Package ‘simex’

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Description

Package *simex* is an implementation of the SIMEX–algorithm by Cook and Stephanski and the MCSIMEX–Algorithm by Küchenhoff, Mwalili and Lesaffre.

Details

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The package includes first of all the implementation for the SIMEX– and MCSIMEX–Algorithms. Jackknife and asymptotic variance estimation are implemented. Various methods and analytic tools are provided for a simple and fast access to the SIMEX– and MCSIMEX–Algorithm.

Functions *simex()* and *mcsimex()* can be used on models issued from *lm()* , *glm()* with asymptotic estimation. Models from *nls()* , *gam()* (package *mgcv*), *polr()* (package *MASS*), *lme()* , *nlme()* (package *nlme*) and *coxph()* (package *survival*) can also be corrected with these algorithms, but without asymptotic estimations.

Author(s)

Wolfgang Lederer, Heidi Seibold, Helmut Küchenhoff

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References

See Also

simex, mcsimex, misclass

and for functions generating the initial naive models: lm, glm, nls, gam, lme, nlme, polr, coxph

Examples

# See example(simex) and example(mcsimex)

## Seed
set.seed(49494)

## simulating the measurement error standard deviations
sd_me1 <- 0.3
sd_me2 <- 0.4
temp <- runif(100, min = 0, max = 0.6)
sd_me_het1 <- sort(temp)
temp2 <- rnorm(100, sd = 0.1)
sd_me_het2 <- abs(sd_me_het1 + temp2)

## simulating the independent variables x (real and with measurement error):
x_real1 <- rnorm(100)
x_real2 <- rpois(100, lambda = 2)
x_real3 <- -4*x_real1 + runif(100, min = -2, max = 2)  # correlated to x_real

x_measured1 <- x_real1 + sd_me1 * rnorm(100)
x_measured2 <- x_real2 + sd_me2 * rnorm(100)
x_het1 <- x_real1 + sd_me_het1 * rnorm(100)
x_het2 <- x_real3 + sd_me_het2 * rnorm(100)

## calculating dependent variable y:
y1 <- x_real1 + rnorm(100, sd = 0.05)
y2 <- x_real1 + 2*x_real2 + rnorm(100, sd = 0.08)
y3 <- x_real1 + 2*x_real3 + rnorm(100, sd = 0.08)

### one variable with homoscedastic measurement error
(model_real <- lm(y1 ~ x_real1))
(model_naiv <- lm(y1 ~ x_measured1, x = TRUE))

(model_simex <- simex(model_naiv, SIMEXvariable = "x_measured1", measurement.error = sd_me1))
plot(model_simex)

### two variables with homoscedastic measurement errors
(model_real2 <- lm(y2 ~ x_real1 + x_real2))

(model_naiv2 <- lm(y2 ~ x_measured1 + x_measured2, x = TRUE))

(model_simex2 <- simex(model_naiv2, SIMEXvariable = c("x_measured1", "x_measured2"),
measurement.error = cbind(sd_me1, sd_me2)))
```
plot(model_simex2)

### one variable with increasing heteroscedastic measurement error
model_real

(mod_naiv1 <- lm(y1 ~ x_het1, x = TRUE))
(mod_simex1 <- simex(mod_naiv1, SIMEXvariable = "x_het1",
                     measurement.error = sd_me_het1, asymptotic = FALSE))
plot(mod_simex1)

## Not run:

### two correlated variables with heteroscedastic measurement errors
(model_real3 <- lm(y3 ~ x_real1 + x_real3))
(mod_naiv2 <- lm(y3 ~ x_het1 + x_het2, x = TRUE))
(mod_simex2 <- simex(mod_naiv2, SIMEXvariable = c("x_het1", "x_het2"),
                     measurement.error = cbind(sd_me_het1, sd_me_het2), asymptotic = FALSE))
plot(mod_simex2)

### two variables, one with homoscedastic, one with heteroscedastic measurement error
model_real2

(mod_naiv3 <- lm(y2 ~ x_measured1 + x_het2, x = TRUE))
(mod_simex3 <- simex(mod_naiv3, SIMEXvariable = c("x_measured1", "x_het2"),
                     measurement.error = cbind(sd_me1, sd_me_het2), asymptotic = FALSE))

### glm: two variables, one with homoscedastic, one with heteroscedastic measurement error
t <- x_real1 + 2*x_real2
g <- 1 / (1 + exp(-t))
u <- runif(100)
ybin <- as.numeric(u < g)

(logit_real <- glm(ybin ~ x_real1 + x_real2, family = binomial))
(logit_naiv <- glm(ybin ~ x_measured1 + x_het2, x = TRUE, family = binomial))
(logit_simex <- simex(logit_naiv, SIMEXvariable = c("x_measured1", "x_het2"),
                      measurement.error = cbind(sd_me1, sd_me_het2), asymptotic = FALSE))
summary(logit_simex)
print(logit_simex)
plot(logit_simex)

## End(Not run)
```

diag.block  Constructs a block diagonal matrix

Description

The function takes a list and constructs a block diagonal matrix with the elements of the list on the diagonal. If d is not a list then d will be repeated n times and written on the diagonal (a wrapper for kronecker())

Usage

diag.block(d, n)

Arguments

d          a list of matrices or vectors, or a matrix or vector
n          number of repetitions

Value

returns a matrix with the elements of the list or the repetitions of the supplied matrix or vector on the diagonal.

Author(s)

Wolfgang Lederer, <wolfgang.lederer@gmail.com>

See Also

diag, kronecker

Examples

a <- matrix(rep(1, 4), nrow = 2)
b <- matrix(rep(2, 6), nrow = 2)
e <- c(3, 3, 3, 3)
f <- t(e)
d <- list(a, b, e, f)
diag.block(d)
diag.block(a, 3)
Build and check misclassification matrices from empirical estimations

Description
Empirical misclassification matrices to the power of lambda may not exist for small values of lambda. These functions provide methods to estimate the nearest version of the misclassification matrix that satisfies the conditions a misclassification matrix has to fulfill, and to check it (existence for exponents smaller than 1).

Usage
build.mc.matrix(mc.matrix, method = "series",
                tuning = sqrt(.Machine$double.eps), diag.cor = FALSE,
                tol = .Machine$double.eps, max.iter = 100)

Arguments
- mc.matrix: an empirical misclassification matrix
- method: method used to estimate the generator for the misclassification matrix. One of "series", "log" or "jlt" (see Details)
- tuning: security parameter for numerical reasons
- diag.cor: should corrections be substracted from the diagonal or from all values corresponding to the size?
- tol: tolerance level for series method for convergence
- max.iter: maximal number of iterations for the series method to converge. Ignored if method is not "series"

Details
Method "series" constructs a generator via the series
\[(Pi - I) - (Pi - I)^2/2 + (Pi - I)^3/3 - \ldots\]
Method "log" constructs the generator via taking the log of the misclassification matrix. Small negative off-diagonal values are corrected and set to \((0 + tuning)\). The amount used to correct for negative values is added to the diagonal element if diag.cor = TRUE and distributed among all values if diag.cor = FALSE.
Method "jlt" uses the method described by Jarrow et al. (see Israel et al.).

Value
- build.mc.matrix() returns a misclassification matrix that is the closest estimate for a working misclassification matrix.
- check.mc.matrix() returns a vector of logicals.
mcsimex

Author(s)

Wolfgang Lederer, <wolfgang.lederer@gmail.com>

References


See Also

mcsimex, misclass, diag.block

Examples

Pi <- matrix(data = c(0.989, 0.01, 0.001, 0.17, 0.829, 0.001, 0.001, 0.18, 0.819),
nrow = 3, byrow = FALSE)
check.mc.matrix(list(Pi))
check.mc.matrix(list(build.mc.matrix(Pi)))
build.mc.matrix(Pi)

Pi3 <- matrix(c(0.8, 0.2, 0, 0, 0.8, 0.1, 0.1, 0.8, 0.1, 0, 0, 0.3, 0.7), nrow = 4)
check.mc.matrix(list(Pi3))
build.mc.matrix(Pi3)
check.mc.matrix(list(build.mc.matrix(Pi3)))
P1 <- matrix(c(1, 0, 0, 1), nrow = 2)
P2 <- matrix(c(0.8, 0.15, 0, 0.2, 0.7, 0.2, 0, 0.15, 0.8), nrow = 3, byrow = TRUE)
P3 <- matrix(c(0.4, 0.6, 0.6, 0.4), nrow = 2)
mc.matrix <- list(P1, P2, P3)
check.mc.matrix(mc.matrix) # TRUE FALSE FALSE

---

mcsimex

*Misclassification in models using MCSIMEX*

Description

Implementation of the misclassification MCSIMEX algorithm as described by Küchenhoff, Mwalili and Lesaffre.

Usage

```r
mcsimex(model, SIMEXvariable, mc.matrix, lambda = c(0.5, 1, 1.5, 2),
B = 100, fitting.method = "quadratic",
jackknife.estimation = "quadratic", asymptotic = TRUE)
```

## S3 method for class 'mcsimex'
plot(x, xlab = expression((1 + lambda)),
ylab = colnames(b)[-1], ask = FALSE, show = rep(TRUE, NCOL(b) - 1),
```
...)
## S3 method for class 'mcsimex'
predict(object, newdata, ...)

## S3 method for class 'mcsimex'
print(x, digits = max(3,getOption("digits") - 3), ...)

## S3 method for class 'summary.mcsimex'
print(x, digits = max(3,getOption("digits") - 3), ...)

## S3 method for class 'mcsimex'
summary(object, ...)

## S3 method for class 'mcsimex'
refit(object, fitting.method = "quadratic",
jackknife.estimation = "quadratic", asymptotic = TRUE, ...)

Arguments

model          the naive model, the misclassified variable must be a factor
SIMEXvariable vector of names of the variables for which the MCSIMEX-method should be applied
mc.matrix      if one variable is misclassified it can be a matrix. If more than one variable is misclassified it must be a list of the misclassification matrices, names must match with the SIMEXvariable names, column- and row-names must match with the factor levels. If a special misclassification is desired, the name of a function can be specified (see details)
lambda         vector of exponents for the misclassification matrix (without 0)
B               number of iterations for each lambda
fitting.method linear, quadratic and loglinear are implemented (first 4 letters are enough)
jackknife.estimation specifying the extrapolation method for jackknife variance estimation. Can be set to FALSE if it should not be performed
asymptotic     logical, indicating if asymptotic variance estimation should be done, the option x = TRUE must be enabled in the naive model
x               object of class 'mcsimex'
xlab           optional name for the X-Axis
ylab           vector containing the names for the Y-Axis
ask             logical. If TRUE, the user is asked for input, before a new figure is drawn
show           vector of logicals indicating for which variables a plot should be produced
arguments passed to other functions
object object of class ‘mcsimex’
newdata optionally, a data frame in which to look for variables with which to predict. If omitted, the fitted linear predictors are used
digits number of digits to be printed

Details

If mc.matrix is a function the first argument of that function must be the whole dataset used in the naive model, the second argument must be the exponent (lambda) for the misclassification. The function must return a data.frame containing the misclassified SIMEXvariable. An example can be found below.

Asymptotic variance estimation is only implemented for lm and glm

The loglinear fit has the form $g(\lambda, \text{GAMMA}) = \exp(\gamma_0 + \gamma_1 \cdot \lambda)$. It is realized via the log() function. To avoid negative values the minimum +1 of the dataset is added and after the prediction later subtracted $\exp(\text{predict}(\ldots)) - \min(\text{data}) - 1$.

The 'log2' fit is fitted via the nls() function for direct fitting of the model $y \sim \exp(\gamma_0 + \gamma_1 \cdot \lambda)$. As starting values the results of a LS-fit to a linear model with a log transformed response are used. If nls does not converge, the model with the starting values is returned.

refit() refits the object with a different extrapolation function.

Value

An object of class ‘mcsimex’ which contains:

coefficients corrected coefficients of the MCSIMEX model,
SIMEX.estimates the MCSIMEX-estimates of the coefficients for each lambda,
lambda the values of lambda,
model the naive model,
mc.matrix the misclassification matrix,
B the number of iterations,
extrapolation the model object of the extrapolation step,
fitting.method the fitting method used in the extrapolation step,
SIMEXvariable name of the SIMEXvariables,
call the function call,
variance.jackknife the jackknife variance estimates,
extrapolation.variance the model object of the variance extrapolation,
mcsimex

variance.jackknife.lambda
  the data set for the extrapolation,
variance.asymptotic
  the asymptotic variance estimates,
theta
  all estimated coefficients for each lambda and B,

... 

Methods (by generic)

• plot: Plots of the simulation and extrapolation
• predict: Predict with mcsimex correction
• print: Nice printing
• print: Print summary nicely
• summary: Summary for mcsimex
• refit: Refits the model with a different extrapolation function

Author(s)

Wolfgang Lederer, <wolfgang.lederer@gmail.com>

References


See Also

misclass, simex

Examples

```r
x <- rnorm(200, 0, 1.142)
z <- rnorm(200, 0, 2)
y <- factor(rbinom(200, 1, (1 / (1 + exp(-1 * (-2 + 1.5 * x -0.5 * z))))))
Pi <- matrix(data = c(0.9, 0.1, 0.3, 0.7), nrow = 2, byrow = FALSE)
dimnames(Pi) <- list(levels(y), levels(y))
ystar <- misclass(data.frame(y), list(y = Pi), k = 1)
naive.model <- glm(ystar ~ x + z, family = binomial, x = TRUE, y = TRUE)
true.model <- glm(y ~ x + z, family = binomial)
simex.model <- mcsimex(naive.model, mc.matrix = Pi, SIMEXvariable = "ystar")
op <- par(mfrow = c(2, 3))
invisible(lapply(simex.model$theta, boxplot, notch = TRUE, outline = FALSE,
```
names = c(0.5, 1, 1.5, 2)))
plot(simex.model)

simex.model2 <- refit(simex.model, "line")
plot(simex.model2)
par(op)

# example using polr from the MASS package
## Not run:
if(require(MASS)) {
  yord <- cut((1 / (1 + exp(-1 * (-2 + 1.5 * x -0.5 * z)))), 3, ordered=TRUE)
  Pi3 <- matrix(data = c(0.8, 0.1, 0.1, 0.2, 0.7, 0.1, 0.1, 0.2, 0.7), nrow = 3, byrow = FALSE)
  dimnames(Pi3) <- list(levels(yord), levels(yord))
  ystarord <- misclass(data.frame(yord), list(yord = Pi3), k = 1)[, 1]
  naive.ord.model <- polr(ystarord ~ x + z, Hess = TRUE)
  simex.ord.model <- mcsimex(naive.ord.model, mc.matrix = Pi3,
                          SIMEXvariable = "ystarord", asymptotic=FALSE)
}
## End(Not run)

# example for a function which can be supplied to the function mcsimex()
# "ystar" is the variable which is to be misclassified
# using the example above
## Not run:
my.misclass <- function (datas, k) {
  ystar <- datas"ystar"
  p1 <- matrix(data = c(0.75, 0.25, 0.25, 0.75), nrow = 2, byrow = FALSE)
  colnames(p1) <- levels(ystar)
  rownames(p1) <- levels(ystar)
  p0 <- matrix(data = c(0.8, 0.2, 0.2, 0.8), nrow = 2, byrow = FALSE)
  colnames(p0) <- levels(ystar)
  rownames(p0) <- levels(ystar)
  ystar[datas$x < 0] <- misclass(data.frame(ystar = ystar[datas$x < 0]), list(ystar = p1), k = k)[, 1]
  ystar[datas$x > 0] <- misclass(data.frame(ystar = ystar[datas$x > 0]), list(ystar = p0), k = k)[, 1]
  ystar <- factor(ystar)
  return(data.frame(ystar))}

simex.model.differential <- mcsimex(naive.model, mc.matrix = "my.misclass", SIMEXvariable = "ystar")
## End(Not run)

misclass

Generates misclassified data
Description

Takes a data.frame and produces misclassified data. Probabilities for the misclassification are given in mc.matrix.

Usage

misclass(data.org, mc.matrix, k = 1)

Arguments

data.org data.frame containing the factor variables. Must be factors.
mc.matrix a list of matrices giving the probabilities for the misclassification. Names of the list must correspond to the variable names in data.org. The colnames must be named according to the factor levels.
k the exponent for the misclassification matrix

Value

A data.frame containing the misclassified variables

Author(s)

Wolfgang Lederer, <wolfgang.lederer@gmail.com>

See Also

mcsimex, mc.matrix, diag.block

Examples

x1 <- factor(rbinom(100, 1, 0.5))
x2 <- factor(rbinom(100, 2, 0.5))

p1 <- matrix(c(1, 0, 0, 1), nrow = 2)
p2 <- matrix(c(0.8, 0.1, 0.1, 0.1, 0.8, 0.1, 0.1, 0.1, 0.8), nrow = 3)
colnames(p1) <- levels(x1)
colnames(p2) <- levels(x2)

x <- data.frame(x1 = x1, x2 = x2)
matrix <- list(x1 = p1, x2 = p2)

x.mc <- misclass(data.org = x, mc.matrix = matrix, k = 1)

identical(x[, 1], x.mc[, 1]) # TRUE
identical(x[, 2], x.mc[, 2]) # FALSE
Measurement error in models using SIMEX

Description

Implementation of the SIMEX algorithm for measurement error models according to Cook and Stefanski

Usage

```r
simex(model, SIMEXvariable, measurement.error, lambda = c(0.5, 1, 1.5, 2), B = 100, fitting.method = "quadratic", jackknife.estimation = "quadratic", asymptotic = TRUE)
```

Arguments

- **model** the naive model
- **SIMEXvariable** character or vector of characters containing the names of the variables with measurement error
- **measurement.error** given standard deviations of measurement errors. In case of homoskedastic measurement error it is a matrix with dimension 1xlength(SIMEXvariable). In case of heteroskedastic error for at least one SIMEXvariable it is a matrix of dimension nx
lambda vector of lambdas for which the simulation step should be done (without 0)
B number of iterations for each lambda
fitting.method fitting method for the extrapolation. linear, quadratic, nonlinear are implemented. (first 4 letters are enough)
jackknife.estimation specifying the extrapolation method for jackknife variance estimation. Can be set to FALSE if it should not be performed
asymptotic logical, indicating if asymptotic variance estimation should be done, in the naive model the option x = TRUE has to be set
x object of class ’simex’
xlab optional name for the X-Axis
ylab vector containing the names for the Y-Axis
ask logical. If TRUE, the user is asked for input, before a new figure is drawn
show vector of logicals indicating for which variables a plot should be produced
... arguments passed to other functions
object of class ’simex’
ewdata optionally, a data frame in which to look for variables with which to predict. If omitted, the fitted linear predictors are used
digits number of digits to be printed

Details

Nonlinear is implemented as described in Cook and Stefanski, but is numerically instable. It is not advisable to use this feature. If a nonlinear extrapolation is desired please use the refit() method.

Asymptotic is only implemented for naive models of class lm or glm with homoscedastic measurement error.

refit() refits the object with a different extrapolation function.

Value

An object of class ’simex’ which contains:

coefficients the corrected coefficients of the SIMEX model,
SIMEX.estimates the estimates for every lambda,
model the naive model,
measurement.error the known error standard deviations,
B the number of iterations,
extrapolation the model object of the extrapolation step,
fitting.method
the fitting method used in the extrapolation step,
residuals
the residuals of the main model,
fbitted.values
the fitted values of the main model,
call
the function call,
variance.jackknife
the jackknife variance estimate,
extrapolation.variance
the model object of the variance extrapolation,
variance.jackknife.lambda
the data set for the extrapolation,
variance.asymptotic
the asymptotic variance estimates,
theta
the estimates for every B and lambda,

Methods (by generic)
• plot: Plot the simulation and extrapolation step
• predict: Predict using simex correction
• print: Print simex nicely
• print: Print summary nicely
• refit: Refits the model with a different extrapolation function
• summary: Summary of simulation and extrapolation

Author(s)
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References
See Also

`mcsimex` for discrete data with misclassification, `lm`, `glm`

Examples

```r
## Seed
set.seed(49494)

## simulating the measurement error standard deviations
sd_me <- 0.3
sd_me2 <- 0.4
temp <- runif(100, min = 0, max = 0.6)
sd_me_het1 <- sort(temp)
temp2 <- rnorm(100, sd = 0.1)
sd_me_het2 <- abs(sd_me_het1 + temp2)

## simulating the independent variables x (real and with measurement error):

x_real <- rnorm(100)
x_real2 <- rpois(100, lambda = 2)
x_real3 <- -4*x_real + runif(100, min = -10, max = 10) # correlated to x_real

x_measured <- x_real + sd_me * rnorm(100)
x_measured2 <- x_real2 + sd_me2 * rnorm(100)
x_het1 <- x_real + sd_me_het1 * rnorm(100)
x_het2 <- x_real3 + sd_me_het2 * rnorm(100)

## calculating dependent variable y:
y <- x_real + rnorm(100, sd = 0.05)
y2 <- x_real + 2*x_real2 + rnorm(100, sd = 0.08)
y3 <- x_real + 2*x_real3 + rnorm(100, sd = 0.08)

### one variable with homoscedastic measurement error
(model_real <- lm(y ~ x_real))

(model_naiv <- lm(y ~ x_measured, x = TRUE))

(model_simex <- simex(model_naiv, SIMEXvariable = "x_measured", measurement.error = sd_me))
plot(model_simex)

### two variables with homoscedastic measurement errors
(model_real2 <- lm(y2 ~ x_real + x_real2))
(model_naiv2 <- lm(y2 ~ x_measured + x_measured2, x = TRUE))
(model_simex2 <- simex(model_naiv2, SIMEXvariable = c("x_measured", "x_measured2"),
                      measurement.error = cbind(sd_me, sd_me2)))
plot(model_simex2)

## Not run:
### one variable with increasing heteroscedastic measurement error
model_real
```

```
(mod_naiv1 <- lm(y ~ x_het1, x = TRUE))
(mod_simex1 <- simex(mod_naiv1, SIMEXvariable = "x_het1",
                     measurement.error = sd_me_het1, asymptotic = FALSE))

plot(mod_simex1)

### two correlated variables with heteroscedastic measurement errors
(model_real3 <- lm(y3 ~ x_real + x_real3))
(mod_naiv2 <- lm(y3 ~ x_het1 + x_het2, x = TRUE))
(mod_simex2 <- simex(mod_naiv2, SIMEXvariable = c("x_het1", "x_het2"),
                     measurement.error = cbind(sd_me_het1, sd_me_het2), asymptotic = FALSE))

plot(mod_simex2)

### two variables, one with homoscedastic, one with heteroscedastic measurement error
(model_real2 <- lm(y2 ~ x_measured + x_het2, x = TRUE))
(mod_simex3 <- simex(mod_naiv3, SIMEXvariable = c("x_measured", "x_het2"),
                     measurement.error = cbind(sd_me, sd_me_het2), asymptotic = FALSE))

### glm: two variables, one with homoscedastic, one with heteroscedastic measurement error

### polr: two variables, one with homoscedastic, one with heteroscedastic measurement error
if(require("MASS")) {  # Requires MASS
  yerr <- jitter(y, amount=1)
yfactor <- cut(yerr, 3, ordered_result=TRUE)

  (logit_real <- glm(ybin ~ x_real + x_real2, family = binomial))
  (logit_naiv <- glm(y ~ x_measured + x_het2, x = TRUE, family = binomial))
  (logit_simex <- simex(logit_naiv, SIMEXvariable = c("x_measured", "x_het2"),
                         measurement.error = cbind(sd_me, sd_me_het2), asymptotic = FALSE))

  summary(logit_simex)
  print(logit_simex)
  plot(logit_simex)
}

## End(Not run)