## Package 'DImodels'

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Author Rafael de Andrade Moral [aut, cre], John Connolly [aut], Rishabh Vishwakarma [ctb], Caroline Brophy [aut]

Maintainer Rafael de Andrade Moral <rafael.deandrademoral@mu.ie>

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Description The 'DImodels' package is suitable for analysing data from biodiversity and ecosystem function studies using the Diversity-Interactions (DI) modelling approach introduced by Kirwan et al. (2009) <doi:10.1890/08-1684.1>. Suitable data will contain proportions for each species and a community-level response variable, and may also include additional factors, such as blocks or treatments. The package can perform data manipulation tasks, such as computing pairwise interactions (the DI\_data() function), can perform an automated model selection process (the autoDI() function) and has the flexibility to fit a wide range of user-defined DI models (the DI() function).

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DImodels-package Diversity-Interactions (DI) Models

## Description

The 'DImodels' package is suitable for analysing data from biodiversity and ecosystem function studies using the Diversity-Interactions (DI) modelling approach introduced by Kirwan et al. (2009) <doi:10.1890/08-1684.1>. Suitable data will contain proportions for each species and a community-level response variable, and may also include additional factors, such as blocks or treatments. The package can perform data manipulation tasks, such as computing pairwise interactions (the DI\_data() function), can perform an automated model selection process (the autoDI() function) and has the flexibility to fit a wide range of user-defined DI models (the DI() function).

#### Details

#### Introduction to Diversity-Interactions models

Diversity-Interactions (DI) models (Kirwan et al 2009) are a set of tools for analysing and interpreting data from experiments that explore the effects of species diversity on community-level responses; for example, the effect of increasing community diversity on biomass production in a grassland ecosystem. Most analyses of diversity experiments quantify community diversity in terms of species richness, the number of species present. The DI method modifies this presence/absence approach in mixed communities by taking species relative abundance in the community into account. So, instead of ignoring differences in community responses across communities with the same species but with different species relative abundances, the DI approach aims to understand and explain these differences.

#### What variables will a suitable dataset contain?

The DI approach assesses the effect of species diversity on a community response over a period of time. For data from a biodiversity study with *S* species to be suited to the DI approach, the variables that are required on each experimental unit are:

- 1. A set of proportions p1, p2, ..., pS that characterise the proportions of each species at a defined starting point in time. These proportions (or relative abundances) of species in the community (pi for the ith species) range between 0 (absence) and 1 (monoculture the only species present) and the sum of all the pi values for a community is always 1.
- 2. A community-level response variable, recorded a period of time after the initial species proportions were recorded.

The dataset may also contain other variables such as a block, density or treatments.

#### What are Diversity-Interactions models?

A DI model typically has three components and takes the form:

$$y = Identities + Interactions + Structures + \epsilon$$

where y is a community-level response, the *Identities* are the effects of species identities and enter the model as individual species proportions at the beginning of the time period, the *Interactions* are the interactions among the species proportions, while *Structures* include other experimental structures such as blocks, treatments or density. In a three species system, with an experimental blocking structure, a possible DI model is:

$$y = \beta_1 p 1 + \beta_2 p 2 + \beta_3 p 3 + \delta_{12} p 1 p 2 + \delta_{13} p 1 p 3 + \delta_{23} p 2 p 3 + \alpha_k + \epsilon$$

Where p1, p2 and p3 are the species proportions of species 1, 2 and 3 respectively, and  $\alpha_k$  is the effect of block k. The error term  $\epsilon$  is usually assumed to be normally distributed with mean 0 and constant variance (and assumed independent and identically distributed).

In a monoculture of the ith species, the expected performance of y in block k is  $\beta_i$ . In mixture, the *Identities* component provides the expected performance as a weighted average of monoculture responses, and the *Interactions* component is added to it to give the overall expected performance of the mixed community. The *Interactions* component addresses the question: do mixed communities perform differently from what might be expected from the weighted averaging of monoculture performances? Note that in Kirwan et al 2009 the *Interactions* component is referred to as the

diversity effect, however, here we use the more general term "*Interactions*", since the interpretation of how species diversity affects the response is a combination of both the *Identities* and *Interactions* components. The community with the best overall performance may depend on both the *Identities* and *Interactions* and will rarely be the community with the largest net interactions effect. The equation above provides an example of a DI model where there is a unique interaction term for each pair of species. It is possible to test various constraints among interactions, some of which may be motivated by the context of the data (Kirwan et al 2009).

The *Interactions* component may also include an non-linear exponent parameter  $\theta$  on each *pipj* term, where a value different to one allows the importance and impact of interaction terms to be altered (Connolly et al 2013).

#### What can the DImodels package do?

The DI approach is a full regression method where the response of the community is characterised by the effects of diversity variables such as *Identities* and *Interactions* components, and by experimental structural variables such as blocks, density and treatments. All of these may be important determinants of response and so should be included in the analysis of community responses. The DImodels package aims to make it easier to analyse data using DI models.

Currently, the DImodels package contains three main functions: autoDI, DI and DI\_data. Here we give a brief overview of each, and link to the respective help files for further information.

auto\_DI: This function gives a simple overview of the successive contribution of the *Structures*, *Identities* and *Interactions* components to the model via an automated model selection process. It will identify the 'best' model from a (limited) subset of all possible DI models. However, autoDI may need to be supplemented by more refined analysis, for example, auto\_DI does not test for interactions between the terms in the *Structures* and *Identities* components. It can also only facilitate one block, one density and one treatment variable. However, it is a very useful starting point for DI model exploration. Further information at: autoDI.

DI: This function can fit a wide range of DI models and includes the flexibility to test for multiple treatments or additional interactions, for example, between terms in the *Identities* and *Structures* components. The DI function fits one user-defined DI model at a time, and it allows for flexibility in the form of the model through a combination of in-built argument options and additional user-defined options. Further information at: DI.

DI\_data: This function can compute various forms of interactions among the *pi* variables. This function is not required when using autoDI, or for the in-built argument options in DI, but may be needed when specifying additional user-defined options in DI. Further information at: DI\_data and for examples of when it is required see DI.

There are three other functions:

- 1. theta\_CI can fit a confidence interval to the parameter theta, when it has been estimated using either autoDI or DI,
- 2. DI\_compare that can compare a fitted DI model to the 'reference' model (see autoDI) for details about the reference model), and
- 3. update\_DI that can update a fitted DI model passing different values to one or more arguments (see update\_DI) for details).

#### Challenges with fitting and interpreting Diversity-Interactions models

Analysing data using DI methods can be tricky for people familiar with ordinary regression models and the DImodels package aims to make analysis easier. The difficulties lie in:

- 1. The lack of familiarity in dealing with the *Identities* component variables *pi*, which must sum to 1. This constraint can lead to interpretative issues, and estimation problems with some widely used R software.
- 2. The novelty of specifying the *Interactions* components in terms of many pairwise interaction terms whose numbers may greatly increase with *S*. The number of pairwise terms can often be reduced by identifying biologically meaningful patterns among them, for example, through functional grouping of species. This may greatly reduce the number of coefficients to be estimated and interpreted in the model (Kirwan et al, 2009).
- 3. The introduction of a power coefficient theta ( $\theta$ ) for all pairwise interaction terms (Connolly et al, 2013). This parameter can be very useful in describing the effect of community evenness on community response, i.e., whether response changes rapidly or slowly across communities where the relative abundance of species changes from being equal for all species to dominance by one or more species.

#### Limitations of the DImodels package

Currently, the DImodels package does not support multivariate responses or repeated measurements on the same experimental unit. It also does not currently support the random effects approach to modelling pairwise interactions that was developed by Brophy et al 2017.

#### Author(s)

Rafael de Andrade Moral [aut, cre], John Connolly [aut], Rishabh Vishwakarma [ctb], Caroline Brophy [aut]

Maintainer: Rafael de Andrade Moral <rafael.deandrademoral@mu.ie>

#### References

Brophy C, A Dooley, L Kirwan, JA Finn, J McDonnell, T Bell, MW Cadotte and J Connolly. (2017) Biodiversity and ecosystem function: Making sense of numerous species interactions in multi-species communities. Ecology 98, 1771-1778.

Connolly J, T Bell, T Bolger, C Brophy, T Carnus, JA Finn, L Kirwan, F Isbell, J Levine, A Lüscher, V Picasso, C Roscher, MT Sebastia, M Suter and A Weigelt (2013) An improved model to predict the effects of changing biodiversity levels on ecosystem function. Journal of Ecology, 101, 344-355.

Kirwan L, J Connolly, JA Finn, C Brophy, A Lüscher, D Nyfeler and MT Sebastia (2009) Diversityinteraction modelling - estimating contributions of species identities and interactions to ecosystem function. Ecology, 90, 2032-2038.

#### See Also

## autoDI DI DI\_data theta\_CI

Example datasets: The Bell dataset. The sim1 dataset. The sim2 dataset. The sim3 dataset. The sim3 dataset. The sim5 dataset. The Switzerland dataset.

## Examples

## Load the Switzerland data
 data(Switzerland)

```
## Check that the proportions sum to 1 (required for DI models)
## p1 to p4 are in the 4th to 7th columns in Switzerland
 Switzerlandsums <- rowSums(Switzerland[4:7])</pre>
 summary(Switzerlandsums)
## Example of autoDI
 auto1 <- autoDI(y = "yield", density = "density", prop = c("p1","p2","p3","p4"),</pre>
                  treat = "nitrogen", FG = c("G","G","L","L"), data = Switzerland,
                  selection = "Ftest")
 summary(auto1)
## Example of DI
 m1 <- DI(y = "yield", density = "density", prop = 4:7, treat = "nitrogen",</pre>
           FG = c("G", "G", "L", "L"), DImodel = "FG", data = Switzerland)
 summary(m1)
## Example of DI_data.
## Create interaction variables and incorporate them into a new data frame Switzerland2.
## Switzerland2 will contain the new variables: AV, E, p1_add, p2_add, p3_add, p4_add,
## bfg_G_L, wfg_G, wfg_L.
 FG_matrix <- DI_data(prop = c("p1", "p2", "p3", "p4"), FG = c("G", "G", "L", "L"),</pre>
                        data = Switzerland, what = "FG")
 Switzerland2 <- data.frame(Switzerland, FG_matrix)</pre>
```

autoDI

Automated Diversity-Interactions Model Fitting

## Description

This function provides an automated way to fit a (limited) range of Diversity-Interactions (DI) models. Using one of several selection criteria, autoDI will identify the best DI model from the range fitted via a three-step selection process (see Details for more information). While autoDI can be a useful starting point for fitting DI models, its range of models is not exhaustive and additional model fitting or testing via DI is likely to be required. For instance, autoDI does not test for interactions of a treatment with other variables in the model.

## Usage

```
autoDI(y, prop, data, block, density, treat, ID, FG = NULL,
    selection = c("Ftest","AIC","AICc","BIC","BICC"),
    step0 = FALSE, step4 = TRUE)
```

## Arguments

У	The column name of the response vector, which must be in quotes, for example, y = "yield".
block	The name of the block variable (if present), which must be in quotes, for example, block = "block". If no blocking variable, omit this argument.

density	The name of the density variable (if present), which must be in quotes, for example, density = "density". If no density variable, omit this argument.
prop	A vector of <i>s</i> column names identifying the species proportions in each row in the dataset. For example, if the species proportions columns are labelled p1 to p4, then prop = $c("p1", "p2", "p3", "p4")$ . Alternatively, the column numbers can be specified, for example, prop = 4:7, where the species proportions are in the 4th to 7th columns.
treat	The name of a column in the dataset containing the value of a treatment factor or covariate. The treatment name must be included in quotes, for example, treat = "nitrogen". (Only one treatment or covariate is permitted in autoDI, but see DI for options involving more than one treatment.) If the treatment is a factor, the variable must already be specified as a factor prior to using autoDI.
ID	This argument takes a text list (of length <i>s</i> ) dsecirbing groupings for the identity effects of the species. For example, if there are four species and you wish to group the identity effects all four species into a single term: ID could be ID = $c("ID1", "ID1", "ID1", "ID1")$ , where "ID1" is the name of the ID group. Similarly if the we wish to have two identity effect groups where identity effect of species 1 and 3, and species 2 and 4 are grouped together: ID could be ID = $c("ID1", "ID2", "ID1", "ID2")$ , where "ID1" and "ID2" are the names of the ID groups. These ideas expand to any number of species and any number or combination of groups. Finally, the ID groups do not have to be named "ID1" and "ID2", the user can specify any name for the groups.
	• If the ID argument is not specified, each species will be assumed to have a separate identity effect.
	<ul> <li>Specify an grouping for the ID does not affect the interaction terms. The interactions are still calculated using the individual species proportions.</li> <li>The ID argument is defunct when using the custom_formula argument, since species identity effects must be included directly in the custom_formula argument.</li> </ul>
FG	If species are classified by g functional groups, this parameter gives a text list (of length s) of the functional group to which each species belongs. For example, for four grassland species with two grasses and two legumes: FG could be $FG = c("G", "G", "L", "L")$ , where G stands for grass and L stands for legume.
data	Specify the dataset, for example, data = Switzerland. The dataset name should not appear in quotes.
selection	Selection method to be used in the automated model selection process. Options are "Ftest", "AIC", "AICC", "BIC" and "BICC". The default is selection = "Ftest".
step0	By default, autoDI outputs steps 1 - 4, however, an initial step 0 can be included by specifying step0 = TRUE. This will fit a model with an intercept only, and will sequentially add in and test the inclusion of block, density and treat, if they are specified in the autoDI arguments.
step4	Step 4 performs a lack of fit test for the final model selected by steps 1 - 3. By default, step4 = TRUE, but it can be omitted by specifying step4 = FALSE.

#### Details

#### What are Diversity-Interactions models?

Diversity-Interactions (DI) models (Kirwan et al 2009) are a set of tools for analysing and interpreting data from experiments that explore the effects of species diversity on community-level responses. We recommend that users of the DImodels package read the short introduction to DI models (available at: DImodels). Further information on DI models is available in Kirwan et al 2009 and Connolly et al 2013.

#### Checks on data prior to using autoDI.

Before using autoDI, check that the species proportions for each row in your dataset sum to one. See the 'Examples' section for code to do this. An error message will be generated if the proportions don't sum to one.

## How does the autoDI function work?

The autoDI function identifies the 'best' Diversity-Interactions (DI) model from a specific range of proposed models using a three-step process of selection (Steps 1 to 3) and performs a lack of fit test on the selected model (Step 4). Only a limited subset of all possible models are examined under autoDI, for example, interactions involving experiment structural terms (block, density, treat) are not explored. The autoDI function can provide an excellent initial analysis, but often additional modelling and exploration will be required using the DI function.

Steps 1-3 outlined below provide details on the automated model selection process followed by autoDI. Step 4 is a lack of fit test for the selected model. Step 0 may also be included (step0 = TRUE) as an initial step to sequentially test the inclusion of experiment structural variables (block, density, treat), prior to fitting the DI models in Step 1.

The default selection method used is selection = "Ftest", which will return the appropriate F test statistic value(s) and p-value(s) in each step. When any of the information theoretic approaches ("AIC", "AICc", "BIC" or "BICC") are specified, the model with the lowest value is selected in each step, even if it is only the lowest by a tiny margin; therefore, it is recommended to examine the information theoretic values across all models.

## Step 1

The AV model is fitted twice: considering the non-linear parameter theta equal to 1, and estimating it by maximising the profile likelihood. For example, for a design with 4 species, for the AV model, the parameter theta enters the model as:

 $AV_theta = (p1*p2)^theta + (p1*p3)^theta + (p1*p4)^theta + (p2*p3)^theta + (p2*p4)^theta + (p3*p4)^theta$ 

In the profile likelihood estimation, theta is tested across the range 0.01 to 1.5. Then, the two models (with theta estimated and with theta set to 1) are compared using the method specified by the selection argument.

Details on DI models that include theta are described in Connolly et al 2013.

Step 2

Five models are fitted, sequentially, each building on the previous model, and compared. If in Step 1 the conclusion is that theta is not different from 1, all models are fitted without estimating theta. If, however, in Step 1 the conclusion is that theta is different from 1, all models are fitted by fixing theta to its estimate obtained in Step 1.

#### autoDI

If the experiment structural variables treat, block or density are specified, they will be included as an additive factor or covariate in **each** of the five models, but interactions between them and the DI model terms will not be included or tested.

Assume that FG (functional groups) have been specified. The five DI models are:

- STR: This model contains an intercept, and block, density and treatment if present; STR stand for 'structural' and represents experiment structural variables.
- ID: The species proportions are added to the STR model. The proportions sum to 1, and are included in the model as 0 + p1 + ... + ps, where s is the number of species in the pool, as specified in the prop option.
- AV: The terms in the ID model, plus a single 'average' pairwise interaction term. For the Switzerland dataset, the single variable that is added to the model is computed as: AV = p1\*p2 + p1\*p3 + p1\*p4 + p2\*p3 + p2\*p4 + p3\*p4.
- FG: The terms in the ID model, plus interaction terms related to functional groups. These terms describe the average effects of interaction between pairs of species within each functional group, and between pairs of species from different functional groups. For example, in the Switzerland dataset there are four species with FG = c("Grass", "Grass", "Legume", "Legume"), and there are six pairwise interactions, one between the two grasses, one between the two legumes, and four between grass and legume species. Grouping these interactions gives three terms, one for interactions between grasses, one for interactions between legumes and one for between a grass and a legume species. The model assumes that any grass will interaction with any legume in the same way and the 'between functional group grass-legume' variable is computed as: bfg\_G\_L = p1\*p3 + p1\*p4 + p2\*p3 + p2\*p4. If there were more than two grasses in the dataset, this model would assume that any pair of grasses interact in the same way, similarly for legumes. If the FG argument is not specified, this model is omitted from Step 1.
- FULL: The terms in the ID model, plus an interaction term for each pair of species. When there are *s* species, there are *s*\*(*s*-1)/2 pairwise interaction terms, i.e., for the Switzerland dataset with four species, there are six interactions that are each added to the model (in R formula syntax: p1:p2, p1:p3, p1:p4, p2:p3, p2:p4 and p3:p4).

If the FG argument is omitted, the FG model will be replaced by:

• ADD: The terms in the ID model, plus a species specific 'additive' interaction term for each species. These terms measure the interactive contribution of each species with any other species and are denoted  $\lambda_i$  for the *i*th species. The interaction between any pair of species *i* and *j* is computed as  $\lambda_i + \lambda_j$ .

If selection by information criteria is specified, both ADD and FG models will be fitted and compared using the selected information criterion.

Step 3

If treat is specified, the selected model in Step 2 includes the treat variable (since all models in Step 2 include treat if present). Here, the selected model from Step 2 is re-fitted without treat and the models with and without the treatment are compared using the method specified by the selection argument.

If treat was not specified, this step is redundant.

Step 4

Step 4 provides a lack of fit test for the model selected by Steps 1 to 3. A factor called 'community' is created that has a level for each unique setting of the species proportions (as specified in the prop argument). The 'reference' model includes all terms in the model that was selected by Steps 1 to 3, plus the factor community. The reference model is compared to the model selected by Steps 1 to 3 via an F-test (regardless of the selection argument value), thus providing a lack of fit test.

Note, that the reference model is never intended to be a candidate model, it is only fitted for the purpose of testing lack of fit. If the test result is significant, it indicates that there is a lack of fit in the Diversity-Interactions model selected by autoDI.

Note also, that the test will not work if all combinations of the species proportions are unique. In this instance, the option Step4 = FALSE should be selected.

## Value

The function returns the final selected model, an object of class DI.

#### Author(s)

Rafael A. Moral, John Connolly, Rishabh Vishwakarma and Caroline Brophy

## References

Connolly J, T Bell, T Bolger, C Brophy, T Carnus, JA Finn, L Kirwan, F Isbell, J Levine, A Lüscher, V Picasso, C Roscher, MT Sebastia, M Suter and A Weigelt (2013) An improved model to predict the effects of changing biodiversity levels on ecosystem function. Journal of Ecology, 101, 344-355.

Kirwan L, J Connolly, JA Finn, C Brophy, A Lüscher, D Nyfeler and MT Sebastia (2009) Diversityinteraction modelling - estimating contributions of species identities and interactions to ecosystem function. Ecology, 90, 2032-2038.

## See Also

#### DI

Other examples using autoDI: The sim1 dataset examples. The sim2 dataset examples. The sim3 dataset examples. The sim4 dataset examples. The sim5 dataset examples. The Switzerland dataset examples.

#### Examples

```
## Load the Switzerland data
    data(Switzerland)
## Summarise the Switzerland data
    summary(Switzerland)
## Check that the proportions sum to 1 (required for DI models)
## p1 to p4 are in the 4th to 7th columns in Switzerland
    Switzerlandsums <- rowSums(Switzerland[4:7])</pre>
```

summary(Switzerlandsums)

## Perform automated model fitting on the Switzerland dataset

```
## Model selection by F-test
 auto1 <- autoDI(y = "yield", density = "density", prop = c("p1","p2","p3","p4"),</pre>
                  treat = "nitrogen", FG = c("G", "G", "L", "L"), data = Switzerland,
                  selection = "Ftest")
 summary(auto1)
## Running autoDI after grouping identity effects using the "ID" argument
 auto2 <- autoDI(y = "yield", density = "density",</pre>
                  prop = c("p1","p2","p3","p4"),
                  treat = "nitrogen", ID = c("ID1", "ID1", "ID1", "ID1"),
                  FG = c("G", "G", "L", "L"), data = Switzerland,
                  selection = "Ftest")
 summary(auto2)
## Using column numbers to indicate which columns contain the proportions and including Step 0
 auto2 <- autoDI(y = "yield", density = "density", prop = 4:7, treat = "nitrogen",</pre>
            FG = c("G", "G", "L", "L"), data = Switzerland, selection = "Ftest", step0 = TRUE)
 summary(auto2)
## Exclude the FG (functional group) argument to include the additive species "ADD" model in Step 1
 auto3 <- autoDI(y = "yield", density = "density", prop = 4:7, treat = "nitrogen",</pre>
                  data = Switzerland, selection = "Ftest")
 summary(auto3)
```

Bell

The "Bell" Dataset

## Description

This dataset comes from a bacterial biodiversity experiment (Bell et al 2005). The bacterial ecosystems used were from semi-permanent rainpools that form in bark-lined depressions near the base of large European beech trees (*Fagus sylvatica*). Microcosms consisting of sterile beech leaf disks and 10 ml of liquid (phosphate buffer) were inoculated with random combinations of 72 bacterial species isolated from these ecosystems. A total of 1,374 microcosms were constructed at richness levels of 1, 2, 3, 4, 6, 8, 9, 12, 18, 24, 36 and 72 species. The daily respiration rate of the bacterial community in each microcosm was measured over three time intervals (days 0-7, 7-14 and 14-28) and the average over the three time intervals was recorded.

## Usage

```
data("Bell")
```

## Format

A data frame with 1374 observations on the following 76 variables:

- id A numeric vector uniquely identifying each row of the dataset.
- community A numeric vector identifying each unique community, i.e., two rows with the same community value also share the same set of p1 to p72 values.
- richness The number of species included in the initial composition, i.e., the number of proportions from p1 to p72 that are >0.
- p1 A numeric vector indicating the initial proportion of species 1 in the community.
- p2 A numeric vector indicating the initial proportion of species 2 in the community.
- p3 A numeric vector indicating the initial proportion of species 3 in the community.
- p4 A numeric vector indicating the initial proportion of species 4 in the community.
- p5 A numeric vector indicating the initial proportion of species 5 in the community.
- p6 A numeric vector indicating the initial proportion of species 6 in the community.
- p7 A numeric vector indicating the initial proportion of species 7 in the community.
- p8 A numeric vector indicating the initial proportion of species 8 in the community.
- p9 A numeric vector indicating the initial proportion of species 9 in the community.
- p10 A numeric vector indicating the initial proportion of species 10 in the community.
- p11 A numeric vector indicating the initial proportion of species 11 in the community.
- p12 A numeric vector indicating the initial proportion of species 12 in the community.
- p13 A numeric vector indicating the initial proportion of species 13 in the community.
- p14 A numeric vector indicating the initial proportion of species 14 in the community.
- p15 A numeric vector indicating the initial proportion of species 15 in the community.
- p16 A numeric vector indicating the initial proportion of species 16 in the community.
- p17 A numeric vector indicating the initial proportion of species 17 in the community.
- p18 A numeric vector indicating the initial proportion of species 18 in the community.
- p19 A numeric vector indicating the initial proportion of species 19 in the community.
- p20 A numeric vector indicating the initial proportion of species 20 in the community.
- p21 A numeric vector indicating the initial proportion of species 21 in the community.
- p22 A numeric vector indicating the initial proportion of species 22 in the community.
- p23 A numeric vector indicating the initial proportion of species 23 in the community. p24 A numeric vector indicating the initial proportion of species 24 in the community.
- p25 A numeric vector indicating the initial proportion of species 25 in the community.
- p26 A numeric vector indicating the initial proportion of species 26 in the community.
- p27 A numeric vector indicating the initial proportion of species 27 in the community.
- p28 A numeric vector indicating the initial proportion of species 27 in the community.
- p29 A numeric vector indicating the initial proportion of species 29 in the community.
- p30 A numeric vector indicating the initial proportion of species 30 in the community.
- p31 A numeric vector indicating the initial proportion of species 31 in the community.
- p32 A numeric vector indicating the initial proportion of species 32 in the community.
- p33 A numeric vector indicating the initial proportion of species 33 in the community.

A numeric vector indicating the initial proportion of species 34 in the community. p34 p35 A numeric vector indicating the initial proportion of species 35 in the community. p36 A numeric vector indicating the initial proportion of species 36 in the community. A numeric vector indicating the initial proportion of species 37 in the community. p37 A numeric vector indicating the initial proportion of species 38 in the community. p38 A numeric vector indicating the initial proportion of species 39 in the community. p39 A numeric vector indicating the initial proportion of species 40 in the community. p40 A numeric vector indicating the initial proportion of species 41 in the community. p41 p42 A numeric vector indicating the initial proportion of species 42 in the community. A numeric vector indicating the initial proportion of species 43 in the community. p43 A numeric vector indicating the initial proportion of species 44 in the community. p44 A numeric vector indicating the initial proportion of species 45 in the community. p45 A numeric vector indicating the initial proportion of species 46 in the community. p46 A numeric vector indicating the initial proportion of species 47 in the community. p47 A numeric vector indicating the initial proportion of species 48 in the community. p48 A numeric vector indicating the initial proportion of species 49 in the community. p49 A numeric vector indicating the initial proportion of species 50 in the community. p50 A numeric vector indicating the initial proportion of species 51 in the community. p51 A numeric vector indicating the initial proportion of species 52 in the community. p52 A numeric vector indicating the initial proportion of species 53 in the community. p53 A numeric vector indicating the initial proportion of species 54 in the community. p54 p55 A numeric vector indicating the initial proportion of species 55 in the community. A numeric vector indicating the initial proportion of species 56 in the community. p56 A numeric vector indicating the initial proportion of species 57 in the community. p57 p58 A numeric vector indicating the initial proportion of species 58 in the community. p59 A numeric vector indicating the initial proportion of species 59 in the community. A numeric vector indicating the initial proportion of species 60 in the community. p60 A numeric vector indicating the initial proportion of species 61 in the community. p61 p62 A numeric vector indicating the initial proportion of species 62 in the community. p63 A numeric vector indicating the initial proportion of species 63 in the community. A numeric vector indicating the initial proportion of species 64 in the community. p64 A numeric vector indicating the initial proportion of species 65 in the community. p65 A numeric vector indicating the initial proportion of species 66 in the community. p66 p67 A numeric vector indicating the initial proportion of species 67 in the community. p68 A numeric vector indicating the initial proportion of species 68 in the community. A numeric vector indicating the initial proportion of species 69 in the community. p69 A numeric vector indicating the initial proportion of species 70 in the community. p70 p71 A numeric vector indicating the initial proportion of species 71 in the community.

p72 A numeric vector indicating the initial proportion of species 72 in the community.

response A numeric vector giving the average daily respiration rate of the bacterial community.

## Details

#### What are Diversity-Interactions (DI) models?

Diversity-Interactions (DI) models (Kirwan et al 2009) are a set of tools for analysing and interpreting data from experiments that explore the effects of species diversity on community-level responses. We strongly recommend that users read the short introduction to Diversity-Interactions models (available at: DImodels). Further information on Diversity-Interactions models is also available in Kirwan et al 2009 and Connolly et al 2013.

The Bell dataset is analysed using Diversity-Interactions models in both Brophy et al 2017 and Connolly et al 2013.

## Source

Bell T, JA Newman, BW Silverman, SL Turner and AK Lilley (2005) The contribution of species richness and composition to bacterial services. Nature, 436, 1157-1160.

#### References

Brophy C, A Dooley, L Kirwan, JA Finn, J McDonnell, T Bell, MW Cadotte and J Connolly (2017) Biodiversity and ecosystem function: Making sense of numerous species interactions in multi-species communities. Ecology, 98, 1771-1778.

Connolly J, T Bell, T Bolger, C Brophy, T Carnus, JA Finn, L Kirwan, F Isbell, J Levine, A Lüscher, V Picasso, C Roscher, MT Sebastia, M Suter and A Weigelt (2013) An improved model to predict the effects of changing biodiversity levels on ecosystem function. Journal of Ecology, 101, 344-355.

Kirwan L, J Connolly, JA Finn, C Brophy, A Lüscher, D Nyfeler and MT Sebastia (2009) Diversityinteraction modelling - estimating contributions of species identities and interactions to ecosystem function. Ecology, 90, 2032-2038.

## Examples

```
## Load the Bell data
    data(Bell)
## View the first five entries
    head(Bell)
## Explore the variabes in sim1
    str(Bell)
## Check that the proportions sum to 1 (required for DI models)
## p1 to p72 are in the 4th to 75th columns in Bell
    Bellsums <- rowSums(Bell[4:75])
    summary(Bellsums)
## Check characteristics of Bell
    hist(Bell$response)
    summary(Bell$response)
    plot(Bell$richness, Bell$response)</pre>
```

```
## Fit the average pairwise model using DI and the AV tag, with theta estimated
 m1 <- DI(y = "response", prop = 4:75, DImodel = "AV", estimate_theta = TRUE, data = Bell)
 summary(m1)
 CI_95 <- theta_CI(m1, conf = .95)
 CI_95
 plot(m1)
 library(hnp)
 hnp(m1)
## Graph the profile likelihood
 library(ggplot2)
 ggplot(m1$profile_loglik, aes(x = grid, y = prof)) +
    theme_bw() +
    geom_line() +
   xlim(0, 1.5) +
   xlab(expression(theta)) +
   ylab("Log-likelihood") +
   geom_vline(xintercept = CI_95, lty = 3) +
   labs(title = " Log-likelihood versus theta",
        caption = "dotted vertical lines are upper and lower bounds of 95% CI for theta")
```

```
contrasts_DI Compute contrasts for Diversity Interactions (DI) models
```

## Description

This function calculates and tests contrasts using glht for a model object created by the DI or autoDI functions.

## Usage

```
contrasts_DI(object, contrast, contrast_vars, ...)
```

## Arguments

object	A DI or autoDI model object.
contrast	The coefficients to generate the contrast. There are three options to specify these coefficients:
	A list with each element being a vector of the same length as the number of linear coefficients in the model. The list can be named for tracking the contrasts.
	A matrix with the same number of columns as the number of linear coefficients in the model. The matrix can be given row names to track the different contrasts.
	A numeric vector with the length being a multiple of the number of coefficients in the matrix.
	Overrides contrast_vars if specified.

contrast_vars	A quicker and easier way to specify contrast coefficients for testing categorical variables. A nested named list with same names as the categorical variables in the model and same lengths as levels of those variables can be specified and the contrast will be calculated without the user having to specify the remaining variables.
	Will be overridden if contrast is specified.
	Recommended for only testing cateogrical variables in the model.
	Additional arguments passed to the glht function

## Details

The contrasts are calculated and tested using the glht function in the multcomp package.

#### Value

An object of class glht is returned

#### Author(s)

Rafael A. Moral, John Connolly, Rishabh Vishwakarma and Caroline Brophy

## References

Kirwan L, J Connolly, JA Finn, C Brophy, A Lüscher, D Nyfeler and MT Sebastia (2009) Diversityinteraction modelling - estimating contributions of species identities and interactions to ecosystem function. Ecology, 90, 2032-2038.

Torsten Hothorn, Frank Bretz and Peter Westfall (2008). Simultaneous Inference in General Parametric Models. Biometrical Journal 50(3), 346–363.

## See Also

DI autoDI glht

## Examples

#### describe\_model

describe\_model Describe DI models

#### Description

This function accepts a DImodel (i.e., regression models fit using the DI or autoDI functions) object and returns a short text summary describing the model.

## Usage

describe\_model(model)

#### Arguments

model A DI or autoDI regression model object.

#### Value

A short text describing the supplied DImodel object.

## Author(s)

Rafael A. Moral, John Connolly, Rishabh Vishwakarma and Caroline Brophy

## References

Kirwan L, J Connolly, JA Finn, C Brophy, A Lüscher, D Nyfeler and MT Sebastia (2009) Diversityinteraction modelling - estimating contributions of species identities and interactions to ecosystem function. Ecology, 90, 2032-2038.

## See Also

DI autoDI

#### Examples

design\_a

*The "design\_a" Dataset* 

#### Description

This dataset contains a set of proportions p1 to p9 where each row sums to 1. It is used as the design matrix for simulating other datasets in the DImodels package.

## Usage

data("design\_a")

## Format

A data frame with 206 observations on the following 11 variables:

- community A numeric vector identifying each unique community, i.e., two rows with the same community value also share the same set of p1 to p9 values.
- richness A numeric vector indicating the number of species in the initial composition, i.e., the number of proportions from p1 to p9 that are >0.
- p1 A numeric vector indicating a proportion (of species 1).
- p2 A numeric vector indicating a proportion (of species 2).
- p3 A numeric vector indicating a proportion (of species 3).
- p4 A numeric vector indicating a proportion (of species 4).

## design\_b

- p5 A numeric vector indicating a proportion (of species 5).
- p6 A numeric vector indicating a proportion (of species 6).
- p7 A numeric vector indicating a proportion (of species 7).
- p8 A numeric vector indicating a proportion (of species 8).
- p9 A numeric vector indicating a proportion (of species 9).

## Details

The columns p1 to p9 form a simplex space.

#### Examples

```
## Load the design_a data
    data(design_a)
## View the first five entries
    head(design_a)
## Explore the variables in design_a
    str(design_a)
## Check that the proportions sum to 1 (required for DI models)
## p1 to p9 are in the 3rd to 11th columns in design_a
    design_a_sums <- rowSums(design_a[3:11])
    summary(design_a_sums)</pre>
```

design\_b The "design\_b" Dataset

#### Description

This dataset contains a set of proportions p1 to p6 where each row sums to 1. It is used as the design matrix for simulating other datasets in the DImodels package.

#### Usage

data("design\_b")

## Format

A data frame with 47 observations on the following seven variables:

- richness A numeric vector indicating the number of species in the initial composition, i.e., the number of proportions from p1 to p6 that are >0.
- p1 A numeric vector indicating a proportion (of species 1).
- p2 A numeric vector indicating a proportion (of species 2).
- p3 A numeric vector indicating a proportion (of species 3).
- p4 A numeric vector indicating a proportion (of species 4).
- p5 A numeric vector indicating a proportion (of species 5).
- p6 A numeric vector indicating a proportion (of species 6).

## Details

The columns p1 to p6 form a simplex space.

## Examples

```
## Load the design_b data
data(design_b)
## View the first five entries
head(design_b)
## Explore the variables in design_b
str(design_b)
## Check that the proportions sum to 1 (required for DI models)
## p1 to p6 are in the 2nd to 7th columns in design_b
design_b_sums <- rowSums(design_b[2:7])
summary(design_b_sums)
```

DI

#### Diversity-Interactions Model Fitting

## Description

This function will fit a wide range of Diversity-Interactions (DI) models, one at a time. It provides some assisted automated ways to fit DI models, and includes the flexibility to extend DI models in several directions.

#### Usage

## Arguments

The minimum required arguments to use DI are either:

- Argument DImodel with data, y and prop, or
- Argument custom\_formula with data.

The DImodel argument allows fitting of DI models via a range of 'tag' options that determine the form of the species interactions terms (the tags, described below, are STR, ID, AV, FG, ADD and FULL) and extra terms can be added to the model using the extra\_formula argument. Using the argument custom\_formula requires full specification of the model to be fitted using standard lm or glm syntax.

y The column name of the response vector, which must be in quotes, for example, y = "yield".

block	The name of the block variable (if present), which must be in quotes, for example, block = "block". If no blocking variable, omit this argument.
density	The name of the density variable (if present), which must be in quotes, for example, density = "density". If no density variable, omit this argument.
prop	A vector of <i>s</i> column names identifying the species proportions in each commu- nity in the dataset. For example, if the species proportions columns are labelled p1 to p4, then prop = $c("p1", "p2", "p3", "p4")$ . Alternatively, the column numbers can be specified, for example, prop = 4:7, where species proportions are in the 4th to 7th columns.
treat	The name of a column in the dataset containing the value of a treatment factor or covariate. The treatment name must be included in quotes, for example, treat = "nitrogen". If the treatment is a factor, the variable must already be specified as a factor prior to using DI.
	<ul> <li>When used in conjunction with DImodel, the treatment will be included in the model as an additive factor or covariate, for example, specifying treat = nitrogen, DImodel = ID will fit the model p1 + p2 + + ps + nitrogen. Additional treatments, or interactions between the treatment and other model terms can be included via the extra_formula argument.</li> <li>The treat argument is defunct when using the custom_formula argument, and any treatment must be included directly in the custom_formula argu- ment.</li> </ul>
ID	This argument takes a text list (of length <i>s</i> ) dsecirbing groupings for the identity effects of the species. For example, if there are four species and you wish to group the identity effects all four species into a single term: ID could be ID = $c("ID1", "ID1", "ID1", "ID1")$ , where "ID1" is the name of the ID group. Similarly if the we wish to have two identity effect groups where identity effect of species 1 and 3, and species 2 and 4 are grouped together: ID could be ID = $c("ID1", "ID2", "ID1", "ID2")$ , where "ID1" and "ID2" are the names of the ID groups. These ideas expand to any number of species and any number or combination of groups. Finally, the ID groups do not have to be named "ID1" and "ID2", the user can specify any name for the groups.
	<ul> <li>If the ID argument is not specified, each species will be assumed to have a separate identity effect.</li> <li>Specify an grouping for the ID does not affect the interaction terms. The interactions are still calculated using the individual species proportions.</li> <li>The ID argument is defunct when using the custom_formula argument, since species identity effects must be included directly in the custom_formula</li> </ul>
	argument.
FG	It species are classified by g functional groups, this argument takes a text list (of length s) of the functional group to which each species belongs. For example, for four grassland species with two grasses and two legumes: FG could be FG = $c("G", "G", "L", "L")$ , where G stands for grass and L stands for legume.
	<ul> <li>The FG argument is required if DImodel = "FG" is specified.</li> <li>The FG argument is defined when using the system formula.</li> </ul>
	• The FG argument is defunct when using the custom_formula argument, since species interactions must be included directly in the custom_formula argument.

• STR (no identity or interaction effects, only an intercept is fitted, plus the experiment structural variables block, density and treat, if specified).

Each of the following includes the species proportions as specified in prop, the interaction variables according to the tag, plus block, density and treat if specified.

- ID (no interaction terms),
- AV (a single average species pairwise interaction variable),
- FG (functional group interaction variables, the FG argument must be specified to use this option),
- ADD (the additive species interaction variables),
- FULL (all pairwise interaction variables).

The DImodel tag should appear in quotes, for example, DImodel = "STR".

- extra\_formula In conjunction with DImodel, additional terms can be added using extra\_formula. A ~ must be included before specifying the terms. For example, if DImodel = "AV" has been specified, adding extra\_formula = ~ I(AV\*\*2) will add a quadratic average pairwise interaction variable or extra\_formula = ~ treatment: AV will add an interaction between the average pairwise species interaction variable and the treatment. Any variable included directly in extra\_formula must already be contained in the dataset (interaction variables can be created using the function DI\_data, if required).
- custom\_formula To specify your own DI model, write your own model formula using the custom\_formula argument. The standard notation from 1m and g1m is used here, for example, custom\_formula = yield ~ 0 + p1:treatment + p2:treatment + p3:treatment + p4: treatment will fit the DI model with the identity effects each crossed with treatment, where treatment is a variable in the dataset. The custom\_formula argument is recommended when the DImodel and extra\_formula arguments are not sufficient. Any variable included directly in custom\_formula must be already contained in the dataset (interaction variables can be created using the function DI\_data, if required).
- data Specify the dataset, for example, data = Switzerland. The dataset name should not appear in quotes.
- estimate\_theta By default, theta (the power parameter on all pi \* pj components of each interaction variable in the model) is set equal to one. Specify estimate\_theta = TRUE to include the estimation of  $\theta$  in the specified model. The estimate\_theta argument can only be used in conjunction with the DImodel argument; if the custom\_formula is used, then theta estimation is not available and the default estimate\_theta = FALSE must be used.
- theta Users may specify a value of theta different than 1 to fit the DI model. Note that if estimate\_theta = TRUE, then theta will be estimated via maximum profile log-likelihood and the value specified for theta will be overridden.

DImodel

#### Details

#### What are Diversity-Interactions models?

Diversity-Interactions (DI) models (Kirwan et al 2009) are a set of tools for analysing and interpreting data from experiments that explore the effects of species diversity on community-level responses. We recommend that users of the DImodels package read the short introduction to DI models (available at: DImodels). Further information on DI models is available in Kirwan et al 2009 and Connolly et al 2013.

#### Checks on data prior to using DI.

Before using DI, check that the species proportions for each row in your dataset sum to one. See the 'Examples' section for code to do this. An error message will be generated if the proportions don't sum to one.

## How does the DI function work?

The DI function provides wide flexibility in the types of Diversity-Interactions (DI) models that can be fitted. There are two ways to fit models in DI: 1) using DImodel, possibly augmented by extra\_formula, or 2) using custom\_formula. Models are estimated using iteratively reweighted least squares, via the glm package, when the option estimate\_theta = FALSE.

Consider the following DI model, for example (in R formula syntax):  $y \sim p1 + p2 + p3 + treatment + p1:p2 + p1:p3 + p2:p3 + p1:p2:treatment + p1:p3:treatment + p2:p3:treatment$ 

This model can be fitted using DImodel and extra\_formula: DI(y = "y", prop = c("p1", "p2", "p3"), treat = "nitrogen", DImodel = "FULL", extra\_formula = ~ p1:p2:treatment + p1:p3:treatment + p2:p3:treatment, data = datasetname)

or, by specifying all of the terms in the model using custom\_formula: DI(custom\_formula = y ~
p1 + p2 + p3 + treatment + p1:p2 + p1:p3 + p2:p3 + p1:p2:treatment + p1:p3:treatment + p2:p3:treatment,
data = datasetname)

We recommend to use DImodel where possible, to augment with extra\_formula where required, and to only use custom\_formula when DImodel plus extra\_formula is insufficient.

#### Including theta in DI models

A non-linear parameter  $\theta$  can be included in DI models as a power on all pi \* pj components of each pairwise interaction variable. For example (in R formula syntax):  $y \sim p1 + p2 + p3 + (p1:p2)^{theta} + (p1:p3)^{theta} + (p2:p3)^{theta}$  for the full pairwise interaction model. Including  $\theta$  alters the contribution of the interaction term to the response (Connolly et al 2013).

By default, the value of  $\theta$  is 1. By specifying estimate\_theta = TRUE within DI, a value of  $\theta$  will be estimated using profile likelihood over the space  $\theta = 0.01$  to 1.5. The option estimate\_theta = TRUE can only be used with DImodel, it is not available when using custom\_formula.

As a general guideline to testing if  $\theta$  is required, we recommend:

1) finding the best form of the species interaction terms assuming theta = 1, and then,

2) testing if theta differs from 1.

If no species interaction terms are needed, then there is no need to do any testing for theta.

## Value

A model object of class "glm" including the components detailed in glm, plus the following:

DIcall the call of the DI function

## DI

DIinternalcall an internal call made within the DI model fitting process

## Author(s)

Rafael A. Moral, John Connolly and Caroline Brophy

## References

Connolly J, T Bell, T Bolger, C Brophy, T Carnus, JA Finn, L Kirwan, F Isbell, J Levine, A Lüscher, V Picasso, C Roscher, MT Sebastia, M Suter and A Weigelt (2013) An improved model to predict the effects of changing biodiversity levels on ecosystem function. Journal of Ecology, 101, 344-355.

Kirwan L, J Connolly, JA Finn, C Brophy, A Lüscher, D Nyfeler and MT Sebastia (2009) Diversityinteraction modelling - estimating contributions of species identities and interactions to ecosystem function. Ecology, 90, 2032-2038.

## See Also

## autoDI theta\_CI

Other examples using DI: The Bell dataset examples. The sim1 dataset examples. The sim2 dataset examples. The sim3 dataset examples. The sim4 dataset examples. The sim5 dataset examples. The Switzerland dataset examples.

## Examples

```
## Load the Switzerland data
data(Switzerland)
## Check that the proportions sum to 1 (required for DI models)
## p1 to p4 are in the 4th to 7th columns in Switzerland
Switzerlandsums <- rowSums(Switzerland[4:7])</pre>
summary(Switzerlandsums)
## Fit the a simple AV DImodel with theta = 1
mod <- DI(y = "yield", prop = c("p1", "p2", "p3", "p4"),</pre>
         DImodel = "AV", data = Switzerland)
summary(mod)
## Fit the same model but group the 4 species identity effect into 2 groups
mod <- DI(y = "yield", prop = c("p1", "p2", "p3", "p4"),</pre>
         ID = c("ID1", "ID1", "ID2", "ID2"), DImodel = "AV",
         data = Switzerland)
summary(mod)
## Combine the four identity effects into a single term and estimate theta
estimate_theta = TRUE, data = Switzerland)
summary(mod)
```

## Fit the FG DImodel, with factors density and treatment, and with theta = 1

## DImodels-internal

```
m1 <- DI(y = "yield", density = "density", prop = 4:7, treat = "nitrogen",
         FG = c("G", "G", "L", "L"), DImodel = "FG", data = Switzerland)
summary(m1)
## Fit the FG DImodel, with factors density and treatment, and a fixed value of theta not equal to 1
m2 <- DI(y = "yield", density = "density", prop = 4:7, treat = "nitrogen",</pre>
         FG = c("G", "G", "L", "L"), DImodel = "FG", data = Switzerland,
         theta = 0.5)
summary(m2)
## Test if the identity effects interact with nitrogen (and main effect of nitrogen excluded)
m3 <- DI(y = "yield", density = "density", prop = 4:7, FG = c("G", "G", "L", "L"), DImodel = "FG",
         extra_formula = ~ (p1 + p2 + p3 + p4):nitrogen, data = Switzerland)
summary(m3)
## Fit the average pairwise model and check for a quadratic term using extra_formula.
## Need to create AV variable to be included in extra_formula and put in new dataset Switzerland2.
 AV_variable <- DI_data(prop = c("p1","p2","p3","p4"), data = Switzerland, what = "AV")
 Switzerland2 <- data.frame(Switzerland, "AV" = AV_variable)</pre>
 m4 <- DI(y = "yield", density = "density", prop = 4:7, DImodel = "AV",
           extra_formula = ~ I(AV**2), data = Switzerland2)
 summary(m4)
## Using the custom_formula option to fit some, but not all, of the FG interactions.
## Fit the FG DImodel using custom_formula, with factors density and treatment, and theta = 1.
## Need to create functional group interaction variables for inclusion in custom_formulaand put
## in new dataset Switzerland3.
 FG_matrix <- DI_data(prop = 4:7, FG = c("G", "G", "L", "L"), data = Switzerland, what = "FG")
 Switzerland3 <- data.frame(Switzerland, FG_matrix)</pre>
 m5 <- DI(y = "yield", prop = c("p1","p2","p3","p4"),</pre>
           custom_formula = yield ~ 0 + p1 + p2 + p3 + p4 + bfg_G_L + wfg_G
           + density + nitrogen,
           data = Switzerland3)
  summary(m5)
```

DImodels-internal Internal Functions

#### Description

Internal functions used within the DI and autoDI functions.

#### Author(s)

Rafael A. Moral, John Connolly, Rishabh Vishwakarma and Caroline Brophy

DI\_compare

## Description

This function fits the reference model internally and compares a DI model fit to it using anova.

#### Usage

DI\_compare(model, ...)

#### Arguments

model	A DI model object.
	Further arguments passed to anova.

## Details

This function takes a DI model object as input, fits the reference model internally and compares the two models using anova. The reference model includes an additive effect of community (each unique combination of species proportions) in the linear predictor. For more details on the reference model, see Connolly et al. (2013).

## Value

The function returns the reference model, a glm model object.

## Author(s)

Rafael A. Moral, John Connolly and Caroline Brophy

## References

Connolly J, T Bell, T Bolger, C Brophy, T Carnus, JA Finn, L Kirwan, F Isbell, J Levine, A Lüscher, V Picasso, C Roscher, MT Sebastia, M Suter and A Weigelt (2013) An improved model to predict the effects of changing biodiversity levels on ecosystem function. Journal of Ecology, 101, 344-355.

## See Also

DI autoDI

#### DI\_data\_manipulation

## Examples

```
## Load the sim1 data
    data(sim1)
## Fit the FULL model
    m1 <- DI(y = "response", block = "block", prop = 3:6,
        DImodel = "FULL", data = sim1)
## Compare with the reference model
    DI_compare(m1, test = "F")</pre>
```

DI\_data\_manipulation Data manipulation function

#### Description

This function can be used to compute additional variables for the various types of interactions among pairs of species proportions. These variables are defined following Kirwan et al 2007 and 2009, and Connolly et al 2013.

The variables are denoted:

AV and E: the average pairwise interaction variable (AV) and a scaled version of it (E), each a single variable. The variable AV is the sum of products of the proportions of each pair of species in the mixture. The variable E is a scaled version of AV that ranges between 0 (for a monoculture community) to 1 for the equi-proportional mixture of all species in the pool.

FG: the functional group interaction variables. There is a variable for (within) each functional group and one for (between) each pair of functional groups, i.e., if there are two functional groups, there will be three functional group interaction variables, while if there are three functional groups, there will be six functional group interaction variables.

ADD: the additive species interaction variables, one for each species.

FULL: all individual pairwise interactions. There will be s \* (s - 1)/2 new variables created, where s is the number of species in the pool.

By default, the interaction variables described above are created with theta = 1, but a different value of theta can also be specified (Connolly et al 2013).

## Usage

DI\_data(prop, FG, data, theta = 1, what = c("E", "AV", "FG", "ADD", "FULL"))

## Arguments

prop

A vector of column names identifying the species proportions in the dataset. For example, if the species proportions columns are labelled p1 to p4, then prop = c("p1", "p2", "p3", "p4"). The column numbers in which the proportions are stored can also be referred to, for example, prop = 4:7 for the Switzerland data.

FG	If species are classified by <i>g</i> functional groups, this argument takes a text list (of length <i>s</i> ) of the functional group to which each species belongs. For example, for four grassland species with two grasses and two legumes, it could be $FG = c("G", "G", "L", "L")$ , where G stands for grass and L stands for legume. This argument is required when "FG" is included in the what argument.
data	Specify the dataset, for example, data = Switzerland. The dataset name should not appear in quotes.
theta	Interaction variables will be computed with the theta power, equal to the value specified, on all $pi * pj$ components of each interaction variable, with default value one. For example, with three species AV = p1*p2 + p1*p3 + p2*p3 and if computed with theta = 0.5, this becomes $(p1*p2)^0.5 + (p1*p3)^0.5 + (p2*p3)^0.5$ .
what	The interactions to be computed. By default each set of variables will be computed: AV, E, FG (if FG argument specified), ADD and FULL. Individual sets can be selected. For example, what = $c("FULL")$ or what = $c("AV", "FULL")$ .

## Details

## What are Diversity-Interactions models?

Diversity-Interactions (DI) models (Kirwan et al 2009) are a set of tools for analysing and interpreting data from experiments that explore the effects of species diversity on community-level responses. We recommend that users of the DImodels package read the short introduction to DI models (available at: DImodels). Further information on DI models is available in Kirwan et al 2009 and Connolly et al 2013.

## Checks on data prior to using the DI\_data function.

Before using the DI\_data function, check that the species proportions in each row of your dataset sum to one. See the 'Examples' section for code to do this. An error message will be generated if the proportions don't sum to one.

#### When is the DI\_data function needed?

It is not required to use the DI\_data function if using the autoDI function, or the DImodel option in the DI function, as they will automatically create the species interaction variables needed. If using species interaction variables in the extra\_formula or custom\_formula options in DI, then it is required to have the variables already in the dataset and DI\_data can do that.

#### Short worked example to illustrate how the DI\_data function works

The code to implement this example is provided in the 'Examples' section.

Assume four species with initial proportions in two communities: (0.1, 0.2, 0.3, 0.4) and (0.25, 0.25, 0.25), with FG = c("G", "G", "L", "L").

For community 1: (0.1, 0.2, 0.3, 0.4), assuming theta = 1, the data preparation functions will compute the following additional variables (details in Kirwan et al 2007 and 2009):

$$AV = 0.1*0.2 + 0.1*0.3 + 0.1*0.4 + 0.2*0.3 + 0.2*0.4 + 0.3*0.4 = 0.35$$

E = (2s/(s-1))\*AV = 0.9333

 $p1_add = 0.1 * (1 - 0.1) = 0.09$ 

 $p2_add = 0.2 * (1 - 0.2) = 0.16$ 

 $p3\_add = 0.3 * (1 - 0.3) = 0.21$   $p4\_add = 0.4 * (1 - 0.4) = 0.24$   $bfg\_G\_L = 0.1*0.3 + 0.1*0.4 + 0.2*0.3 + 0.2*0.4 = 0.21$   $wfg\_G = 0.1*0.2 = 0.02$  $wfg\_L = 0.3*0.4 = 0.12$ 

For community 1: (0.1, 0.2, 0.3, 0.4), assuming theta = 0.5, the data preparation functions will compute the follow additional variables (details in Connolly et al 2013):

 $AV = (0.1*0.2)^{0.5} + (0.1*0.3)^{0.5} + (0.1*0.4)^{0.5} + (0.2*0.3)^{0.5} + (0.2*0.4)^{0.5} + (0.3*0.4)^{0.5} = 1.3888$ 

E = (2s/(s-1))\*AV = 3.7035

 $p1_add = 0.1^{0.5} * (0.2^{0.5} + 0.3^{0.5} + 0.4^{0.5}) = 0.5146$ 

 $p2_add = 0.2^{0.5} * (0.1^{0.5} + 0.3^{0.5} + 0.4^{0.5}) = 0.6692$ 

 $p3_add = 0.3^{0.5} * (0.1^{0.5} + 0.2^{0.5} + 0.4^{0.5}) = 0.7646$ 

 $p4_add = 0.4^{0.5} * (0.1^{0.5} + 0.2^{0.5} + 0.3^{0.5}) = 0.8293$ 

 $bfg\_G\_L = (0.1*0.3)^{0.5} + (0.1*0.4)^{0.5} + (0.2*0.3)^{0.5} + (0.2*0.4)^{0.5} = 0.9010$ 

wfg\_G =  $(0.1*0.2)^0.5 = 0.1414$ 

 $wfg_L = (0.3*0.4)^0.5 = 0.3464$ 

When using the DI\_data function to create interactions for theta values for a value different from 1, it is recommended to rename the new interaction variables to include \_theta.

The data manipulation values for community 2 (0.25, 0.25, 0.25, 0.25) can be seen when the 'Examples' section code is run.

#### Value

DI\_data returns a named list with one or more the following components (depending on the specification of the what argument:

AV a numeric vector containing the average pairwise interaction variabl	e
FG a matrix containing the functional group-related interaction variable	S
ADD a matrix containing the additive species contributions interaction var	riables
FULL a matrix containing all pairwise interactions	

## Author(s)

Rafael A. Moral, John Connolly and Caroline Brophy

#### References

Connolly J, T Bell, T Bolger, C Brophy, T Carnus, JA Finn, L Kirwan, F Isbell, J Levine, A Lüscher, V Picasso, C Roscher, MT Sebastia, M Suter and A Weigelt (2013) An improved model to predict the effects of changing biodiversity levels on ecosystem function. Journal of Ecology, 101, 344-355.

Kirwan L, A Lüscher, MT Sebastia, JA Finn, RP Collins, C Porqueddu, A Helgadottir, OH Baadshaug, C Brophy, C Coran, S Dalmannsdottir, I Delgado, A Elgersma, M Fothergill, BE Frankow-Lindberg, P Golinski, P Grieu, AM Gustavsson, M Höglind, O Huguenin-Elie, C Iliadis, M Jørgensen, Z Kadziuliene, T Karyotis, T Lunnan, M Malengier, S Maltoni, V Meyer, D Nyfeler, P Nykanen-Kurki, J Parente, HJ Smit, U Thumm, & J Connolly (2007) Evenness drives consistent diversity effects in intensive grassland systems across 28 European sites. Journal of Ecology, 95, 530-539.

Kirwan L, J Connolly, JA Finn, C Brophy, A Lüscher, D Nyfeler and MT Sebastia (2009) Diversityinteraction modelling - estimating contributions of species identities and interactions to ecosystem function. Ecology, 90, 2032-2038.

## See Also

#### DI autoDI

Other examples using the DI\_data function: The sim2 dataset examples. The sim3 dataset examples. The sim4 dataset examples. The sim5 dataset examples. The Switzerland dataset examples.

#### Examples

#### 

#### Data manipulation for the Switzerland dataset

```
## Load the Switzerland data
    data(Switzerland)
```

```
## Check that the proportions sum to 1 (required for DI models)
## p1 to p4 are in the 4th to 7th columns in Switzerland
Switzerlandsums <- rowSums(Switzerland[4:7])
summary(Switzerlandsums)</pre>
```

```
## Create FG interaction variables and incorporate them into a new data frame Switzerland3.
## Use theta = 0.5.
FG_matrix <- DI_data(prop = c("p1","p2","p3","p4"), FG = c("G","G","L","L"),</pre>
```

```
data = Switzerland, what = "FG", theta = 0.5)
Switzerland3 <- data.frame(Switzerland, FG_matrix)
## Add "_theta" to the new interaction variables to differentiate from when theta = 1</pre>
```

```
names(Switzerland3)[9:11] <- paste0(names(Switzerland3)[9:11], "_theta")</pre>
```

#### All interactions can be added to a new dataset all together: ## Create all interactions and add them to a new data frame called Switzerland4 newlist <- DI\_data(prop = c("p1", "p2", "p3", "p4"), FG = c("G", "G", "L", "L"), data = Switzerland,</pre> what = c("E", "AV", "FG", "ADD", "FULL")) Switzerland4 <- data.frame(Switzerland, "E" = newlist\$E, "AV" = newlist\$AV, newlist\$FG, newlist\$ADD, newlist\$FULL) #### Or the various interactions can also be added to a new dataset individually: ## Create the average pairwise interaction and evenness variables ## and store them in a new data frame called Switzerland5. ## Switzerland5 will contain the new variables: AV, E E\_variable <- DI\_data(prop = c("p1","p2","p3","p4"), data = Switzerland, what = "E")</pre> AV\_variable <- DI\_data(prop = c("p1","p2","p3","p4"), data = Switzerland, what = "AV") Switzerland5 <- data.frame(Switzerland, "AV" = AV\_variable, "E" = E\_variable)</pre> ## Create the functional group variables and add them to Switzerland5. ## In the FG names vector: G stands for grass, L stands for legume. ## Switzerland5 will contain: bfg\_G\_L, wfg\_G and wfg\_L FG\_matrix <- DI\_data(prop = 4:7, FG = c("G", "G", "L", "L"), data = Switzerland, what = "FG") Switzerland5 <- data.frame(Switzerland5, FG\_matrix)</pre> ## Create the additive species variables and add them to Switzerland5. ## Switzerland5 will contain the new variables: p1\_add, p2\_add, p3\_add and p4\_add. ADD\_matrix <- DI\_data(prop = c("p1","p2","p3","p4"), data = Switzerland, what = "ADD") Switzerland5 <- data.frame(Switzerland5, ADD\_matrix)</pre> ## Create all pairwise interaction variables and add them to Switzerland5. ## Switzerland5 will contain the new variables: p1.p2, p1.p3, p1.p4, p2.p3, p2.p4, p3.p4. FULL\_matrix <- DI\_data(prop = c("p1","p2","p3","p4"), data = Switzerland, what = "FULL")</pre> Switzerland5 <- data.frame(Switzerland5, FULL\_matrix)</pre> #### Short worked example (as illustrated the Details section) ## Create a dataframe p1 <- c(0.1, 0.25) p2 <- c(0.2, 0.25) p3 <- c(0.3, 0.25) p4 <- c(0.4, 0.25)

```
minidataset1 <- data.frame(p1,p2,p3,p4)</pre>
```

```
## Check the rows sum to 1
rowSums(minidataset1[1:4])
```

#### 

DI\_methods

#### Methods for DI Objects

#### Description

Different methods that can be used with objects of class DI.

## Usage

```
## S3 method for class 'DI'
anova(object, ...)
## S3 method for class 'DI'
AIC(object, ...)
## S3 method for class 'DI'
BIC(object, ...)
## S3 method for class 'DI'
AICc(obj)
## S3 method for class 'DI'
BICc(obj)
## S3 method for class 'DI'
logLik(object, ...)
## S3 method for class 'DI'
fortify(model, data, ...)
```

## Arguments

object	a DI model object
obj	a DI model object
model	a DI model object

## extract

data	data to which to add model fit statistics. Defaults to the model frame.
	further arguments passed to anova, AIC, BIC, loglik, or fortify

## Author(s)

Rafael A. Moral, John Connolly, Rishabh Vishwakarma and Caroline Brophy

## See Also

autoDI

extract

Extract terms from a DI or autoDI model object

## Description

Extracts terms from a DI or autoDI model object that were calculated using the data preparation functions prior to the model fitting procedure.

## Usage

```
extract(obj, what = c("FULL","ADD","FG","AV","E"))
## S3 method for class 'DI'
extract(obj, what = c("FULL","ADD","FG","AV","E"))
## S3 method for class 'autoDI'
extract(obj, what = c("FULL","ADD","FG","AV","E"))
```

#### Arguments

obj	a DI or autoDI model object
what	the variable(s) to be extracted from the object.

## Value

A list containing one or more of the following elements:

E	the evenness interaction variable
AV	the average pairwise interaction variable
FG	the functional group-related interaction variables
ADD	the additive species contributions interaction variables
FULL	all pairwise interactions

## Author(s)

Rafael A. Moral, John Connolly and Caroline Brophy

## References

Connolly J, T Bell, T Bolger, C Brophy, T Carnus, JA Finn, L Kirwan, F Isbell, J Levine, A Lüscher, V Picasso, C Roscher, MT Sebastia, M Suter and A Weigelt (2013) An improved model to predict the effects of changing biodiversity levels on ecosystem function. Journal of Ecology, 101, 344-355.

Kirwan L, J Connolly, JA Finn, C Brophy, A Lüscher, D Nyfeler and MT Sebastia (2009) Diversityinteraction modelling - estimating contributions of species identities and interactions to ecosystem function. Ecology, 90, 2032-2038.

#### See Also

DI

## Examples

predict.DI

```
Predict Method for Diversity-Interactions (DI) Models
```

## Description

Generates predictions for a fitted DI models object and, optionally, the associated standard errors for those predictions.

## Usage

```
## S3 method for class 'DI'
predict(object, newdata, se.fit = FALSE,
interval = c("none", "confidence", "prediction"),
level = 0.95, weights = 1,
type = c("link", "response", "terms"), ...)
```

## Arguments

object	a DI or autoDI model object.
newdata	optionally, a data frame in which to look for variables with which to predict. If omitted, predictions will be made for data used to fit the model.
se.fit	A logical switch indicating whether to calculate the associated standard errors.

## predict.DI

interval	The type of interval to be calculated. Accepts one of "none", "confidence" or "prediction", with "none"" being the default.
level	The level (1 - $\alpha$ ) at which to calculate the interval. Defaults to 0.95, giving a 95% interval.
weights	The variance weights for calculating the prediction intervals. By default all values get the same weight of 1. Can also specify a numeric vector of same length as number of rows in newdata.
type	the type of prediction required. One of "link", "response" or "terms". The default "link" is on the scale of the linear predictors while "response" is on the scale of the response variable. The "terms" option returns a matrix giving the fitted values of each term in the model formula on the linear predictor scale.
	further arguments passed to or from other methods. For eg: dispersion or na.action arguments from predict.glm function.

## Details

If newdata doesn't contain all predictors from the model, necessary numeric predictors will be added in with a value of 0, while categorical predictors will be added in with their baseline value. See examples for more information.

## Value

if se.fit = FALSE, a vector of predictions is returned.	
if se.fit = TRUE, a list with the following components is returned.	
fit	Predictions, as for se.fit = FALSE.
se.fit	Estimated standard error for each prediction
residual.scale	A scalar giving the square root of the dispersion used in computing the standard errors.

## Author(s)

Rafael A. Moral, John Connolly, Rishabh Vishwakarma and Caroline Brophy

#### References

Connolly J, T Bell, T Bolger, C Brophy, T Carnus, JA Finn, L Kirwan, F Isbell, J Levine, A Luescher, V Picasso, C Roscher, MT Sebastia, M Suter and A Weigelt (2013) An improved model to predict the effects of changing biodiversity levels on ecosystem function. Journal of Ecology, 101, 344-355.

Kirwan L, J Connolly, JA Finn, C Brophy, A Luescher, D Nyfeler and MT Sebastia (2009) Diversityinteraction modelling - estimating contributions of species identities and interactions to ecosystem function. Ecology, 90, 2032-2038.

## See Also

DI autoDI predict.glm

## Examples

```
## Load the Switzerland data
 data(Switzerland)
## Summarise the Switzerland data
 summary(Switzerland)
## Fit a DI model
 m1 <- DI(y = "yield", prop = 4:7, treat = 'nitrogen', DImodel = 'AV',</pre>
 density = 'density', estimate_theta = TRUE, data = Switzerland)
 summary(m1)
## Prediction without newdata, full dataset from model fit will be used
 predict(m1, se.fit = TRUE)
## Prediction with newdata
 newdata1 <- data.frame('p1' = c(1,0), 'p2' = c(0,1), 'p3' = c(0,0), 'p4' = c(0,0),
                         'nitrogen' = c(50, 150), 'density' = c('low', 'high'))
 predict(m1, newdata = newdata1, se.fit = TRUE)
## If any categorical variable is missing, the baseline level
## of the variable is used for prediction
 newdata2 <- newdata1[, -5]</pre>
 print(newdata2)
 predict(m1, newdata = newdata2)
## If a numerical variable is missing, the value 0 is used for it
 newdata3 <- newdata1[, -c(3,4)]
 print(newdata3)
 predict(m1, newdata = newdata3)
```

richness\_vs\_DI Comparing the Richness Model with DI Alternatives

## Description

This function provides an automated way to fit the richness model and a (limited) range of Diversity-Interactions (DI) models.

## Usage

richness\_vs\_DI(y, prop, data, extra\_formula)

## Arguments

У	The column name of the response vector, which must be in quotes, for example, y = "yield".
prop	A vector of $s$ column names identifying the species proportions in each row in the detest. For example, if the species proportions columns are labelled pl to
	p4, then prop = $c("p1", "p2", "p3", "p4")$ . Alternatively, the column numbers

	can be specified, for example, prop = 4:7, where the species proportions are in the 4th to 7th columns.
data	Specify the dataset, for example, data = Switzerland. The dataset name should not appear in quotes.
extra_formula	Additional terms can be added using extra_formula. A ~ must be included before specifying the terms. For example, extra_formula = ~ treatment:AV will add a treatment effect. Any variable included directly in extra_formula must already be contained in the dataset (interaction variables can be created using the function DI_data, if required).

#### Details

Connolly et al. (2013; Appendix 1) shows that there is an equivalence between DI models and different types of richness models (linear and nonlinear predictors using richness in different scales).

This function fits four models and compares them using AIC. The four models are:

1. The richness model

$$y = Intercept + Slope * Richness + \epsilon;$$

2. The average pairwise interactions (AV) DI model with common identity effects and theta equal to 0.5 (which is equivalent to model 1 when communities are all equi-proportional);

3. The average pairwise interactions (AV) DI model with common identity effects and estimating theta;

4. The average pairwise interactions (AV) DI model allowing for unique identity effects, but maintaining theta equal to 0.5;

5. The average pairwise interactions (AV) DI model allowing for unique identity effects, and estimating theta.

The function prints a table with AIC, AICc, BIC, and associated degrees of freedom for each of the four models above, and returns the model with the smallest AIC.

#### Value

The function returns the final selected model, an object of class DI or 1m.

## Author(s)

Rafael A. Moral, John Connolly, Rishabh Vishwakarma and Caroline Brophy

## References

Connolly J, T Bell, T Bolger, C Brophy, T Carnus, JA Finn, L Kirwan, F Isbell, J Levine, A Lüscher, V Picasso, C Roscher, MT Sebastia, M Suter and A Weigelt (2013) An improved model to predict the effects of changing biodiversity levels on ecosystem function. Journal of Ecology, 101, 344-355.

## See Also

DI autoDI

## Examples

```
## Load the Switzerland data
    data(Switzerland)
## compare the richness model with DI alternatives
    richness_vs_DI(y = "yield", prop = 4:7, data = Switzerland)
## include the density effects in the linear predictors of the four models
    richness_vs_DI(y = "yield", prop = 4:7, data = Switzerland, extra_formula = ~ density)
```

sim0

The Simulated "sim0" Dataset

## Description

The sim0 dataset was simulated. There are four replicates and three species that vary in proportions (p1 - p3). There are 16 unique sets of proportions identified by the variable community. The response was simulated assuming that there were species identity effects and separate pairwise interactions effects.

#### Usage

data(sim0)

## Format

A data frame with 64 observations on the following six variables:

- community A numeric vector identifying each unique community, i.e., two rows with the same community value also share the same set of p1 to p3 values.
- richness A numeric vector indicating the number of species in the initial composition, i.e., the number of proportions from p1 to p3 that are >0.
- p1 A numeric vector indicating the initial proportion of species 1.
- p2 A numeric vector indicating the initial proportion of species 2.
- p3 A numeric vector indicating the initial proportion of species 3.

response A numeric vector giving the simulated response variable.

#### Details

#### What are Diversity-Interactions (DI) models?

Diversity-Interactions (DI) models (Kirwan et al 2009) are a set of tools for analysing and interpreting data from experiments that explore the effects of species diversity on community-level responses. We strongly recommend that users read the short introduction to Diversity-Interactions

models (available at: DImodels). Further information on Diversity-Interactions models is also available in Kirwan et al 2009 and Connolly et al 2013.

## Parameter values for the simulation

DI models take the general form of:

$$y = Identities + Interactions + Structures + \epsilon$$

where *y* is a community-level response, the *Identities* are the effects of species identities and enter the model as individual species proportions at the beginning of the time period, the *Interactions* are the interactions among the species proportions, while *Structures* include other experimental structures such as blocks, treatments or density.

The dataset sim0 was simulated with:

- identity effects for the four species with values = 25, 20, 15
- all 3 pairwise interaction effects with values: 30, 20, 40 (for pairs of species 1-2, 1-3, and 2-3, respectively).
- $\epsilon$  assumed normally distributed with mean 0 and standard deviation 2.

## References

Connolly J, T Bell, T Bolger, C Brophy, T Carnus, JA Finn, L Kirwan, F Isbell, J Levine, A Lüscher, V Picasso, C Roscher, MT Sebastia, M Suter and A Weigelt (2013) An improved model to predict the effects of changing biodiversity levels on ecosystem function. Journal of Ecology, 101, 344-355.

Kirwan L, J Connolly, JA Finn, C Brophy, A Lüscher, D Nyfeler and MT Sebastia (2009) Diversityinteraction modelling - estimating contributions of species identities and interactions to ecosystem function. Ecology, 90, 2032-2038.

## Examples

## Check goodness-of-fit using a half-normal plot with a simulated envelope
library(hnp)
hnp(m1)

sim0\_design

## Description

This dataset contains a set of proportions p1 to p3 where each row sums to 1. It is used as the design matrix for simulating other datasets in the DImodels package.

## Usage

```
data("sim0_design")
```

#### Format

A data frame with 16 observations on the following 5 variables:

- community A numeric vector identifying each unique community, i.e., two rows with the same community value also share the same set of p1 to p3 values.
- richness A numeric vector indicating the number of species in the initial composition, i.e., the number of proportions from p1 to p3 that are >0.
- p1 A numeric vector indicating a proportion (of species 1).
- p2 A numeric vector indicating a proportion (of species 2).
- p3 A numeric vector indicating a proportion (of species 3).

## Details

The columns p1 to p3 form a simplex space.

## Examples

```
## Load the sim0_design data
    data(sim0_design)
## View the first five entries
    head(sim0_design)
## Explore the variables in design_a
    str(sim0_design)
```

```
## Check that the proportions sum to 1 (required for DI models)
## p1 to p3 are in the 3rd to 5th columns in sim0_design
   sim0_design_sums <- rowSums(sim0_design[3:5])
   summary(sim0_design)</pre>
```

#### Description

The sim1 dataset was simulated. There are four blocks and four species that vary in proportions (p1 - p4). There are 15 unique sets of proportions identified by the variable community. Each unique community appears once in each block. The response was simulated assuming that there were species identity effects and block effects, but no diversity effects.

#### Usage

data(sim1)

#### Format

A data frame with 60 observations on the following seven variables:

community A numeric vector identifying each unique community, i.e., two rows with the same community value also share the same set of p1 to p4 values.

block A factor taking values 1 to 4 indicating block membership.

p1 A numeric vector indicating the initial proportion of species 1.

p2 A numeric vector indicating the initial proportion of species 2.

p3 A numeric vector indicating the initial proportion of species 3.

p4 A numeric vector indicating the initial proportion of species 4.

response A numeric vector giving the simulated response variable.

## Details

#### What are Diversity-Interactions (DI) models?

Diversity-Interactions (DI) models (Kirwan et al 2009) are a set of tools for analysing and interpreting data from experiments that explore the effects of species diversity on community-level responses. We strongly recommend that users read the short introduction to Diversity-Interactions models (available at: DImodels). Further information on Diversity-Interactions models is also available in Kirwan et al 2009 and Connolly et al 2013.

#### Parameter values for the simulation

DI models take the general form of:

#### $y = Identities + Interactions + Structures + \epsilon$

where y is a community-level response, the *Identities* are the effects of species identities and enter the model as individual species proportions at the beginning of the time period, the *Interactions* are the interactions among the species proportions, while *Structures* include other experimental structures such as blocks, treatments or density.

The dataset sim1 was simulated with:

# sim1

- identity effects for the four species with values = 10, 9, 8, 7
- block effects for the four blocks with values = 1, 1.5, 2, 0
- no interaction effects
- $\epsilon$  assumed normally distributed with mean 0 and standard deviation 1.1.

#### References

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Connolly J, T Bell, T Bolger, C Brophy, T Carnus, JA Finn, L Kirwan, F Isbell, J Levine, A Lüscher, V Picasso, C Roscher, MT Sebastia, M Suter and A Weigelt (2013) An improved model to predict the effects of changing biodiversity levels on ecosystem function. Journal of Ecology, 101, 344-355.

Kirwan L, J Connolly, JA Finn, C Brophy, A Lüscher, D Nyfeler and MT Sebastia (2009) Diversityinteraction modelling - estimating contributions of species identities and interactions to ecosystem function. Ecology, 90, 2032-2038.

## Examples

## Simulate dataset sim1 with species identity effects and block effects, but no interaction effect

```
## Use the proportions from the first fifteen plots in Switzerland
 data(Switzerland)
## Repeat the 15 plots over four blocks.
## Give each community type a unique (community) number.
 sim1 <- data.frame(community = rep(1:15, each = 4),</pre>
                   block = factor(rep(1:4, times = 15)),
                   p1 = rep(Switzerland p1[1:15], each = 4),
                   p2 = rep(Switzerland p2[1:15], each = 4),
                   p3 = rep(Switzerland p3[1:15], each = 4),
                   p4 = rep(Switzerland p4[1:15], each = 4))
## To simulate the response, first create a matrix of predictors that includes
## p1-p4 and the four block dummy variables.
 X <- model.matrix(~ p1 + p2 + p3 + p4 + block -1, data = sim1)
## Create a vector of 'known' parameter values for simulating the response.
## The first four are the p1-p4 parameters, the second four are the block effects.
 sim1_coeff <- c(10,9,8,7, 1,1.5,2,0)</pre>
## Create response and add normally distributed error
 sim1$response <- as.numeric(X %*% sim1_coeff)</pre>
 set.seed(2020)
 r <- rnorm(n = 60, mean = 0, sd = 1.1)
 sim1$response <- round(sim1$response + r, digits = 3)</pre>
```

```
## Analyse the sim1 dataset
## Load the sim1 data
 data(sim1)
## View the first few entries
 head(sim1)
## Explore the variables in sim1
 str(sim1)
## Check that the proportions sum to 1 (required for DI models)
## p1 to p4 are in the 3rd to 6th columns in sim1
 sim1sums <- rowSums(sim1[3:6])</pre>
 summary(sim1sums)
## Check characteristics of sim1
 hist(sim1$response)
 summary(sim1$response)
 plot(sim1$p1, sim1$response)
 plot(sim1$p2, sim1$response)
 plot(sim1$p3, sim1$response)
 plot(sim1$p4, sim1$response)
## Find the best DI model using autoDI and F-test selection
 auto1 <- autoDI(y = "response", prop = c("p1","p2","p3","p4"), block = "block", data = sim1,</pre>
                  selection = "Ftest")
 summary(auto1)
## Fit the identity model using DI and the ID tag
 m1 <- DI(y = "response", prop = c("p1","p2","p3","p4"), block = "block", DImodel = "ID",</pre>
           data = sim1)
 summary(m1)
 plot(m1)
## Check goodness-of-fit using a half-normal plot with a simulated envelope
 library(hnp)
 hnp(m1)
## Fit the identity model using DI and custom_formula
 m^2 < -DI(y = "response", custom_formula = response ~ 0 + p1 + p2 + p3 + p4 + block, data = sim1)
 summary(m2)
```

#### Description

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The sim2 dataset was simulated. There are four blocks and four species that vary in proportions (p1 - p4). There are 15 unique sets of proportions identified by the variable community. Each unique community appears once in each block. The response was simulated assuming that there were species identity effects, block effects, an average pairwise interaction effect and a theta value of 0.5.

## Usage

data(sim2)

#### Format

A data frame with 60 observations on the following seven variables:

community A numeric vector identifying each unique community, i.e., two rows with the same community value also share the same set of p1 to p4 values.

block A factor taking values 1 to 4 indicating block membership.

p1 A numeric vector indicating the initial proportion of species 1.

p2 A numeric vector indicating the initial proportion of species 2.

p3 A numeric vector indicating the initial proportion of species 3.

p4 A numeric vector indicating the initial proportion of species 4.

response A numeric vector giving the simulated response variable.

#### Details

#### What are Diversity-Interactions (DI) models?

Diversity-Interactions (DI) models (Kirwan et al 2009) are a set of tools for analysing and interpreting data from experiments that explore the effects of species diversity on community-level responses. We strongly recommend that users read the short introduction to Diversity-Interactions models (available at: DImodels). Further information on Diversity-Interactions models is also available in Kirwan et al 2009 and Connolly et al 2013.

#### Parameter values for the simulation

DI models take the general form of:

 $y = Identities + Interactions + Structures + \epsilon$ 

where *y* is a community-level response, the *Identities* are the effects of species identities and enter the model as individual species proportions at the beginning of the time period, the *Interactions* are the interactions among the species proportions, while *Structures* include other experimental structures such as blocks, treatments or density.

The dataset sim2 was simulated with:

- identity effects for the four species with values = 10, 9, 8, 7
- block effects for the four blocks with values = 1, 1.5, 2, 0

- an average pairwise interaction effect = 8
- theta = 0.5 (where  $\theta$  is a non-linear parameter included as a power on each *pipj* product within interaction variables, see Connolly et al 2013 for details)
- $\epsilon$  assumed normally distributed with mean 0 and standard deviation 1.1.

#### References

Connolly J, T Bell, T Bolger, C Brophy, T Carnus, JA Finn, L Kirwan, F Isbell, J Levine, A Lüscher, V Picasso, C Roscher, MT Sebastia, M Suter and A Weigelt (2013) An improved model to predict the effects of changing biodiversity levels on ecosystem function. Journal of Ecology, 101, 344-355.

Kirwan L, J Connolly, JA Finn, C Brophy, A Lüscher, D Nyfeler and MT Sebastia (2009) Diversityinteraction modelling - estimating contributions of species identities and interactions to ecosystem function. Ecology, 90, 2032-2038.

## Examples

```
## Simulate dataset sim2 with species identity effects, block effects and
## an average pairwise interaction effect with theta=0.5.
## Use the proportions from the first fifteen plots in Switzerland
 data(Switzerland)
## Repeat the 15 plots over four blocks.
## Give each community type a unique (community) number.
 sim2 <- data.frame(community = rep(1:15, each = 4),</pre>
                   block = factor(rep(1:4, times = 15)),
                   p1 = rep(Switzerland p1[1:15], each = 4),
                   p2 = rep(Switzerland p2[1:15], each = 4),
                   p3 = rep(Switzerland$p3[1:15], each = 4),
                   p4 = rep(Switzerland p4[1:15], each = 4))
## Create the average pairwise interaction variable, with theta = 0.5
 AV_variable <- DI_data(prop = c("p1", "p2", "p3", "p4"), data = sim2,
                         theta = 0.5, what = "AV")
 sim2 <- data.frame(sim2, "AV_theta" = AV_variable)</pre>
## To simulate the response, first create a matrix of predictors that includes p1-p4 and
## the four block variables and the average pairwise interaction variable with theta=0.5.
 X <- model.matrix(~ p1 + p2 + p3 + p4 + block + AV_theta -1, data = sim2)
## Create a vector of 'known' parameter values for simulating the response.
## The first four are the p1-p4 parameters, the second four are the block effects and
## the last one is the interaction parameter.
 sim2_coeff <- c(10,9,8,7, 1,1.5,2,0,</pre>
                                            8)
```

## Create response and add normally distributed error

```
sim2$response <- as.numeric(X %*% sim2_coeff)</pre>
 set.seed(328781)
 r <- rnorm(n = 60, mean = 0, sd = 1.1)
 sim2$response <- round(sim2$response + r, digits = 3)</pre>
 sim2$AV_theta <- NULL</pre>
## sim2
## Analyse the sim2 dataset
## Load the sim2 data
 data(sim2)
## View the first few entries
 head(sim2)
## Explore the variables in sim2
 str(sim2)
## Check that the proportions sum to 1 (required for DI models)
## p1 to p4 are in the 3rd to 6th columns in sim2
 sim2sums <- rowSums(sim2[3:6])</pre>
 summary(sim2sums)
## Check characteristics of sim2
 hist(sim2$response)
 summary(sim2$response)
 plot(sim2$p1, sim2$response)
 plot(sim2$p2, sim2$response)
 plot(sim2$p3, sim2$response)
 plot(sim2$p4, sim2$response)
## Find the best DI model using autoDI and F-test selection
 auto1 <- autoDI(y = "response", prop = c("p1", "p2", "p3", "p4"), block = "block", data = sim2,</pre>
               selection = "Ftest")
 summary(auto1)
 ## Fit the average pairwise model, including theta, using DI and the AV tag
 m1 <- DI(y = "response", prop = c("p1","p2","p3","p4"), block = "block", DImodel = "AV",</pre>
         estimate_theta = TRUE, data = sim2)
 summary(m1)
 CI_95 <- theta_CI(m1, conf = .95)
 CI_95
 plot(m1)
 library(hnp)
```

## Check goodness-of-fit using a half-normal plot with a simulated envelope
library(hnp)

sim3

hnp(m1)

## Graph the profile likelihood

xlab(expression(theta)) + ylab("Log-likelihood") +

geom\_vline(xintercept = CI\_95, lty = 3) +

library(ggplot2)

 $theme_bw() +$ geom\_line() + xlim(0, 1.5) +

```
ggplot(m1$profile_loglik, aes(x = grid, y = prof)) +
```

```
labs(title = " Log-likelihood versus theta",
      caption = "dotted vertical lines are upper and lower bounds of 95% CI for theta")
## Fit the average pairwise model, including theta, using DI and custom_formula
## A value of theta must be 'chosen'. Take: 0.4533437 from m1. The 'estimate_theta' option is not
## available with custom_formula.
 AV_variable <- DI_data(prop = c(3:6), data = sim2, theta = 0.4533437, what = "AV")
 sim2a <- data.frame(sim2, "AV_theta" = AV_variable)</pre>
 m^2 < -DI(y = "response", custom_formula = response ~ 0 + p1 + p2 + p3 + p4 + AV_theta + block,
           data = sim2a)
## This will adjust the standard errors in m2 for the 'estimation' of theta
 m2$df.residual <- m2$df.residual - 1</pre>
## This will adjust the AIC in m2 for the 'estimation' of theta
 m2$aic <- m2$aic + 2
 summary(m2)
```

sim3

The Simulated "sim3" Dataset

#### Description

The sim3 dataset was simulated. There are two treatments and nine species that vary in proportions (p1 - p9). It is assumed that species 1 to 5 come from functional group 1, species 6 and 7 from functional group 2 and species 8 and 9 from functional group 3. The response was simulated assuming that there were species identity effects and functional group specific interaction effects.

#### Usage

data(sim3)

## Format

A data frame with 412 observations on the following 13 variables:

community A numeric vector identifying each unique community, i.e., two rows with the same community value also share the same set of p1 to p9 values.

richness A numeric vector identifying the number of species in the initial composition.

treatment A factor with levels A or B.

- p1 A numeric vector indicating the initial proportion of species 1.
- p2 A numeric vector indicating the initial proportion of species 2.
- p3 A numeric vector indicating the initial proportion of species 3.
- p4 A numeric vector indicating the initial proportion of species 4.
- p5 A numeric vector indicating the initial proportion of species 5.
- p6 A numeric vector indicating the initial proportion of species 6.
- p7 A numeric vector indicating the initial proportion of species 7.
- p8 A numeric vector indicating the initial proportion of species 8.
- p9 A numeric vector indicating the initial proportion of species 9.

response A numeric vector giving the simulated response variable.

#### Details

#### What are Diversity-Interactions (DI) models?

Diversity-Interactions (DI) models (Kirwan et al 2009) are a set of tools for analysing and interpreting data from experiments that explore the effects of species diversity on community-level responses. We strongly recommend that users read the short introduction to Diversity-Interactions models (available at: DImodels). Further information on Diversity-Interactions models is also available in Kirwan et al 2009 and Connolly et al 2013.

#### Parameter values for the simulation

DI models take the general form of:

$$y = Identities + Interactions + Structures + \epsilon$$

where *y* is a community-level response, the *Identities* are the effects of species identities and enter the model as individual species proportions at the beginning of the time period, the *Interactions* are the interactions among the species proportions, while *Structures* include other experimental structures such as blocks, treatments or density.

The dataset sim3 was simulated with:

- identity effects for the nine species with values = 10, 9, 8, 7, 11, 6, 5, 8, 9
- treatment effects = 3, 0
- functional group specific interact effects; assume functional groups are labelled FG1, FG2 and FG3, then the interaction parameter values are: between FG1 and FG2 = 4, between FG1 and FG3 = 9, between FG2 and FG3 = 3, within FG1 = 2, within FG2 = 3 and within FG3 = 1
- theta = 1 (where  $\theta$  is a non-linear parameter included as a power on each *pipj* product within interaction variables, see Connolly et al 2013 for details)
- $\epsilon$  assumed normally distributed with mean 0 and standard deviation 1.2.

#### sim3

#### References

Connolly J, T Bell, T Bolger, C Brophy, T Carnus, JA Finn, L Kirwan, F Isbell, J Levine, A Lüscher, V Picasso, C Roscher, MT Sebastia, M Suter and A Weigelt (2013) An improved model to predict the effects of changing biodiversity levels on ecosystem function. Journal of Ecology, 101, 344-355.

Kirwan L, J Connolly, JA Finn, C Brophy, A Lüscher, D Nyfeler and MT Sebastia (2009) Diversityinteraction modelling - estimating contributions of species identities and interactions to ecosystem function. Ecology, 90, 2032-2038.

## Examples

```
## Simulate dataset sim3 with 9 species, three functional groups and two levels of a treatment.
## The species 1-5 are FG1, species 6-7 are FG2 and species 8-9 are FG3.
## Assume ID effects and the FG interaction model, with a treatment (factor with two levels).
```

```
## Set up proportions
  data("design_a")
  sim3a <- design_a</pre>
```

```
# Replicate the design over two treatments
sim3b <- sim3a[rep(seq_len(nrow(sim3a)), each = 2), ]
sim3c <- data.frame(treatment = factor(rep(c("A","B"), times = 206)))
sim3 <- data.frame(sim3b[,1:2], sim3c, sim3b[,3:11])
row.names(sim3) <- NULL</pre>
```

```
## To simulate the response, first create a matrix of predictors that includes p1-p9, the treatment
## and the interaction variables.
```

```
## Create a vector of 'known' parameter values for simulating the response.
## The first nine are the p1-p9 parameters, and the second set of two are the treatment effects
## and the third set of six are the interaction parameters.
sim3_coeff <- c(10,9,8,7,11, 6,5, 8,9, 3,0, 4,9,3, 2,3,1)</pre>
```

```
## Create response and add normally distributed error
sim3$response <- as.numeric(X %*% sim3_coeff)
set.seed(1657914)
r <- rnorm(n = 412, mean = 0, sd = 1.2)
sim3$response <- round(sim3$response + r, digits = 3)</pre>
```

sim3

```
sim3[,13:18] <- NULL
```

```
## Analyse the sim3 dataset
## Load the sim3 data
 data(sim3)
## View the first few entries
 head(sim3)
## Explore the variables in sim3
 str(sim3)
## Check characteristics of sim3
 hist(sim3$response)
 summary(sim3$response)
 plot(sim3$richness, sim3$response)
 plot(sim3$p1, sim3$response)
 plot(sim3$p2, sim3$response)
 plot(sim3$p3, sim3$response)
 plot(sim3$p4, sim3$response)
 plot(sim3$p5, sim3$response)
 plot(sim3$p6, sim3$response)
 plot(sim3$p7, sim3$response)
 plot(sim3$p8, sim3$response)
 plot(sim3$p9, sim3$response)
## What model fits best? Selection using F-test in autoDI
 auto1 <- autoDI(y = "response", prop = 4:12, treat = "treatment",</pre>
             FG = c("FG1", "FG1", "FG1", "FG1", "FG2", "FG2", "FG3", "FG3"), data = sim3,
                  selection = "Ftest")
 summary(auto1)
## Fit the functional group model, with treatment, using DI and the FG tag
 m1 <- DI(y = "response", prop = 4:12,</pre>
       FG = c("FG1", "FG1", "FG1", "FG1", "FG1", "FG2", "FG2", "FG3", "FG3"), treat = "treatment",
          DImodel = "FG", data = sim3)
 summary(m1)
 plot(m1)
## Check goodness-of-fit using a half-normal plot with a simulated envelope
 library(hnp)
 hnp(m1)
## Create the functional group interactions and store them in a new dataset
```

```
sim3a <- data.frame(sim3, FG_matrix)
## Test if the FG interaction variables interact with treatment using 'extra_formula'
m2 <- DI(y = "response", prop = 4:12,
            FG = c("FG1", "FG1", "FG1", "FG1", "FG2", "FG2", "FG3", "FG3"),
            treat = "treatment", DImodel = "FG", extra_formula = ~ bfg_FG1_FG2:treatment
            + bfg_FG1_FG3:treatment + bfg_FG2_FG3:treatment + wfg_FG1:treatment + wfg_FG3:treatment, data = sim3a)
    summary(m2)
## Fit the functional group model using DI and custom_formula
## Set up a dummy variable for treatment first (required).
    sim3a$treatmentA <- as.numeric(sim3a$treatment=="A")
m3 <- DI(y = "response", custom_formula = response ~ 0 + p1 + p2 + p3 + p4 + p5 + p6 + p7 + p8
            + p9 + treatmentA + bfg_FG1_FG2 + bfg_FG1_FG3 + bfg_FG2_FG3 + wfg_FG1 + wfg_FG2
            + wfg_FG3, data = sim3a)
    summary(m3)</pre>
```

```
sim4
```

#### The Simulated "sim4" Dataset

#### Description

The sim4 dataset was simulated. There is a covariate treatment and six species that vary in proportions (p1 - p6). It is assumed that species 1 and 2 come from functional group 1, species 3 and 4 from functional group 2 and species 5 and 6 from functional group 3. The response was simulated assuming that there were species identity effects, separate pairwise interaction effects and a covariate effect.

## Usage

data(sim4)

#### Format

A data frame with 141 observations on the following nine variables:

richness A numeric vector identifying the number of species in the initial composition.

treatment A covariate taking values 50, 150 or 250.

- p1 A numeric vector indicating the initial proportion of species 1.
- p2 A numeric vector indicating the initial proportion of species 2.
- p3 A numeric vector indicating the initial proportion of species 3.
- p4 A numeric vector indicating the initial proportion of species 4.
- p5 A numeric vector indicating the initial proportion of species 5.
- p6 A numeric vector indicating the initial proportion of species 6.

response A numeric vector giving the simulated response variable.

## Details

#### What are Diversity-Interactions (DI) models?

Diversity-Interactions (DI) models (Kirwan et al 2009) are a set of tools for analysing and interpreting data from experiments that explore the effects of species diversity on community-level responses. We strongly recommend that users read the short introduction to Diversity-Interactions models (available at: DImodels). Further information on Diversity-Interactions models is also available in Kirwan et al 2009 and Connolly et al 2013.

#### Parameter values for the simulation

DI models take the general form of:

## $y = Identities + Interactions + Structures + \epsilon$

where y is a community-level response, the *Identities* are the effects of species identities and enter the model as individual species proportions at the beginning of the time period, the *Interactions* are the interactions among the species proportions, while *Structures* include other experimental structures such as blocks, treatments or density.

The dataset sim4 was simulated with:

- identity effects for the six species with values = 25, 16, 18, 20, 10, 12
- a covariate effect = 0.03
- all 15 pairwise interaction effects with values: 30, 27, 20, 15, 10, 9, 14, 18, 36, 17, 26, 32, 9, 21, 16 (for pairs of species 1-2, 1-3, 1-4, 1-5, 1-6, 2-3, 2-4, ..., 5-6 respectively).
- theta = 1 (where  $\theta$  is a non-linear parameter included as a power on each *pipj* product within interaction variables, see Connolly et al 2013 for details)
- $\epsilon$  assumed normally distributed with mean 0 and standard deviation 2.

### References

Connolly J, T Bell, T Bolger, C Brophy, T Carnus, JA Finn, L Kirwan, F Isbell, J Levine, A Lüscher, V Picasso, C Roscher, MT Sebastia, M Suter and A Weigelt (2013) An improved model to predict the effects of changing biodiversity levels on ecosystem function. Journal of Ecology, 101, 344-355.

Kirwan L, J Connolly, JA Finn, C Brophy, A Lüscher, D Nyfeler and MT Sebastia (2009) Diversityinteraction modelling - estimating contributions of species identities and interactions to ecosystem function. Ecology, 90, 2032-2038.

#### Examples

## Simulate dataset sim4 with 6 species, three functional groups and three levels of a covariate
## The species 1-2 are FG1, species 3-4 are FG2 and species 5-6 are FG3.

## Assume ID effects and the full pairwise interaction model, with a covariate.

## Set up proportions

```
data("design_b")
 sim4a <- design_b</pre>
# Replicate the design for three values of a covariate
 sim4b <- sim4a[rep(seq_len(nrow(sim4a)), times = 3), ]</pre>
 sim4c <- data.frame(treatment = rep(c(50, 150, 250), each = 47))
 sim4 <- data.frame(richness = sim4b[,1], sim4c, sim4b[,2:7])</pre>
 row.names(sim4) <- NULL</pre>
## To simulate the response, first create a matrix of predictors that includes p1-p6, the treatment
## and all pairwise interaction variables
 X <- model.matrix(~ p1 + p2 + p3 + p4 + p5 + p6 + treatment + (p1 + p2 + p3 + p4 + p5 + p6)^2 -1,
                    data = sim4)
## Create a vector of 'known' parameter values for simulating the response.
## The first six are the p1-p6 parameters, and the second set of one is the treatment parameter
## and the third set of 15 are the interaction parameters.
 sim4_coeff <- c(25,16,18,20,10,12, 0.03,
                                               30, 27, 20, 15, 10, 9, 14, 18, 36, 17, 26, 32, 9, 21, 16)
## Create response and add normally distributed error
 sim4$response <- as.numeric(X %*% sim4_coeff)</pre>
 set.seed(34261)
 r <- rnorm(n = 141, mean = 0, sd = 2)
 sim4$response <- round(sim4$response + r, digits = 3)</pre>
## Analyse the sim4 dataset
## Load the sim4 data
 data(sim4)
## View the first few entries
 head(sim4)
## Explore the variables in sim4
 str(sim4)
## Check characteristics of sim4
 hist(sim4$response)
 summary(sim4$response)
 plot(sim4$richness, sim4$response)
 plot(sim4$richness[sim4$treatment==50], sim4$response[sim4$treatment==50], ylim=c(0,40))
 plot(sim4$richness[sim4$treatment==150], sim4$response[sim4$treatment==150], ylim=c(0,40))
 plot(sim4$richness[sim4$treatment==250], sim4$response[sim4$treatment==250], ylim=c(0,40))
 plot(sim4$p1, sim4$response)
 plot(sim4$p2, sim4$response)
 plot(sim4$p3, sim4$response)
 plot(sim4$p4, sim4$response)
 plot(sim4$p5, sim4$response)
 plot(sim4$p6, sim4$response)
```

```
## What model fits best? Selection using F-test
 auto1 <- autoDI(y = "response", prop = 3:8, treat = "treatment",</pre>
            FG = c("FG1", "FG1", "FG2", "FG2", "FG3", "FG3"), data = sim4, selection = "Ftest")
 summary(auto1)
## Ignore functional groups (will replace FG model with ADD model in Step 1 selection)
 auto2 <- autoDI(y = "response", prop = 3:8, treat = "treatment", data = sim4, selection = "Ftest")
 summary(auto2)
## Fit the functional group model using DI and the FG tag
 m1 <- DI(y = "response", prop = 3:8, treat = "treatment",</pre>
           FG = c("FG1", "FG1", "FG2", "FG2", "FG3", "FG3"), DImodel = "FG", data = sim4)
 summary(m1)
## Fit the additive species model using DI and the ADD tag
 m2 <- DI(y = "response", prop = 3:8, treat = "treatment", DImodel = "ADD", data = sim4)
 summary(m2)
## Fit the full pairwise model using DI and the FULL tag
 m3 <- DI(y = "response", prop = 3:8, treat = "treatment", DImodel = "FULL", data = sim4)
 summary(m3)
 plot(m3)
## Check goodness-of-fit using a half-normal plot with a simulated envelope
 library(hnp)
 hnp(m3)
## Create the functional group and additive species interaction variables,
## and store in a new data frame called sim4a
 newlist <- DI_data(prop = 3:8, FG = c("FG1", "FG1", "FG2", "FG2", "FG3", "FG3"),</pre>
                     data = sim4, what = c("FG", "ADD")
 sim4a <- data.frame(sim4, newlist$FG, newlist$ADD)</pre>
## Fit the functional group model using DI and custom_formula (equivalent to m1)
 m4 <- DI(custom_formula = response ~ 0 + p1 + p2 + p3 + p4 + p5 + p6 + bfg_FG1_FG2
        + bfg_FG1_FG3 + bfg_FG2_FG3 + wfg_FG1 + wfg_FG2 + wfg_FG3 + treatment, data = sim4a)
 summary(m4)
## Fit the additive species model using DI and custom_formula (equivalent to m2)
 m5 <- DI(custom_formula = response ~ 0 + p1 + p2 + p3 + p4 + p5 + p6 + p1_add
           + p2_add + p3_add + p4_add + p5_add + p6_add + treatment, data = sim4a)
 summary(m5)
## Fit the full pairwise model using DI and custom_formula (equivalent to m3)
 m6 <- DI(custom_formula = response ~ 0 + p1 + p2 + p3 + p4 + p5 + p6</pre>
           + (p1 + p2 + p3 + p4 + p5 + p6)<sup>2</sup> + treatment, data = sim4a)
 summary(m6)
```

#### Description

The sim5 dataset was simulated. There are nine species that vary in proportions (p1 - p9). It is assumed that species 1 to 5 come from functional group 1, species 6 and 7 from functional group 2 and species 8 and 9 from functional group 3. The response was simulated assuming that there were species identity effects and functional group specific interaction effects, with theta = 0.7.

#### Usage

data(sim5)

## Format

A data frame with 206 observations on the following 12 variables:

community A numeric vector identifying each unique community, i.e., two rows with the same community value also share the same set of p1 to p9 values.

richness A numeric vector identifying the number of species in the initial composition.

p1 A numeric vector indicating the initial proportion of species 1.

p2 A numeric vector indicating the initial proportion of species 2.

p3 A numeric vector indicating the initial proportion of species 3.

p4 A numeric vector indicating the initial proportion of species 4.

p5 A numeric vector indicating the initial proportion of species 5.

p6 A numeric vector indicating the initial proportion of species 6.

p7 A numeric vector indicating the initial proportion of species 7.

p8 A numeric vector indicating the initial proportion of species 8.

p9 A numeric vector indicating the initial proportion of species 9.

response A numeric vector giving the simulated response variable.

#### **Details**

#### What are Diversity-Interactions (DI) models?

Diversity-Interactions (DI) models (Kirwan et al 2009) are a set of tools for analysing and interpreting data from experiments that explore the effects of species diversity on community-level responses. We strongly recommend that users read the short introduction to Diversity-Interactions models (available at: DImodels). Further information on Diversity-Interactions models is also available in Kirwan et al 2009 and Connolly et al 2013.

## Parameter values for the simulation

DI models take the general form of:

sim5

where y is a community-level response, the *Identities* are the effects of species identities and enter the model as individual species proportions at the beginning of the time period, the *Interactions* are the interactions among the species proportions, while *Structures* include other experimental structures such as blocks, treatments or density.

The dataset sim5 was simulated with:

- identity effects for the nine species with values = 10, 9, 8, 7, 11, 6, 5, 8, 9
- functional group specific interaction effects; assume functional groups are labelled FG1, FG2 and FG3, then the interaction parameter values are: between FG1 and FG2 = 8, between FG1 and FG3 = 3, between FG2 and FG3 = 6, within FG1 = 6, within FG2 = 4 and within FG3 = 5
- theta = 0.7 (where  $\theta$  is a non-linear parameter included as a power on each *pipj* product within interaction variables, see Connolly et al 2013 for details)
- $\epsilon$  assumed normally distributed with mean 0 and standard deviation 1.2.

## References

Connolly J, T Bell, T Bolger, C Brophy, T Carnus, JA Finn, L Kirwan, F Isbell, J Levine, A Lüscher, V Picasso, C Roscher, MT Sebastia, M Suter and A Weigelt (2013) An improved model to predict the effects of changing biodiversity levels on ecosystem function. Journal of Ecology, 101, 344-355.

Kirwan L, J Connolly, JA Finn, C Brophy, A Lüscher, D Nyfeler and MT Sebastia (2009) Diversityinteraction modelling - estimating contributions of species identities and interactions to ecosystem function. Ecology, 90, 2032-2038.

## Examples

```
## Simulate dataset sim5 with 9 species and three functional groups.
## The species 1-5 are FG1, species 6-7 are FG2 and species 8-9 are FG3.
## Assume ID effects and the FG interactions model, with theta = 0.7.
## Set up proportions
data("design_a")
sim5 <- design_a
## Create the functional group interaction variables, with theta = 0.7.
FG_matrix <- DI_data(prop = 3:11, FG = c("FG1", "FG1", "FG1", "FG1", "FG1", "FG2", "FG2", "FG3", "FG3"),
data = sim5, theta = 0.7, what = "FG")
sim5 <- data.frame(sim5, FG_matrix)
names(sim5)[12:17] <- paste0(names(sim5)[12:17], "_theta")
## To simulate the response, first create a matrix of predictors that includes p1-p9, the
## treatment and the interaction variables.
X <- model.matrix(~ p1 + p2 + p3 + p4 + p5 + p6 + p7 + p8 + p9</pre>
```

```
+ bfg_FG1_FG2_theta + bfg_FG1_FG3_theta + bfg_FG2_FG3_theta
                    + wfg_FG1_theta + wfg_FG2_theta + wfg_FG3_theta -1, data = sim5)
## Create a vector of 'known' parameter values for simulating the response.
## The first nine are the p1-p9 parameters, and the second set of six are the interaction
## parameters.
 sim5_coeff <- c(10,9,8,7,11, 6,5, 8,9,
                                          8,3,6, 6,4,5)
##Create response and add normally distributed error
 sim5$response <- as.numeric(X %*% sim5_coeff)</pre>
 set.seed(35748)
 r <- rnorm(n = 206, mean = 0, sd = 1.2)
 sim5$response <- round(sim5$response + r, digits = 3)</pre>
 sim5[,12:17] <- NULL
## Analyse the sim5 dataset
## Load the sim5 data
 data(sim5)
## View the first few entries
 head(sim5)
## Explore the variables in sim5
 str(sim5)
## Check characteristics of sim5
 hist(sim5$response)
 summary(sim5$response)
 plot(sim5$richness, sim5$response)
 plot(sim5$p1, sim5$response)
 plot(sim5$p2, sim5$response)
 plot(sim5$p3, sim5$response)
 plot(sim5$p4, sim5$response)
 plot(sim5$p5, sim5$response)
 plot(sim5$p6, sim5$response)
 plot(sim5$p7, sim5$response)
 plot(sim5$p8, sim5$response)
 plot(sim5$p9, sim5$response)
## What model fits best? Selection using F-test in autoDI
 auto1 <- autoDI(y = "response", prop = 3:11,</pre>
                  FG = c("FG1", "FG1", "FG1", "FG1", "FG2", "FG2", "FG3", "FG3"),
                  data = sim5, selection = "Ftest")
 summary(auto1)
## Fit the functional group model, with theta, using DI and the FG tag
 m1 <- DI(y = "response", prop = 3:11,</pre>
          FG = c("FG1", "FG1", "FG1", "FG1", "FG1", "FG2", "FG2", "FG3", "FG3"), DImodel = "FG",
           estimate_theta = TRUE, data = sim5)
```

```
summary(m1)
 CI_95 <- theta_CI(m1, conf = .95)
 CI_95
 plot(m1)
## Check goodness-of-fit using a half-normal plot with a simulated envelope
 library(hnp)
 hnp(m1)
## Graph the profile likelihood
 library(ggplot2)
 ggplot(m1$profile_loglik, aes(x = grid, y = prof)) +
   theme_bw() +
   geom_line() +
   xlim(0, 1.5) +
   xlab(expression(theta)) +
   ylab("Log-likelihood") +
   geom_vline(xintercept = CI_95, lty = 3) +
   labs(title = " Log-likelihood versus theta",
         caption = "dotted vertical lines are upper and lower bounds of 95% CI for theta")
## Fit the functional group model, with theta set equal to the estimate from m1, and custom_formula.
## Note, it is not possible to estimate theta with custom_formula (only select a 'known' value).
## First, create the functional group interactions (theta value as estimated from m1),
## store them in a new dataset and rename them with a theta indicator.
 FG_matrix <- DI_data(prop = 3:11, FG=c("FG1", "FG1", "FG1", "FG1", "FG2", "FG2", "FG3", "FG3"),</pre>
                      theta = 0.7296887, data = sim5, what = "FG")
 sim5new <- data.frame(sim5, FG_matrix)</pre>
 names(sim5new)[13:18] <- paste0(names(sim5new)[13:18], "_theta")</pre>
 m2 <- DI(custom_formula = response ~ 0 + p1 + p2 + p3 + p4 + p5 + p6 + p7 + p8 + p9 +
        bfg_FG1_FG2_theta + bfg_FG1_FG3_theta + bfg_FG2_FG3_theta
         + wfg_FG1_theta + wfg_FG2_theta + wfg_FG3_theta, data = sim5new)
## This will adjust the standard errors in m2 for the 'estimation' of theta
 m2$df.residual <- m2$df.residual - 1
## This will adjust the AIC in m2 for the 'estimation' of theta
 m2$aic <- m2$aic + 2
 summary(m2)
```

Switzerland

The "Switzerland" Dataset

#### Description

This dataset comes from a grassland biodiversity experiment that was conducted in Switzerland as part of the "Agrodiversity Experiment" (Kirwan et al 2014). A total of 68 grassland plots were established across a gradient of species diversity, and two additional treatments (nitrogen fertiliser and total seed density) were also manipulated. The proportions of four species were varied across

#### Switzerland

the plots: there were plots with 100% of a single species, and 2- and 4-species mixtures with varying proportions (e.g., (0.5, 0.5, 0, 0) and (0.7, 0.1, 0.1, 0.1)). Nitrogen fertiliser was either 50 or 100 kg N per annum and total seed density was either low or high. Total annual yield per plot was recorded for the first year after establishment. An analysis of the Switzerland dataset is presented in Kirwan et al 2009.

## Usage

data("Switzerland")

#### Format

A data frame with 68 observations on the following 8 variables:

- plot A numeric vector uniquely identifying each of the 68 plots.
- nitrogen A factor with two levels: "50" or "150" to indicate the level of nitrogen fertiliser (kg N per annum) applied to the plot.
- density A factor with two levels: "low" and "high" to indicate the level of total seed density used when sowing the plot.
- p1 A numeric vector indicating the proportion of species 1 in the plot. Species 1 was the grass species *Lolium perenne*.
- p2 A numeric vector indicating the proportion of species 2 in the plot. Species 2 was the grass species *Dactylis glomerata*.
- p3 A numeric vector indicating the proportion of species 3 in the plot. Species 3 was the legume species *Trifolium pratense*.
- p4 A numeric vector indicating the proportion of species 4 in the plot. Species 4 was the legume species *Trifolium repens*.
- yield A numeric vector giving the total dry matter yield for the plot (tonnes per hectare per annum).

#### Details

#### What are Diversity-Interactions (DI) models?

Diversity-Interactions (DI) models (Kirwan et al 2009) are a set of tools for analysing and interpreting data from experiments that explore the effects of species diversity on community-level responses. We strongly recommend that users read the short introduction to Diversity-Interactions models (available at: DImodels). Further information on Diversity-Interactions models is also available in Kirwan et al 2009 and Connolly et al 2013.

#### Functional groups

In Ecology, species can be categorised into 'functional groups' based on their traits and functions. Here, the four species comprise two grasses (species 1 and 2) and two legumes (species 3 and 4); this is one possible 'functional group' categorisation of the four species.

#### Source

Kirwan L, J Connolly, C Brophy, O Baadshaug, G Belanger, A Black, T Carnus, R Collins, J Čop, I Delgado, A De Vliegher, A Elgersma, B Frankow-Lindberg, P Golinski, P Grieu, AM Gustavsson, Á Helgadóttir, M Höglind, O Huguenin-Elie, M Jørgensen, Ž Kadžiuliene, T Lunnan, A Lüscher, P Kurki, C Porqueddu, MT Sebastia, U Thumm, D Walmsley and JA Finn (2014) The Agrodiversity Experiment: three years of data from a multisite study in intensively managed grasslands. Ecology, 95, 2680.

## References

Connolly J, T Bell, T Bolger, C Brophy, T Carnus, JA Finn, L Kirwan, F Isbell, J Levine, A Lüscher, V Picasso, C Roscher, MT Sebastia, M Suter and A Weigelt (2013) An improved model to predict the effects of changing biodiversity levels on ecosystem function. Journal of Ecology, 101, 344-355.

Kirwan L, J Connolly, JA Finn, C Brophy, A Lüscher, D Nyfeler and MT Sebastia (2009) Diversityinteraction modelling - estimating contributions of species identities and interactions to ecosystem function. Ecology, 90, 2032-2038.

## Examples

```
## Load the Switzerland data
 data(Switzerland)
## View the first few entries
 head(Switzerland)
## Explore the variables in Switzerland
 str(Switzerland)
## Histogram of the response variable yield
 hist(Switzerland$yield)
## Explore the marginal relationship between yield and each predictor
 plot(Switzerland$p1, Switzerland$yield)
 plot(Switzerland$p2, Switzerland$yield)
 plot(Switzerland$p3, Switzerland$yield)
 plot(Switzerland$p4, Switzerland$yield)
 boxplot(yield ~ nitrogen, data = Switzerland)
 boxplot(yield ~ density, data = Switzerland)
## Check that the proportions sum to 1 (required for DI models)
## p1 to p4 are in the 4th to 7th columns in Switzerland
 Switzerlandsums <- rowSums(Switzerland[4:7])</pre>
 summary(Switzerlandsums)
## Model selection by F-test
 auto1 <- autoDI(y = "yield", density = "density", prop = c("p1","p2","p3","p4"),</pre>
                  treat = "nitrogen", FG = c("G", "G", "L", "L"), data = Switzerland,
                  selection = "Ftest")
  summary(auto1)
## Fit the model chosen by autoDI using DI
 m1 <- DI(y = "yield", density = "density", prop = 4:7, DImodel = "FG", FG = c("G", "G", "L", "L"),
           data = Switzerland)
 summary(m1)
```

```
theta_CI
```

#### Compute Confidence Interval for Theta

#### Description

This function allows the computation of a confidence interval for theta from a model object created from DI that includes the argument estimate\_theta = TRUE, or from certain model objects created from autoDI.

A description of the non-linear parameter theta is available in Connolly et al 2013.

## Usage

theta\_CI(obj, conf = .95, n =100)

## Arguments

obj	DI model object.
conf	Confidence level of the interval. The default is 0.95.
n	Number of subintervals in which the root is sought. The default is 100

## Details

The confidence interval calculated here is based on the values obtained when profiling the loglikelihood function for different values of theta. It is obtained in four steps:

1. define a grid of values for theta ranging from 0.01 to 2.5 of length 101 including the profile likelihood estimate of theta

2. fit the DI model setting theta equal to each value in the grid and obtain the log-likelihood value corresponding to each value of theta

3. obtain linear interpolations between the log-likelihood (l) values (here we use approxfun)

4. calculate the lower and upper values of the CI by obtaining the values of theta corresponding to a log-likelihood value of  $max_{\theta}(l) - 0.5 * \chi_{(1 - \alpha; 1)}^2$ , where  $max_{\theta}(l)$  is the maximum value of the profile log-likelihood obtained in the grid and  $\chi_{(conf; 1)}^2$  is the conf \* 100% percentile of the chi-squared distribution with 1 d.f.

When fitting any DI model setting estimate\_theta = TRUE, steps 1 and 2 are automatically done within the DI function call. The theta\_CI function performs steps 3 and 4 above to return the CI.

Note that when maximising the log-likelihood to find the estimate for theta, the parametric space is limited between 0.01 and 1.5. The larger grid (up to 2.5) is constructed to allow for obtaining the upper bound of the confidence interval in case the estimate of theta is close to 1.5.

## Value

The function returns a named numeric vector with two values: the lower and upper limits of the conf\*100% CI for theta.

## Author(s)

Rafael A. Moral, John Connolly and Caroline Brophy

#### References

Connolly J, T Bell, T Bolger, C Brophy, T Carnus, JA Finn, L Kirwan, F Isbell, J Levine, A Lüscher, V Picasso, C Roscher, MT Sebastia, M Suter and A Weigelt (2013) An improved model to predict the effects of changing biodiversity levels on ecosystem function. Journal of Ecology, 101, 344-355.

## See Also

#### DI autoDI

Other examples using the theta\_CI function: The Bell dataset examples. The sim2 dataset examples. The sim5 dataset examples.

#### Examples

```
## Load the sim5 data
    data(sim5)
## View the first five entries
    head(sim5)
## Explore the variables in sim5
    str(sim5)
## Fit the functional group model, with theta, using DI and the FG tag
    m1 <- DI(y = "response", prop = 3:11,
            FG = c("FG1", "FG1", "FG1", "FG1", "FG2", "FG2", "FG3", "FG3"), DImodel = "FG",
            estimate_theta = TRUE, data = sim5)
    summary(m1)</pre>
```

## update\_DI

```
CI_95 <- theta_CI(m1, conf = .95)
CI_95
## Graph the profile likelihood
library(ggplot2)
ggplot(m1$profile_loglik, aes(x = grid, y = prof)) +
theme_bw() +
geom_line() +
xlim(0,1.5) +
xlab(expression(theta)) +
ylab("Log-likelihood") +
geom_vline(xintercept = CI_95, lty = 3) +
labs(title = " Log-likelihood versus theta",
caption = "dotted vertical lines are upper and lower bounds of 95% CI for theta")
```

update\_DI

Update DI function call

## Description

Update the call to the DI function. This function allows users to update a previous call to the DI function by only updating the relevant arguments from DI, without the need to write out the full DI code again.

## Usage

update\_DI(object, ...)

#### Arguments

object	a DI model object
	other arguments passed to the DI function

## Value

A model object of class "glm" including the components detailed in glm, plus the following:

DIcall	the call of the DI function
DIinternalcall	an internal call made within the DI model fitting process

## Author(s)

Rafael A. Moral, John Connolly and Caroline Brophy

## References

Connolly J, T Bell, T Bolger, C Brophy, T Carnus, JA Finn, L Kirwan, F Isbell, J Levine, A Lüscher, V Picasso, C Roscher, MT Sebastia, M Suter and A Weigelt (2013) An improved model to predict the effects of changing biodiversity levels on ecosystem function. Journal of Ecology, 101, 344-355.

Kirwan L, J Connolly, JA Finn, C Brophy, A Lüscher, D Nyfeler and MT Sebastia (2009) Diversityinteraction modelling - estimating contributions of species identities and interactions to ecosystem function. Ecology, 90, 2032-2038.

#### See Also

DI

## Examples

```
## Load the Switzerland data
    data(Switzerland)
```

## Fit the FG DImodel, with factors density and treatment, and theta estimated m2 <- update\_DI(m1, estimate\_theta = TRUE) summary(m2)

## Fit the FULL DImodel, with factors density and treatment, and theta estimated m3 <- update\_DI(m1, DImodel = "FULL", estimate\_theta = TRUE) summary(m3)

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