Package ‘DHARMa’

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Title Residual Diagnostics for Hierarchical (Multi-Level / Mixed) Regression Models

Version 0.4.4

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Description The 'DHARMa' package uses a simulation-based approach to create readily interpretable scaled (quantile) residuals for fitted (generalized) linear mixed models. Currently supported are linear and generalized linear (mixed) models from 'lme4' (classes 'lmerMod', 'glmerMod'), 'glmmTMB' 'GLMMadaptive' and 'spaMM', generalized additive models ('gam' from 'mgcv'), 'glm' (including 'negbin' from 'MASS', but excluding quasi-distributions) and 'lm' model classes. Moreover, externally created simulations, e.g. posterior predictive simulations from Bayesian software such as 'JAGS', 'STAN', or 'BUGS' can be processed as well. The resulting residuals are standardized to values between 0 and 1 and can be interpreted as intuitively as residuals from a linear regression. The package also provides a number of plot and test functions for typical model misspecification problems, such as over/underdispersion, zero-inflation, and residual spatial and temporal autocorrelation.

Depends R (>= 3.0.2)

Imports stats, graphics, utils, grDevices, Matrix, parallel, gap, lmtest, ape, qgam (>= 1.3.2), lme4

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Enhances phyr, rstan, rjags, BayesianTools

License GPL (>= 3)

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LazyData TRUE

BugReports https://github.com/florianhartig/DHARMa/issues

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createData

This function creates synthetic dataset with various problems such as overdispersion, zero-inflation, etc.

Usage

createData(sampleSize = 100, intercept = 0, fixedEffects = 1, quadraticFixedEffects = NULL, numGroups = 10, randomEffectVariance = 1, overdispersion = 0, family = poisson(), scale = 1, cor = 0, roundPoissonVariance = NULL, pZeroInflation = 0, binomialTrials = 1, temporalAutocorrelation = 0, spatialAutocorrelation = 0, factorResponse = F, replicates = 1, hasNA = F)

Arguments

- sampleSize: sample size of the dataset
- intercept: intercept (linear scale)
- fixedEffects: vector of fixed effects (linear scale)
- quadraticFixedEffects: vector of quadratic fixed effects (linear scale)
- numGroups: number of groups for the random effect
- randomEffectVariance: variance of the random effect (intercept)
- overdispersion: if this is a numeric value, it will be used as the sd of a random normal variate that is added to the linear predictor. Alternatively, a random function can be provided that takes as input the linear predictor.
- family: family
- scale: scale if the distribution has a scale (e.g. sd for the Gaussian)
- cor: correlation between predictors
- roundPoissonVariance: if set, this creates a uniform noise on the poisson response. The aim of this is to create heteroscedasticity
- pZeroInflation: probability to set any data point to zero
- binomialTrials: Number of trials for the binomial. Only active if family == binomial
- temporalAutocorrelation: strength of temporalAutocorrelation
createDHARMA

Create a DHARMA object from hand-coded simulations or Bayesian posterior predictive simulations

spatialAutocorrelation
strength of spatial Autocorrelation

factorResponse should the response be transformed to a factor (intended to be used for 0/1 data)

replicates number of datasets to create

hasNA should an NA be added to the environmental predictor (for test purposes)

Examples

testData = createData(sampleSize = 500, intercept = 2, fixedEffects = c(1),
overdispersion = 0, family = poisson(), quadraticFixedEffects = c(-3),
randomEffectVariance = 0)

par(mfrow = c(1,2))
plot(testData$Environment1, testData$observedResponse)
hist(testData$observedResponse)

# with zero-inflation

testData = createData(sampleSize = 500, intercept = 2, fixedEffects = c(1),
overdispersion = 0, family = poisson(), quadraticFixedEffects = c(-3),
randomEffectVariance = 0, pZeroInflation = 0.6)

par(mfrow = c(1,2))
plot(testData$Environment1, testData$observedResponse)
hist(testData$observedResponse)

# binomial with multiple trials

testData = createData(sampleSize = 40, intercept = 2, fixedEffects = c(1),
overdispersion = 0, family = binomial(), quadraticFixedEffects = c(-3),
randomEffectVariance = 0, binomialTrials = 20)

plot(observedResponse1 / observedResponse0 ~ Environment1, data = testData, ylab = "Proportion 1")

# spatial / temporal correlation

testData = createData(sampleSize = 100, family = poisson(), spatialAutocorrelation = 3,
temporalAutocorrelation = 3)

plot(log(observableResponse) ~ time, data = testData)
plot(log(observableResponse) ~ x, data = testData)
createDHARMa

Description

Create a DHARMa object from hand-coded simulations or Bayesian posterior predictive simulations.

Usage

createDHARMa(simulatedResponse, observedResponse, 
  fittedPredictedResponse = NULL, integerResponse = F, seed = 123, 
  method = c("PIT", "traditional"), rotation = NULL)

Arguments

simulatedResponse
  matrix of observations simulated from the fitted model - row index for observations and column index for simulations

observedResponse
  true observations

fittedPredictedResponse
  optional fitted predicted response. For Bayesian posterior predictive simulations, using the median posterior prediction as fittedPredictedResponse is recommended. If not provided, the mean simulatedResponse will be used.

integerResponse
  if T, noise will be added at to the residuals to maintain a uniform expectations for integer responses (such as Poisson or Binomial). Unlike in simulateResiduals, the nature of the data is not automatically detected, so this MUST be set by the user appropriately

seed
  the random seed to be used within DHARMa. The default setting, recommended for most users, is keep the random seed on a fixed value 123. This means that you will always get the same randomization and thus the same result when running the same code. NULL = no new seed is set, but previous random state will be restored after simulation. FALSE = no seed is set, and random state will not be restored. The latter two options are only recommended for simulation experiments. See vignette for details.

method
  the quantile randomization method used. The two options implemented at the moment are probability integral transform (PIT-) residuals (current default), and the "traditional" randomization procedure, that was used in DHARMa until version 0.3.0. For details, see getQuantile

rotation
  optional rotation of the residual space to remove residual autocorrelation. See details in simulateResiduals, section residual auto-correlation for an extended explanation, and getQuantile for syntax.

Details

The use of this function is to convert simulated residuals (e.g. from a point estimate, or Bayesian p-values) to a DHARMa object, to make use of the plotting / test functions in DHARMa

Note

Either scaled residuals or (simulatedResponse AND observed response) have to be provided
## READING IN HAND-CODED SIMULATIONS

```r
# data
testData = createData(sampleSize = 50, randomEffectVariance = 0)
fittedModel <- glm(observedResponse ~ Environment1, data = testData, family = "poisson")

# in DHARMA, using the simulate.glm function of glm
sims = simulateResiduals(fittedModel)
plot(sims, quantreg = FALSE)

# Doing the same with a handcoded simulate function.
# of course this code will only work with a 1-par glm model
simulateMyfit <- function(n=10, fittedModel){
  int = coef(fittedModel)[1]
  slo = coef(fittedModel)[2]
  pred = exp(int + slo * testData(Environment1))
  predSim = replicate(n, rpois(length(pred), pred))
  return(predSim)
}
sims = simulateMyfit(250, fittedModel)

dharmaRes <- createDHARMa(simulatedResponse = sims,
                         observedResponse = testData(observedResponse),
                         fittedPredictedResponse = predict(fittedModel, type = "response"),
                         integer = TRUE)
plot(dharmaRes, quantreg = FALSE)
```

### DHARMa - Residual Diagnostics for Hierarchical (Multi-level / Mixed) Regression Models

**Description**

The 'DHARMa' package uses a simulation-based approach to create readily interpretable scaled (quantile) residuals for fitted (generalized) linear mixed models. Currently supported are linear and generalized linear (mixed) models from 'lme4' (classes 'lmerMod', 'glmerMod'), 'glmmTMB' and 'spaMM', generalized additive models ('gam' from 'mgcv'), 'glm' (including 'negbin' from 'MASS', but excluding quasi-distributions) and 'lm' model classes. Moreover, externally created simulations, e.g. posterior predictive simulations from Bayesian software such as 'JAGS', 'STAN', or 'BUGS' can be processed as well. The resulting residuals are standardized to values between 0 and 1 and can be interpreted as intuitively as residuals from a linear regression. The package also provides a number of plot and test functions for typical model misspecification problems, such as over/underdispersion, zero-inflation, and residual spatial and temporal autocorrelation.

### Details

See index / vignette for details
getFitted

See Also

simulateResiduals

Examples

vignette("DHARMa", package="DHARMa")

getFitted

Get fitted / predicted values

Description

Wrapper to get the fitted / predicted response of model at the response scale

Usage

getFitted(object, ...)

## Default S3 method:
getFitted(object, ...)

## Default S3 method:
getResiduals(object, ...)

## S3 method for class 'gam'
getFitted(object, ...)

## S3 method for class 'HLfit'
getFitted(object, ...)

## S3 method for class 'MixMod'
getFitted(object, ...)

Arguments

object

a fitted model

...

additional parameters to be passed on, usually to the simulate function of the respective model class

Details

The purpose of this wrapper is to standardize extract the fitted values, which is implemented via predict(model, type = "response") for most model classes.

If you implement this function for a new model class, you should include an option to modifying which REs are included in the predictions. If this option is not available, it is essential that predictions are provided marginally / unconditionally, i.e. without the random effect estimates (because of https://github.com/florianhartig/DHARMa/issues/43), which corresponds to re-form = ~0 in lme4
Author(s)
Florian Hartig

See Also
getObservedResponse, getSimulations, getRefit, getFixedEffects

Examples

testData = createData(sampleSize = 400, family = gaussian())
fittedModel <- lm(observedResponse ~ Environment1, data = testData)

# response that was used to fit the model
getObservedResponse(fittedModel)

# predictions of the model for these points
getFitted(fittedModel)

# extract simulations from the model as matrix
getSimulations(fittedModel, nsim = 2)

# extract simulations from the model for refit (often requires different structure)
x = getSimulations(fittedModel, nsim = 2, type = "refit")

getRefit(fittedModel, x[[1]])

getRefit(fittedModel, getObservedResponse(fittedModel))

getFixedEffects

Get fixed effects of a supported model

Description
A wrapper to extract fixed effects of a supported model

Usage
getFixedEffects(fittedModel)

getFixedEffects.MixMod(fittedModel)

Arguments
fittedModel a fitted model

See Also
getObservedResponse, getSimulations, getRefit, getFitted
getObservedResponse

Examples

testData = createData(sampleSize = 400, family = gaussian())

fittedModel <- lm(observedResponse ~ Environment1, data = testData)

# response that was used to fit the model
getObservedResponse(fittedModel)

# predictions of the model for these points
getFitted(fittedModel)

# extract simulations from the model as matrix
getSimulations(fittedModel, nsim = 2)

# extract simulations from the model for refit (often requires different structure)
x = getSimulations(fittedModel, nsim = 2, type = "refit")

getRefit(fittedModel, x[[1]])

getRefit(fittedModel, getObservedResponse(fittedModel))

getObservedResponse  Get model response

Description

Extract the response of a fitted model

Usage

getObservedResponse(object, ...)

## Default S3 method:
getObservedResponse(object, ...)

## S3 method for class 'HLfit'
getObservedResponse(object, ...)

Arguments

object  a fitted model

...  additional parameters

Details

The purpose of this function is to safely extract the observed response (dependent variable) of the fitted model classes
getQuantile

Author(s)
Florian Hartig

See Also
getRefit, getSimulations, getFixedEffects, getFitted

Examples

testData = createData(sampleSize = 400, family = gaussian())
fittedModel <- lm(observedResponse ~ Environment1, data = testData)

# response that was used to fit the model
getObservedResponse(fittedModel)

# predictions of the model for these points
getFitted(fittedModel)

# extract simulations from the model as matrix
getSimulations(fittedModel, nsim = 2)

# extract simulations from the model for refit (often requires different structure)
x = getSimulations(fittedModel, nsim = 2, type = "refit")
getRefit(fittedModel, x[[1]])
getRefit(fittedModel, getObservedResponse(fittedModel))

---

getQuantile calculate quantiles

Description
calculates residual quantiles from a given simulation

Usage
getQuantile(simulations, observed, integerResponse, method = c("PIT", "traditional"), rotation = NULL)

Arguments

- simulations: a matrix with simulations from a fitted model. Rows = observations, columns = replicate simulations
- observed: a vector with the observed data
- integerResponse: is the response integer-valued. Only has an effect for method = "traditional"
The function calculates residual quantiles from the simulated data. For continuous distributions, this will simply the the value of the ecdf.

**Randomization procedure for discrete data**

For discrete data, there are two options implemented. The current default (available since DHARMa 0.3.1) are probability integral transform (PIT-) residuals (Smith, 1985; Dunn & Smyth, 1996; see also also Warton, et al., 2017).

Before DHARMa 0.3.1, a different randomization procedure was used, in which the a U(-0.5, 0.5) distribution was added on observations and simulations for discrete distributions. For a completely discrete distribution, the two procedures should deliver equivalent results, but the second method has the disadvantage that a) one has to know if the distribution is discrete (DHARMa tries to recognize this automatically), and b) that it leads to inefficiencies for some distributions such as the the Tweedie, which are partly continuous, partly discrete (see e.g. https://github.com/florianhartig/DHARMa/issues/168).

**Rotation (optional)**

The getQuantile function includes an additional option to rotate residuals. The purpose is to de-correlated residuals in case of residual autocorrelation. If the expected residual autocorrelation is known (e.h. when fitting gls type models), it can be provided as a covariance matrix. If that is note the case, the option "estimated" will try to estimate the covariance from the data simulated by the model. Note, however, that this approximation will tend to have considerable error and may be slow to compute for high-dimensional data.

**References**


Usage

getRandomState(seed = NULL)

Arguments

seed seed argument to set.seed(), typically a number. Additional options: NULL = no seed is set, but return includes function for restoring random seed. F = function does nothing, i.e. neither seed is changed, nor does the returned function do anything

Details

This function is intended for two (not mutually exclusive tasks)
a) record the current random state
b) change the current random state in a way that the previous state can be restored

Value

a list with various infos about the random state that after function execution, as well as a function to restore the previous state before the function execution

Author(s)

Florian Hartig

Examples

set.seed(13)
runif(1)

# testing the function in standard settings
currentSeed = .Random.seed
x = getRandomState(123)
runif(1)
x$restoreCurrent()
all(.Random.seed == currentSeed)

# if no seed was set in env, this will also be restored

rm(.Random.seed) # now, there is no random seed
x = getRandomState(123)
exists(".Random.seed") # TRUE
runif(1)
x$restoreCurrent()
exists(".Random.seed") # False
runif(1) # re-create a seed

# with seed = false
currentSeed = .Random.seed
```r
x = getRandomState(FALSE)
runif(1)
x$restoreCurrent()
all(.Random.seed == currentSeed)

# with seed = NULL
currentSeed = .Random.seed
x = getRandomState(NULL)
runif(1)
x$restoreCurrent()
all(.Random.seed == currentSeed)
```

---

### getRefit

**Get model refit**

#### Description

Wrapper to refit a fitted model
checks if the fitted model excluded NA values

#### Usage

```r
getRefit(object, newresp, ...)
```

## Default S3 method:
```
getRefit(object, newresp, ...)
```

## S3 method for class 'lm'
```
getRefit(object, newresp, ...)
```

## S3 method for class 'glmmTMB'
```
getRefit(object, newresp, ...)
```

## S3 method for class 'HLfit'
```
getRefit(object, newresp, ...)
```

## S3 method for class 'MixMod'
```
getRefit(object, newresp, ...)
```

#### Arguments

- **object** a fitted model
- **newresp** the new response that should be used to refit the model
- **...** additional parameters to be passed on to the refit or update class that is used to refit the model
Details

The purpose of this wrapper is to standardize the refit of a model. The behavior of this function
depends on the supplied model. When available, it uses the refit method, otherwise it will use
update. For glmmTMB: since version 1.0, glmmTMB has a refit function, but this didn’t work, so
I switched back to this implementation, which is a hack based on the update function.
Checks if the fitted model excluded NA values

Author(s)

Florian Hartig

See Also

getObservedResponse, getSimulations, getFixedEffects

Examples

testData = createData(sampleSize = 400, family = gaussian())

fittedModel <- lm(observedResponse ~ Environment1, data = testData)

# response that was used to fit the model
getObservedResponse(fittedModel)

# predictions of the model for these points
getFitted(fittedModel)

# extract simulations from the model as matrix
getSimulations(fittedModel, nsim = 2)

# extract simulations from the model for refit (often requires different structure)
x = getSimulations(fittedModel, nsim = 2, type = "refit")

getRefit(fittedModel, x[[1]])

getRefit(fittedModel, getObservedResponse(fittedModel))

---

table

| getResiduals | Get model residuals |

Description

Wrapper to get the residuals of a fitted model

Usage

getResiduals(object, ...)

## S3 method for class 'MixMod'
getResiduals(object, ...)


**getSimulations**

Arguments

- object: a fitted model
- ...: additional parameters to be passed on, usually to the residual function of the respective model class

Details

The purpose of this wrapper is to standardize extract the model residuals. Similar to some other functions, a key question is whether to calculate those conditional or unconditional on the fitted REs.

Author(s)

Florian Hartig

See Also

getObservedResponse, getSimulations, getRefit, getFixedEffects, getFitted

Examples

```r
testData = createData(sampleSize = 400, family = gaussian())
fittedModel <- lm(observedResponse ~ Environment1 , data = testData)

# response that was used to fit the model
getObservedResponse(fittedModel)

# predictions of the model for these points
getFitted(fittedModel)

# extract simulations from the model as matrix
getSimulations(fittedModel, nsim = 2)

# extract simulations from the model for refit (often requires different structure)
x = getSimulations(fittedModel, nsim = 2, type = "refit")

getRefit(fittedModel, x[[1]])
getRefit(fittedModel, getObservedResponse(fittedModel))
```

---

**Description**

Wrapper to simulate from a fitted model
Usage

getSimulations(object, nsim = 1, type = c("normal", "refit"), ...)

## Default S3 method:
getSimulations(object, nsim = 1, type = c("normal", "refit"), ...)

## S3 method for class 'negbin'
getSimulations(object, nsim = 1, type = c("normal", "refit"), ...)

## S3 method for class 'lmerMod'
getSimulations(object, nsim = 1, type = c("normal", "refit"), ...)

## S3 method for class 'glmmTMB'
getSimulations(object, nsim = 1, type = c("normal", "refit"), ...)

## S3 method for class 'HLfit'
getSimulations(object, nsim = 1, type = c("normal", "refit"), ...)

## S3 method for class 'MixMod'
getSimulations(object, nsim = 1, type = c("normal", "refit"), ...)

Arguments

object      a fitted model
nsim        number of simulations
type        if simulations should be prepared for getQuantile or for refit
...          additional parameters to be passed on, usually to the simulate function of the
             respective model class

Details

The purpose of this wrapper for the simulate function is to return the simulations from a model
in a standardized way.

The purpose of this function is to wrap or implement the simulate function of different model classes
and thus return simulations from fitted models in a standardized way.

Note: GLMM and other regression packages often differ in how simulations are produced, and
which parameters can be used to modify this behavior.

One important difference is how to modify which hierarchical levels are held constant, and which
are re-simulated. In lme4, this is controlled by the re.form argument (see \texttt{lme4::simulate.merMod}).
For other packages, please consort the help.

If the model was fit with weights and the respective model class does not include the weights in
the simulations, getSimulations will throw a warning. The background is if weights are used on
the likelihood directly, then what is fitted is effectively a pseudo likelihood, and there is no way to
directly simulate from the specified likelihood. Whether or not residuals can be used in this case
depends very much on what is tested and how weights are used. I’m sorry to say that it is hard
to give a general recommendation, you have to consult someone that understands how weights are
processed in the respective model class.
Value

a matrix with simulations

Author(s)

Florian Hartig

See Also

getObservedResponse, getRefit, getFixedEffects, getFitted

Examples

testData = createData(sampleSize = 400, family = gaussian())
fittedModel <- lm(observedResponse ~ Environment1, data = testData)

# response that was used to fit the model
getObservedResponse(fittedModel)

# predictions of the model for these points
getFitted(fittedModel)

# extract simulations from the model as matrix
getSimulations(fittedModel, nsim = 2)

# extract simulations from the model for refit (often requires different structure)
x = getSimulations(fittedModel, nsim = 2, type = "refit")
getRefit(fittedModel, x[[1]])
getRefit(fittedModel, getObservedResponse(fittedModel))

---

hist.DHARMa  

Histogram of DHARMa residuals

Description

The function produces a histogram from a DHARMa output

Usage

## S3 method for class 'DHARMa'
hist(x, breaks = seq(-0.02, 1.02, len = 53),
     col = c("red", rep("lightgrey", 50), "red"),
     main = "Hist of DHARMa residuals",
     xlab = "Residuals (outliers are marked red)", cex.main = 1, ...)
Arguments

- `x`: a DHARMa simulation output (class DHARMa)
- `breaks`: breaks for hist() function
- `col`: col for hist bars
- `main`: plot main
- `xlab`: plot xlab
- `cex.main`: plot cex.main
- `...`: other arguments to be passed on to hist

See Also

- `plotSimulatedResiduals`, `plotResiduals`

Examples

```r
testdata = createData(sampleSize = 200, family = poisson(),
  randomEffectVariance = 1, numGroups = 10)
fittedModel <- glm(observedResponse ~ Environment1,
  family = "poisson", data = testData)
simulationOutput <- simulateResiduals(fittedModel = fittedModel)

######### main plotting function #############
# for all functions, quantreg = T will be more
# informative, but slower
plot(simulationOutput, quantreg = FALSE)

############# Distribution ######################
plotQQunif(simulationOutput = simulationOutput,
  testDispersion = FALSE,
  testUniformity = FALSE,
  testOutliers = FALSE)
hist(simulationOutput)

############# residual plots ####################

# rank transformation, using a simulationOutput
plotResiduals(simulationOutput, rank = TRUE, quantreg = FALSE)

# smooth scatter plot - usually used for large datasets, default for n > 10000
plotResiduals(simulationOutput, rank = TRUE, quantreg = FALSE, smoothScatter = TRUE)

# residual vs predictors, using explicit values for pred, residual
plotResiduals(simulationOutput, form = testData$Environment1,
  quantreg = FALSE)
```
# if pred is a factor, or if asFactor = T, will produce a boxplot
plotResiduals(simulationOutput, form = testData$group)

# All these options can also be provided to the main plotting function

# If you want to plot summaries per group, use
simulationOutput = recalculateResiduals(simulationOutput, group = testData$group)
plot(simulationOutput, quantreg = FALSE)

# we see one residual point per RE

<table>
<thead>
<tr>
<th>hurricanes</th>
<th>Hurricanes</th>
</tr>
</thead>
</table>

**Description**

A data set on hurricane strength and fatalities in the US between 1950 and 2012. The data originates from the study by Jung et al., PNAS, 2014, who claim that the masculinity / femininity of a hurricane name has a causal effect on fatalities, presumably through a different perception of danger caused by the names.

**Format**

A 'data.frame': 93 obs. of 14 variables

**Year** Year of the hurricane (1950-2012)

**Name** Name of the hurricane

**MasFem** Masculinity-femininity rating of the hurricane’s name in the range 1 = very masculine, 11 = very feminine

**MinPressure_before** Minimum air pressure (909-1002)

**Minpressure_Updated_2014** Updated minimum air pressure (909-1003)

**Gender_MF** Binary gender (male/female) based on MasFem (male = 0, female = 1)

**Category** Strength of the hurricane in categories (1:7). (1 = not at all, 7 = very intense)

**alldeaths** Deaths occurred (1:256)

**NDAM** normalized damage in millions (1:75,000). The raw (dollar) amounts of property damage caused by hurricanes were obtained, and the unadjusted dollar amounts were normalized to 2013 monetary values by adjusting them to inflation, wealth and population density

**_elapsed_Yrs** elapsed since the occurrence of hurricanes (1:63)

**Source** MWR/wikipedia ()

**ZMasFem** scaled (MasFem)

**ZMinPressure_A** scaled (Minpressure_Updated_2014)

**ZNDAM** scaled (NDAM) ...
References


Examples

```r
## Not run:
# Loading hurricanes dataset

library(DHARMa)

data(hurricanes)

str(hurricanes)

# this is the model fit by Jung et al.
library(glmmTMB)

originalModelGAM = glmmTMB(alldeaths ~ scale(MasFem) * 
(scale(Minpressure_Updated_2014) + scale(NDAM)), 
        data = hurricanes, family = nbinom2)

# no significant deviation in the general DHARMa plot
res <- simulateResiduals(originalModelGAM)
plot(res)

# but residuals ~ NDAM looks funny, which was pointed
# out by Bob O'Hara in a blog post after publication of the paper
plotResiduals(res, hurricanes$NDAM)

# we also find temporal autocorrelation
res2 = recalculateResiduals(res, group = hurricanes$Year)
testTemporalAutocorrelation(res2, time = unique(hurricanes$Year))

# task: try to address these issues - in many instances, this will
# make the MasFem predictor n.s.

## End(Not run)
```

---

### outliers

**Return outliers**

Returns the outliers of a DHARMa object

**Usage**

```r
outliers(object, lowerQuantile = 0, upperQuantile = 1, 
        return = c("index", "logical"))
```
plot.DHARMa

Arguments

- **object**: an object with simulated residuals created by `simulateResiduals`
- **lowerQuantile**: lower threshold for outliers. Default is zero = outside simulation envelope
- **upperQuantile**: upper threshold for outliers. Default is 1 = outside simulation envelope
- **return**: whether to return an indices of outliers or a logical vector

Details

First of all, note that the standard definition of outlier in the DHARMa plots and outlier tests is an observation that is outside the simulation envelope. How far outside that is depends a lot on how many simulations you do. If you have 100 data points and to 100 simulations, you would expect to have one "outlier" on average, even with a perfectly fitting model. This is in fact what the outlier test tests.

Thus, keep in mind that for a small number of simulations, outliers are mostly a technical term: these are points that are outside our simulations, but we don’t know how far away they are.

If you are seriously interested in HOW FAR outside the expected distribution a data point is, you should increase the number of simulations in `simulateResiduals` to be sure to get the tail of the data distribution correctly. In this case, it may make sense to adjust `lowerQuantile` and `upperQuantile`, e.g. to 0.025, 0.975, which would define outliers as values outside the central 95% of the distribution.

Also, note that outliers are particularly concerning if they have a strong influence on the model fit. One could test the influence, for example, by removing them from the data, or by some measures of leverage, e.g. generalisations for Cook’s distance as in Pinho, L. G. B., Nobre, J. S., & Singer, J. M. (2015). Cook’s distance for generalized linear mixed models. Computational Statistics & Data Analysis, 82, 126–136. doi:10.1016/j.csda.2014.08.008. At the moment, however, no such function is provided in DHARMa.

---

plot.DHARMa  
DHARMa standard residual plots

Description

This S3 function creates standard plots for the simulated residuals contained in an object of class DHARMa, using `plotQQunif` (left panel) and `plotResiduals` (right panel)

Usage

```r
## S3 method for class 'DHARMa'
plot(x, ...)
```

Arguments

- **x**: an object of class DHARMa with simulated residuals created by `simulateResiduals`
- **...**: further options for `plotResiduals`. Consider in particular parameters quantreg, rank and asFactor. xlab, ylab and main cannot be changed when using `plot.DHARMa`, but can be changed when using `plotResiduals`. 
The function creates a plot with two panels. The left panel is a uniform qq plot (calling `plotQQunif`), and the right panel shows residuals against predicted values (calling `plotResiduals`), with outliers highlighted in red.

Very briefly, we would expect that a correctly specified model shows:

a) a straight 1-1 line, as well as n.s. of the displayed tests in the qq-plot (left) -> evidence for an the correct overall residual distribution (for more details on the interpretation of this plot, see `plotQQunif`)

b) visual homogeneity of residuals in both vertical and horizontal direction, as well as n.s. of quantile tests in the res ~ predictor plot (for more details on the interpretation of this plot, see `plotResiduals`)

Deviations from these expectations can be interpreted similar to a linear regression. See the vignette for detailed examples.

Note that, unlike `plotResiduals`, plot.DHARMa command uses the default rank = T.

### Examples

```r
testData = createData(sampleSize = 200, family = poisson(),
    randomEffectVariance = 1, numGroups = 10)
fittedModel <- glm(observedResponse ~ Environment1,
    family = "poisson", data = testData)
simulationOutput <- simulateResiduals(fittedModel = fittedModel)

# for all functions, quantreg = T will be more informative, but slower
plot(simulationOutput, quantreg = FALSE)

plotQQunif(simulationOutput = simulationOutput,
    testDispersion = FALSE,
    testUniformity = FALSE,
    testOutliers = FALSE)

hist(simulationOutput)

plotResiduals(simulationOutput, rank = TRUE, quantreg = FALSE)

# smooth scatter plot - usually used for large datasets, default for n > 10000
```
plot.DHARMaBenchmark

The function plots the result of an object of class DHARMaBenchmark, created by runBenchmarks

Usage

## S3 method for class 'DHARMaBenchmark'
plot(x, ...)

Arguments

x object of class DHARMaBenchmark, created by runBenchmarks

... parameters to pass to the plot function

Details

The function will create two types of plots, depending on whether the run contains only a single value (or no value) of the control parameter, or whether a vector of control values was provided.

If a single or no value of the control parameter was provided, the function will create box plots of the estimated p-values, with the number of significant p-values plotted to the left.

If a control parameter was provided, the function will plot the proportion of significant p-values against the control parameter, with 95% CIs based on the performed replicates displayed as confidence bands.

See Also

runBenchmarks
plotConventionalResiduals

Conventional residual plot

Description
Convenience function to draw conventional residual plots

Usage
plotConventionalResiduals(fittedModel)

Arguments
fittedModel a fitted model object

plotQQunif

Quantile-quantile plot for a uniform distribution

Description
The function produces a uniform quantile-quantile plot from a DHARMa output

Usage
plotQQunif(simulationOutput, testUniformity = T, testOutliers = T, testDispersion = T, ...)

Arguments
simulationOutput a DHARMa simulation output (class DHARMa)
testUniformity if T, the function testUniformity will be called and the result will be added to the plot
testOutliers if T, the function testOutliers will be called and the result will be added to the plot
testDispersion if T, the function testDispersion will be called and the result will be added to the plot
... arguments to be passed on to qqunif

Details
the function calls qqunif from the R package gap to create a quantile-quantile plot for a uniform distribution, and overlays tests for particular distributional problems as specified.
See Also

`plotSimulatedResiduals, plotResiduals`

Examples

testData = createData(sampleSize = 200, family = poisson(),
                      randomEffectVariance = 1, numGroups = 10)
fittedModel <- glm(observedResponse ~ Environment1,
                   family = "poisson", data = testData)
simulationOutput <- simulateResiduals(fittedModel = fittedModel)

############## main plotting function ##############
# for all functions, quantreg = T will be more
# informative, but slower
plot(simulationOutput, quantreg = FALSE)

############### Distribution ###################
plotQQunif(simulationOutput = simulationOutput,
           testDispersion = FALSE,
           testUniformity = FALSE,
           testOutliers = FALSE)

hist(simulationOutput)

############# residual plots #################
# rank transformation, using a simulationOutput
plotResiduals(simulationOutput, rank = TRUE, quantreg = FALSE)

# smooth scatter plot - usually used for large datasets, default for n > 10000
plotResiduals(simulationOutput, rank = TRUE, quantreg = FALSE, smoothScatter = TRUE)

# residual vs predictors, using explicit values for pred, residual
plotResiduals(simulationOutput, form = testData$Environment1,
              quantreg = FALSE)

# if pred is a factor, or if asFactor = T, will produce a boxplot
plotResiduals(simulationOutput, form = testData$group)

# All these options can also be provided to the main plotting function

# If you want to plot summaries per group, use
simulationOutput = recalculateResiduals(simulationOutput, group = testData$group)
plot(simulationOutput, quantreg = FALSE)
# we see one residual point per RE
plotResiduals

Generic res ~ pred scatter plot with spline or quantile regression on top

Description

The function creates a generic residual plot with either spline or quantile regression to highlight patterns in the residuals. Outliers are highlighted in red.

Usage

plotResiduals(simulationOutput, form = NULL, quantreg = NULL, rank = T, asFactor = NULL, smoothScatter = NULL, quantiles = c(0.25, 0.5, 0.75), ...)

Arguments

simulationOutput
- an object, usually a DHARMa object, from which residual values can be extracted. Alternatively, a vector with residuals or a fitted model can be provided, which will then be transformed into a DHARMa object.

form
- optional predictor against which the residuals should be plotted. Default is to use the predicted(simulationOutput)

quantreg
- whether to perform a quantile regression based on testQuantiles or a smooth spline around the mean. Default NULL chooses T for nObs < 2000, and F otherwise.

rank
- if T, the values provided in form will be rank transformed. This will usually make patterns easier to spot visually, especially if the distribution of the predictor is skewed. If form is a factor, this has no effect.

asFactor
- should a numeric predictor provided in form be treated as a factor. Default is to choose this for < 10 unique values, as long as enough predictions are available to draw a boxplot.

smoothScatter
- if T, a smooth scatter plot will plotted instead of a normal scatter plot. This makes sense when the number of residuals is very large. Default NULL chooses T for nObs < 10000, and F otherwise.

quantiles
- for a quantile regression, which quantiles should be plotted

... additional arguments to plot / boxplot.

Details

The function plots residuals against a predictor (by default against the fitted value, extracted from the DHARMa object, or any other predictor).

Outliers are highlighted in red (for information on definition and interpretation of outliers, see testOutliers).
To provide a visual aid in detecting deviations from uniformity in y-direction, the plot function calculates an (optional) quantile regression of the residuals, by default for the 0.25, 0.5 and 0.75 quantiles. As the residuals should be uniformly distributed for a correctly specified model, the theoretical expectations for these regressions are straight lines at 0.25, 0.5 and 0.75, which are displayed as dashed black lines on the plot. Some deviations from these expectations are to be expected by chance, however, even for a perfect model, especially if the sample size is small. The function therefore tests if deviation of the fitted quantile regression from the expectation is significant, using `testQuantiles`. If so, the significant quantile regression will be highlighted as red, and a warning will be displayed in the plot.

The quantile regression can take some time to calculate, especially for larger datasets. For that reason, `quantreg = F` can be set to produce a smooth spline instead. This is default for n > 2000. If form is a factor, a boxplot will be plotted instead of a scatter plot. The distribution for each factor level should be uniformly distributed, so the box should go from 0.25 to 0.75, with the median line at 0.5 (within-group). To test if deviations from those expectations are significant, KS-tests per group and a Levene test for homogeneity of variances is performed. See `testCategorical` for details.

**Value**

if quantile tests are performed, the function returns them invisibly.

**Note**

if nObs > 10000, the scatter plot is replaced by `graphics::smoothScatter`

**See Also**

`plotQQunif`, `testQuantiles`, `testOutliers`

**Examples**

testData = createData(sampleSize = 200, family = poisson(),
        randomEffectVariance = 1, numGroups = 10)
fittedModel <- glm(observedResponse ~ Environment1,
        family = "poisson", data = testData)
simulationOutput <- simulateResiduals(fittedModel = fittedModel)

######### main plotting function #############
# for all functions, quantreg = T will be more
# informative, but slower
plot(simulationOutput, quantreg = FALSE)

############ Distribution ####################
plotQQunif(simulationOutput = simulationOutput,
        testDispersion = FALSE, testUniformity = FALSE, testOutliers = FALSE)
hist(simulationOutput)

# rank transformation, using a simulationOutput
plotResiduals(simulationOutput, rank = TRUE, quantreg = FALSE)

# smooth scatter plot - usually used for large datasets, default for n > 10000
plotResiduals(simulationOutput, rank = TRUE, quantreg = FALSE, smoothScatter = TRUE)

# residual vs predictors, using explicit values for pred, residual
plotResiduals(simulationOutput, form = testData$Environment1,
               quantreg = FALSE)

# if pred is a factor, or if asFactor = T, will produce a boxplot
plotResiduals(simulationOutput, form = testData$group)

# All these options can also be provided to the main plotting function

# If you want to plot summaries per group, use
simulationOutput = recalculateResiduals(simulationOutput, group = testData$group)
plot(simulationOutput, quantreg = FALSE)
# we see one residual point per RE

plotSimulatedResiduals

DHARMa standard residual plots

Description
DEPRECATED, use plot() instead

Usage
plotSimulatedResiduals(simulationOutput, ...)

Arguments
simulationOutput
an object with simulated residuals created by simulateResiduals

... further options for plotResiduals. Consider in particular parameters quantreg, rank and asFactor. xlab, ylab and main cannot be changed when using plotSimulatedResiduals, but can be changed when using plotResiduals.

Note
This function is deprecated. Use plot.DHARMa
### print.DHARMa

**Print simulated residuals**

**Description**

Print simulated residuals

**Usage**

```r
## S3 method for class 'DHARMa'
print(x, ...)
```

**Arguments**

- `x` an object with simulated residuals created by `simulateResiduals`
- `...` optional arguments for compatibility with the generic function, no function implemented

### recalculateResiduals

**Recalculate residuals with grouping**

**Description**

The purpose of this function is to recalculate scaled residuals per group, based on the simulations done by `simulateResiduals`

**Usage**

```r
recalculateResiduals(simulationOutput, group = NULL, aggregateBy = sum, sel = NULL, seed = 123, method = c("PIT", "traditional"), rotation = NULL)
```

**Arguments**

- `simulationOutput` an object with simulated residuals created by `simulateResiduals`
- `group` group of each data point
- `aggregateBy` function for the aggregation. Default is sum. This should only be changed if you know what you are doing. Note in particular that the expected residual distribution might not be flat any more if you choose general functions, such as sd etc.
recalculateResiduals

sel

an optional vector for selecting the data to be aggregated

seed

the random seed to be used within DHARMa. The default setting, recommended for most users, is keep the random seed on a fixed value 123. This means that you will always get the same randomization and thus the same result when running the same code. NULL = no new seed is set, but previous random state will be restored after simulation. FALSE = no seed is set, and random state will not be restored. The latter two options are only recommended for simulation experiments. See vignette for details.

method

the quantile randomization method used. The two options implemented at the moment are probability integral transform (PIT-) residuals (current default), and the "traditional" randomization procedure, that was used in DHARMa until version 0.3.0. For details, see getQuantile

rotation

optional rotation of the residual space to remove residual autocorrelation. See details in simulateResiduals, section residual auto-correlation for an extended explanation, and getQuantile for syntax.

Value

an object of class DHARMa, similar to what is returned by simulateResiduals, but with additional outputs for the new grouped calculations. Note that the relevant outputs are 2x in the object, the first is the grouped calculations (which is returned by $name access), and later another time, under identical name, the original output. Moreover, there is a function 'aggregateByGroup', which can be used to aggregate predictor variables in the same way as the variables calculated here

Examples

library(lme4)

testData = createData(sampleSize = 100, overdispersion = 0.5, family = poisson())
fittedModel <- glmer( observedResponse ~ Environment1 + (1|group),
 family = "poisson", data = testData)

simulationOutput <- simulateResiduals(fittedModel = fittedModel)

# standard plot
plot(simulationOutput)

# one of the possible test, for other options see ?testResiduals / vignette
testDispersion(simulationOutput)

# the calculated residuals can be accessed via
residuals(simulationOutput)

# transform residuals to other pdf, see ?residuals.DHARMa for details
residuals(simulationOutput, quantileFunction = qnorm, outlierValues = c(-7,7))

# get residuals that are outside the simulation envelope
outliers(simulationOutput)

# calculating aggregated residuals per group
residuals.DHARMa

Return residuals of a DHARMa simulation

Description

Return residuals of a DHARMa simulation

Usage

## S3 method for class 'DHARMa'
residuals(object, quantileFunction = NULL, outlierValues = NULL, ...)

Arguments

object an object with simulated residuals created by simulateResiduals
quantileFunction optional - a quantile function to transform the uniform 0/1 scaling of DHARMa to another distribution
outlierValues if a quantile function with infinite support (such as dnorm) is used, residuals that are 0/1 are mapped to -Inf / Inf. outlierValues allows to convert -Inf / Inf values to an optional min / max value.
... optional arguments for compatibility with the generic function, no function implemented

Details

the function accesses the slot $scaledResiduals in a fitted DHARMa object, and optionally transforms the standard DHARMa quantile residuals (which have a uniform distribution) to a particular pdf.

Note

some of the papers on simulated quantile residuals transforming the residuals (which are natively uniform) back to a normal distribution. I presume this is because of the larger familiarity of most users with normal residuals. Personally, I never considered this desirable, for the reasons explained in https://github.com/florianhartig/DHARMa/issues/39, but with this function, I wanted to give users the option to plot normal residuals if they so wish.
Examples

library(lme4)

testData = createData(sampleSize = 100, overdispersion = 0.5, family = poisson())
fittedModel <- glmer(observedResponse ~ Environment1 + (1|group),
family = "poisson", data = testData)

simulationOutput <- simulateResiduals(fittedModel = fittedModel)

# standard plot
plot(simulationOutput)

# one of the possible test, for other options see ?testResiduals / vignette
testDispersion(simulationOutput)

# the calculated residuals can be accessed via
residuals(simulationOutput)

# transform residuals to other pdf, see ?residuals.DHARMa for details
residuals(simulationOutput, quantileFunction = qnorm, outlierValues = c(-7,7))

# get residuals that are outside the simulation envelope
outliers(simulationOutput)

# calculating aggregated residuals per group
simulationOutput2 = recalculateResiduals(simulationOutput, group = testData$group)
plot(simulationOutput2, quantreg = FALSE)

# calculating residuals only for subset of the data
simulationOutput3 = recalculateResiduals(simulationOutput, sel = testData$group == 1)
plot(simulationOutput3, quantreg = FALSE)

---

runBenchmarks

**Benchmark calculations**

Description

This function runs statistical benchmarks, including Power / Type I error simulations for an arbitrary test with a control parameter

Usage

runBenchmarks(calculateStatistics, controlValues = NULL, nRep = 10,
alpha = 0.05, parallel = FALSE, ...)

Arguments

calculateStatistics

the statistics to be benchmarked. Should return one value, or a vector of values. If controlValues are given, must accept a parameter control
runBenchmarks

controlValues  optionally, a vector with a control parameter (e.g. to vary the strength of a problem the test should be specific to). See help for an example
nRep  number of replicates per level of the controlValues
alpha  significance level
parallel  whether to use parallel computations. Possible values are F, T (sets the cores automatically to number of available cores -1), or an integer number for the number of cores that should be used for the cluster
...  additional parameters to calculateStatistics

Value

A object with list structure of class DHARMaBenchmark. Contains an entry simulations with a matrix of simulations, and an entry summaries with an list of summaries (significant (T/F), mean, p-value for KS-test uniformity). Can be plotted with plot.DHARMaBenchmark

Note

The benchmark function in DHARMa are intended for development purposes, and for users that want to test / confirm the properties of functions in DHARMa. If you are running an applied data analysis, they are probably of little use.

Author(s)

Florian Hartig

See Also

plot.DHARMaBenchmark

Examples

# define a function that will run a simulation and return a number of statistics, typically p-values
returnStatistics <- function(control = 0){
  testData = createData(sampleSize = 20, family = poisson(), overdispersion = control,
                randomEffectVariance = 0)
  fittedModel <- glm(observedResponse ~ Environment1, data = testData, family = poisson())
  res <- simulateResiduals(FittedModel = fittedModel, n = 250)
  out <- c(testUniformity(res, plot = FALSE)$p.value, testDispersion(res, plot = FALSE)$p.value)
  return(out)
}

# testing a single return
returnStatistics()

# running benchmark for a fixed simulation, increase nRep for sensible results
out = runBenchmarks(returnStatistics, nRep = 5)

# plotting results depend on whether a vector or a single value is provided for control
plot(out)
# running benchmark with varying control values
# out = runBenchmarks(returnStatistics, controlValues = c(0, 0.5, 1), nRep = 100)
# plot(out)

# running benchmark can be done using parallel cores
# out = runBenchmarks(returnStatistics, nRep = 100, parallel = TRUE)
# out = runBenchmarks(returnStatistics, controlValues = c(0, 0.5, 1), nRep = 10, parallel = TRUE)

# Alternative plot function using vioplot, provides nicer pictures
# plot.DHARMaBenchmark <- function(x, ...){
#   # if(length(x$controlValues)== 1){
#   #   vioplot::vioplot(x$simulations[,x$nSummaries:1], las = 2, horizontal = T, side = "right",
#   #       areaEqual = F,
#   #       main = "p distribution under H0",
#   #       ylim = c(-0.15,1), ...) 
#   #   abline(v = 1, lty = 2)
#   #   abline(v = c(0.05, 0), lty = 2, col = "red")
#   #   text(-0.1, x$nSummaries:1, labels = x$summaries$propSignificant[-1])
#   # }
#   # else{
#   #   res = x$summaries$propSignificant
#   #   matplot(res$controlValues, res[, -1], type = "l",
#   #       main = "Power analysis", ylab = "Power", ...)
#   #   legend("bottomright", colnames(res[, -1]),
#   #       col = 1:x$nSummaries, lty = 1:x$nSummaries, lwd = 2)
#   # }
# #}

simulateResiduals Create simulated residuals

Description

The function creates scaled residuals by simulating from the fitted model. Residuals can be extracted with residuals.DHARMA. See testResiduals for an overview of residual tests, plot.DHARMA for an overview of available plots.

Usage

simulateResiduals(fittedModel, n = 250, refit = F, 
integerResponse = NULL, plot = F, seed = 123, method = c("PIT", 
"traditional"), rotation = NULL, ...)

Arguments

fittedModel a fitted model of a class supported by DHARMA
number of simulations. The smaller the number, the higher the stochastic error on the residuals. Also, for very small n, discretization artefacts can influence the tests. Default is 250, which is a relatively safe value. You can consider increasing to 1000 to stabilize the simulated values.

if FALSE, new data will be simulated and scaled residuals will be created by comparing observed data with new data. If TRUE, the model will be refit on the simulated data (parametric bootstrap), and scaled residuals will be created by comparing observed with refitted residuals.

if TRUE, noise will be added at to the residuals to maintain a uniform expectations for integer responses (such as Poisson or Binomial). Usually, the model will automatically detect the appropriate setting, so there is no need to adjust this setting.

if TRUE, plotResiduals will be directly run after the residuals have been calculated.

the random seed to be used within DHARMa. The default setting, recommended for most users, is keep the random seed on a fixed value 123. This means that you will always get the same randomization and thus the same result when running the same code. NULL = no new seed is set, but previous random state will be restored after simulation. FALSE = no seed is set, and random state will not be restored. The latter two options are only recommended for simulation experiments. See vignette for details.

for refit = F, the quantile randomization method used. The two options implemented at the moment are probability integral transform (PIT-) residuals (current default), and the "traditional" randomization procedure, that was used in DHARMa until version 0.3.0. Refit = T will always use "traditional", respectively of the value of method. For details, see getQuantile.

optional rotation of the residual space prior to calculating the quantile residuals. The main purpose of this is to remove residual autocorrelation. See details below, section residual auto-correlation, and help of getQuantile.

parameters to pass to the simulate function of the model object. An important use of this is to specify whether simulations should be conditional on the current random effect estimates, e.g. via re.form. Note that not all models support syntax to specify conditional or unconditional simulations. See also details

Details

There are a number of important considerations when simulating from a more complex (hierarchical) model:

**Re-simulating random effects / hierarchical structure:** in a hierarchical model, we have several stochastic processes aligned on top of each other. Specifically, in a GLMM, we have a lower level stochastic process (random effect), whose result enters into a higher level (e.g. Poisson distribution). For other hierarchical models such as state-space models, similar considerations apply.

In such a situation, we have to decide if we want to re-simulate all stochastic levels, or only a subset of those. For example, in a GLMM, it is common to only simulate the last stochastic level (e.g. Poisson) conditional on the fitted random effects. This is often referred to as a conditional
Simulate residuals. For controlling how many levels should be re-simulated, the simulateResiduals function allows to pass on parameters to the simulate function of the fitted model object. Please refer to the help of the different simulate functions (e.g. `simulate.merMod`) for details. For merMod (lme4) model objects, the relevant parameters are parameters are `use.u` and `re.form`.

If the model is correctly specified, the simulated residuals should be flat regardless how many hierarchical levels we re-simulate. The most thorough procedure would therefore be to test all possible options. If testing only one option, I would recommend to re-simulate all levels, because this essentially tests the model structure as a whole. This is the default setting in the DHARMa package. A potential drawback is that re-simulating the lower-level random effects creates more variability, which may reduce power for detecting problems in the upper-level stochastic processes. In particular dispersion tests may produce different results when switching from conditional to unconditional simulations, and often the conditional simulation is more sensitive.

**Refitting or not:** a third issue is how residuals are calculated. simulateResiduals has two options that are controlled by the refit parameter:

1. if refit = FALSE (default), new data is simulated from the fitted model, and residuals are calculated by comparing the observed data to the new data
2. if refit = TRUE, a parametric bootstrap is performed, meaning that the model is refit on the new data, and residuals are created by comparing observed residuals against refitted residuals. I advise against using this method per default (see more comments in the vignette), unless you are really sure that you need it.

**Residuals per group:** In many situations, it can be useful to look at residuals per group, e.g. to see how much the model over/underpredicts per plot, year or subject. To do this, use `recalculateResiduals`, together with a grouping variable (see also help).

**Transformation to other distributions:** DHARMa calculates residuals for which the theoretical expectation (assuming a correctly specified model) is uniform. To transform this residuals to another distribution (e.g. so that a correctly specified model will have normal residuals) see `residuals.DHARMa`.

**Integer responses:** this is only relevant if method = "traditional", in which case it activates the randomization of the residuals. Usually, this does not need to be changed, as DHARMa will try to automatically if the fitted model has an integer or discrete distribution via the family argument. However, in some cases the family does not allow to uniquely identify the distribution type. For example, a tweedie distribution can be inter or continuous. Therefore, DHARMa will additionally check the simulation results for repeated values, and will change the distribution type if repeated values are found (a message is displayed in this case).

**Residual auto-correlation:** a common problem is residual autocorrelation. Spatial, temporal and phylogenetic autocorrelation can be tested with `testSpatialAutocorrelation` and `testTemporalAutocorrelation`. If simulations are unconditional, residual correlations will be maintained, even if the autocorrelation is addressed by an appropriate CAR structure. This may be a problem, because autocorrelation may create apparently systematic patterns in plots or tests such as `testUniformity`. To reduce this problem, either simulate conditional on fitted correlated REs, or you could try to rotate residuals via the rotation parameter (the latter will likely only work in approximately linear models). See `getQuantile` for details on the rotation.
Value

An S3 class of type "DHARMa". Implemented S3 functions include `plot.DHARMa`, `print.DHARMa` and `residuals.DHARMa`. For other functions that can be used on a DHARMa object, see section "See Also" below.

See Also

testResiduals, plotResiduals, recalculateResiduals, outliers

Examples

```r
library(lme4)

testData = createData(sampleSize = 100, overdispersion = 0.5, family = poisson())
fittedModel <- glmer(observedResponse ~ Environment1 + (1|group),
                      family = "poisson", data = testData)

simulationOutput <- simulateResiduals(fittedModel = fittedModel)

# standard plot
plot(simulationOutput)

# one of the possible test, for other options see ?testResiduals / vignette
testDispersion(simulationOutput)

# the calculated residuals can be accessed via
residuals(simulationOutput)

# transform residuals to other pdf, see ?residuals.DHARMa for details
residuals(simulationOutput, quantileFunction = qnorm, outlierValues = c(-7,7))

# get residuals that are outside the simulation envelope
outliers(simulationOutput)

# calculating aggregated residuals per group
simulationOutput2 = recalculateResiduals(simulationOutput, group = testData$group)
plot(simulationOutput2, quantreg = FALSE)

# calculating residuals only for subset of the data
simulationOutput3 = recalculateResiduals(simulationOutput, sel = testData$group == 1)
plot(simulationOutput3, quantreg = FALSE)
```

description

This function tests if there are problems in a res ~ group structure. It performs two tests: test for within-group uniformity, and test for between-group homogeneity of variances.
Usage

testCategorical(simulationOutput, catPred, quantiles = c(0.25, 0.5, 0.75), plot = T)

Arguments

simulationOutput
an object of class DHARMa, either created via `simulateResiduals` for supported models or by `createDHARMa` for simulations created outside DHARMa, or a supported model. Providing a supported model directly is discouraged, because simulation settings cannot be changed in this case.

catPred
a categorical predictor with the same dimensions as the residuals in simulationOutput

quantiles
whether to draw the quantile lines.

plot
if T, the function will create an additional plot

Details

The function tests for two common problems: are residuals within each group distributed according to model assumptions, and is the variance between group heterogeneous.

The test for within-group uniformity is performed via multipe KS-tests, with adjustment of p-values for multiple testing. If the plot is drawn, problematic groups are highlighted in red, and a corresponding message is displayed in the plot.

The test for homogeneity of variances is done with a Levene test. A significant p-value means that group variances are not constant. In this case, you should consider modelling variances, e.g. via ~dispformula in glmmTMB.

Author(s)

Florian Hartig

See Also

testResiduals, testUniformity, testOutliers, testDispersion, testZeroInflation, testGeneric, testTemporalAutocorrelation, testSpatialAutocorrelation, testQuantiles, testCategorical

Examples

testData = createData(sampleSize = 100, overdispersion = 0.5, randomEffectVariance = 0)
fittedModel <- glm(observedResponse ~ Environment1, family = "poisson", data = testData)
simulationOutput <- simulateResiduals(fittedModel = fittedModel)

# the plot function runs 4 tests
# i) KS test ii) Dispersion test iii) Outlier test iv) quantile test
plot(simulationOutput, quantreg = TRUE)

# testResiduals tests distribution, dispersion and outliers
# testResiduals(simulationOutput)
### Individual tests ###

# KS test for correct distribution of residuals
testUniformity(simulationOutput)

# KS test for correct distribution within and between groups

testCategorical(simulationOutput, testData$group)

# Dispersion test - for details see ?testDispersion

testDispersion(simulationOutput)  # tests under and overdispersion

# Outlier test (number of observations outside simulation envelope)
# Use type = "bootstrap" for exact values, see ?testOutliers

testOutliers(simulationOutput, type = "binomial")

# testing zero inflation

testZeroInflation(simulationOutput)

# testing generic summaries

countOnes <- function(x) sum(x == 1)  # testing for number of 1s

testGeneric(simulationOutput, summary = countOnes)  # 1-inflation

testGeneric(simulationOutput, summary = countOnes, alternative = "less")  # 1-deficit

means <- function(x) mean(x)  # testing if mean prediction fits

testGeneric(simulationOutput, summary = means)

spread <- function(x) sd(x)  # testing if mean sd fits

testGeneric(simulationOutput, summary = spread)

---

**testDispersion**

**DHARMa dispersion tests**

**Description**

This function performs simulation-based tests for over/underdispersion. If type = "DHARMa" (default and recommended), simulation-based dispersion tests are performed. Their behavior differs depending on whether simulations are done with refit = F, or refit = T, and whether data is simulated conditional (e.g. re.form ~0 in lme4) (see below). If type = "PearsonChisq", a chi2 test on Pearson residuals is performed.

**Usage**

```r
testDispersion(simulationOutput, alternative = c("two.sided", "greater", "less"), plot = T, type = c("DHARMa", "PearsonChisq"), ...)
```

**Arguments**

- `simulationOutput`: an object of class DHARMa, either created via `simulateResiduals` for supported models or by `createDHARMa` for simulations created outside DHARMa,
or a supported model. Providing a supported model directly is discouraged, because simulation settings cannot be changed in this case.

alternative

a character string specifying whether the test should test if observations are "greater", "less" or "two.sided" compared to the simulated null hypothesis. Greater corresponds to testing only for overdispersion. It is recommended to keep the default setting (testing for both over and underdispersion)

plot

whether to provide a plot for the results

type

which test to run. Default is DHARMa, other options are PearsonChisq (see details)

... arguments to pass on to testGeneric

Details

Over / underdispersion means that the observed data is more / less dispersed than expected under the fitted model. There is no unique way to test for dispersion problems, and there are a number of different dispersion tests implemented in various R packages. This function implements several dispersion tests.

Simulation-based dispersion tests (type == "DHARMa")

If type = "DHARMa" (default and recommended), simulation-based dispersion tests are performed. Their behavior differs depending on whether simulations are done with refit = F, or refit = T, and whether data is simulated conditional (e.g. re.form ~0 in lme4)

If refit = F, the function uses testGeneric to compare the variance of the observed raw residuals (i.e. var(observed - predicted), displayed as a red line) against the variance of the simulated residuals (i.e. var(observed - simulated), histogram). The variances are scaled to the mean simulated variance. A significant ratio > 1 indicates overdispersion, a significant ratio < 1 underdispersion.

If refit = T, the function compares the approximate deviance (via squared pearson residuals) with the same quantity from the models refitted with simulated data. Applying this is much slower than the previous alternative. Given the computational cost, I would suggest that most users will be satisfied with the standard dispersion test.

Important: for either refit = T or F, the results of type = "DHARMa" dispersion test will differ depending on whether simulations are done conditional (= conditional on fitted random effects) or unconditional (= REs are re-simulated). How to change between conditional or unconditional simulations is discussed in simulateResiduals. The general default in DHARMa is to use unconditional simulations, because this has advantages in other situations, but dispersion tests for models with strong REs specifically may increase substantially in power / sensitivity when switching to conditional simulations. I therefore recommend checking dispersion with conditional simulations if supported by the used regression package.

Analytical dispersion tests (type == "PearsonChisq")

This is the test described in https://bbolker.github.io/mixedmodels-misc/glmmFAQ.html#overdispersion, identical to performance::check_overdispersion. Works only if the fitted model provides df.residual and Pearson residuals.

The test statistics is biased to lower values under quite general conditions, and will therefore tend to test significant for underdispersion. It is recommended to use this test only for overdispersion, i.e. use alternative == "greater". Also, obviously, it requires that Pearson residuals are available for the chosen model, which will not be the case for all models / packages.
Note

For particular model classes / situations, there may be more powerful and thus preferable over the DHARMa test. The advantage of the DHARMa test is that it directly targets the spread of the data (unless other tests such as dispersion/df, which essentially measure fit and may thus be triggered by problems other than dispersion as well), and it makes practically no assumptions about the fitted model, other than the availability of simulations.

Author(s)

Florian Hartig

See Also

testResiduals, testUniformity, testOutliers, testDispersion, testZeroInflation, testGeneric, testTemporalAutocorrelation, testSpatialAutocorrelation, testQuantiles, testCategorical

Examples

library(lme4)
set.seed(123)
testData = createData(sampleSize = 100, overdispersion = 0.5, randomEffectVariance = 1)
fittedModel <- glmer(observedResponse ~ Environment1 + (1|group),
                      family = "poisson", data = testData)
simulationOutput <- simulateResiduals(fittedModel = fittedModel)
# default DHARMa dispersion test - simulation-based
testDispersion(simulationOutput)
testDispersion(simulationOutput, alternative = "less", plot = FALSE) # only underdispersion

# for mixed models, the test is usually more powerful if residuals are calculated
# conditional on fitted REs
simulationOutput <- simulateResiduals(fittedModel = fittedModel, re.form = NULL)
testDispersion(simulationOutput)

# DHARMa also implements the popular Pearson-chisq test that is also on the glmmWiki by Ben Bolker
# The issue with this test is that it requires the df of the model, which are not well defined
# for GLMMs. It is biased towards underdispersion, with bias getting larger with the number
# of RE groups. In doubt, only test for overdispersion

# if refit = T, a different test on simulated Pearson residuals will calculated (see help)
simulationOutput2 <- simulateResiduals(fittedModel = fittedModel, refit = TRUE, seed = 12, n = 20)
testDispersion(simulationOutput2)

# often useful to test dispersion per group (in particular for binomial data, see vignette)
simulationOutputAggregated = recalculateResiduals(simulationOutput2, group = testData$group)
testDispersion(simulationOutputAggregated)
testGeneric

Generic simulation test of a summary statistic

Description

This function tests if a user-defined summary differs when applied to simulated / observed data.

Usage

testGeneric(simulationOutput, summary, alternative = c("two.sided", "greater", "less"), plot = T, methodName = "DHARMa generic simulation test")

Arguments

- **simulationOutput**: an object of class DHARMa, either created via `simulateResiduals` for supported models or by `createDHARMa` for simulations created outside DHARMa, or a supported model. Providing a supported model directly is discouraged, because simulation settings cannot be changed in this case.
- **summary**: a function that can be applied to simulated / observed data. See examples below
- **alternative**: a character string specifying whether the test should test if observations are "greater", "less" or "two.sided" compared to the simulated null hypothesis
- **plot**: whether to plot the simulated summary
- **methodName**: name of the test (will be used in plot)

Details

This function tests if a user-defined summary differs when applied to simulated / observed data. The function can easily be remodeled to apply summaries on the residuals, by simply defining f = function(x) summary(x - predictions), as done in `testDispersion`

Note

The function that you supply is applied on the data as it is represented in your fitted model, which may not always correspond to how you think. This is important in particular when you use k/n binomial data, and want to test for 1-inflation. As an example, if have k/20 observations, and you provide your data via `cbind(y, y-20)`, you have to test for 20-inflation (because this is how the data is represented in the model). However, if you provide data via y/20, and weights = 20, you should test for 1-inflation. In doubt, check how the data is internally represented in `model.frame(model)`, or via `simulate(model)`

Author(s)

Florian Hartig
See Also

testResiduals, testUniformity, testOutliers, testDispersion, testZeroInflation, testGeneric,
testTemporalAutocorrelation, testSpatialAutocorrelation, testQuantiles, testCategorical

Examples

testData = createData(sampleSize = 100, overdispersion = 0.5, randomEffectVariance = 0)
fittedModel <- glm( observedResponse ~ Environment1, family = "poisson", data = testData)
simulationOutput <- simulateResiduals(fittedModel = fittedModel)

# the plot function runs 4 tests
# i) KS test i) Dispersion test iii) Outlier test iv) quantile test
plot(simulationOutput, quantreg = TRUE)

# testResiduals tests distribution, dispersion and outliers
# testResiduals(simulationOutput)

##### Individual tests ######
# KS test for correct distribution of residuals
testUniformity(simulationOutput)

# KS test for correct distribution within and between groups
testCategorical(simulationOutput, testData$group)

# Dispersion test - for details see ?testDispersion
testDispersion(simulationOutput) # tests under and overdispersion

# Outlier test (number of observations outside simulation envelope)
# Use type = "bootstrap" for exact values, see ?testOutliers
testOutliers(simulationOutput, type = "binomial")

# testing zero inflation
testZeroInflation(simulationOutput)

# testing generic summaries
countOnes <- function(x) sum(x == 1) # testing for number of 1s
testGeneric(simulationOutput, summary = countOnes) # 1-inflation
testGeneric(simulationOutput, summary = countOnes, alternative = "less") # 1-deficit

means <- function(x) mean(x) # testing if mean prediction fits
testGeneric(simulationOutput, summary = means)

spread <- function(x) sd(x) # testing if mean sd fits
testGeneric(simulationOutput, summary = spread)

---

testOutliers  Test for outliers
Description

This function tests if the number of observations outside the simulation envelope are larger or smaller than expected.

Usage

testOutliers(simulationOutput, alternative = c("two.sided", "greater", "less"), margin = c("both", "upper", "lower"), type = c("default", "bootstrap", "binomial"), nBoot = 100, plot = T)

Arguments

- simulationOutput: an object of class DHARMa, either created via simulateResiduals for supported models or by createDHARMa for simulations created outside DHARMa, or a supported model. Providing a supported model directly is discouraged, because simulation settings cannot be changed in this case.
- alternative: a character string specifying whether the test should test if observations are "greater", "less" or "two.sided" (default) compared to the simulated null hypothesis.
- margin: whether to test for outliers only at the lower, only at the upper, or both sides (default) of the simulated data distribution.
- type: either default, bootstrap or binomial. See details.
- nBoot: number of bootstrap replicates. Only used if type = "bootstrap".
- plot: if T, the function will create an additional plot.

Details

DHARMa residuals are created by simulating from the fitted model, and comparing the simulated values to the observed data. It can occur that all simulated values are higher or smaller than the observed data, in which case they get the residual value of 0 and 1, respectively. I refer to these values as simulation outliers, or simply outliers.

Because no data was simulated in the range of the observed value, we don’t know "how strongly" these values deviate from the model expectation, so the term "outlier" should be used with a grain of salt. It is not a judgment about the magnitude of the residual deviation, but simply a dichotomous sign that we are outside the simulated range. Moreover, the number of outliers will decrease as we increase the number of simulations.

To test if the outliers are a concern, testOutliers implements 2 options (bootstrap, binomial), which can be chosen via the parameter "type". The third option (default) chooses bootstrap for integer-valued distributions with nObs < 500, and else binomial.

The binomial test considers that under the null hypothesis that the model is correct, and for continuous distributions (i.e. data and the model distribution are identical and continuous), the probability that a given observation is higher than all simulations is 1/(nSim +1), and binomial distributed. The testOutlier function can test this null hypothesis via type = "binomial". In principle, it would be nice if we could extend this idea to integer-valued distributions, which are randomized via the PIT procedure (see simulateResiduals), the rate of "true" outliers is more difficult to calculate, and
in general not \(1/(nSim +1)\). The testOutlier function implements a small tweak that calculates the rate of residuals that are closer than \(1/(nSim+1)\) to the 0/1 border, which roughly occur at a rate of \(nData /(nSim +1)\). This approximate value, however, is generally not exact, and may be particularly off non-bounded integer-valued distributions (such as Poisson or neg binom).

For this reason, the testOutlier function implements an alternative procedure that uses the bootstrap to generate a simulation-based expectation for the outliers. It is recommended to use the bootstrap for integer-valued distributions (and integer-valued only, because it has no advantage for continuous distributions, ideally with reasonably high values of nSim and nBoot (I recommend at least 1000 for both). Because of the high runtime, however, this option is switched off for type = default when nObs > 500.

Both binomial or bootstrap generate a null expectation, and then test for an excess or lack of outliers. Per default, testOutliers() looks for both, so if you get a significant p-value, you have to check if you have to many or too few outliers. An excess of outliers is to be interpreted as too many values outside the simulation envelope. This could be caused by overdispersion, or by what we classically call outliers. A lack of outliers would be caused, for example, by underdispersion.

Author(s)

Florian Hartig

See Also

testResiduals, testUniformity, testOutliers, testDispersion, testZeroInflation, testGeneric, testTemporalAutocorrelation, testSpatialAutocorrelation, testQuantiles, testCategorical

deprecated, switch your code to using the testDispersion function
testOverdispersionParametric

Parametric overdispersion tests

Description
Parametric overdispersion tests

Usage
testOverdispersionParametric(...)

Arguments
... arguments will be ignored, the parametric tests is no longer recommend

Details
Deprecated, switch your code to using the testDispersion function.

testPDistribution

Plot distribution of p-values

Description
Plot distribution of p-values

Usage
testPDistribution(x, plot = T,
    main = "p distribution \n expected is flat at 1", ...)

Arguments
x vector of p values
plot should the values be plotted
main title for the plot
... additional arguments to hist

Author(s)
Florian Hartig
Description

This function tests

Usage

testQuantiles(simulationOutput, predictor = NULL, quantiles = c(0.25, 0.5, 0.75), plot = T)

Arguments

- `simulationOutput`: an object of class DHARMa, either created via `simulateResiduals` for supported models or by `createDHARMa` for simulations created outside DHARMa, or a supported model. Providing a supported model directly is discouraged, because simulation settings cannot be changed in this case.
- `predictor`: an optional predictor variable to be used, instead of the predicted response (default)
- `quantiles`: the quantiles to be tested
- `plot`: if T, the function will create an additional plot

Details

The function fits quantile regressions (via package qgam) on the residuals, and compares their location to the expected location (because of the uniform distribution, the expected location is 0.5 for the 0.5 quantile).

A significant p-value for the splines means the fitted spline deviates from a flat line at the expected location (p-values of intercept and spline are combined via Benjamini & Hochberg adjustment to control the FDR).

The p-values of the splines are combined into a total p-value via Benjamini & Hochberg adjustment to control the FDR.

Author(s)

Florian Hartig

See Also

testResiduals, testUniformity, testOutliers, testDispersion, testZeroInflation, testGeneric, testTemporalAutocorrelation, testSpatialAutocorrelation, testQuantiles, testCategorical
Examples

testData = createData(sampleSize = 200, overdispersion = 0.0, randomEffectVariance = 0)
fittedModel <- glm(observedResponse ~ Environment1, family = "poisson", data = testData)
simulationOutput <- simulateResiduals(fittedModel = fittedModel)

# run the quantile test
x = testQuantiles(simulationOutput)
x # the test shows a combined p-value, corrected for multiple testing

## Not run:
# accessing results of the test
x$pvals # pvalues for the individual quantiles
x$qgamFits # access the fitted quantile regression
summary(x$qgamFits[[1]]) # summary of the first fitted quantile

# possible to test user-defined quantiles
testQuantiles(simulationOutput, quantiles = c(0.7))

# example with missing environmental predictor
fittedModel <- glm(observedResponse ~ 1, family = "poisson", data = testData)
simulationOutput <- simulateResiduals(fittedModel = fittedModel)
testQuantiles(simulationOutput, predictor = testData$Environment1)

plot(simulationOutput)
plotResiduals(simulationOutput)

## End(Not run)

testResiduals

---

**testResiduals**

*DHARMa general residual test*

**Description**

Calls both uniformity and dispersion test

**Usage**

```r
testResiduals(simulationOutput, plot = T)
```

**Arguments**

- `simulationOutput`:
  - an object of class DHARMa, either created via `simulateResiduals` for supported models or by `createDHARMa` for simulations created outside DHARMa, or a supported model. Providing a supported model directly is discouraged, because simulation settings cannot be changed in this case.

- `plot`:
  - if T, plots functions of the tests are called
Details

This function is a wrapper for the various test functions implemented in DHARMa. Currently, this function calls the `testUniformity` and the `testDispersion` functions. All other tests (see list below) have to be called by hand.

Author(s)

Florian Hartig

See Also

testResiduals, testUniformity, testOutliers, testDispersion, testZeroInflation, testGeneric, testTemporalAutocorrelation, testSpatialAutocorrelation, testQuantiles, testCategorical

Examples

testData = createData(sampleSize = 100, overdispersion = 0.5, randomEffectVariance = 0)
fittedModel <- glm(observedResponse ~ Environment1, family = "poisson", data = testData)
simulationOutput <- simulateResiduals(fittedModel = fittedModel)

# the plot function runs 4 tests
# i) KS test i) Dispersion test iii) Outlier test iv) quantile test
plot(simulationOutput, quantreg = TRUE)

# testResiduals tests distribution, dispersion and outliers
# testResiduals(simulationOutput)

######## Individual tests ########

# KS test for correct distribution of residuals
testUniformity(simulationOutput)

# KS test for correct distribution within and between groups
testCategorical(simulationOutput, testData$group)

# Dispersion test - for details see ?testDispersion
testDispersion(simulationOutput) # tests under and overdispersion

# Outlier test (number of observations outside simulation envelope)
# Use type = "bootstrap" for exact values, see ?testOutliers
testOutliers(simulationOutput, type = "binomial")

# testing zero inflation
testZeroInflation(simulationOutput)

# testing generic summaries
countOnes <- function(x) sum(x == 1) # testing for number of 1s
testGeneric(simulationOutput, summary = countOnes) # 1-inflation
testGeneric(simulationOutput, summary = countOnes, alternative = "less") # 1-deficit

means <- function(x) mean(x) # testing if mean prediction fits
testGeneric(simulationOutput, summary = means)
spread <- function(x) sd(x) # testing if mean sd fits
testGeneric(simulationOutput, summary = spread)

testSimulatedResiduals

Residual tests

Description
Residual tests

Usage

  testSimulatedResiduals(simulationOutput)

Arguments

  simulationOutput
    an object of class DHARMa, either created via simulateResiduals for supported models or by createDHARMa for simulations created outside DHARMa, or a supported model. Providing a supported model directly is discouraged, because simulation settings cannot be changed in this case.

Details

  Deprecated, switch your code to using the testResiduals function

Author(s)

  Florian Hartig

testSpatialAutocorrelation

Test for distance-based (spatial, phylogenetic or similar) autocorrelation

Description

  This function performs a Moran’s I test for distance-based (spatial, phylogenetic or similar) autocorrelation on the calculated quantile residuals

Usage

  testSpatialAutocorrelation(simulationOutput, x = NULL, y = NULL, distMat = NULL, alternative = c("two.sided", "greater", "less"), plot = T)
testSpatialAutocorrelation

Arguments

simulationOutput
an object of class DHARMa, either created via simulateResiduals for supported models or by createDHARMa for simulations created outside DHARMa, or a supported model. Providing a supported model directly is discouraged, because simulation settings cannot be changed in this case.

x
the x coordinate, in the same order as the data points. Must be specified unless distMat is provided.

y
the y coordinate, in the same order as the data points. Must be specified unless distMat is provided.

distMat
optional distance matrix. If not provided, euclidean distances based on x and y will be calculated. See details for explanation

alternative
a character string specifying whether the test should test if observations are "greater", "less" or "two.sided" compared to the simulated null hypothesis

plot
whether to plot output

Details

The function performs Moran.I test from the package ape on the DHARMa residuals. If a distance matrix (distMat) is provided, calculations will be based on this distance matrix, and x,y coordinates will only used for the plotting (if provided). If distMat is not provided, the function will calculate the euclidean distances between x,y coordinates, and test Moran.I based on these distances.

Testing for spatial autocorrelation requires unique x,y values - if you have several observations per location, either use the recalculateResiduals function to aggregate residuals per location, or extract the residuals from the fitted object, and plot / test each of them independently for spatially repeated subgroups (a typical scenario would repeated spatial observation, in which case one could plot / test each time step separately for temporal autocorrelation). Note that the latter must be done by hand, outside testSpatialAutocorrelation.

Note

Standard DHARMa simulations from models with (temporal / spatial / phylogenetic) conditional autoregressive terms will still have the respective temporal / spatial / phylogenetic correlation in the DHARMa residuals, unless the package you are using is modelling the autoregressive terms as explicit REs and is able to simulate conditional on the fitted REs. This has two consequences

1. If you check the residuals for such a model, they will still show significant autocorrelation, even if the model fully accounts for this structure.
2. Because the DHARMa residuals for such a model are not statistically independent any more, other tests (e.g. dispersion, uniformity) may have inflated type I error, i.e. you will have a higher likelihood of spurious residual problems.

There are three (non-exclusive) routes to address these issues when working with spatial / temporal / other autoregressive models:

1. Simulate conditional on the fitted CAR structures (see conditional simulations in the help of simulateResiduals)
2. Rotate simulations prior to residual calculations (see parameter rotation in \texttt{simulateResiduals})
3. Use custom tests / plots that explicitly compare the correlation structure in the simulated data to the correlation structure in the observed data.

\textbf{Author(s)}

Florian Hartig

\textbf{See Also}

testResiduals, testUniformity, testOutliers, testDispersion, testZeroInflation, testGeneric, testTemporalAutocorrelation, testSpatialAutocorrelation, testQuantiles, testCategorical

\textbf{Examples}

testData = createData(sampleSize = 40, family = gaussian())
fittedModel <- lm(observedResponse ~ Environment1, data = testData)
res = simulateResiduals(fittedModel)

# Standard use
testSpatialAutocorrelation(res, x = testData$x, y = testData$y)

# Alternatively, one can provide a distance matrix
dM = as.matrix(dist(cbind(testData$x, testData$y)))
testSpatialAutocorrelation(res, distMat = dM)

# You could add a spatial variogram via
# library(gstat)
# dat = data.frame(res = residuals(res), x = testData$x, y = testData$y)
# coordinates(dat) = ~x+y
# vario = variogram(res~1, data = dat, alpha=c(0,45,90,135))
# plot(vario, ylim = c(-1,1))

# if there are multiple observations with the same x values,
# create first ar group with unique values for each location
# then aggregate the residuals per location, and calculate
# spatial autocorrelation on the new group

# modifying x, y, so that we have the same location per group
# just for completeness
testData$x = as.numeric(testData$group)
 testData$y = as.numeric(testData$group)

calculating x, y positions per group
groupLocations = aggregate(testData[, 6:7], list(testData$group), mean)

calculating residuals per group
res2 = recalculateResiduals(res, group = testData$group)

# running the spatial test on grouped residuals
testSpatialAutocorrelation(res2, groupLocations$x, groupLocations$y)
# careful when using REs to account for spatially clustered (but not grouped) data. this originates from https://github.com/florianhartig/DHARMa/issues/81

# Assume our data is divided into clusters, where observations are close together but not at the same point, and we suspect that observations in clusters are autocorrelated

clusters = 100
subsamples = 10
size = clusters * subsamples

testData = createData(sampleSize = size, family = gaussian(), numGroups = clusters)
testData$x = rnorm(clusters)[testData$group] + rnorm(size, sd = 0.01)
testData$y = rnorm(clusters)[testData$group] + rnorm(size, sd = 0.01)

# It's a good idea to use a RE to take out the cluster effects. This accounts for the autocorrelation within clusters

library(lme4)
fittedModel <- lmer(observedResponse ~ Environment1 + (1|group), data = testData)

# DHARMa default is to re-simulated REs - this means spatial pattern remains because residuals are still clustered

res = simulateResiduals(fittedModel)
testSpatialAutocorrelation(res, x = testData$x, y = testData$y)

# However, it should disappear if you just calculate an aggregate residuals per cluster because at least how the data are simulated, cluster are spatially independent

res2 = recalculateResiduals(res, group = testData$group)
testSpatialAutocorrelation(res2, x = aggregate(testData$x, list(testData$group), mean)$x, y = aggregate(testData$y, list(testData$group), mean)$x)

# For lme4, it's also possible to simulated residuals conditional on fitted REs (re.form). Conditional on the fitted REs (i.e. accounting for the clusters) the residuals should now be independent. The remaining RSA we see here is probably due to the RE shrinkage

res = simulateResiduals(fittedModel, re.form = NULL)
testSpatialAutocorrelation(res, x = testData$x, y = testData$y)

---

testTemporalAutocorrelation

Test for temporal autocorrelation
Description

This function performs a standard test for temporal autocorrelation on the simulated residuals.

Usage

testTemporalAutocorrelation(simulationOutput, time, alternative = c("two.sided", "greater", "less"), plot = T)

Arguments

- **simulationOutput**: an object of class DHARMa, either created via `simulateResiduals` for supported models or by `createDHARMa` for simulations created outside DHARMa, or a supported model. Providing a supported model directly is discouraged, because simulation settings cannot be changed in this case.
- **time**: the time, in the same order as the data points.
- **alternative**: a character string specifying whether the test should test if observations are "greater", "less" or "two.sided" compared to the simulated null hypothesis
- **plot**: whether to plot output

Details

The function performs a Durbin-Watson test on the uniformly scaled residuals, and plots the residuals against time. The DB test was originally be designed for normal residuals. In simulations, I didn’t see a problem with this setting though. The alternative is to transform the uniform residuals to normal residuals and perform the DB test on those.

Testing for temporal autocorrelation requires unique time values - if you have several observations per time value, either use `recalculateResiduals` function to aggregate residuals per time step, or extract the residuals from the fitted object, and plot / test each of them independently for temporally repeated subgroups (typical choices would be location / subject etc.). Note that the latter must be done by hand, outside `testTemporalAutocorrelation`.

Note

Standard DHARMa simulations from models with (temporal / spatial / phylogenetic) conditional autoregressive terms will still have the respective temporal / spatial / phylogenetic correlation in the DHARMa residuals, unless the package you are using is modelling the autoregressive terms as explicit REs and is able to simulate conditional on the fitted REs. This has two consequences:

1. If you check the residuals for such a model, they will still show significant autocorrelation, even if the model fully accounts for this structure.
2. Because the DHARMa residuals for such a model are not statistically independent any more, other tests (e.g. dispersion, uniformity) may have inflated type I error, i.e. you will have a higher likelihood of spurious residual problems.

There are three (non-exclusive) routes to address these issues when working with spatial / temporal / other autoregressive models:
1. Simulate conditional on the fitted CAR structures (see conditional simulations in the help of `simulateResiduals`)
2. Rotate simulations prior to residual calculations (see parameter rotation in `simulateResiduals`)
3. Use custom tests / plots that explicitly compare the correlation structure in the simulated data to the correlation structure in the observed data.

**Author(s)**

Florian Hartig

**See Also**

`testResiduals, testUniformity, testOutliers, testDispersion, testZeroInflation, testGeneric, testTemporalAutocorrelation, testSpatialAutocorrelation, testQuantiles, testCategorical`

**Examples**

```r
testData = createData(sampleSize = 40, family = gaussian(),
                      randomEffectVariance = 0)
fittedModel <- lm(observedResponse ~ Environment1, data = testData)
res = simulateResiduals(fittedModel)

# Standard use
testTemporalAutocorrelation(res, time = testData$time)

# If you have several observations per time step, e.g.
# because you have several locations, you will have to
# aggregate

timeSeries1 = createData(sampleSize = 40, family = gaussian(),
                         randomEffectVariance = 0)
timeSeries1$location = 1
timeSeries2 = createData(sampleSize = 40, family = gaussian(),
                         randomEffectVariance = 0)
timeSeries2$location = 2
testData = rbind(timeSeries1, timeSeries2)
fittedModel <- lm(observedResponse ~ Environment1, data = testData)
res = simulateResiduals(fittedModel)

# Will not work because several residuals per time
# testTemporalAutocorrelation(res, time = testData$time)

# aggregating residuals by time
res = recalculateResiduals(res, group = testData$time)
testTemporalAutocorrelation(res, time = unique(testData$time))

# testing only subgroup location 1, could do same with loc 2
res = recalculateResiduals(res, sel = testData$location == 1)
testTemporalAutocorrelation(res, time = unique(testData$time))
```

# example to demonstrate problems with strong temporal correlations and
# how to possibly remove them by rotating residuals

## Not run:

```r
set.seed(1)
C <- exp(-as.matrix(dist(seq(0,50,by=.5))))
obs <- as.numeric(mvtnorm::rmvnorm(1,sigma=C))

opar <- par(mfrow = c(1,2))
image(C, main = "Specified autocorrelation (covariance)"
plot(obs, type = "l", main = "Time series")
par(opar)

# calculate standard DHARMa residuals

## simulations from the model:
```n
x = replicate(1000, as.numeric(mvtnorm::rmvnorm(1,sigma=C)))
```
res <- createDHARMa(x, obs, integerResponse = F)
plot(res)
testTemporalAutocorrelation(res, time = 1:length(res$scaledResiduals))

# calculated rotated DHARMa residuals to remove temporal correlation
# this only works if the autocorrelation is homogeneous / stationary
res <- createDHARMa(x, obs, integerResponse = F, rotation = C)
testUniformity(res)
testTemporalAutocorrelation(res, time = 1:length(res$scaledResiduals))

# the same, but with a covariance based on simulations
res <- createDHARMa(x, obs, integerResponse = F, rotation = "estimated")
testUniformity(res)
testTemporalAutocorrelation(res, time = 1:length(res$scaledResiduals))

## End(Not run)

---

**testUniformity**

### Description

This function tests the overall uniformity of the simulated residuals in a DHARMa object

### Usage

```r
testUniformity(simulationOutput, alternative = c("two.sided", "less", "greater"), plot = T)
```
Arguments

simulationOutput

an object of class DHARMa, either created via \texttt{simulateResiduals} for supported models or by \texttt{createDHARMa} for simulations created outside DHARMa, or a supported model. Providing a supported model directly is discouraged, because simulation settings cannot be changed in this case.

alternative

a character string specifying whether the test should test if observations are "greater", "less" or "two.sided" compared to the simulated null hypothesis. See \texttt{ks.test} for details

plot

if \( T \), plots calls \texttt{plotQQunif} as well

Details

The function applies a \texttt{ks.test} for uniformity on the simulated residuals.

Author(s)

Florian Hartig

See Also

testResiduals, testUniformity, testOutliers, testDispersion, testZeroInflation, testGeneric, testTemporalAutocorrelation, testSpatialAutocorrelation, testQuantiles, testCategorical

Examples

testData = createData(sampleSize = 100, overdispersion = 0.5, randomEffectVariance = 0)
fittedModel <- glm(observedResponse ~ Environment1, family = "poisson", data = testData)
simulationOutput <- simulateResiduals(fittedModel = fittedModel)

# the plot function runs 4 tests
# i) KS test i) Dispersion test iii) Outlier test iv) quantile test
plot(simulationOutput, quantreg = TRUE)

# testResiduals tests distribution, dispersion and outliers
# testResiduals(simulationOutput)

######## Individual tests ########

# KS test for correct distribution of residuals
testUniformity(simulationOutput)

# KS test for correct distribution within and between groups
testCategorical(simulationOutput, testData$group)

# Dispersion test - for details see \texttt{testDispersion}
testDispersion(simulationOutput) # tests under and overdispersion

# Outlier test (number of observations outside simulation envelope)
# Use type = "bootstrap" for exact values, see \texttt{testOutliers}
testOutliers(simulationOutput, type = "binomial")

# testing zero inflation
testZeroInflation(simulationOutput)

# testing generic summaries
countOnes <- function(x) sum(x == 1)  # testing for number of 1s
testGeneric(simulationOutput, summary = countOnes)  # 1-inflation
testGeneric(simulationOutput, summary = countOnes, alternative = "less")  # 1-deficit

means <- function(x) mean(x)  # testing if mean prediction fits
testGeneric(simulationOutput, summary = means)

spread <- function(x) sd(x)  # testing if mean sd fits
testGeneric(simulationOutput, summary = spread)

testZeroInflation  # Tests for zero-inflation

Description
This function compares the observed number of zeros with the zeros expected from simulations.

Usage

testZeroInflation(simulationOutput, ...)

Arguments

simulationOutput
  an object of class DHARMa, either created via simulateResiduals for supported models or by createDHARMa for simulations created outside DHARMa, or a supported model. Providing a supported model directly is discouraged, because simulation settings cannot be changed in this case.

... further arguments to testGeneric

Details

The plot shows the expected distribution of zeros against the observed values, the ratioObsSim shows observed vs. simulated zeros. A value < 1 means that the observed data has less zeros than expected, a value > 1 means that it has more zeros than expected (aka zero-inflation). Per default, the function tests both sides.

Some notes about common problems / questions:

- Zero-inflation tests after fitting the model are crucial to see if you have zero-inflation. Just because there are a lot of zeros doesn’t mean you have zero-inflation, see Warton, D. I. (2005). Many zeros does not mean zero inflation: comparing the goodness-of-fit of parametric models to multivariate abundance data. Environmetrics 16(3), 275-289.
That being said, zero-inflation tests are often not a reliable guide to decide whether to add a zi term or not. In general, model structures should be decided on ideally a priori, if that is not possible via model selection techniques (AIC, BIC, WAIC, Bayes Factor). A zero-inflation test should only be run after that decision, and to validate the decision that was taken.

Note

This function is a wrapper for `testGeneric`, where the summary argument is set to `function(x) sum(x == 0)`

Author(s)

Florian Hartig

See Also

`testResiduals, testUniformity, testOutliers, testDispersion, testZeroInflation, testGeneric, testTemporalAutocorrelation, testSpatialAutocorrelation, testQuantiles, testCategorical`

Examples

testData = createData(sampleSize = 100, overdispersion = 0.5, randomEffectVariance = 0)
fittedModel <- glm(observedResponse ~ Environment1, family = "poisson", data = testData)
simulationOutput <- simulateResiduals(fittedModel = fittedModel)

# the plot function runs 4 tests
# i) KS test i) Dispersion test iii) Outlier test iv) quantile test
plot(simulationOutput, quantreg = TRUE)

# testResiduals tests distribution, dispersion and outliers
# testResiduals(simulationOutput)

####### Individual tests #######

# KS test for correct distribution of residuals
testUniformity(simulationOutput)

# KS test for correct distribution within and between groups
testCategorical(simulationOutput, testData$group)

# Dispersion test - for details see ?testDispersion
testDispersion(simulationOutput) # tests under and overdispersion

# Outlier test (number of observations outside simulation envelope)
# Use type = "bootstrap" for exact values, see ?testOutliers
testOutliers(simulationOutput, type = "binomial")

# testing zero inflation
testZeroInflation(simulationOutput)

# testing generic summaries
countOnes <- function(x) sum(x == 1) # testing for number of 1s
testGeneric(simulationOutput, summary = countOnes) # 1-inflation
# 1-deficit

means <- function(x) mean(x) # testing if mean prediction fits
testGeneric(simulationOutput, summary = means)

spread <- function(x) sd(x) # testing if mean sd fits
testGeneric(simulationOutput, summary = spread)

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### transformQuantiles

*Transform quantiles to pdf (deprecated)*

#### Description

The purpose of this function was to transform the DHARMa quantile residuals (which have a uniform distribution) to a particular pdf. Since DHARMa 0.3.0, this functionality is integrated in the `residuals.DHARMa` function. Please switch to using this function.

#### Usage

```r
transformQuantiles(res, quantileFunction = qnorm, outlierValue = 7)
```

#### Arguments

- `res` an object with simulated residuals created by `simulateResiduals`
- `quantileFunction` optional - a quantile function to transform the uniform 0/1 scaling of DHARMa to another distribution
- `outlierValue` if a quantile function with infinite support (such as dnorm) is used, residuals that are 0/1 are mapped to -Inf / Inf. `outlierValues` allows to convert -Inf / Inf values to an optional min / max value.
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