x, ann = NULL, rep = 1, ...)

Arguments

х	A quarry object.
ann	The neural network used to estimate the interaction index. By default, if set to NULL, it uses a neural network provided by the package. The neural network is an object of class nn.
rep	The repetition of ann to be used.
	Further arguments passed to or from other methods. For instance, see compute of the package neuralnet .

Details

The neural network provided with the package has a feed-forward design and has a hidden layer of 7 nodes. It takes as an input a quarry constructed with the function "quarry" using the default parameters. This neural network is fully detailed in "Interaction prediction between groundwater and quarry extension using discrete choice models and artificial neural networks" (Barthelemy et al., 2016).

It is possible to use another neural network that has been trained with the function train.ann.

Value

A list whose elements are:

low	The output of the ann for a low interaction level.
medium	The output of the ann for a medium interaction level.
high	The output of the ann for a high interaction level.
very.high	The output of the ann for a very high interaciton level.
idx	a string with the level of interaction (low, medium, high or very high).

6

The quarry x must have been created by the quarry. It can accept custom ranges for the parameters values but they must be consistent with what has been used to train the neural network ann.

Author(s)

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References

Barthelemy, J., Carletti, T., Collier L., Hallet, H., Moriame, M., Sartenaer, A. (2016) Interaction prediction between groundwater and quarry extension using discrete choice models and artificial neural networks *Environmental Earth Sciences* (in press)

Collier, L., Barthelemy, J., Carletti, T., Moriame, M., Sartenaer, A., Hallet, H. (2015) Calculation of an Interaction Index between the Extractive Activity and Groundwater Resources *Energy Procedia* 76, 412-420

Krieselm, D. (2007) A Brief Introduction to Neural Networks. On-line available at http://www.dkriesel.com

Ripley, B. (1996) Pattern recognition and neural networks Cambridge university press

See Also

compute.dc to compute an interaction index based on a discrete choice model and compute.interaction to predict the interaction between the quarry and the groundwater using both the discrete choice-based index and the neural network-based index.

train.ann to train a neural network and use it as an input for this function.

compute and neuralnet of the package **neuralnet** for optional additional parameters and details about objects of class nn.

Examples

computing the interaction index using the default neural network
inter.idx <- compute.ann(q)</pre>

compute.dc

Description

Given an object of type quarry, the function computes the probabilities of each level of interaction (low, medium, high and very high) using a Logit discrete choice model.

Usage

S3 method for class 'quarry'
compute.dc(x, ...)

Arguments

Х	An object of type quarry.
	Further arguments passed to or from other methods.

Details

The model parameters have been estimated with BIOGEME and has an adjusted ρ^2 of 0.609. The model is fully detailed in the paper "Interaction prediction between groundwater and quarry extension using discrete choice models and artificial neural networks" (Barthelemy et al., 2016).

Value

A list whose elements are:

p.low	The probability of a low interaction level.
p.medium	The probability of a medium interaction level.
p.high	The probability of a high interaction level.
p.very.high	The probability of a very high interaciton level.

Note

In order to use the function, the quarry must have been constructed with the function quarry using the default parameters.

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References

Barthelemy, J., Carletti, T., Collier L., Hallet, V., Moriame, M., Sartenaer, A. (2016) Interaction prediction between groundwater and quarry extension using discrete choice models and artificial neural networks *Environmental Earth Sciences* (in press)

Collier, L., Barthelemy, J., Carletti, T., Moriame, M., Sartenaer, A., Hallet, V. (2015) Calculation of an Interaction Index between the Extractive Activity and Groundwater Resources *Energy Procedia* 76, 412-420

Bierlaire, M. (2003) BIOGEME: a free package for the estimation of discrete choice models. *Swiss Transport Research Conference* TRANSP-OR-CONF-2006-048

See Also

compute.ann to compute an interaction index based on an artificial neural network and compute.interaction to predict the interaction between the quarry and the groundwater using both the discrete choice-based index and the neural network-based index.

Examples

compute.interaction Compute the Interaction Index for a Quarry

Description

Computes the interaction indices between a quarry and groundwater and returns an object of class interaction.index. The function implements 2 indices based on hazard and vulnerability parameters. The levels of each index are low, medium, high and very high.

Usage

Arguments

х	A quarry object.
method	A string specifying the method to use for computing the index. Possible values are: dc for the discrete choice, ann for the neural network, all for both methods. Default is all.

fun.ann	Specify which function to be used for the neural network method. By default it is compute.ann, but it can be replaced by any function returning the same outputs.
fun.dc	Specify which function to be used for the discrete choice method. By default it is compute.dc, but it can be replaced by any function returning the same outputs.
	Further arguments passed to or from other methods. For instance, For instance the parameter ann of the function compute.ann can be passed to use a neural network different from the default one.

Value

An interaction.index object consisting of a list whose elements are

method	The selected method for computing the interaction index.
dc	The discrete choice-based interaction index computed by the function specified in fun.dc (if method = "all" or "dc").
ann	The neural network-based interaction index computed by the function specified in fun.ann (if method = "all" or "ann").
call	The matched call.

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References

Barthelemy, J., Carletti, T., Collier L., Hallet, V., Moriame, M., Sartenaer, A. (2016) Interaction prediction between groundwater and quarry extension using discrete choice models and artificial neural networks *Environmental Earth Sciences* (in press)

Collier, L., Barthelemy, J., Carletti, T., Moriame, M., Sartenaer, A., Hallet, V. (2015) Calculation of an Interaction Index between the Extractive Activity and Groundwater Resources *Energy Procedia* 76, 412-420

Bierlaire, M. (2003) BIOGEME: a free package for the estimation of discrete choice models. *Swiss Transport Research Conference* TRANSP-OR-CONF-2006-048

Krieselm, D. (2007) A Brief Introduction to Neural Networks. On-line available at http://www. dkriesel.com

Ripley, B. (1996) Pattern recognition and neural networks Cambridge university press

See Also

compute.ann and compute.dc for more details about the different interaction indices and the outputs of the corresponding functions.

train. ann to train a neural network that can be used with this function.

print to print a interaction. index object.

Examples

int.in.range Check if an object is an integer in a given range

Description

This function checks if an object is an integer in the range [low.bound, up.bound].

Usage

int.in.range(x, low.bound = 1, up.bound = 4)

Arguments

х	An object to be tested.
low.bound	The lower bound. Default value is 1.
up.bound	The upper bound. Default value is 4.

Value

TRUE if x is an integer in [low.bound, up.bound], FALSE otherwise.

Author(s)

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Examples

```
# test if x in [0,10]
x <- 5
int.in.range(x, low.bound = 0, up.bound = 10)
# test if y in [1,4]
y <- 10
int.in.range(y)</pre>
```

10

quarries

Description

Each record of the data frame details a quarry and a groudwater as well as their level of interaction. This level of interaction correspond to the environmental risk, or potential impact of the quarry on the regional hydrology.

Depending on the parameters of the quarry and the groundwater, there will be a *low*, *medium*, *high* or *very high* level of interaction. Hence, the interaction determines the level of investigation of the feasibility study to undertake before considering any extension of the quarry:

- low hydrogeology characterization;
- medium low + piezometric monitoring;
- high medium + steady state (static) mathematical model;
- very high high + transient state (dynamic) mathematical model.

The 6 retained parameters are grouped in 2 categories:

- the geological, hydrogeological and piezometric contexts defining the hazard that a quarry represents;
- the relative position of the quarry and the water catchments, the production of the catchments and the potential quality of the groundwater characterising the vulnerability of the groundwater resources.

Each of those parameters is classified into 4 modalities.

Usage

data("quarries")

Format

A data frame with 3327 observations on the following 36 variables.

ID The id of the observation.

INTERACTION An integer in [1, 4] giving the interaction level.

1. Low.

2. Medium.

3. High.

4. Very high.

- H An integer in [1, 4]. Hydrogeological context. Refers to the combinations of geological formations according to their hydrodynamic characteristics.
 - 1. Aquiclude formation.
 - 2. Aquitard formation.

- 3. Aquifer formation.
- 4. Carbonate aquifer formation.
- Z An integer in [1, 4]. Piezometric context: altimetric level of the quarry floor. Characterizes the relative position between the quarry pit bottom and the groundwater piezometric level.
 - 1. Higher than the piezometric level of the water table.
 - 2. Lower than the piezometric level of the water table but higher than the river thalweg which is the regional base level.
 - 3. Lower than the piezometric level of the water table and the altimetric level of the river thalweg which is the regional base level.
 - 4. Lower than the piezometric level of the water table and the altimetric level of the river thalweg which is not the regional level any more (the river is perched).
- G An integer in [1, 4]. Geological context. Characterizes the lithology and extension of the geological formation exploited in the quarry and those of the neighbouring geological formations that will govern the groundwater flow directions.
 - 1. Completely isolated by other formations with low permeability.
 - 2. Limited extension and partly compartmentalized.
 - 3. Local extension.
 - 4. Regional extension.
- C An integer in [1, 4]. Relative position of the quarry and the water catchments. Catchments (well, spring, gallery, etc.) for public distribution of drinking water are threatened by various sources of pollution. Closer a quarry gets to the catchment, greater its impact may be important. Consequently, 4 successive perimeters, within which the activities and facilities are regulated, are set up around the catchment based on the velocity of groundwater (transfert time).
 - 1. Outside the drainage zone of a catchment.
 - 2. In the drainage zone of a catchment.
 - 3. In the distant prevention area of a catchment (50 days of delay in case of aquifer contamination).
 - 4. In the close prevention area of a catchment (24 hours of delay in case of aquifer contamination).
- T An integer in [1, 4]. Production of the catchments. Volume exploited in catchments for public distribution in the hydrogeological formation near the quarry.
 - 1. Lower than 2 m3/h.
 - 2. Between 2 and 10 m3/h.
 - 3. Between 10 and 30 m3/h.
 - 4. Greater than 30 m3/h.
- L An integer in [1, 4]. Potential quality of the catchments. Quality and the potability of the ground-water.
 - 1. Poor quality.
 - 2. Water potabilisable with minor treatment.
 - 3. Good quality water.
 - 4. Water of exceptional quality (mineral water).

low An integer set to 1 if INTERACTION = 1, 0 otherwhise.

quarries

- medium An integer set to 1 if INTERACTION = 2, 0 otherwhise.
- high An integer set to 1 if INTERACTION = 3, 0 otherwhise.
- very.high An integer set to 1 if INTERACTION = 4, 0 otherwhise.
- H1 An integer set to 1 if H = 1, 0 otherwhise.
- H2 An integer set to 1 if H = 2, 0 otherwhise.
- H3 An integer set to 1 if H = 3, 0 otherwhise.
- H4 An integer set to 1 if H = 4, 0 otherwhise.
- Z1 An integer set to 1 if Z = 1, 0 otherwhise.
- Z2 An integer set to 1 if Z = 2, 0 otherwhise.
- Z3 An integer set to 1 if Z = 3, 0 otherwhise.
- Z4 An integer set to 1 if Z = 4, 0 otherwhise.
- G1 An integer set to 1 if G = 1, 0 otherwhise.
- G2 An integer set to 1 if G = 2, 0 otherwhise.
- G3 An integer set to 1 if G = 3, 0 otherwhise.
- G4 An integer set to 1 if G = 4, 0 otherwhise.
- C1 An integer set to 1 if C = 1, 0 otherwhise.
- C2 An integer set to 1 if C = 2, 0 otherwhise.
- C3 An integer set to 1 if C = 3, 0 otherwhise.
- C4 An integer set to 1 if C = 4, 0 otherwhise.
- T1 An integer set to 1 if T = 1, 0 otherwhise.
- T2 An integer set to 1 if T = 2, 0 otherwhise.
- T3 An integer set to 1 if T = 3, 0 otherwhise.
- T4 An integer set to 1 if T = 4, 0 otherwhise.
- L1 An integer set to 1 if L = 1, 0 otherwhise.
- L2 An integer set to 1 if L = 2, 0 otherwhise.
- L3 An integer set to 1 if L = 3, 0 otherwhise.
- L4 An integer set to 1 if L = 4, 0 otherwhise.

Source

Department of Geology, University of Namur, Namur, Belgium - https://www.unamur.be/en/ sci/geology

References

Barthelemy, J., Carletti, T., Collier L., Hallet, V., Moriame, M., Sartenaer, A. (2016) Interaction prediction between groundwater and quarry extension using discrete choice models and artificial neural networks *Environmental Earth Sciences* (in press)

Collier, L., Barthelemy, J., Carletti, T., Moriame, M., Sartenaer, A., Hallet, V. (2015) Calculation of an Interaction Index between the Extractive Activity and Groundwater Resources *Energy Procedia* 76, 412-420

quarry

Examples

```
data(quarries)
# histogram of INTERACTION levels
barplot(table(quarries$INTERACTION))
```

quarry

Create a Quarry Object

Description

This function create a S3 object of type quarry characterizing a quarry and the groundwater in the quarry's area.

A quarry object has 6 attributes, each classified (by default) in 4 modalities coded as an integer in the range [1, 4]. These attributes are grouped in 2 distinct categories:

- the geological (geological.context), hydrological (hydrogeological.context) and piezometric (piezometric.context) contexts defining the hazard that a quarry represents;
- the relative position of the quarry and the water catchments (quarry.position), the production of the catchments (production.catchment) and the potential quality (quality.catchment) of the groundwater characterising the vulnerability of the groundwater ressources.

The possible values for each attribue are described in the Argument Section.

Usage

Arguments

geological.context

The geological context of the quarry. Characterizes the lithology and extension of the geological formation exploited in the quarry and those of the neighbouring geological formations that will govern the groundwater flow directions. By default the possible values are:

- 1: completely isolated by other formations with low permeability (default);
- 2: limited extension and partly compartmentalized;
- 3: local extension;
- 4: regional extension.

14

hydrogeological.context

The hydrogeological context of the quarry. Refers to the combinations of geological formations according to their hydrodynamic characteristics. By default the possible values are:

- 1: aquiclude formation (default);
- 2: aquitard formation;
- 3: aquifer formation;
- 4: carbonate aquifer formation.

piezometric.context

The piezometric context of the quarry, i.e. the altimetric level of the quarry floor. Characterizes the relative position between the quarry pit bottom and the groundwater piezometric level. By default the possible values are:

- 1: higher than the piezometric level of the water table (default);
- 2: lower than the piezometric level of the water table but higher than the river thalweg which is the regional base level;
- 3: lower than the piezometric level of the water table and the altimetric level of the river thalweg which is the regional base level;
- 4: lower than the piezometric level of the water table and the altimetric level of the river thalweg which is not the regional level any more (the river is perched).
- quarry.position

Relative position of the quarry and the water catchments. By default the possible values are:

- 1: outside the drainage zone of a catchment (default);
- 2: in the drainage zone of a catchment;
- 3: in the distant prevention area of a catchment;
- 4: in the close prevention area of a catchment.

production.catchment

Production of the catchments. Volume exploited in catchments for public distribution in the hydrogeological formation near the quarry. By default the possible values are:

- 1: lower than 2 m3/h (default);
- 2: between 2 and 10 m3/h;
- 3: between 10 and 30 m3/h;
- 4: greater than 30 m3/h.

quality.catchment

Potential quality of the catchments. Quality and the potability of the groundwater. By default the possible values are:

- 1: poor quality (default);
- 2: water potabilisable with minor treatment
- 3: good quality water;
- 4: water of exceptional quality (mineral water).

verbose

If set to TRUE, then the print method will print the description of parameters' values instead of the integer value. Default is FALSE. Note that this parameter is only meaningfull when the parameters have values in the default range [1, 4].

	Further arguments passed to or from other methods. For instance if the val-
	ues of the variables must be in the range [1, u] instead of [1, 4], then it can
	be achieved using low.bound = 1 and up.bound = u as the function relies on int.in.range.
	inc.in. alge.
х	An object of type quarry.

Value

A quarry object consisting of a list whose elements are

G	The geological context of the quarry.
Н	The hydrogeological context of the quarry.
Z	The piezometric context of the quarry.
С	The relative position of the quarry and the water catchment.
Т	The production of the water catchments.
L	The potential quality of the water catchments.
G.dummy	A vector of binary components for the dummy variable encoding of ${\tt G}.$
H.dummy	A vector of binary components for the dummy variable encoding of $\ensuremath{H}.$
Z.dummy	A vector of binary components for the dummy variable encoding of Z.
C.dummy	A vector of binary components for the dummy variable encoding of C.
T.dummy	A vector of binary components for the dummy variable encoding of $T.$
L.dummy	A vector of binary components for the dummy variable encoding of L.

Note

By default, the modalities are integer in [1,4], but that can be changed to be an integer in any given range by passing in . . . the arguments low.bound and up.bound of the function int.in.range.

Author(s)

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References

Barthelemy, J., Carletti, T., Collier L., Hallet, V., Moriame, M., Sartenaer, A. (2016) Interaction prediction between groundwater and quarry extension using discrete choice models and artificial neural networks *Environmental Earth Sciences* (sumbitted)

Collier, L., Barthelemy, J., Carletti, T., Moriame, M., Sartenaer, A., Hallet, V. (2015) Calculation of an Interaction Index between the Extractive Activity and Groundwater Resources *Energy Procedia* 76, 412-420

train.ann

See Also

int.in.range to a use custom range for the values of the paramters.

print to print a quarry object.

as.data.frame to coerce a quarry to a data frame.

compute.interaction to predict the interaction between the quarry and the groundwater.

Examples

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Training an Artificial Neural Network for Interaction Prediction.

Description

The function trains a neural network to be used with the functions compute.interaction and compute.ann. The neural network can then be used to predict whether the level of interaction between a quarry and the groundwater is *low*, *medium*, *high* or *very high*.

The user can specify:

- the explanatory variables to be used;
- the data frame used to train and validate the network;
- the structure of the hidden layers;
- the number of repetitions for the neural network training.

Usage

Arguments

var	The explanatory variable to be used. By default, all the variables in the default data frame are used. Note that the variables must be categorical (coded with integers) and will be transformed in dummy variables. For instance if X has 5 possible values $(1,2,3,4,5)$, then it will be replaced by the binary variables X1, X2, X3, X4, X5.
data	The training and validation dataframe. It must contain the variables listed in "var" and the dependent binary variables "low", "medium", "high" and "very.high" representing the interaction level. By default, it uses the dataframe "quarries" from the package.
hidden	A vector of integer detailing the structure of the hidden layers. For instance if we want 2 hidden layers with 4 and 2 nodes respectively, then it must be it to (2, 4). The default is 7, i.e. 1 hidden layer of 7 nodes.
rep	The number of repetition of the neural network to be computed.
	Further arguments passed to or from other methods. See the documentation of "neuralnet" from the package "neuralnet".

Value

A list whose elements are:

ann	A nn object containing the trained neural network.
prop.correct.p	rediction
	A list detailing for each repetition of the neural network the proportion of correct predictions.

Author(s)

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References

Barthelemy, J., Carletti, T., Collier L., Hallet, V., Moriame, M., Sartenaer, A. (2016) Interaction prediction between groundwater and quarry extension using discrete choice models and artificial neural networks *Environmental Earth Sciences* (in press)

Collier, L., Barthelemy, J., Carletti, T., Moriame, M., Sartenaer, A., Hallet, V. (2015) Calculation of an Interaction Index between the Extractive Activity and Groundwater Resources *Energy Procedia* 76, 412-420

Krieselm, D. (2007) A Brief Introduction to Neural Networks. On-line available at http://www.dkriesel.com

Ripley, B. (1996) Pattern recognition and neural networks Cambridge university press

train.ann

See Also

The function relies on the function neuralnet of the **neuralnet** package to generate an object of type nn containing the trained neural network.

compute.interaction and compute.ann to use the trained neural network.

The data frame quarries.

Examples

19

Index

* data frame as.data.frame.quarry,4 * datasets quarries, 11 * data as.data.frame.quarry,4 * discrete choice compute.dc, 7compute.interaction, 8 quarrint-package, 2 * geology quarrint-package, 2 * hydrogeology quarrint-package, 2 * integer int.in.range, 10 * interaction quarrint-package, 2 * manip as.data.frame.quarry,4 * math int.in.range, 10 * models compute.dc, 7 compute.interaction, 8 quarrint-package, 2 * neural compute.ann, 5 compute.dc, 7 compute.interaction, 8 quarrint-package, 2 train.ann, 17 * package quarrint-package, 2 * quarry quarry, 14 * range int.in.range, 10

ann.interactions (compute.ann), 5

as.data.frame, 4, 17 as.data.frame.quarry,4 compute, 5, 6 compute.ann, 3, 5, 8, 9, 17, 19 compute.dc, *3*, *6*, *7*, *9* compute.interaction, *3*, *6*, *8*, *8*, *17*, *19* int.in.range, *3*, 10, *16*, *17* interaction.index (compute.interaction), 8 neuralnet, 3, 6, 19 print, 9, 15, 17 print.interaction.index (compute.interaction), 8 print.quarry (quarry), 14 quarries, 2, 11, 19 quarrint(quarrint-package), 2 quarrint-package, 2 quarry, 3, 6, 7, 14 train.ann, 3, 5, 6, 9, 17