Package ‘pbkrttest’

February 20, 2020

Version 0.4-8.6
Title Parametric Bootstrap and Kenward Roger Based Methods for Mixed Model Comparison
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Description Test in mixed effects models. Attention is on mixed effects models as implemented in the 'lme4' package. This package implements a parametric bootstrap test and a Kenward Roger modification of F-tests for linear mixed effects models and a parametric bootstrap test for generalized linear mixed models.
URL http://people.math.aau.dk/~sorenh/software/pbkrttest/
Depends R (>= 3.6.0), lme4 (>= 1.1.10)
Imports Matrix (>= 1.2.3), parallel, magrittr, MASS, methods
Encoding UTF-8
ZipData no
License GPL (>= 2)
RoxygenNote 7.0.2
LazyData true
NeedsCompilation no
Repository CRAN
Date/Publication 2020-02-20 21:40:02 UTC

R topics documented:

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**Description**

Yield and sugar percentage in sugar beets from a split plot experiment. Data is obtained from a split
plot experiment. There are 3 blocks and in each of these the harvest time defines the "whole plot"
and the sowing time defines the "split plot". Each plot was $25m^2$ and the yield is recorded in kg.
See 'details' for the experimental layout.

**Usage**

beets

**Format**

A dataframe with 5 columns and 30 rows.

**Details**

<table>
<thead>
<tr>
<th>Experimental plan</th>
<th>Sowing times</th>
<th>Harvest times</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td></td>
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<td>4</td>
<td>4</td>
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<tr>
<td></td>
<td>5</td>
<td>5</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Plots allocation:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Block 1</td>
</tr>
<tr>
<td>---------</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>Plot</td>
</tr>
<tr>
<td>1-15</td>
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<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>Plot</td>
</tr>
<tr>
<td>16-30</td>
</tr>
<tr>
<td></td>
</tr>
</tbody>
</table>
data-budworm

References


Examples

data(beets)

beets$bh <- with(beets, interaction(block, harvest))
summary(aov(yield ~ block + sow + harvest + Error(bh), beets))
summary(aov(sugpct ~ block + sow + harvest + Error(bh), beets))

Description

Effect of Insecticide on survivial of tobacco budworms number of killed budworms exposed to an insecticidepp mortality of the moth tobacco budworm 'Heliothis virescens' for 6 doses of the pyrethroid trans-cypermethrin differentiated with respect to sex

Usage

budworm

Format

This data frame contains 12 rows and 4 columns:

sex: sex of the budworm
dose: dose of the insecticide trans-cypermethrin in $[\mu g]$
ndead: budworms killed in a trial
ntotal: total number of budworms exposed per trial

Source


References

Examples

```r
data(budworm)

## function to caculate the empirical logits
empirical.logit <- function(nevent, ntotal) {
  y <- log((nevent + 0.5) / (ntotal - nevent + 0.5))
  y
}

# plot the empirical logits against log-dose
log.dose <- log(budworm$dose)
emp.logit <- empirical.logit(budworm$ndead, budworm$ntotal)
plot(log.dose, emp.logit, type="n", xlab="log-dose", ylab="empirical logit")
title("budworm: empirical logits of probability to die ")
male <- budworm$sex=='male'
female <- budworm$sex=='female'
lines(log.dose[male], emp.logit[male], type='b', lty=1, col=1)
lines(log.dose[female], emp.logit[female], type='b', lty=2, col=2)
legend(0.5, 2, legend=c("male", "female"), lty=c(1,2), col=c(1,2))

## Not run:
* SAS example;
data budworm;
infile budworm.txt firstobs=2;
input sex dose ndead ntotal;
run;
## End(Not run)
```

getkr

Extract (or "get") components from a KRmodcomp object.

Description

Extract (or "get") components from a KRmodcomp object, which is the result of the KRmodcomp function.

Usage

```r
getKR(
  object,
  name = c("ndf", "ddf", "Fstat", "p.value", "F.scaling", "FstatU", "p.valueU", "aux")
)
```
get_ddf_Lb

Arguments

  object  A KRmodcomp object, which is the result of the KRmodcomp function
  name    The available slots. If name is missing or NULL then everything is returned.

Author(s)

Søren Højsgaard <sorenh@math.aau.dk>

References


See Also

  KRmodcomp, PBmodcomp, vcovAdj

Examples

data(beets, package='pbkrtest')
lg <- lmer(sugpct ~ block + sow + harvest + (1|block:harvest),
          data=beets, REML=FALSE)
sm <- update(lg, .~. - harvest)
modcomp <- KRmodcomp(lg, sm)
getKR(modcomp, "ddf") # get denominator degrees of freedom.

Description

Get adjusted denominator degrees of freedom for testing Lb=0 in a linear mixed model where L is a restriction matrix.

Usage

get_Lb_ddf(object, L)

## S3 method for class 'lmerMod'
get_Lb_ddf(object, L)

Lb_ddf(L, V0, Vadj)
get_ddf_Lb

## S3 method for class 'lmerMod'
get_ddf_Lb(object, Lcoef)

ddf_Lb(VVa, Lcoef, VV0 = VVa)

Arguments

object
A linear mixed model object.

L
A vector with the same length as fixef(object) or a matrix with the same
number of columns as the length of fixef(object)

VV0, Vadj
Unadjusted and adjusted covariance matrix for the fixed effects parameters.
Unadjusted covariance matrix is obtained with vcov() and adjusted with vcovAdj().

Lcoef
Linear contrast matrix

VVa
Adjusted covariance matrix

VV0
Unadjusted covariance matrix

Value

Adjusted degrees of freedom (adjustment made by a Kenward-Roger approximation).

Author(s)

Søren Højsgaard, <sorenh@math.aau.dk>

References

Ulrich Halekoh, Søren Højsgaard (2014)., A Kenward-Roger Approximation and Parametric Boot-
strap Methods for Tests in Linear Mixed Models - The R Package pbkrtest., Journal of Statistical
Software, 58(10), 1-30., http://www.jstatsoft.org/v59/i09/

See Also

KRmodcomp, vcovAdj, model2restrictionMatrix, restrictionMatrix2model

Examples

(fmLarge <- lmer(Reaction ~ Days + (Days|Subject), sleepstudy))
## removing Days
(fmSmall <- lmer(Reaction ~ 1 + (Days|Subject), sleepstudy))
anova(fmLarge, fmSmall)

KRmodcomp(fmLarge, fmSmall)  ## 17 denominator df's
get_Lb_ddf(fmLarge, c(0,1))  ## 17 denominator df's

# Notice: The restriction matrix L corresponding to the test above
# can be found with
L <- model2restrictionMatrix(fmLarge, fmSmall)
L

internal

Internal functions for the pbkrtest package

Description

These functions are not intended to be called directly.

internal-pbkrtest

pbkrtest internal

Description

pbkrtest internal

kr-modcomp

F-test and degrees of freedom based on Kenward-Roger approximation

Description

An approximate F-test based on the Kenward-Roger approach.

Usage

KRmodcomp(largeModel, smallModel, betaH = 0, details = 0)

## S3 method for class 'lmerMod'
KRmodcomp(largeModel, smallModel, betaH = 0, details = 0)

## S3 method for class 'mer'
KRmodcomp(largeModel, smallModel, betaH = 0, details = 0)

Arguments

largeModel An lmer model
smallModel An lmer model or a restriction matrix
betaH A number or a vector of the beta of the hypothesis, e.g. L beta= L betaH. betaH=0 if modelSmall is a model not a restriction matrix.
details If larger than 0 some timing details are printed.
Details

The model object must be fitted with restricted maximum likelihood (i.e. with \( \text{REML=TRUE} \)). If the object is fitted with maximum likelihood (i.e. with \( \text{REML=FALSE} \)) then the model is refitted with \( \text{REML=TRUE} \) before the p-values are calculated. Put differently, the user needs not worry about this issue.

An F test is calculated according to the approach of Kenward and Roger (1997). The function works for linear mixed models fitted with the \text{lmer} function of the \text{nlme4} package. Only models where the covariance structure is a sum of known matrices can be compared.

The \text{largeModel} may be a model fitted with \text{lmer} either using \( \text{REML=TRUE} \) or \( \text{REML=FALSE} \). The \text{smallModel} can be a model fitted with \text{lmer}. It must have the same covariance structure as \text{largeModel}. Furthermore, its linear space of expectation must be a subspace of the space for \text{largeModel}. The model \text{smallModel} can also be a restriction matrix \( L \) specifying the hypothesis \( L\beta = L\beta_H \), where \( L \) is a \( k \times p \) matrix and \( \beta \) is a \( p \) column vector the same length as \( \text{fixef(largeModel)} \).

The \( \beta_H \) is a \( p \) column vector.

Notice: if you want to test a hypothesis \( L\beta = c \) with a \( k \) vector \( c \), a suitable \( \beta_H \) is obtained via \( \beta_H = Lc \) where \( L_n \) is a g-inverse of \( L \).

Notice: It cannot be guaranteed that the results agree with other implementations of the Kenward-Roger approach!

Note

This functionality is not thoroughly tested and should be used with care. Please do report bugs etc.

Author(s)

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References


See Also

\text{getKR, lmer, vcovAdj, PBmodcomp}

Examples

\begin{verbatim}
(fmLarge <- lmer(Reaction ~ Days + (Days|Subject), sleepstudy))
## removing Days
(fmSmall <- lmer(Reaction ~ 1 + (Days|Subject), sleepstudy))
anova(fmLarge,fmSmall)
KRmodcomp(fmLarge,fmSmall)
\end{verbatim}
## The same test using a restriction matrix
L <- cbind(0,1)
KRmodcomp(fmLarge, L)

## Same example, but with independent intercept and slope effects:
m.large <- lmer(Reaction ~ Days + (1|Subject) + (0+Days|Subject), data = sleepstudy)
m.small <- lmer(Reaction ~ 1 + (1|Subject) + (0+Days|Subject), data = sleepstudy)
anova(m.large, m.small)
KRmodcomp(m.large, m.small)

---

kr-vcov

### Adjusted covariance matrix for linear mixed models according to Kenward and Roger

**Description**

Kenward and Roger (1997) describe an improved small sample approximation to the covariance matrix estimate of the fixed parameters in a linear mixed model.

**Usage**

```r
covAdj(object, details = 0)
```

**Arguments**

- `object`: An `lmer` model
- `details`: If larger than 0 some timing details are printed.

**Value**

- `phiA`: the estimated covariance matrix, this has attributed P, a list of matrices used in `KR_adjust` and the estimated matrix W of the variances of the covariance parameters of the random effects
- `SigmaG`: list: Sigma: the covariance matrix of Y; G: the G matrices that sum up to Sigma; n.ggamma: the number (called M in the article) of G matrices

**Note**

If $N$ is the number of observations, then the `vcovAdj()` function involves inversion of an $N \times N$ matrix, so the computations can be relatively slow.
Author(s)

Ulrich Halekoh <uhalekoh@health.sdu.dk>, Søren Højsgaard <sorenh@math.aau.dk>

References


See Also

getKR, KRmodcomp, lmer, PBmodcomp, vcovAdj

Examples

fm1 <- lmer(Reaction ~ Days + (Days|Subject), sleepstudy)
class(fm1)

## Here the adjusted and unadjusted covariance matrices are identical,  
## but that is not generally the case:

v1 <- vcov(fm1)
v2 <- vcovAdj(fm1, details=0)
v2 / v1

## For comparison, an alternative estimate of the variance-covariance  
## matrix is based on parametric bootstrap (and this is easily 
## parallelized):

## Not run:
nsim <- 100
sim <- simulate(fm.ml, nsim)
B <- lapply(sim, function(newy) try(fixef(refit(fm.ml, newresp=newy))))
B <- do.call(rbind, B)
v3 <- cov.wt(B)$cov
v2/v1
v3/v1

## End(Not run)
Conversion between a model object and a restriction matrix

Description

Testing a small model under a large model corresponds to imposing restrictions on the model matrix of the larger model, and these restrictions come in the form of a restriction matrix. These functions convert a model to a restriction matrix and vice versa.

Usage

model2restrictionMatrix(largeModel, smallModel)

restrictionMatrix2model(largeModel, LL)

Arguments

largeModel, smallModel
  Model objects of the same "type". Possible types are linear mixed effects models and linear models (including generalized linear models)

LL
  A restriction matrix.

Value


Note

That these functions are visible is a recent addition; minor changes may occur.

Author(s)

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References


See Also

PBmodcomp, PBrefdist, KRmodcomp
Examples

library(pbkrtest)

data("beets", package = "pbkrtest")
sug <- lm(sugpct ~ block + sow + harvest, data=beets)
sug.h <- update(sug, .~- harvest)
sug.s <- update(sug, .~- sow)

## Construct restriction matrices from models
L.h <- model2restrictionMatrix(sug, sug.h); L.h
L.s <- model2restrictionMatrix(sug, sug.s); L.s

## Construct submodels from restriction matrices
mod.h <- restrictionMatrix2model(sug, L.h); mod.h
mod.s <- restrictionMatrix2model(sug, L.s); mod.s

## The models have the same fitted values
plot(fitted(mod.h), fitted(sug.h))
plot(fitted(mod.s), fitted(sug.s))

## and the same log likelihood
logLik(mod.h)
logLik(sug.h)
logLik(mod.s)
logLik(sug.s)

pb-modcomp

Model comparison using parametric bootstrap methods.

Description

Model comparison of nested models using parametric bootstrap methods. Implemented for some commonly applied model types.

Usage

seqPBmodcomp(largeModel, smallModel, h = 20, nsim = 1000, cl = 1)

PBmodcomp(
  largeModel,
  smallModel,
  nsim = 1000,
  ref = NULL,
  seed = NULL,
  cl = NULL,
  details = 0
)

## S3 method for class 'merMod'
PBmodcomp(
    largeModel,
    smallModel,
    nsim = 1000,
    ref = NULL,
    seed = NULL,
    cl = NULL,
    details = 0
)

## S3 method for class 'lm'
PBmodcomp(
    largeModel,
    smallModel,
    nsim = 1000,
    ref = NULL,
    seed = NULL,
    cl = NULL,
    details = 0
)

Arguments

largeModel A model object. Can be a linear mixed effects model or generalized linear mixed effects model (as fitted with lmer() and glmer() function in the lme4 package) or a linear normal model or a generalized linear model. The largeModel must be larger than smallModel (see below).

smallModel A model of the same type as largeModel or a restriction matrix.

h For sequential computing for bootstrap p-values: The number of extreme cases needed to generate before the sampling process stops.

nsim The number of simulations to form the reference distribution.

cl A vector identifying a cluster; used for calculating the reference distribution using several cores. See examples below.

ref Vector containing samples from the reference distribution. If NULL, this vector will be generated using PBrefdist().

seed A seed that will be passed to the simulation of new datasets.

details The amount of output produced. Mainly relevant for debugging purposes.

Details

The model object must be fitted with maximum likelihood (i.e. with REML=FALSE). If the object is fitted with restricted maximum likelihood (i.e. with REML=TRUE) then the model is refitted with REML=FALSE before the p-values are calculated. Put differently, the user needs not worry about this issue.

Under the fitted hypothesis (i.e. under the fitted small model) nsim samples of the likelihood ratio test statistic (LRT) are generated.
Then p-values are calculated as follows:
LRT: Assuming that LRT has a chi-square distribution.
PBtest: The fraction of simulated LRT-values that are larger or equal to the observed LRT value.
Bartlett: A Bartlett correction is of LRT is calculated from the mean of the simulated LRT-values
Gamma: The reference distribution of LRT is assumed to be a gamma distribution with mean and variance determined as the sample mean and sample variance of the simulated LRT-values.
F: The LRT divided by the number of degrees of freedom is assumed to be F-distributed, where the denominator degrees of freedom are determined by matching the first moment of the reference distribution.

Note
It can happen that some values of the LRT statistic in the reference distribution are negative. When this happens one will see that the number of used samples (those where the LRT is positive) are reported (this number is smaller than the requested number of samples).
In theory one can not have a negative value of the LRT statistic but in practice on can: We speculate that the reason is as follows: We simulate data under the small model and fit both the small and the large model to the simulated data. Therefore the large model represents - by definition - an overfit; the model has superfluous parameters in it. Therefore the fit of the two models will for some simulated datasets be very similar resulting in similar values of the log-likelihood. There is no guarantee that the the log-likelihood for the large model in practice always will be larger than for the small (convergence problems and other numerical issues can play a role here).
To look further into the problem, one can use the PBrefdist() function for simulating the reference distribution (this reference distribution can be provided as input to PBmodcomp()). Inspection sometimes reveals that while many values are negative, they are numerically very small. In this case one may try to replace the negative values by a small positive value and then invoke PBmodcomp() to get some idea about how strong influence there is on the resulting p-values. (The p-values get smaller this way compared to the case when only the originally positive values are used).

Author(s)
Søren Højsgaard <sorenh@math.aau.dk>

References
http://www.jstatsoft.org/v59/i09/

See Also
KRmodcomp, PBrefdist

Examples

data(beets, package="pbkrtest")
head(beets)
## Linear mixed effects model:
sug <- lmer(sugpct ~ block + sow + harvest + (1|block:harvest),
             data=beets, REML=FALSE)
sug.h <- update(sug, .~. -harvest)
sug.s <- update(sug, .~. -sow)

anova(sug, sug.h)
PBmodcomp(sug, sug.h, nsim=50, cl=1)

anova(sug, sug.h)
PBmodcomp(sug, sug.s, nsim=50, cl=1)

## Linear normal model:
sug <- lm(sugpct ~ block + sow + harvest, data=beets)
sug.h <- update(sug, .~. -harvest)
sug.s <- update(sug, .~. -sow)

anova(sug, sug.h)
PBmodcomp(sug, sug.h, nsim=50, cl=1)

anova(sug, sug.s)
PBmodcomp(sug, sug.s, nsim=50, cl=1)

## Generalized linear model
counts <- c(18,17,15,20,10,20,25,13,12)
outcome <- gl(3,1,9)
treatment <- gl(3,3)
d.AD <- data.frame(treatment, outcome, counts)
head(d.AD)
glm.D93 <- glm(counts ~ outcome + treatment, family = poisson())
glm.D93.o <- update(glm.D93, .~. -outcome)
glm.D93.t <- update(glm.D93, .~. -treatment)

anova(glm.D93, glm.D93.o, test="Chisq")
PBmodcomp(glm.D93, glm.D93.o, nsim=50, cl=1)

anova(glm.D93, glm.D93.t, test="Chisq")
PBmodcomp(glm.D93, glm.D93.t, nsim=50, cl=1)

## Generalized linear mixed model (it takes a while to fit these)
## Not run:
(gm1 <- glmer(cbind(incidence, size - incidence) ~ period + (1 | herd),
              data = cbpp, family = binomial))
(gm2 <- update(gm1, .~.-period))

anova(gm1, gm2)
PBmodcomp(gm1, gm2, cl=2)

## End(Not run)

## Not run:
(fmLarge <- lmer(Reaction ~ Days + (Days|Subject), sleepstudy))
## removing Days
(fmSmall <- lmer(Reaction ~ 1 + (Days|Subject), sleepstudy))

anova(fmLarge, fmSmall)
PBmodcomp(fmLarge, fmSmall, cl=1)

## The same test using a restriction matrix
L <- cbind(0,1)
PBmodcomp(fmLarge, L, cl=1)

## Vanilla
PBmodcomp(beet0, beet_no.harv, nsim=1000, cl=1)

## Simulate reference distribution separately:
refdist <- PBrefdist(beet0, beet_no.harv, nsim=1000)
PBmodcomp(beet0, beet_no.harv, ref=refdist, cl=1)

## Do computations with multiple processors:
## Number of cores:
(nc <- detectCores())
## Create clusters
cl <- makeCluster(rep("localhost", nc))
## Then do:
PBmodcomp(beet0, beet_no.harv, cl=cl)

## Or in two steps:
refdist <- PBrefdist(beet0, beet_no.harv, nsim=1000, cl=cl)
PBmodcomp(beet0, beet_no.harv, ref=refdist)

## It is recommended to stop the clusters before quitting R:
stopCluster(cl)

## End(Not run)

---

**pb-refdist**

*Calculate reference distribution using parametric bootstrap*

---

**Description**

Calculate reference distribution of likelihood ratio statistic in mixed effects models using parametric bootstrap

**Usage**

```
PBrefdist(
  largeModel,  # required
  smallModel,  # required
  nsim = 1000,  # simulates reference distribution
  seed = NULL,  # required
  cl = NULL,  # required
  details = 0
)
```
## S3 method for class 'lm'
PBrefdist(
  largeModel,
  smallModel,
  nsim = 1000,
  seed = NULL,
  cl = NULL,
  details = 0
)

## S3 method for class 'merMod'
PBrefdist(
  largeModel,
  smallModel,
  nsim = 1000,
  seed = NULL,
  cl = NULL,
  details = 0
)

### Arguments

- **largeModel**: A linear mixed effects model as fitted with the `lmer()` function in the `lme4` package. This model must be larger than `smallModel` (see below).
- **smallModel**: A linear mixed effects model as fitted with the `lmer()` function in the `lme4` package. This model must be smaller than `largeModel` (see above).
- **nsim**: The number of simulations to form the reference distribution.
- **seed**: Seed for the random number generation.
- **cl**: Used for controlling parallel computations. See sections 'details' and 'examples' below.
- **details**: The amount of output produced. Mainly relevant for debugging purposes.

### Details

The model object must be fitted with maximum likelihood (i.e. with `REML=FALSE`). If the object is fitted with restricted maximum likelihood (i.e. with `REML=TRUE`) then the model is refitted with `REML=FALSE` before the p-values are calculated. Put differently, the user needs not worry about this issue.

The argument 'cl' (originally short for 'cluster') is used for controlling parallel computations. 'cl' can be NULL (default), positive integer or a list of clusters.

Special care must be taken on Windows platforms (described below) but the general picture is this: the recommended way of controlling cl is to specify the component `pbcl` in options() with e.g. `options("pbcl"=4)`.

If cl is NULL, the function will look at if the `pbcl` has been set in the options list with `getOption("pbcl")`. If cl=N then N cores will be used in the computations. If cl is NULL then the function will look for
Value

A numeric vector

Author(s)

Søren Højsgaard <sorenh@math.aau.dk>

References


See Also

PBmodcomp, KRmodcomp

Examples

data(beets)
head(beets)
beet0 <- lmer(sugpct ~ block + sow + harvest + (1|block:harvest), data=beets, REML=FALSE)
beet_no.harv <- update(beet0, . ~ . - harvest)
rd <- PBrefdist(beet0, beet_no.harv, nsim=20, cl=1)
rd

## Not run:
## Note: Many more simulations must be made in practice.

# Computations can be made in parallel using several processors:

# 1: On OSs that fork processes (that is, not on windows):
# ---------------------------------------------
if (Sys.info()["sysname"] != "Windows"){
  N <- 2 ## Or N <- parallel::detectCores()
  # N cores used in all calls to function in a session
  options("mc.cores"=N)
  rd <- PBrefdist(beet0, beet_no.harv, nsim=20)
  # N cores used just in one specific call (when cl is set,
  # options("mc.cores") is ignored):
  rd <- PBrefdist(beet0, beet_no.harv, nsim=20, cl=N)
}

# In fact, on Windows, the approach above also work but only when setting the
# number of cores to 1 (so there is to parallel computing)

# In all calls:
# options("mc.cores"=1)
# rd <- PBrefdist(beet0, beet_no.harv, nsim=20)
# Just once
# rd <- PBrefdist(beet0, beet_no.harv, nsim=20, cl=1)

# 2. On all platforms (also on Windows) one can do
# ------------------------------------------------
library(parallel)
N <- 2  ## Or N <- detectCores()
clus <- makeCluster(rep("localhost", N))

# In all calls in a session
options("pb.cl"=clus)
rd <- PBrefdist(beet0, beet_no.harv, nsim=20)

# Just once:
rd <- PBrefdist(beet0, beet_no.harv, nsim=20, cl=clus)
stopCluster(clus)

## End(Not run)
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