# Package 'OEFPIL'

March 7, 2021

Type Package

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coef.OEFPIL

Extract model coefficients from OEFPIL

# **Description**

Function which extracts the estimated model coefficients from an object of class "OEFPIL".

# Usage

```
## S3 method for class 'OEFPIL'
coef(object, ...)
```

# **Arguments**

```
object an object of class "OEFPIL" (a result of a call to OEFPIL). . . . other arguments.
```

### Value

A named vector of estimated model coefficients extracted from an "OEFPIL" object.

# See Also

**OEFPIL** 

```
##Creating a data file (using steam data from MASS library)
library(MASS)
steamdata <- steam
colnames(steamdata) <- c("x","y")
startsteam <- list(b1 = 5, b2 = 8, b3 = 200)
k <- nrow(steamdata)
CM <- diag(rep(0.1,2*k))

##Creating an OEFPIL object
st1 <- OEFPIL(steamdata, y ~ b1 * 10^(b2 * x/ (b3 + x)), startsteam, CM, useNLS = FALSE)
##Use of coef function
coef(st1)</pre>
```

confBands.OEFPIL 3

confBands.OEFPIL $C$	Confidence and prediction bands for OEFPIL object
----------------------	---

# **Description**

Function calculates pointwise confidence bands and prediction bands of estimated function from an object of class "OEFPIL".

# Usage

```
## S3 method for class 'OEFPIL'
confBands(object, xx, signif.level = 0.05, new.obs.variance)
```

# **Arguments**

object an object of class "OEFPIL" (a result of a call to OEFPIL).

xx a sequence of x-coordinates of points for computing confidence and prediction

intervals. If missing, the default sequence seq(from = min(x), to = max(x), length.out

= 301) is used.

signif.level a numerical value or a vector of significance levels for confidence bands. If

missing, the default value 0.05 is used.

new.obs.variance

the variance of a new observation for prediction interval computing.

### **Details**

An argument signif.level can be one numerical value or vector of numerical values of significance levels for confidence intervals.

# Value

Returns an object of type list containing the following components.

xx a numerical vector of points where intervals are calculated. yy a numerical vector with values of estimated function in xx.

PointwiseCB a matrix of confidence intervals at points xx.

PredictCB a matrix of prediction intervals at points xx.

# See Also

```
OEFPIL, plot.OEFPIL
```

```
##-- Continuing the coef.OEFPIL(.) example:
##Use of confBands function with default parameters
a <- confBands(st1)
str(a)
##Computing two different confidence bands in one step</pre>
```

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```
b \leftarrow confBands(st1, signif.level = c(0.01,0.05))
str(b)
```

confInt.OEFPIL

Confidence intervals for OEFPIL parameters

### **Description**

Function computes confidence intervals for the parameters counted by OEFPIL function.

# Usage

```
confInt.OEFPIL(object, signif.level = object$contents$signif.level, parm)
```

# **Arguments**

object an object of class "OEFPIL" (a result of a call to OEFPIL).

signif.level a numerical value or a vector of significance levels for confidence intervals. If

missing, a value from the input "OEFPIL" object is used.

parm a specification of which parameters are to be given confidence intervals, either

a vector of numbers or a vector of names. If missing, all parameters are consid-

ered.

# **Details**

The confidence intervals are computing under normality assumption.

### Value

A matrix of estimated confidence intervals for model coefficients from an "OEFPIL" object. The matrix contains lower and upper confidence limits (columns) for each parameter (rows).

#### See Also

**OEFPIL** 

```
##-- Continuing the coef.OEFPIL(.) example:
##Use of confint function
#one numerical value
confInt.OEFPIL(st1)

#vector of numerical values
confInt.OEFPIL(st1, signif.level = c(0.01,0.05,0.1))

#estimation of specified parameters
confInt.OEFPIL(st1, signif.level = c(0.01,0.05,0.1), parm = c('b1','b2'))
```

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curvplot.OEFPIL

Plot of estimated curve for OEFPIL object

### **Description**

Function for plotting the estimated curve with pointwise confidence bands for an object of class "OEFPIL".

# Usage

```
curvplot.OEFPIL(object, signif.level, xx)
```

#### **Arguments**

object an object of class "OEFPIL" (a result of a call to OEFPIL).

signif.level a numeric value or a vector of significance levels for pointwise confidence bands.

If missing, the estimated curve is plotted without confidence bands.

xx a sequence of x-coordinates of points for computing and plotting confidence

bands. If missing, the default sequence seq(from = min(x), to = max(x), length.out)

= 301) is used.

#### Value

A ggplot graph of the estimated curve with pointwise confidence bands. The result can be edit using other ggplot components as usually.

### See Also

```
OEFPIL, paramplot.OEFPIL and plot.OEFPIL.
```

```
library(MASS)
library(ggplot2)
##Creating a data file
steamdata <- steam
colnames(steamdata) <- c("x","y")</pre>
n <- nrow(steamdata)</pre>
CM1 <- diag(rep(10,2*n))
CM2 \leftarrow diag(c(rep(12,n), rep(14,n)))
##Creating OEFPIL objects
st1 \leftarrow OEFPIL(steamdata, y \sim b1 * 10^(b2 * x/ (b3 + x)), list(b1 = 5, b2 = 8, b3 = 200),
              CM1, useNLS = FALSE)
st2 \leftarrow OEFPIL(steamdata, y \sim b1 * 10^(b2 * x/ (b3 + x)), list(b1 = 5, b2 = 8, b3 = 200),
              CM2, useNLS = FALSE)
##Use of curvplot.OEFPIL function on an object of class 'OEFPIL'
curvplot.OEFPIL(st1, signif.level = 0.05)
##Use of curvplot.OEFPIL function on an object of class 'OEFPIL' with different arguments
curvplot.0EFPIL(st2, signif.level = c(0.01,0.05), xx = seq(0,110,1))
```

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```
##Use of curvplot.OEFPIL function with additional arguments as for ggplot2
curvplot.OEFPIL(st1, signif.level = 0.05) +
  labs(x = "New x label") +
  labs(title = "New graph title")
```

NanoIndent.OEFPIL

Estimation of parameters in nanoindentation

# Description

Fitting the unloading curve in nanoindentation process by power law function with parameters estimated by iterated linearization algorithm (OEFPIL). The special case of OEFPIL function customized for using in nanoindentation (see 'Details').

### Usage

#### **Arguments**

data an object of type data. frame with 2 named columns or list with 2 elements.

alpha.start a starting value of the fitting constant alpha.

m. start a starting value of the exponent m.

hp.start a starting value of the permanent indentation depth hp.

unload.data a logical value (default FALSE) indicating the structure of data. If TRUE, an input

data contains only unloading part of the curve. If FALSE, an input data contains

complete loading, hold and unloading parts of an indentation process.

ucut a numerical value, indicating the upper bound of cut off.

lcut a numerical value, indicating the lower bound of cut off.

CM a covariance matrix of the input data. See 'Details' for more information.

uh standard deviation of depth.

uF standard deviation of load.

max.iter maximum number of iterations.

see.iter.val logical. If TRUE, all the partial results of the OEFPIL algorithm are displayed

and saved. The default value is FALSE.

save.file.name a name of the file for saving results. If missing, no output file is saved.

th a numerical value, indicating threshold necessary for the iteration stoppage.

signif.level a significance level for the confidence interval.

useNLS logical. If TRUE (the default value), function will set up starting parameters

calculated by nlsLM function (nonlinear least square estimation).

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#### **Details**

In this special case of the OEFPIL function, the dependence of parameters is fixed in the form:  $F = \alpha * (h - h_p)^m$ , where F is load and h depth measured within a nanoindentation process. It is possible to set own starting values of the parameters, in the other case these values are calculated by the algorithm and printing into the console.

A selection of the part of the unloading curve fitted by a power law function is provided with 1cut and ucut arguments. The default values 0.4 and 0.98 corresponds to the range 40 - 98%  $F_max$  (maximum force) as recommended in ISO 14577 standard.

The CM has to be a 2n covariance matrix (where n is length of data) of following structure: first n elements of the diagonal correspond to the variance of depth and other to the variance of load. If argument CM is missing, the input covariance matrix is set to a diagonal matrix with variance of depth and load (calculated from uh and uF) on the diagonal. If standard deviations are missing too, the default values (uh=0.5, uF=0.001) are used.

The estimations and confidence intervals are computed under normality assumption (see OEFPIL 'Details').

#### Value

Returns an object of class "OEFPIL". It is a list containing at least the following components

name\_Est estimations of model parameters.

name\_upgraded.start.val

modified starting values of estimating parameters (result from nlsLM function).

cov.m\_Est estimated covariance matrix of parameters.

it\_num number of iterations.

CI\_parameters a list of confidence intervals for estimated parameters (a significance level is

based on signif.level argument).

logs warnings or messages of events, which happen during the run of the algorithm.

.. for other components specification see OEFPIL.

contents a list of outputs as original values of data and other characteristics, which are

usable in plotting or other operations with model results.

If useNLS argument is set to FALSE, the name\_upgraded.start.val are the same as start.values (no nlsLM procedure for starting value fitting is performed).

#### References

ISO/IEC: 14577-1:2015 Metallic materials – Instrumented indentation test for hardness and materials parameters – Part 1: Test method (ISO/IEC, Internation Organisation for Standardisation, 2015).

Anna Charvátová Campbell, Petr Grolich, Radek Šlesinger. *Niget: Nanoindentation general evaluation tool.* SoftwareX (2019), **Vol. 9**: 248–254. https://doi.org/10.1016/j.softx.2019.03.

Köning, R., Wimmer, G. and Witkovský, V. *Ellipse fitting by nonlinear constraints to demodulate quadrature homodyne interferometer signals and to determine the statistical uncertainty of the interferometric phase*. Measurement Science and Technology (2014).

# See Also

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### **Examples**

```
##Use of NanoIndent function for data file "silicaBerk.RData" (a part of the OEFPIL package)
signif.level = 0.05
output.form.NI <- NanoIndent.OEFPIL(silicaBerk, unload.data = TRUE, ucut = 0.98, lcut = 0.2,
uh = 0.5, uF = 0.001, signif.level = signif.level)
##The output is an object of class 'OEFPIL', supplementary functions for this class are available
##Use of summary function
summary(output.form.NI)
##Plot of estimated unloading curve
plot(output.form.NI, signif.level = signif.level)
```

**OEFPIL** 

Optimal Estimation of Parameters by Iterated Linearization

# **Description**

Function for computing optimal estimate of parameters of a nonlinear function by iterated linearization (using Taylor expansion). The model considers measurements errors in both (dependent and independent) variables.

# Usage

```
OEFPIL(data, form, start.val, CM, max.iter = 100, see.iter.val = FALSE,
       save.file.name, th, signif.level, useNLS = TRUE)
```

# **Arguments**

data	a data file can be any object of type data. frame with 2 named columns or list with 2 elements.
form	an object of class formula (or one that can be coerced to that class): a symbolic description of the model to be fitted. The details of model specification are given under 'Details'.
start.val	a named list of starting values of estimating parameters.
CM	a covariance matrix of data (See 'Details' for the information about required structure.).
max.iter	maximum number of iterations.
see.iter.val	logical. If TRUE, all the partial results of the algorithm are displayed and saved. The default value is FALSE.
save.file.name	a name of the file for saving results. If missing, no output file is saved.
th	a numerical value, indicating threshold necessary for the iteration stoppage. The default value is .Machine\$double.eps ^ (2 / 3).
signif.level	a significance level for the confidence interval. If missing, the default value $0.05$ is used.
useNLS	logical. If TRUE (the default value), function will set up starting parameters

calculated by nlsLM function (nonlinear least square estimation).

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#### **Details**

Models for OEPFIL function are specified symbolically. A typical model has the form  $y \sim f(x, a_1, \dots, a_n)$ , where

- y is the (numerical) response vector,
- x is the predictor,
- terms a\_1, ..., a\_n are parameters of specified model.

Function f is known nonlinear function with continuous second partial derivatives with respect to x and parameters  $a_1, \dots a_n$  (for more details see  $Kub\acute{a}\check{c}ek$ ).

All calculations are performed assuming normality of a response vector and measurements errors.

In the data entry of type data. frame, both columns must be named as variables in formula. The same holds for elements of list.

A choice of start.val is important for the convergence of the algorithm. If the OEFPIL algorithm does not converge, starting values modified by nlsLM function (useNLS = TRUE) are recommended (see Example 3).

The CM has to be a 2n covariance matrix (where n is length of data) of following structure: first n elements of the diagonal correspond to the variance of independent variable (x) and other to the variance of dependent variable (y). If argument CM is missing, the input covariance matrix is set to a diagonal variance matrix with sample variance on the main diagonal.

#### Value

Returns an object of class "OEFPIL". It is a list containing the following components

name\_Est estimations of model parameters.

name\_upgraded.start.val

modified starting values of estimating parameters (result from nlsLM function).

cov.m\_Est estimated covariance matrix of parameters.

cov.m\_nlsLM a covariance matrix of starting values of parameters from nlsLM function (if

useNLS was set to TRUE).

it\_num number of iterations.

name\_previous.step

the parameter values from the previous iterative step.

CI\_parameters a list of confidence intervals for estimated parameters (a significance level is

based on signif.level argument).

logs warnings or messages of events, which happen during the run of the algorithm.

contents a list of outputs as original values of data and other characteristics, which are

usable in plotting or other operations with model results.

If useNLS argument is set to FALSE, the name\_upgraded.start.val are the same as start.values (no nlsLM procedure for starting value fitting is performed).

### Note

The symbol pi is reserved for the Ludolf's constant. So naming one of the model's parameters by this symbol results in constant entry of the model.

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#### References

Kubáček, L. and Kubáčková, L. Statistika a metrologie (2000). Univerzita Palackého v Olomouci.

Köning, R., Wimmer, G. and Witkovský, V. *Ellipse fitting by nonlinear constraints to demodulate quadrature homodyne interferometer signals and to determine the statistical uncertainty of the interferometric phase*. Measurement Science and Technology (2014).

#### See Also

NanoIndent.OEFPIL and function nlsLM from minipack.lm package for nonlinear least square algorithms.

```
##Example 1 - Use of OEFPIL function for steam data from MASS library
library(MASS)
steamdata <- steam
colnames(steamdata) \leftarrow c("x","y")
k <- nrow(steamdata)</pre>
CM <- diag(rep(5,2*k))</pre>
st1 <- OEFPIL(steamdata, y \sim b1 * 10 ^{\wedge} (b2 * x/ (b3 + x)),
list(b1 = 5, b2 = 8, b3 = 200), CM, useNLS = FALSE)
## Displaying results using summary function
summary(st1)
## Plot of estimated function
plot(st1, signif.level = 0.05)
## Example 2 - Use of OEFPIL for nanoindentation data "silica2098.RData"
## (which is part of the OEFPIL package)
## Preparing arguments for OEFPIL function
max.iter = 100
see.iter.val = FALSE
signif.level = 0.05
useNLS = TRUE
## Creating a list with starting values for parameters
start.val <- list(alpha=0.1, m=1.5, hp=0.9)
names(start.val) \leftarrow c("alpha", "m", "hp")
## Imputed formula
form <- Load \sim alpha * (Depth - hp) ^{n} m
k <- length(silica2098[,1])</pre>
CM \leftarrow diag(c(rep(0.5^2,k),rep(0.001^2,k)))
## Use of OEFPIL function with defined arguments
output.form <- OEFPIL(silica2098, form, start.val, CM = CM, max.iter = max.iter,</pre>
 see.iter.val = see.iter.val, signif.level = signif.level, useNLS = useNLS)
## Displaying results with summary (the result is the same as in NanoIndent.OEFPIL function)
summary(output.form)
```

ortresiduals.OEFPIL 11

ortresiduals.OEFPIL Orthogonal residuals from an OEFPIL object

# **Description**

Function for calculating orthogonal residuals of an "OEFPIL" object (i.e. the shortest Euclidean distance between data points and the estimated function from OEFPIL).

# Usage

```
ortresiduals.OEFPIL(object, min.c)
```

# **Arguments**

object an object of class "OEFPIL" (a result of a call to OEFPIL).

min.c a numeric value, for defining minimization interval for the optimize function

(if not defined, default value 0.05 \* range(x) is used). Must be positive.

### Value

Returns an object of type list containing following components

x.ores a numerical vector of x coordinates of points, where the minimal distance is

realized.

o.resid a numerical vector of orthogonal residuals (minimal Euclidean distances be-

tween data points and estimated function).

SSort the orthogonal sum of squares.

#### Note

The value min.c should not be too small. In that case the minimization interval is too narrow and the result can be misleading (see Example 3).

### See Also

**OEFPIL** 

```
##-- Continuing the coef.OEFPIL(.) example:

##Example 1 Use ortresiduals.OEFPIL function on the OEFPIL object, with specified value 'min.c'
ortresiduals.OEFPIL(st1,5)

##Example 2 Use ortresiduals.OEFPIL function without value 'min.c' (defaut.value = 0.05 * range(x))
ortresiduals.OEFPIL(st1)

##Example 3 Choice of too narrow interval. Misleading result!
ortresiduals.OEFPIL(st1,0.5)
```

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paramplot.OEFPIL

Plot parameters of an OEFPIL object

### **Description**

Function for plotting the estimated values of the parameters with error bars (plus minus standard deviation) using ggplot for an object (or list of objects) of class "OEFPIL".

# Usage

```
paramplot.OEFPIL(object)
```

# **Arguments**

object

an object or a list of objects of class "OEFPIL" (a result of a call to OEFPIL).

#### **Details**

The input list has to be without NaN, NA, Inf or -Inf values in the estimated parameters or covariance matrix in the source "OEFPIL" object. In that case the function returns a warning message and no graph is plotted.

#### Value

A ggplot graph of the estimated parameter values with error bars. The result can be edit using other ggplot components as usually.

#### Note

Due to possible large differences in units of estimated parameters, the scale argument for facetting in the ggplot graph is set to "free". It should be taken into account when interpreting the results.

# See Also

```
OEFPIL, curvplot.OEFPIL and plot.OEFPIL.
```

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plot.OEFPIL	Plot the estimate from an OEPFIL object	

# **Description**

Plot of the iterated linearization estimate of a function from an "OEFPIL" object with pointwise confidence and prediction bands.

# Usage

```
## S3 method for class 'OEFPIL'
plot(x, xx, signif.level, interval, new.obs.variance, ...)
```

# **Arguments**

х	an object of class "OEFPIL" (a result of a call to OEFPIL).	
xx	a sequence of x-coordinates of points for computing and plotting confidence bands. If missing, the default sequence $seq(from = min(x), to = max(x), length.out = 301)$ is used.	
signif.level	a numerical value or a vector of significance levels for confidence bands.	
interval	a character vector. It states type of an interval to draw. Following values are possible: "conf" for confidence interval, "pred" for prediction interval or c("conf", "pred") for both. If missing, no intervals are plotted.	
new.obs.variance		
	the variance of a new observation for prediction interval computing.	
• • •	additional arguments (same as in plot function) affecting the plot.	

# Details

If the signif.level argument is missing, even though an interval argument is set to "conf", the default value 0.05 is used. The line type is set to 'dashed' for confidence bands and 'dotted' for prediction bands. The confidence and prediction bands are computed under normality assumption.

### Value

Returns an object of type list containing at least the following components

xx a numerical vector of points where bands are calculated.

yy a numerical vector with values of estimated function in xx.

PointwiseCB a matrix of confidence intervals at points xx.

PredictCB a matrix of prediction intervals at points xx.

# See Also

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### **Examples**

```
library(MASS)
##Use of plot function with default parameters
##(only estimation of the function is plotted, without confidence or prediction bands)
steamdata <- steam
colnames(steamdata) <- c("x","y")</pre>
n <- nrow(steamdata)</pre>
CM1 <- diag(rep(10,2*n))</pre>
st1 <- OEFPIL(steamdata, y \sim b1 * 10^{\circ}(b2 * x/(b3 + x)), list(b1 = 5, b2 = 8, b3 = 200),
             CM1, useNLS = FALSE)
plot(st1)
##Use of plot function for plotting confidence bands
plot(st1, seq(0,113,0.1), signif.level = c(0.01,0.05), interval = "conf",
main = "Graph of estimated function")
##Use of plot function for plotting prediction bands
plot(st1, seq(0,113,0.1), interval = "pred", new.obs.variance = 15)
##Return values of plot function
(a <- plot(st1, signif.level = 0.05, interval = "conf"))</pre>
```

print.OEFPIL

Print function for an object of class 'OEFPIL'

### **Description**

Function prints the information about an object of class "OEFPIL".

# Usage

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

# Arguments

```
x an object of class "OEFPIL" (a result of a call to OEFPIL). . . . other arguments.
```

# **Details**

Function prints the formula and estimated parameters of the model from an OEFPIL object.

# See Also

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#### **Examples**

```
##-- Continuing the coef.OEFPIL(.) example:
##Use of print function
print(st1)
```

silica2098

Nanoindentation measurements data

# **Description**

Load and depth measured with Berkovich diamond tip on fused silica material. Data contains only cutted part of unloading indentation curve from silicaBerk data (20 - 98%, as recommended in ISO 14577 standard). The relationship between Load (F) and Depth (h) is given by equation  $F = \alpha (h - h_p)^m$ , where  $h_p$  is permanent indentation depth after removal of the load,  $\alpha$  is fitting constant related to the indenter geometry and power law exponent m should be from (1,2) interval.

# Usage

silica2098

# **Format**

The data frame contains two columns:

**Depth** nanoindentation depth, in nanometers.

Load load, in milinewtons.

### **Source**

Czech Metrology Institute, Brno, Czech Republic.

### References

ISO/IEC: 14577-1:2015 Metallic materials – Instrumented indentation test for hardness and materials parameters – Part 1: Test method (ISO/IEC, Internation Organisation for Standardisation, 2015).

```
attach(silica2098)
plot(Depth, Load, main = 'Graph of nanoindentation data', xlab = 'Depth (nm)', ylab = 'Load (mN)',
col = 'darkgreen', cex = 1)
```

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silicaBerk

Nanoindentation measurements data

### **Description**

Load and depth measured with Berkovich diamond tip on fused silica material. Data contains only unloading part of indentation curve. The relationship between Load (F) and Depth (h) is given by equation  $F = \alpha (h - h_p)^m$ , where  $h\_p$  is permanent indentation depth after removal of the load,  $\alpha$  is fitting constant related to the indenter geometry and power law exponent m should be from (1,2) interval.

### Usage

silicaBerk

#### **Format**

The data frame contains two columns:

**Depth** nanoindentation depth, in nanometers.

Load load, in milinewtons.

#### **Source**

Czech Metrology Institute, Brno, Czech Republic.

# **Examples**

```
attach(silicaBerk)
plot(Depth, Load, main = 'Graph of nanoindentation data', xlab = 'Depth (nm)', ylab = 'Load (mN)',
col = 'darkgreen', cex = 1)
```

summary.OEFPIL

Summary from an OEFPIL object

### **Description**

Function for fast and clean output of all basic information of an "OEFPIL" object.

# Usage

```
## S3 method for class 'OEFPIL'
summary(object, signif.level = object$contents$signif.level, print = TRUE, ...)
```

# **Arguments**

```
object an object of class "OEFPIL" (a result of a call to OEFPIL).
```

signif.level a significance level for the confidence interval. If missing, a value from the input

OEFPIL object is used.

print print out result summaries in the console (default TRUE).

... other arguments.

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### Value

Returns an object of type list containing following components

param\_Est the (numerical) vector of estimated model parameters.

sd standard deviations for estimated model parameters.

cov.m\_Est the covariance matrix of estimated model parameters.

it\_num number of iterations.

CI\_parameters the matrix of lower and upper bounds for confidence intervals.

### See Also

**OEFPIL** 

# **Examples**

```
##-- Continuing the coef.OEFPIL(.) example:
##Use of summary function with default parameters
summary(st1)
##Use of summary function with different parameters
summary(st1, signif.level = 0.01, print = FALSE)
```

vcov.OEFPIL

Covariance matrix from an OEFPIL object

# Description

Function for extracting the estimated covariance matrix from an object of class "OEFPIL".

# Usage

```
## S3 method for class 'OEFPIL'
vcov(object, ...)
```

# Arguments

```
object an object of class "OEFPIL" (a result of a call to OEFPIL). . . . other arguments.
```

### Value

A matrix of the estimated covariances between the parameter estimates from an "OEFPIL" object.

# See Also

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```
##-- Continuing the coef.OEFPIL(.) example:
##Use of vcov function
vcov(st1)
```

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