

Package ‘simex’

February 15, 2012

Type Package

Version 1.4

Date 2009-05-26

Depends stats

Suggests mgcv, nlme

Title SIMEX- and MCSIMEX-Algorithm for measurement error models

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Description Implementation of the SIMEX-Algorithm by Cook & Stefanski
and MCSIMEX by Küchenhoff, Mwalili & Lesaffre

License GPL (>= 2)

Encoding latin1

LazyLoad yes

Repository CRAN

Date/Publication 2009-05-27 08:59:33

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simex-package

Error or misclassification correction in models using (MC)SIMEX

Description

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

Details

Package:	simex
Type:	Package
Version:	1.4
Date:	2009-04-19
License:	GPL 2 or above
LazyLoad:	yes

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**), `lme()` and `nlme()` (package **nlme**) can also be corrected with these algorithms, but without asymptotic estimations.

Author(s)

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References

Lederer, W. and Küchenhof, H. (2006) A short introduction to the SIMEX and MCSIMEX. *R News*, **6/4**, 26 – 31

See Also

[simex](#), [mcsimex](#), [misclass](#)

and for functions generating the initial naive models: [lm](#), [glm](#), [nls](#), [gam](#), [lme](#), [nlme](#)

Examples

```
# See example(simex) and example(mcsimex)
```

`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@googlemail.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)
```

mc.matrix

*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)
check.mc.matrix(mc.matrix, tol = .Machine$double.eps)
```

Arguments

mc.matrix	an empirical misclassification matrix
method	method used to estimate the generator for the misclassification matrix (see Details)
tuning	security parameter for numerical reasons
diag.cor	should corrections be subtracted 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 serie method to converge

Details

Method "series" constructs a generator via the series

$$(P_i - I) - (P_i - I)^2/2 + (P_i - I)^3/3 - \dots$$

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 Jarro 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.

Note

Does not always work! So check properly.

Author(s)

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

References

Israel, R.B., Rosenthal, J.S., Wei, J.Z., Finding generators for Markov Chains via empirical transition matrices, with applications to credit ratings, *Mathematical Finance*, **11**, 245–265

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, 0.8, 0.1, 0.1, 0, 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
```

Description

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

Usage

```

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'
print(x, digits = max(3, getOption("digits") - 3), ...)
## S3 method for class 'mcsimex'
summary(object,...)
## 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'
refit(object, fitting.method = "quadratic",
  jackknife.estimation = "quadratic", asymptotic = TRUE, ...)

```

Arguments

<code>model</code>	the naive model, the misclassified variable must be a factor
<code>SIMEXvariable</code>	vector of names of the variables for which the MCSIMEX-method should be applied
<code>mc.matrix</code>	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 <code>SIMEXvariable</code> 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)
<code>lambda</code>	vector of exponents for the misclassification matrix (without 0)
<code>B</code>	number of iterations for each lambda
<code>fitting.method</code>	linear, quadratic and loglinear are implemented (first 4 letters are enough)
<code>jackknife.estimation</code>	specifying the extrapolation method for jackknife variance estimation. Can be set to FALSE if it should not be performed
<code>asymptotic</code>	logical, indicating if asymptotic variance estimation should be done, the option <code>x = TRUE</code> must be enabled in the naive model
<code>x</code>	object of class 'mcsimex'
<code>digits</code>	number of digits to be printed
<code>object</code>	object of class 'mcsimex'
<code>xlab</code>	optional name for the X-Axis
<code>ylab</code>	vector containing the names for the Y-Axis
<code>ask</code>	logical. If TRUE, the user is asked for input, before a new figure is drawn
<code>show</code>	vector of logicals indicating for wich variables a plot should be produced

newdata	optionally, a data frame in which to look for variables with which to predict. If omitted, the fitted linear predictors are used
...	arguments passed to other functions

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 $g(\lambda, \text{GAMMA}) = \exp(\text{gamma0} + \text{gamma1} * \lambda)$. 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 $\exp(\text{predict}(\dots)) - \min(\text{data}) - 1$.

The 'log2' fit is fitted via the `nls()` function for direct fitting of the model $y \sim \exp(\text{gamma.0} + \text{gamma.1} * \lambda)$. 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:

<code>coefficients</code>	corrected coefficients of the MCSIMEX model, SIMEX.estimates
	the MCSIMEX-estimates of the coefficients for each lambda,
<code>lambda</code>	the values of lambda,
<code>model</code>	the naive model,
<code>mc.matrix</code>	the misclassification matrix,
<code>B</code>	the number of iterations,
<code>extrapolation</code>	the model object of the extrapolation step,
<code>fitting.method</code>	the fitting method used in the extrapolation step,
<code>SIMEXvariable</code>	name of the SIMEXvariables,
<code>call</code>	the function call,
<code>variance.jackknife</code>	the jackknife variance estimates,
<code>extrapolation.variance</code>	the model object of the variance extrapolation,
<code>variance.jackknife.lambda</code>	the data set for the extrapolation,
<code>variance.asymptotic</code>	the asymptotic variance estimates,
<code>theta</code>	all estimated coefficients for each lambda and B,
...	

Author(s)

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References

- Küchenhoff, H., Mwalili, S. M. and Lesaffre, E. (2006) A general method for dealing with misclassification in regression: The Misclassification SIMEX. *Biometrics*, **62**, 85 – 96
- Küchenhoff, H., Lederer, W. and E. Lesaffre. (2006) Asymptotic Variance Estimation for the Misclassification SIMEX. *Computational Statistics and Data Analysis*, **51**, 6197 – 6211
- Lederer, W. and Küchenhoff, H. (2006) A short introduction to the SIMEX and MCSIMEX. *R News*, **6(4)**, 26–31

See Also

[misclass](#), [simex](#)

Examples

```
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)[, 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 for a function which can be supplied to the function mcsimex()
# "ystar" is the variable which is to be misclassified
# using the example above
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")

```

misclass	<i>Generates misclassified data</i>
----------	-------------------------------------

Description

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

Usage

```
misclass(data.org, mc.matrix, k)
```

Arguments

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

Value

A data.frame containing the misclassified variables

Author(s)

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

See Also

[mcsimex](#), [build.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)
mc.matrix <- list(x1 = p1, x2 = p2)

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

identical(x[, 1], x.mc[, 1]) # TRUE
identical(x[, 2], x.mc[, 2]) # FALSE

```

simex

Measurement error in models using SIMEX

Description

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

Usage

```

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

```

```

## S3 method for class 'simex'
print(x, digits = max(3, getOption("digits") - 3), ...)
## S3 method for class 'simex'
summary(object,...)
## S3 method for class 'simex'
plot(x, xlab = expression((1 + lambda)), ylab = colnames(b[, -1]),
     ask = FALSE, show = rep(TRUE, NCOL(b) - 1), ...)
## S3 method for class 'simex'
predict(object, newdata, ...)

refit(object, ...)
## S3 method for class 'simex'
refit(object, 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	vector of standard deviations of the known measurement errors
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 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'
digits	number of digits to be printed
object	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 wich variables a plot should be produced
newdata	optionally, a data frame in which to look for variables with which to predict. If omitted, the fitted linear predictors are used
...	arguments passed to other functions

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`.

`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,
fitted.values	the fitted values,
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,
 ...

Author(s)

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

References

Cook, J.R. and Stefanski, L.A. (1994) Simulation-extrapolation estimation in parametric measurement error models. *Journal of American Statistical Association*, **89**, 1314 – 1328
 Carroll, R.J., Küchenhoff, H., Lombard, F. and Stefanski L.A. (1996) Asymptotics for the SIMEX estimator in nonlinear measurement error models. *Journal of the American Statistical Association*, **91**, 242 – 250
 Carrol, R.J., Ruppert, D., Stefanski, L.A. and Crainiceanu, C. (2006). *Measurement error in nonlinear models: A modern perspective.*, Second Edition. London: Chapman and Hall.
 Lederer, W. and Küchenhoff, H. (2006) A short introduction to the SIMEX and MCSIMEX. *R News*, **6(4)**, 26–31

See Also

[mcsimex](#) for discrete data with misclassification, [lm](#), [glm](#)

Examples

```

# to test nonlinear extrapolation
#set.seed(3)
x <- rnorm(200, 0, 100)
u <- rnorm(200, 0, 25)
w <- x + u
y <- x + rnorm(200, 0, 9)
true.model <- lm(y ~ x)
naive.model <- lm(y ~ w, x = TRUE)
simex.model <- simex(model = naive.model, SIMEXvariable = "w",
  measurement.error = 25)
plot(x, y)
abline(true.model, col = "darkblue")
abline(simex.model, col = "red")
abline(naive.model, col = "green")
legend(min(x), max(y), legend = c("True Model", "SIMEX model", "Naive Model"),

```

```
col = c("darkblue", "red", "green"), lty = 1)

plot(simex.model, mfrow = c(2, 2))

simex.model2 <- refit(simex.model, "line")
plot(simex.model2, mfrow = c(2, 2))
```

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