Package ‘sensitivity’

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Description A collection of functions for factor screening, global sensitivity analysis and reliability sensitivity analysis. Most of the functions have to be applied on model with scalar output, but several functions support multi-dimensional outputs.
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The sensitivity package implements some global sensitivity analysis methods:

- Linear regression coefficients: SRC and SRRC (`src`), PCC and PRCC (`pcc`);
- Bettonvil’s sequential bifurcations (Bettonvil and Kleijnen, 1996) (`sb`);
- Morris’s “OAT” elementary effects screening method (`morris`);
- Derived-based Global Sensitivity Measures:
  - Poincare constants for Derived-based Global Sensitivity Measures (DGSM) (Roustant et al., 2014) (`poincareconstant`),
  - Distributed Evaluation of Local Sensitivity Analysis (DELSA) (Rakovec et al., 2014) (`delsa`);
- Variance-based sensitivity indices (Sobol’ indices):
  - Monte Carlo estimation of Sobol’ indices (also called pick-freeze method):
    * Sobol’ scheme (Sobol, 1993) to compute the indices given by the variance decomposition up to a specified order (`sobol`),
*Saltelli’s scheme (Saltelli, 2002) to compute first order and total indices with a reduced cost (sobol2002),
*Mauntz-Kucherenko’s scheme (Sobol et al., 2007) to compute first order and total indices using improved formulas for small indices (sobol2007),
*Jansen-Sobol’s scheme (Jansen, 1999) to compute first order and total indices using improved formulas (soboljansen),
*Martinez’s scheme using correlation coefficient-based formulas (Martinez, 2011; touati, 2016) to compute first order and total indices, associated with theoretical confidence intervals (sobolmartinez and soboltouati),
*Janon-Monod’s scheme (Monod et al., 2006; Janon et al., 2013) to compute first order indices with optimal asymptotic variance (soboleff),
*Mara’s scheme (Mara and Joseph, 2008) to compute first order indices with a cost independent of the dimension, via a unique-matrix permutations (sobolmara),
*Owen’s scheme (Owen, 2013) to compute first order and total indices using improved formulas (via 3 input independent matrices) for small indices (sobolowen),
*Total Interaction Indices using Liu-Owen’s scheme (Liu and Owen, 2006) (sobolTIIlol) and pick-freeze scheme (Fruth et al., 2014) (sobolTIIpf),
– Estimation of the Sobol’ first order and closed second order indices using replicated orthogonal array-based Latin hypecube sample (Tissot and Prieur, 2012) (sobolroalhs),
– Estimation of the Sobol’ first order and total indices with Saltelli’s so-called “extended-FAST” method (Saltelli et al., 1999) (fast99),
– Estimation of the Sobol’ first order and total indices with kriging-based global sensitivity analysis (Le Gratiet et al., 2014) (sobolGP);
Support index functions (support) of Fruth et al. (2015); Sensitivity Indices based on Csiszar f-divergence (sensifdiv) (particular cases: Borgonovo’s indices and mutual-information based indices) and Hilbert-Schmidt Independence Criterion (sensihsic) of Da Veiga et al. (2014); Reliability sensitivity analysis by the Perturbed-Law based Indices (PLI) of Lemaitre et al. (2015); Sobol’ indices for multidimensional outputs (sobolMultOut): Aggregated Sobol’ indices (Lamboni et al., 2011; Gamboa et al., 2014) and functional (1D) Sobol’ indices.
Moreover, some utilities are provided: standard test-cases (testmodels) and template file generation (template.replace).

**Model managing**

The *sensitivity* package has been designed to work either models written in R than external models such as heavy computational codes. This is achieved with the input argument model present in all functions of this package.

The argument model is expected to be either a function or a predictor (i.e. an object with a predict function such as lm).

- If model = m where m is a function, it will be invoked once by y <- m(x).
- If model = m where m is a predictor, it will be invoked once by y <- predict(m, x).

X is the design of experiments, i.e. a data.frame with p columns (the input factors) and n lines (each, an experiment), and y is the vector of length n of the model responses.

The model in invoked once for the whole design of experiment.
The argument `model` can be left to `NULL`. This is refered to as the decoupled approach and used with external computational codes that rarely run on the statistician’s computer. See `decoupling`.

**Author(s)**

Gilles Pujol, Bertrand Iooss, Alexandre Janon with contributions from Paul Lemaitre for the `PLI` function, Laurent Gilquin for the `sobolroalhs` function, Loic le Gratiet for the `sobolGP` function, Khalid Boumhaout, Taieb Touati and Bernardo Ramos for the `sobolowen` and `soboltouati` functions, Jana Fruth for the `PoincareConstant` and `support` functions, `sobolTIIlo` and `sobolTIIpf` functions, Sebastien Da veiga for the `sensifdiv` and `sensiHSIC` functions, Joseph Guillaume for the `delsa` and `parameterSets` functions, Frank Weber.

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**References**


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**Description**

tell and ask are S3 generic methods for decoupling simulations and sensitivity measures estimations. In general, they are not used by the end-user for a simple `R` model, but rather for an external computational code. Most of the sensitivity analyses objects of this package overload `tell`, whereas `ask` is overloaded for iterative methods only.

**Usage**

tell(x, y = NULL, ...)
ask(x, ...)
Arguments

- **x**: a typed list storing the state of the sensitivity study (parameters, data, estimates), as returned by sensitivity analyses objects constructors, such as `src`, `morris`, etc.
- **y**: a vector of model responses.
- **...**: additional arguments, depending on the method used.

Details

When a sensitivity analysis method is called with no model (i.e. argument `model = NULL`), it generates an incomplete object `x` that stores the design of experiments (field `x`), allowing the user to launch "by hand" the corresponding simulations. The method `tell` allows to pass these simulation results to the incomplete object `x`, thereafter estimating the sensitivity measures.

When the method is iterative, the data to simulate are not stored in the sensitivity analysis object `x`, but generated at each iteration with the `ask` method; see for example `sb`.

Value

- **`tell`** doesn’t return anything. It computes the sensitivity measures, and stores them in the list `x`.
- **Side effect**: `tell` modifies its argument `x`.

- **`ask`** returns the set of data to simulate.

Author(s)

Gilles Pujol

Examples

```r
# Example of use of fast99 with "model = NULL"
x <- fast99(model = NULL, factors = 3, n = 1000,
            q = "qunif", q.arg = list(min = -pi, max = pi))
y <- ishigami.fun(x$X)
tell(x, y)
print(x)
plot(x)
```

Description

`delsa` implements Distributed Evaluation of Local Sensitivity Analysis to calculate first order parameter sensitivity at multiple locations in parameter space. The locations in parameter space can either be obtained by a call to `parametersets` or by specifying `x0` directly, in which case the prior variance of each parameter `varprior` also needs to be specified. Via `plot` (which uses functions of the package `ggplot2` and `reshape2`), the indices can be visualized.
Usage

delsa(model = NULL, perturb=1.01,
   par.ranges, samples, method,
   X0, varprior,
   ...)

## S3 method for class 'delsa'
tell(x, y = NULL,...)

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

## S3 method for class 'delsa'
plot(x, which=1:3, ask = dev.interactive(), ...)

Arguments

model  a function, or a model with a predict method, defining the model to analyze.
perturb  Perturbation used to calculate sensitivity at each evaluation location
par.ranges  A named list of minimum and maximum parameter values
samples  Number of samples to generate. For the "grid" and "innergrid" method, corresponds to the number of samples for each parameter, and may be a vector.
method  Sampling scheme. See parameterSets
X0  Parameter values at which to evaluate sensitivity indices. Can be used instead of specifying sampling method
varprior  Prior variance. If X0 is specified, varprior must also be specified.
...  any other arguments for model which are passed unchanged each time it is called.
x  a list of class "delsa" storing the state of the sensitivity study (parameters, data, estimates).
y  a vector of model responses.
which  if a subset of the plots is required, specify a subset of the numbers 1:3
ask  logical; if TRUE, the user is asked before each plot, see par(ask=.)

Details

print shows summary of the first order indices across parameter space.

plot shows: (1) the cumulative distribution function of first order sensitivity across parameter space, (2) variation of first order sensitivity in relation to model response, and (3) sensitivity in relation to parameter value.
**delsa**

**Value**

delsa returns a list of class "delsa", containing all the input arguments detailed before, plus the following components:

- **call**
  the matched call.

- **x**
  a data.frame containing the design of experiments.

- **y**
  a vector of model responses.

- **delsafirst**
  the first order indices for each location in \( x \)

**Author(s)**

Conversion for sensitivity package by Joseph Guillaume, based on original R code by Oldrich Rakovec

**References**


**See Also**

- parameterSets which is used to generate points, sensitivity for other methods in the package

**Examples**

```r
# Test case: the non-monotonic Sobol g-function
# (there are 8 factors, all following the uniform distribution on [0,1])

## Not run:
library(randtoolbox)
x <- delsa(model=sobol.fun,
    par.ranges=replicate(8,c(0,1),simplify=FALSE),
    samples=100,method="sobol")

# Summary of sensitivity indices of each parameter across parameter space
print(x)

library(ggplot2)
library(reshape2)
x11()
plot(x)

## End(Not run)
```
Description

fast99 implements the so-called "extended-FAST" method (Saltelli et al. 1999). This method allows the estimation of first order and total Sobol' indices for all the factors (alltogether $2^p$ indices, where $p$ is the number of factors) at a total cost of $n \times p$ simulations.

Usage

```r
fast99(model = NULL, factors, n, M = 4, omega = NULL,
       q = NULL, q.arg = NULL, ...)
## S3 method for class 'fast99'
tell(x, y = NULL, ...)  
## S3 method for class 'fast99'
print(x, ...) 
## S3 method for class 'fast99'
plot(x, ylim = c(0, 1), ...)
```

Arguments

- **model** a function, or a model with a `predict` method, defining the model to analyze.
- **factors** an integer giving the number of factors, or a vector of character strings giving their names.
- **n** an integer giving the sample size, i.e. the length of the discretization of the s-space (see Cukier et al.).
- **M** an integer specifying the interference parameter, i.e. the number of harmonics to sum in the Fourier series decomposition (see Cukier et al.).
- **omega** a vector giving the set of frequencies, one frequency for each factor (see details below).
- **q** a vector of quantile functions names corresponding to wanted factors distributions (see details below).
- **q.arg** a list of quantile functions parameters (see details below).
- **x** a list of class "fast99" storing the state of the sensitivity study (parameters, data, estimates).
- **y** a vector of model responses.
- **ylim** y-coordinate plotting limits.
- **...** any other arguments for model which are passed unchanged each time it is called.
Details

If not given, the set of frequencies $\omega$ is taken from Saltelli et al. The first frequency of the vector $\omega$ is assigned to each factor $X_i$ in turn (corresponding to the estimation of Sobol’ indices $S_i$ and $S_{T_i}$), other frequencies being assigned to the remaining factors.

If the arguments q and q.args are not given, the factors are taken uniformly distributed on $[0, 1]$. The argument q must be list of character strings, giving the names of the quantile functions (one for each factor), such as qunif, qnorm... It can also be a single character string, meaning same distribution for all. The argument q.arg must be a list of lists, each one being additional parameters for the corresponding quantile function. For example, the parameters of the quantile function qunif could be list(min=1, max=2), giving an uniform distribution on $[1, 2]$. If q is a single character string, then q.arg must be a single list (rather than a list of one list).

Value

fast99 returns a list of class "fast99", containing all the input arguments detailed before, plus the following components:

- call: the matched call.
- x: a data.frame containing the factors sample values.
- y: a vector of model responses.
- v: the estimation of variance.
- D1: the estimations of Variances of the Conditional Expectations (VCE) with respect to each factor.
- Dt: the estimations of VCE with respect to each factor complementary set of factors ("all but $X_i$").

Author(s)

Gilles Pujol

References


Examples

# Test case: the non-monotonic Ishigami function
x <- fast99(model = ishigami.fun, factors = 3, n = 1000,
        q = "qunif", q.arg = list(min = -pi, max = pi))
print(x)
plot(x)
**morris**

*Morris's Elementary Effects Screening Method*

**Description**

*morris* implements the Morris's elementary effects screening method (Morris 1991). This method, based on design of experiments, allows to identify the few important factors at a cost of \( r \times (p + 1) \) simulations (where \( p \) is the number of factors). This implementation includes some improvements of the original method: space-filling optimization of the design (Campolongo et al. 2007) and simplex-based design (Pujol 2009).

**Usage**

```
morris(model = NULL, factors, r, design, binf = 0, bsup = 1, scale = TRUE, ...)
## S3 method for class 'morris'
tell(x, y = NULL, ...)
## S3 method for class 'morris'
print(x, ...)
## S3 method for class 'morris'
plot(x, identify = FALSE, atpen = FALSE, y_col = NULL, y_dim3 = NULL)
```  

**Arguments**

- **model**: a function, or a model with a `predict` method, defining the model to analyze.
- **factors**: an integer giving the number of factors, or a vector of character strings giving their names.
- **r**: either an integer giving the number of repetitions of the design, i.e. the number of elementary effect computed per factor, or a vector of two integers \( c(r1, r2) \) for the space-filling improvement (Campolongo et al.). In this case, \( r1 \) is the wanted design size, and \( r2 (> r1) \) is the size of the (bigger) population in which is extracted the design (this can throw a warning, see below).
- **design**: a list specifying the design type and its parameters:
  - **type**: = "oat" for Morris's OAT design (Morris 1991), with the parameters:
    - **levels**: either an integer specifying the number of levels of the design, or a vector of integers for different values for each factor.
    - **grid.jump**: either an integer specifying the number of levels that are increased/decreased for computing the elementary effects, or a vector of integers for different values for each factor. If not given, it is set to `grid.jump = 1`. Notice that this default value of one does not follow Morris's recommendation of `levels/2`.  

- type = "simplex" for simplex-based design (Pujol 2009), with the parameter:
  - scale.factor: a numeric value, the homothety factor of the (isometric) simplexes. Edges equal one with a scale factor of one.

binf either an integer, specifying the minimum value for the factors, or a vector for different values for each factor.

bsup either an integer, specifying the maximum value for the factors, or a vector for different values for each factor.

scale logical. If TRUE, the input design of experiments is scaled after building the design and before computing the elementary effects so that all factors vary within the range [0,1]. For each factor, the scaling is done relatively to its corresponding bsup and binf.

x a list of class "morris" storing the state of the screening study (parameters, data, estimates).

y a vector of model responses.

identify logical. If TRUE, the user selects with the mouse the factors to label on the \((\mu^*, \sigma)\) graph (see identify).

atpen logical. If TRUE (and identify = TRUE), the user-identified labels (more precisely: their lower-left corners) of the factors are plotted at the place where the user had clicked (if near enough to one of the factor points). If FALSE (and identify = TRUE), the labels are automatically adjusted to the lower, left, upper or right side of the factor point. For further information, see identify. Defaults to FALSE.

y_col an integer defining the index of the column of x$y to be used for plotting the corresponding Morris statistics \(\mu^*\) and \(\sigma\) (only applies if x$y is a matrix or an array). If set to null (as per default) and x$y is a matrix or an array, the first column (respectively the first element in the second dimension) of x$y is used (i.e. y_col = 1).

y_dim3 an integer defining the index in the third dimension of x$y to be used for plotting the corresponding Morris statistics \(\mu^*\) and \(\sigma\) (only applies if x$y is a three-dimensional array). If set to null (as per default) and x$y is a three-dimensional array, the first element in the third dimension of x$y is used (i.e. y_dim3 = 1).

alpha a vector of three values between 0.0 (fully transparent) and 1.0 (opaque) (see rgl.material). The first value is for the cone, the second for the planes.

sphere.size a numeric value, the scale factor for displaying the spheres.

... for morris: any other arguments for model which are passed unchanged each time it is called. For plot.morris: arguments to be passed to plot.default.

**Details**

plot.morris draws the \((\mu^*, \sigma)\) graph.

plot3d.morris draws the \((\mu, \mu^*, \sigma)\) graph (requires the rgl package). On this graph, the points are in a domain bounded by a cone and two planes (application of the Cauchy-Schwarz inequality).

This version of morris also supports matrices and three-dimensional arrays as output of model.
Value

`morris` returns a list of class "morris", containing all the input argument detailed before, plus the following components:

- **call**: the matched call.
- **X**: a data.frame containing the design of experiments.
- **y**: either a vector, a matrix or a three-dimensional array of model responses (depends on the output of `model`).
- **ee**: if `y` is a vector: a \((r \times p)\) - matrix of elementary effects for all the factors.
  - if `y` is a matrix: a \((r \times p \times ncol(y))\) - array of elementary effects for all the factors and all columns of `y`.
  - if `y` is a three-dimensional array: a \((r \times p \times dim(y)[2] \times dim(y)[3])\) - array of elementary effects for all the factors and all elements of the second and third dimension of `y`.

Notice that the statistics of interest \((\mu, \mu^*\) and \(\sigma)\) are not stored. They can be printed by the `print` method, but to extract numerical values, one has to compute them with the following instructions:

If `x$y` is a vector:

```r
mu <- apply(x$ee, 2, mean)
mu.star <- apply(abs(x$ee), 2, function(x) mean(abs(x)))
sigma <- apply(x$ee, 2, sd)
```

If `x$y` is a matrix:

```r
mu <- apply(x$ee, 3, function(M){
  apply(M, 2, mean)
})
mu.star <- apply(abs(x$ee), 3, function(M){
  apply(M, 2, mean)
})
sigma <- apply(x$ee, 3, function(M){
  apply(M, 2, sd)
})
```

If `x$y` is a three-dimensional array:

```r
mu <- sapply(1:dim(x$ee)[4], function(i){
  apply(x$ee[, , i, drop = FALSE], 3, function(M){
    apply(M, 2, mean)
  })
}, simplify = "array")
mu.star <- sapply(1:dim(x$ee)[4], function(i){
  apply(abs(x$ee)[, , i, drop = FALSE], 3, function(M){
    apply(M, 2, mean)
  })
}, simplify = "array")
```
sigma <- sapply(1:dim(x$ee)[4], function(i){
  apply(x$ee[, , , i, drop = FALSE], 3, function(M){
    apply(M, 2, sd)
  })
}, simplify = "array")

It is highly recommended to use the function with the argument `scale = TRUE` to avoid an uncorrect interpretation of factors that would have different orders of magnitude.

**Warning messages**

"keeping r' repetitions out of r" when generating the design of experiments, identical repetitions are removed, leading to a lower number than requested.

**Author(s)**

Gilles Pujol, with contributions from Frank Weber (2016)

**References**


**Examples**

```r
# Test case: the non-monotonic function of Morris
x <- morris(model = morris.fun, factors = 20, r = 4,
             design = list(type = "oat", levels = 5, grid.jump = 3))
print(x)
plot(x)
## Not run: library(rgl)
plot3d.morris(x)  # (requires the package 'rgl')
## End(Not run)

# Only for demonstration purposes: a model function returning a matrix
morris.fun_matrix <- function(X){
  res_vector <- morris.fun(X)
  cbind(res_vector, 2 * res_vector)
}
x <- morris(model = morris.fun_matrix, factors = 20, r = 4,
            design = list(type = "oat", levels = 5, grid.jump = 3))
plot(x, y_col = 2)
title(main = "y_col = 2")
```

# Also only for demonstration purposes: a model function returning a
# three-dimensional array
morris.fun_array <- function(X){
  res_vector <- morris.fun(X)
  res_matrix <- cbind(res_vector, 2 * res_vector)
  array(data = c(res_matrix, 5 * res_matrix),
        dim = c(length(res_vector), 2, 2))
}
x <- morris(model = morris.fun_array, factors = 20, r = 4,
            design = list(type = "simplex", scale.factor = 1))
plot(x, y_col = 2, y_dim3 = 2)
title(main = "y_col = 2, y_dim3 = 2")

---

**ParameterSets**

**Generate parameter sets**

**Description**

Generate parameter sets from given ranges, with chosen sampling scheme

**Usage**

```r
parameterSets(par.ranges, samples, method = c("sobol", "innergrid", "grid"))
```

**Arguments**

- **par.ranges**: A named list of minimum and maximum parameter values
- **samples**: Number of samples to generate. For the "grid" and "innergrid" method, may be a vector of number of samples for each parameter.
- **method**: the sampling scheme; see Details

**Details**

Method "sobol" generates uniformly distributed Sobol low discrepancy numbers, using the sobol function in the randtoolbox package.

Method "grid" generates a grid within the parameter ranges, including its extremes, with number of points determined by samples.

Method "innergrid" generates a grid within the parameter ranges, with edges of the grid offset from the extremes. The offset is calculated as half of the resolution of the grid `diff(par.ranges)/samples/2`.

**Value**

the result is a matrix, with named columns for each parameter in `par.ranges`. Each row represents one parameter set.

**Author(s)**

Joseph Guillaume, based on similar function by Felix Andrews
See Also
delsa, which uses this function

Examples

```r
X.grid <- parameterSets(par.ranges=list(V1=c(1,1000),V2=c(1,4)),
               samples=c(10,10),method="grid")
plot(X.grid)

X.innergrid<-parameterSets(par.ranges=list(V1=c(1,1000),V2=c(1,4)),
               samples=c(10,10),method="innergrid")
points(X.innergrid,col="red")

## Not run:
library(randtoolbox)
X.sobol<-parameterSets(par.ranges=list(V1=c(1,1000),V2=c(1,4)),
               samples=100,method="sobol")
plot(X.sobol)

## End(Not run)
```

---

### pcc

**Partial Correlation Coefficients**

**Description**

pcc computes the Partial Correlation Coefficients (PCC), or Partial Rank Correlation Coefficients (PRCC), which are sensitivity indices based on linear (resp. monotonic) assumptions, in the case of (linearly) correlated factors.

**Usage**

```r
pcc(X, y, rank = FALSE, nboot = 0, conf = 0.95)
## S3 method for class 'pcc'
print(x, ...)  
## S3 method for class 'pcc'
plot(x, ylim = c(-1,1), ...)
```

**Arguments**

- **X**: a data frame (or object coercible by `as.data.frame`) containing the design of experiments (model input variables).
- **y**: a vector containing the responses corresponding to the design of experiments (model output variables).
- **rank**: logical. If TRUE, the analysis is done on the ranks.
- **nboot**: the number of bootstrap replicates.
conf the confidence level of the bootstrap confidence intervals.
x the object returned by pcc.
ylim the y-coordinate limits of the plot.
... arguments to be passed to methods, such as graphical parameters (see par).

Value

pcc returns a list of class "pcc", containing the following components:
call the matched call.
PCC a data frame containing the estimations of the PCC indices, bias and confidence intervals (if rank = TRUE).
PRCC a data frame containing the estimations of the PRCC indices, bias and confidence intervals (if rank = TRUE).

Author(s)

Gilles Pujol

References


See Also

src

Examples

# a 100-sample with X1 ~ U(0.5, 1.5)
#    X2 ~ U(1.5, 4.5)
#    X3 ~ U(4.5, 13.5)
library(boot)
n <- 100
X <- data.frame(X1 = runif(n, 0.5, 1.5),
                 X2 = runif(n, 1.5, 4.5),
                 X3 = runif(n, 4.5, 13.5))

# linear model : Y = X1 + X2 + X3
y <- with(X, X1 + X2 + X3)

# sensitivity analysis
x <- pcc(X, y, nboot = 100)
print(x)
#plot(x) # TODO: find another example...
Description

PLI computes the Perturbed-Law based Indices (PLI), also known as the Density Modification Based Reliability Sensitivity Indices (DMBRSI), which are sensitivity indices related to a probability of exceedence of a model output (i.e. a failure probability), estimated by a Monte Carlo method. See Lemaitre et al. (2015).

Usage

PLI(failurepoints, failureprobabilityhat, samplesize, deltasvector, InputDistributions, type="MOY", samedelta=TRUE)

Arguments

- **failurepoints**: a matrix of failure points coordinates, one column per variable.
- **failureprobabilityhat**: the estimation of failure probability \( P \) through rough Monte Carlo method.
- **samplesize**: the size of the sample used to estimate \( P \). One must have \( P_{\text{chap}} = \text{dim(failurepoints)[1]} / \text{samplesize} \).
- **deltasvector**: a vector containing the values of delta for which the indices will be computed.
- **InputDistributions**: a list of list. Each list contains, as a list, the name of the distribution to be used and the parameters. Implemented cases so far:
  - For a mean perturbation: Gaussian, Uniform, Triangle, Left Truncated Gaussian, Left Truncated Gumbel. Using Gumbel requires the package evd.
  - For a variance perturbation: Gaussian, Uniform.
- **type**: a character string in which the user will specify the type of perturbation wanted. The sense of "deltasvector" varies according to the type of perturbation:
  - type can take the value "MOY", in which case deltasvector is a vector of perturbated means.
  - type can take the value "VAR", in which case deltasvector is a vector of perturbated variances, therefore needs to be positive integers.
- **samedelta**: a boolean used with the value "MOY" for type.
  - If it is set at TRUE, the mean perturbation will be the same for all the variables.
  - If not, the mean perturbation will be new_mean = mean + sigma*delta where mean, sigma are parameters defined in InputDistributions and delta is a value of deltasvector.
Value

PLI returns a list of size 2, including:

• A matrix where the PLI are stored. Each column corresponds to an input, each line corresponds to a twist of amplitude delta.
• A matrix where their standard deviation are stored.

Author(s)

Paul Lemaitre

References


Examples

## Not run:

```r
# Model: Ishigami function with a threshold at -7
# Failure points are those < -7

distributionIshigami = list()
for (i in 1:3){
distributionIshigami[[i]] = list("unif",c(-pi,pi))
distributionIshigami[[i]]$r = "runif"
}

# Monte Carlo sampling to obtain failure points

N = 10^5
X = matrix(rbind(0,ncol=3,nrow=N)
for (i in 1:3){
X[,i] = runif(N,-pi,pi)
}

T = ishigami.fun(X)
s = sum(as.numeric(T < -7)) # Number of failure
pdefchap = s/N # Failure probability
ptsdef = X[T < -7,] # Failure points

# sensitivity indices with perturbation of the mean

v_delta = seq(-3,3,1/20)
toto = PLI(failurepoints=ptsdef,failureprobabilityhat=pdefchap,samplesize=N,
deltasvector=v_delta,inputdistributions=distributionIshigami,type="MOY",
samedelta=TRUE)
```
BIshm = Toto[[1]]
SIshm = Toto[[2]]

par(mar=c(4,5,1,1,1))
plot(v_delta,BIshm[[2]],ylim=c(-4,4),xlab=expression(delta),
ylab=expression(hat(S[i+delta])),pch=19,cex=1.5)
points(v_delta,BIshm[[1]],col="darkgreen",pch=15,cex=1.5)
points(v_delta,BIshm[[3]],col="red",pch=17,cex=1.5)
lines(v_delta,BIshm[[2]]+1.96*SIshm[[2]],col="black")
lines(v_delta,BIshm[[2]]-1.96*SIshm[[2]],col="black")
lines(v_delta,BIshm[[1]]+1.96*SIshm[[1]],col="darkgreen")
lines(v_delta,BIshm[[1]]-1.96*SIshm[[1]],col="darkgreen")
lines(v_delta,BIshm[[3]]+1.96*SIshm[[3]],col="red")
lines(v_delta,BIshm[[3]]-1.96*SIshm[[3]],col="red")
abline(h=0,lty=2)
legend(0.3,legend=c("X1","X2","X3"),
col=c("darkgreen","black","red"),pch=c(15,19,17),cex=1.5)

# sensitivity indices with perturbation of the variance

v_delta = seq(1,5,1/4) # user parameter. (the true variance is 3.29)
Toto = PLI(failurepoints=ptsdef,failureprobability=hat=pdefs,laplace,samplesize=N,
deltasvector=v_delta,InputDistributions=distributionIshigami,type="VAR",
  samedelta=TRUE)
BIshv=Toto[[1]]
SIshv=Toto[[2]]

par(mfrow=c(2,1),mar=c(1,5,1,1)+0.1)
plot(v_delta,BIshv[[2]],ylim=c(-5.5,5.5),xlab=expression(V_f),
ylab=expression(hat(S[i+delta])),pch=19,cex=1.5)
points(v_delta,BIshv[[1]],col="darkgreen",pch=15,cex=1.5)
points(v_delta,BIshv[[3]],col="red",pch=17,cex=1.5)
lines(v_delta,BIshv[[2]]+1.96*SIshv[[2]],col="black")
lines(v_delta,BIshv[[2]]-1.96*SIshv[[2]],col="black")
lines(v_delta,BIshv[[1]]+1.96*SIshv[[1]],col="darkgreen")
lines(v_delta,BIshv[[1]]-1.96*SIshv[[1]],col="darkgreen")
lines(v_delta,BIshv[[3]]+1.96*SIshv[[3]],col="red")
lines(v_delta,BIshv[[3]]-1.96*SIshv[[3]],col="red")

par(mar=c(4,5,1,1,1.1,1.1))
plot(v_delta,BIshv[[2]],ylim=c(-30,7),xlab=expression(V(f)),
ylab=expression(hat(S[i+delta])),pch=19,cex=1.5)
points(v_delta,BIshv[[1]],col="darkgreen",pch=15,cex=1.5)
points(v_delta,BIshv[[3]],col="red",pch=17,cex=1.5)
lines(v_delta,BIshv[[2]]+1.96*SIshv[[2]],col="black")
lines(v_delta,BIshv[[2]]-1.96*SIshv[[2]],col="black")
lines(v_delta,BIshv[[1]]+1.96*SIshv[[1]],col="darkgreen")
lines(v_delta,BIshv[[1]]-1.96*SIshv[[1]],col="darkgreen")
lines(v_delta,BIshv[[3]]+1.96*SIshv[[3]],col="red")
lines(v_delta,BIshv[[3]]-1.96*SIshv[[3]],col="red")
legend(2.5,-10,legend=c("X1","X2","X3"),col=c("darkgreen","black","red"),
pch=c(15,19,17),cex=1.5)
### Description

A DGSM is the product between a Poincare Constant (Roustant et al., 2014) and the integral (over the space domain of the input variables) of the squared derivatives of the model output with respect to one input variable. The DGSM is a maximal bound of the total Sobol’ index corresponding to the same input (Lamboni et al., 2013).

This DGSM depends on the type of probability distribution of the input variable. In the particular case of log-concave distribution, analytical formulas are available by the way of the median value (Lamboni et al., 2013). For truncated log-concave distributions, different formulas are available (Roustant et al., 2014). For general non-truncated distributions (including the non log-concave case), the Poincare constant is computed via a relatively simple optimization process (Lamboni et al., 2013).

**IMPORTANT:** This program is useless for the following two input variable distributions:

- uniform on \([\min, \max]\) interval: The optimal Poincare constant is \(\frac{(\max - \min)^2}{\pi^2}\).
- normal with a standard deviation \(sd\): The optimal Poincare constant is \(sd^2\).

### Usage

```
PoincareConstant(densityfct=dnorm, qfct=qnorm, cdfct, 
    truncated=FALSE, min=0, max=1, 
    logconcave=TRUE, optimize.interval=c(-100, 100), ...)
```

### Arguments

- `densityfct`: the probability density function of the input variable
- `qfct`: the quantile function of the input variable
- `cdfct`: the distribution function of the input variable
- `truncated`: logical value: TRUE for a truncated distribution. Default value is FALSE
- `min`: the minimal bound in the case of a truncated distribution
- `max`: the maximal bound in the case of a truncated distribution
- `logconcave`: logical value: TRUE (default value) for a log-concave distribution
- `optimize.interval`: In the non-log concave case, a vector containing the end-points of the interval to be searched for the maximum of the function to be optimized
- `...`: additional arguments
Value

PoincareConstant returns the value of the Poincare constant.

Author(s)

Jana Fruth and Bertrand Iooss

References


Examples

```r
# Exponential law (log-concave)
PoincareConstant(dexp, qexp, rate=1)

# Weibull law (non log-concave)
PoincareConstant(dweibull, cdfct=pweibull, logconcave=FALSE, optimize.interval=c(0, 15), shape=1, scale=1)

## Not run:
# Triangular law (log-concave)
library(triangle)
PoincareConstant(dtriangle, qtriangle, a=49, b=51, c=50)

# Truncated Gumbel law (log-concave)
library(evd)
PoincareConstant(dgumbel, qgumbel, pgumbel, truncated=TRUE, min=500, max=3000, loc=1013.0, scale=558.0)

## End(Not run)
```

sb

Sequential Bifurcations

Description

sb implements the Sequential Bifurcations screening method (Bettonvil and Kleijnen 1996).
Usage

```r
sb(p, sign = rep("+", p), interaction = FALSE)
```

Arguments

- `p`: number of factors.
- `sign`: a vector of length `p` filled with "+" and "-", giving the (assumed) signs of the factors effects.
- `interaction`: a boolean, `TRUE` if the model is supposed to be with interactions, `FALSE` otherwise.
- `x`: a list of class "sb" storing the state of the screening study at the current iteration.
- `y`: a vector of model responses.
- `i`: an integer, used to force a wanted bifurcation instead of that proposed by the algorithm.
- `...`: not used.

Details

The model without interaction is

\[ Y = \beta_0 + \sum_{i=1}^{p} \beta_i X_i \]

while the model with interactions is

\[ Y = \beta_0 + \sum_{i=1}^{p} \beta_i X_i + \sum_{1 \leq i < j \leq p} \gamma_{ij} X_i X_j \]

In both cases, the factors are assumed to be uniformly distributed on \([-1, 1]\). This is a difference with Bettonvil et al. where the factors vary across \([0, 1]\) in the former case, while \([-1, 1]\) in the latter.

Another difference with Bettonvil et al. is that in the current implementation, the groups are split right in the middle.

Value

`sb` returns a list of class "sb", containing all the input arguments detailed before, plus the following components:

- `i`: the vector of bifurcations.
The vector of observations.

$y_m$ the vector of mirror observations (model with interactions only).

The groups effects can be displayed with the print method.

Author(s)
Gilles Pujol

References

Examples

```r
# a model with interactions
p <- 50
beta <- numeric(length = p)
beta[1:5] <- runif(n = 5, min = 10, max = 50)
beta[6:p] <- runif(n = p - 5, min = 0, max = 0.3)
beta <- sample(beta)
gamma <- matrix(data = runif(n = p^2, min = 0, max = 0.1), nrow = p, ncol = p)
gamma[lower.tri(gamma, diag = TRUE)] <- 0
gamma[1,2] <- 5
gamma[5,9] <- 12
f <- function(x) { return(sum(x * beta) + (x * gamma * x))}

# 10 iterations of SB
sa <- sb(p, interaction = TRUE)
for (i in 1:10) {
  x <- ask(sa)
  y <- list()
  for (i in names(x)) {
    y[[i]] <- f(x[[i]])
  }
  tell(sa, y)
}
print(sa)
plot(sa)
```

Description

tensiFdiv conducts a density-based sensitivity analysis where the impact of an input variable is defined in terms of dissimilarity between the original output density function and the output density function when the input variable is fixed. The dissimilarity between density functions is measured with Csiszar f-divergences. Estimation is performed through kernel density estimation and the function kde of the package ks.
Usage

sensiFdiv(model = NULL, X, fdiv = "TV", nboot = 0, conf = 0.95, ...)
## S3 method for class 'sensiFdiv'
tell(x, y = NULL, ...)
## S3 method for class 'sensiFdiv'
print(x, ...)
## S3 method for class 'sensiFdiv'
plot(x, ylim = c(0, 1), ...)

Arguments

- **model**: a function, or a model with a predict method, defining the model to analyze.
- **X**: a matrix or data.frame representing the input random sample.
- **fdiv**: a string or a list of strings specifying the Csiszar f-divergence to be used. Available choices are "TV" (Total-Variation), "KL" (Kullback-Leibler), "Hellinger" and "Chi2" (Neyman chi-squared).
- **nboot**: the number of bootstrap replicates
- **conf**: the confidence level for confidence intervals.
- **x**: a list of class "sensiFdiv" storing the state of the sensitivity study (parameters, data, estimates).
- **y**: a vector of model responses.
- **ylim**: y-coordinate plotting limits.
- **...**: any other arguments for model which are passed unchanged each time it is called.

Details

Some of the Csiszar f-divergences produce sensitivity indices that have already been studied in the context of sensitivity analysis. In particular, "TV" leads to the importance measure proposed by Borgonovo (2007) (up to a constant), "KL" corresponds to the mutual information (Krzykacz-Hausmann 2001) and "Chi2" produces the squared-loss mutual information. See Da Veiga (2014) for details.

Value

sensiFdiv returns a list of class "sensiFdiv", containing all the input arguments detailed before, plus the following components:

- **call**: the matched call.
- **X**: a data.frame containing the design of experiments.
- **y**: a vector of model responses.
- **S**: the estimations of the Csiszar f-divergence sensitivity indices. If several divergences have been selected, S is a list where each element encompasses the estimations of the sensitivity indices for one of the divergence.
sensiHSIC conducts a sensitivity analysis where the impact of an input variable is defined in terms of the distance between the input/output joint probability distribution and the product of their marginals when they are embedded in a Reproducing Kernel Hilbert Space (RKHS). This distance corresponds to the Hilbert-Schmidt Independence Criterion (HSIC) proposed by Gretton et al. (2005) and serves as a dependence measure between random variables, see Da Veiga (2014) for an illustration in the context of sensitivity analysis.
Usage

```r
sensiHSIC(model = NULL, X, kernelX = "rbf", paramX = NA,
           kernelY = "rbf", paramY = NA, nboot = 0, conf = 0.95, ...)
## S3 method for class 'sensiHSIC'
tell(x, y = NULL, ...)
## S3 method for class 'sensiHSIC'
print(x, ...)
## S3 method for class 'sensiHSIC'
plot(x, ylim = c(0, 1), ...)
```

Arguments

- **model**: a function, or a model with a `predict` method, defining the model to analyze.
- **X**: a matrix or `data.frame` representing the input random sample.
- **kernelX**: a string or a list of strings specifying the reproducing kernel to be used for the input variables. If only one kernel is provided, it is used for all input variables. Available choices are "rbf" (Gaussian), "laplace" (exponential), "dcov" (distance covariance, see details), "raquad" (rationale quadratic), "invmultiquad" (inverse multiquadratic), "linear" (Euclidean scalar product), "matern3" (Matern 3/2), "matern5" (Matern 5/2), "ssanova1" (kernel of Sobolev space of order 1) and "ssanova2" (kernel of Sobolev space of order 2).
- **paramX**: a scalar or a vector of hyperparameters to be used in the input variable kernels. If only one scalar is provided, it is replicated for all input variables. By default `paramX` is equal to the standard deviation of the input variable for "rbf", "laplace", "raquad", "invmultiquad", "matern3" and "matern5" and to 1 for "dcov". Kernels "linear", "ssanova1" and "ssanova2" do not involve hyperparameters. If `kernelX` is a combination of kernels with and without hyperparameters, `paramX` must have a (dummy) value for the hyperparameter-free kernels, see examples below.
- **kernelY**: a string specifying the reproducing kernel to be used for the output variable. Available choices are "rbf" (Gaussian), "laplace" (exponential), "dcov" (distance covariance, see details), "raquad" (rationale quadratic), "invmultiquad" (inverse multiquadratic), "linear" (Euclidean scalar product), "matern3" (Matern 3/2), "matern5" (Matern 5/2), "ssanova1" (kernel of Sobolev space of order 1) and "ssanova2" (kernel of Sobolev space of order 2).
- **paramY**: a scalar to be used in the output variable kernel. By default `paramY` is equal to the standard deviation of the output variable for "rbf", "laplace", "raquad", "invmultiquad", "matern3" and "matern5" and to 1 for "dcov". Kernels "linear", "ssanova1" and "ssanova2" do not involve hyperparameters.
- **nboot**: the number of bootstrap replicates
- **conf**: the confidence level for confidence intervals.
- **x**: a list of class "sensiHSIC" storing the state of the sensitivity study (parameters, data, estimates).
- **y**: a vector of model responses.
- **ylim**: y-coordinate plotting limits.
... any other arguments for `model` which are passed unchanged each time it is called.

Details

The HSIC sensitivity indices are obtained as a normalized version of the Hilbert-Schmidt independence criterion:

\[ S^\text{HSIC}_i = \frac{\text{HSIC}(X_i, Y)}{\sqrt{\text{HSIC}(X_i, X_i) \sqrt{\text{HSIC}(Y, Y)}}}, \]

see Da Veiga (2014) for details. When kernelX="dcov" and kernelY="dcov", the kernel is given by \( k(u, u') = \frac{1}{2}(||u|| + ||u'|| - ||u - u'||) \) and the sensitivity index is equal to the distance correlation introduced by Szekely et al. (2007) as was recently proven by Sejdinovic et al. (2013).

Value

`sensiHSIC` returns a list of class "sensiHSIC", containing all the input arguments detailed before, plus the following components:

- `call` the matched call.
- `x` a data.frame containing the design of experiments.
- `y` a vector of model responses.
- `S` the estimations of HSIC sensitivity indices.

Author(s)

Sebastien Da Veiga, Snecma

References

Da Veiga S. (2014), *Global sensitivity analysis with dependence measures*, Journal of Statistical Computation and Simulation, in press. [http://hal.archives-ouvertes.fr/hal-00903283](http://hal.archives-ouvertes.fr/hal-00903283)


See Also

`kde`, `sensiFdiv`
Examples

```r
## Not run:  
# Test case : the non-monotonic Sobol g-function
# Only one kernel is provided with default hyperparameter value
n <- 100
X <- data.frame(matrix(runif(8 * n), nrow = n))
x <- sensiHSIC(model = sobol.fun, X, kernelX = "raquad", kernelY = "rbf")
print(x)

# Test case : the Ishigami function
# A list of kernels is given with default hyperparameter value
n <- 100
X <- data.frame(matrix(-pi+2*pi+runif(3 * n), nrow = n))
x <- sensiHSIC(model = ishigami.fun, X, kernelX = c("rbf","matern3","dcov"),
               kernelY = "rbf")
print(x)

# A combination of kernels is given and a dummy value is passed for
# the first hyperparameter
x <- sensiHSIC(model = ishigami.fun, X, kernelX = c("ssanova1","matern3","dcov"),
               paramX = c(1,2,1), kernelY = "ssanova1")
print(x)

## End(Not run)
```

---

**sobol**  
*Monte Carlo Estimation of Sobol’ Indices*

**Description**

`sobol` implements the Monte Carlo estimation of the Sobol’ sensitivity indices (standard estimator). This method allows the estimation of the indices of the variance decomposition, sometimes referred to as functional ANOVA decomposition, up to a given order, at a total cost of \((N+1) \times n\) where \(N\) is the number of indices to estimate. This function allows also the estimation of the so-called subset (or group) indices, i.e. the first-order indices with respect to single multidimensional inputs.

**Usage**

```r
sobol(model = NULL, X1, X2, order = 1, nboot = 0, conf = 0.95, ...)
```

```
## S3 method for class 'sobol'
tell(x, y = NULL, return.var = NULL, ...)
```

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

```
## S3 method for class 'sobol'
plot(x, ylim = c(0, 1), ...)
```
Arguments

model a function, or a model with a predict method, defining the model to analyze.
X1 the first random sample.
X2 the second random sample.
order either an integer, the maximum order in the ANOVA decomposition (all indices up to this order will be computed), or a list of numeric vectors, the multidimensional compounds of the wanted subset indices.
nboot the number of bootstrap replicates.
conf the confidence level for bootstrap confidence intervals.
x a list of class "sobol" storing the state of the sensitivity study (parameters, data, estimates).
y a vector of model responses.
return.var a vector of character strings giving further internal variables names to store in the output object x.
ylim y-coordinate plotting limits.
... any other arguments for model which are passed unchanged each time it is called.

Value

sobol returns a list of class "sobol", containing all the input arguments detailed before, plus the following components:

call the matched call.
X a data.frame containing the design of experiments.
y a vector of model responses.
V the estimations of Variances of the Conditional Expectations (VCE) with respect to one factor or one group of factors.
D the estimations of the terms of the ANOVA decomposition (not for subset indices).
S the estimations of the Sobol' sensitivity indices (not for subset indices).

Users can ask more output variables with the argument return.var (for example, bootstrap outputs V.boot, D.boot and S.boot).

Author(s)

Gilles Pujol

References

See Also
sobol2002, sobol2007, soboljansen, sobolmartinez, sobolEff, sobolmara, sobolroalhs, fast99, sobolGP,
sobolRPPR

Examples

# Test case: the non-monotonic Sobol g-function

# The method of sobol requires 2 samples
# (there are 8 factors, all following the uniform distribution on [0,1])
library(boot)
n <- 1000
X1 <- data.frame(matrix(runif(8 * n), nrow = n))
X2 <- data.frame(matrix(runif(8 * n), nrow = n))

# sensitivity analysis
x <- sobol(model = sobol.fun, X1 = X1, X2 = X2, order = 2, nboot = 100)
print(x)

sobol2002

Description

sobol2002 implements the Monte Carlo estimation of the Sobol’ indices for both first-order and total indices at the same time (alltogether $2^p$ indices), at a total cost of $(p+2) \times n$ model evaluations. These are called the Saltelli estimators.

Usage

sobol2002(model = NULL, X1, X2, nboot = 0, conf = 0.95, ...)
## S3 method for class 'sobol2002'
tell(x, y = NULL, return.var = NULL, ...)
## S3 method for class 'sobol2002'
print(x, ...)
## S3 method for class 'sobol2002'
plot(x, ylim = c(0, 1), ...)

Arguments

model a function, or a model with a predict method, defining the model to analyze.
X1 the first random sample.
X2 the second random sample.
nboot the number of bootstrap replicates.
conf the confidence level for bootstrap confidence intervals.
x a list of class “sobol” storing the state of the sensitivity study (parameters, data, estimates).
y  a vector of model responses.

return.var  a vector of character strings giving further internal variables names to store in the output object x.

ylim  y-coordinate plotting limits.

...  any other arguments for model which are passed unchanged each time it is called

Details

BE CAREFUL! This estimator suffers from a conditioning problem when estimating the variances behind the indices computations. This can seriously affect the Sobol’ indices estimates in case of largely non-centered output. To avoid this effect, you have to center the model output before applying "sobol2002". Functions "sobolEff", "soboljansen" and "sobolmartinez" do not suffer from this problem.

Value

sobol2002 returns a list of class "sobol2002", containing all the input arguments detailed before, plus the following components:

call  the matched call.

X  a data.frame containing the design of experiments.

y  the response used

V  the estimations of Variances of the Conditional Expectations (VCE) with respect to each factor and also with respect to the complementary set of each factor ("all but X_i").

S  the estimations of the Sobol’ first-order indices.

T  the estimations of the Sobol’ total sensitivity indices.

Users can ask more output variables with the argument return.var (for example, bootstrap outputs V.boot, S.boot and T.boot).

Author(s)

Gilles Pujol

References


See Also

sobol, sobol2007, soboljansen, sobolmartinez, sobolEff, sobolmara, sobolGP, sobolMultOut
Examples

```
# Test case: the non-monotonic Sobol g-function

# The method of sobol requires 2 samples
# There are 8 factors, all following the uniform distribution
# on [0,1]

library(boot)
n <- 1000
X1 <- data.frame(matrix(runif(8 * n), nrow = n))
X2 <- data.frame(matrix(runif(8 * n), nrow = n))

# sensitivity analysis
x <- sobol2002(model = sobol.fun, X1, X2, nboot = 100)
print(x)
plot(x)
```

sobol2007

*Monte Carlo Estimation of Sobol’ Indices (improved formulas of Mauntz: Sobol et al. (2007) and Saltelli et al. (2010))*

Description

sobol2007 implements the Monte Carlo estimation of the Sobol’ indices for both first-order and total indices at the same time (alltogether $2^p$ indices), at a total cost of $(p+2) \times n$ model evaluations. These are called the Mauntz estimators.

Usage

```
sobol2007(model = NULL, X1, X2, nboot = 0, conf = 0.95, ...)
## S3 method for class 'sobol2007'
tell(x, y = NULL, return.var = NULL, ...)
## S3 method for class 'sobol2007'
print(x, ...)
## S3 method for class 'sobol2007'
plot(x, ylim = c(0, 1), ...)
```

Arguments

- **model**: a function, or a model with a predict method, defining the model to analyze.
- **X1**: the first random sample.
- **X2**: the second random sample.
- **nboot**: the number of bootstrap replicates.
- **conf**: the confidence level for bootstrap confidence intervals.
- **x**: a list of class "sobol" storing the state of the sensitivity study (parameters, data, estimates).
y

a vector of model responses.

return.var

a vector of character strings giving further internal variables names to store in the output object x.

ylim

y-coordinate plotting limits.

any other arguments for model which are passed unchanged each time it is called

Details

This estimator is good for small first-order and total indices.

BE CAREFUL! This estimator suffers from a conditioning problem when estimating the variances behind the indices computations. This can seriously affect the Sobol’ indices estimates in case of largely non-centered output. To avoid this effect, you have to center the model output before applying "sobolRPPW". Functions "sobolEff", "soboljansen" and "sobolmartinez" do not suffer from this problem.

Value

sobolRPPW returns a list of class “sobolRPPW”, containing all the input arguments detailed before, plus the following components:

call

the matched call.

X

a data.frame containing the design of experiments.

y

the response used

V

the estimations of Variances of the Conditional Expectations (VCE) with respect to each factor and also with respect to the complementary set of each factor ("all but X_i").

S

the estimations of the Sobol’ first-order indices.

T

the estimations of the Sobol’ total sensitivity indices.

Users can ask more ouput variables with the argument return.var (for example, bootstrap outputs V.boot, S.boot and T.boot).

Author(s)

Bertrand Iooss

References


See Also

sobol, sobol2002, soboljansen, sobolmartinez, sobolEff, sobolmara,sobolMultOut
Examples

# Test case: the non-monotonic Sobol g-function

# The method of sobol requires 2 samples
# There are 8 factors, all following the uniform distribution
# on [0,1]

library(boot)
n <- 1000
X1 <- data.frame(matrix(runif(8 * n), nrow = n))
X2 <- data.frame(matrix(runif(8 * n), nrow = n))

# sensitivity analysis
x <- sobol2007(model = sobol.fun, X1, X2, nboot = 100)
print(x)
plot(x)

sobolCert  
Monte Carlo Estimation of Sobol' Indices using certified meta-models

Description

sobolCert implements the Monte Carlo estimation of the Sobol' sensitivity indices using certified metamodels using the formulas in Janon et al. (2011).

Usage

sobolCert(model = NULL, X1=NULL, X2=NULL, nboot = 300, conf = 0.95, lambda0 = 0, h = 0)
## S3 method for class 'sobolCert'
print(x, ...)

Arguments

model a function defining the model to analyze. This function must return a list whose components are:

- outmetamodel output.
- errmetamodel output error bound, satisfying

\[ |\text{model output} - \text{metamodel output}| \leq err \]

X1 the first random sample. If NULL, sobolEff ignores model, X1 and X2, and reuse model outputs from the previous sobolCert call.

X2 the second random sample.

nboot the number of bootstrap replicates.

conf the confidence level for confidence intervals.
lambda0
  if lambda0=0, use the method described in Janon et al. (2011) Section 3.1; else use the method of Section 3.2 with lambda0 as penalty parameter.

h
  if lambda0=0, this parameter is ignored; else it is used as the h bandwidth parameter.

x
  a sobolCert object

... currently not used

Value

sobolCert returns a list of class "sobolCert", containing the following components:

call
  the matched call.

S
  the estimations of the Sobol’ sensitivity indices.

penalty
  (only if lambda0>0) value of the smoothing penalty.

Author(s)
Alexandre Janon

References


See Also

sobol, sobol2002, sobol2007

Examples

```r
## Not run:
# Test case

n <- 1000
X1 <- data.frame(matrix(runif(3 * n), nrow = n))
X2 <- data.frame(matrix(runif(3 * n), nrow = n))

# sensitivity analysis
x=sobolCert(model=function(X) { list(out=X[1]+2*X[2]+X[3]+.001*X[1]*runif(1),err=.01); },
    X1, X2, conf=.99, lambda0=.1, h=.1, nboot=30)
print(x)

x=sobolCert(model=NULL, X1=NULL, X2=NULL, conf=.95)
print(x)

## End(Not run)
```
sobolEff  Monte Carlo Estimation of Sobol’ Indices (formulas of Janon-Monod)

Description

sobolEff implements the Monte Carlo estimation of the Sobol’ sensitivity indices using the asymptotically efficient formulas in section 4.2.4.2 of Monod et al. (2006). This method allows the estimation of all first-order p indices at a cost of N*(p+1) model calls, where p is the number of inputs and N is the random sample size, or the estimation of all closed second order indices at a cost of N*(p*(p-1)/2+1) model calls.

Usage

sobolEff(model = NULL, X1, X2, order=1, nboot = 0, conf = 0.95, ...)
## S3 method for class 'sobolEff'
tell(x, y = NULL, ...)
## S3 method for class 'sobolEff'
print(x, ...)  
## S3 method for class 'sobolEff'
plot(x, ylim = c(0, 1), ...)

Arguments

model a function, or a model with a predict method, defining the model to analyze.
X1 the first random sample.
X2 the second random sample.
order an integer specifying the order of the indices (1 or 2).
nboot the number of bootstrap replicates, or zero to use asymptotic standard deviation estimates given in Janon et al. (2012).
conf the confidence level for confidence intervals.
x a list of class "soboleff" storing the state of the sensitivity study (parameters, data, estimates).
y a vector of model responses.
ylim y-coordinate plotting limits.
... any other arguments for model which are passed unchanged each time it is called.

Details

The estimator used by sobolEff is defined in Monod et al. (2006), Section 4.2.4.2 and studied under the name T_N in Janon et al. (2012). This estimator is good for large first-order indices.
sobolGP

Value
sobolEff returns a list of class "sobolEff", containing all the input arguments detailed before, plus the following components:

- call: the matched call.
- X: a data.frame containing the design of experiments.
- y: a vector of model responses.
- S: the estimations of the Sobol’ sensitivity indices.

Author(s)
Alexandre Janon

References

See Also
sobol, sobol2002, sobol2007, soboljansen, sobolmartinez

Examples

```r
# Test case : the non-monotonic Sobol g-function

# The method of sobol requires 2 samples
# (there are 8 factors, all following the uniform distribution on [0,1])

n <- 1000
X1 <- data.frame(matrix(runif(8 * n), nrow = n))
X2 <- data.frame(matrix(runif(8 * n), nrow = n))

# sensitivity analysis
x <- sobolEff(model = sobol.fun, X1 = X1, X2 = X2, nboot = 0)
print(x)
```

sobolGP

Kriging-based sensitivity analysis

Description
Perform a kriging-based global sensitivity analysis taking into account both the meta-model and the Monte-Carlo errors. The Sobol indices are estimated with a Monte-Carlo integration and the true function is substituted by a kriging model. It is built thanks to the function km of the package DiceKriging. The complete conditional predictive distribution of the kriging model is considered (not only the predictive mean).
Usage

sobolGP(
  model,
  type="SK",
  MCmethod="sobol",
  X1,
  X2,
  nsim=100,
  nboot=1,
  conf = 0.95,
  sequential = FALSE,
  candidate,
  sequential.tot=FALSE,
  max_iter = 1000)

## S3 method for class 'sobolGP'
ask(x, tot = FALSE, ...)

## S3 method for class 'sobolGP'
tell(x,y=NULL,xpoint=NULL,newcandidate=NULL, ...)

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

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

Arguments

model an object of class "km" specifying the kriging model built from package "DiceKriging" (see km).

type a character string giving the type of the considered kriging model. "SK" refers to simple kriging and "UK" refers to universal kriging (see km).

MCmethod a character string specifying the Monte-Carlo procedure used to estimate the Sobol indices. The available methods are: "sobol", "sobol2002", "sobol2007", "sobolEff" and "soboljansen".

X1 a matrix representing the first random sample.

X2 a matrix representing the second random sample.

nsim an integer giving the number of samples for the conditional Gaussian process. It is used to quantify the uncertainty due to the kriging approximation.

nboot an integer representing the number of bootstrap replicates. It is used to quantify the uncertainty due to the Monte-Carlo integrations. We recommend to set nboot = 100.

conf a numeric representing the confidence intervals taking into account the uncertainty due to the bootstrap procedure and the Gaussian process samples.
sequential a boolean. If sequential=TRUE, the procedure provides a new point where to perform a simulation. It is the one minimizing the sum of the MAIN effect estimate variances. The variance is taken with respect to the conditional Gaussian process. The new point is selected in the points candidate.

candidate a matrix representing the candidate points where the best new point to be simulated is selected. The lines represent the points and the columns represent the dimension.

sequential.tot a boolean. If sequential.tot=TRUE, the procedure provides a new point where to perform the simulation. It is the one minimizing the sum of the TOTAL effect estimate. The variance is taken with respect to the conditional Gaussian process. The new point is selected in the points candidate.

max_iter a numeric giving the maximal number of iterations for the propagative Gibbs sampler. It is used to simulate the realizations of the Gaussian process.

x an object of class S3 "sobolGP" obtaining from the procedure sobolGP. It stores the results of the Kriging-based global sensitivity analysis.

tot a boolean. If tot=TRUE, the procedure asks provides a point relative to the uncertainty of the total Sobol' indices (instead of first-order ones).

xpoint a matrix representing a new point added to the kriging model.

y a numeric giving the response of the function at xpoint.

newcandidate a matrix representing the new candidate points where the best point to be simulated is selected. If newcandidate=NULL, these points correspond to candidate without the new point xpoint.

... any other arguments to be passed

Details

The function ask provides the new point where the function should be simulated. Furthermore, the function tell performs a new kriging-based sensitivity analysis when the point x with the corresponding observation y is added.

Value

An object of class S3 sobolGP.

• call : a list containing the arguments of the function sobolGP :
  – X1 : X1
  – X2 : X2
  – conf : conf
  – nboot : nboot
  – candidate : candidate
  – sequential : sequential
  – max_iter : max_iter
  – sequential.tot : sequential.tot
  – model : model
  – tot : tot
- method: MCmethod
- type: type
- nsim: nsim

• S: a list containing the results of the kriging-based sensitivity analysis for the MAIN effects:
  - mean: a matrix giving the mean of the Sobol index estimates.
  - var: a matrix giving the variance of the Sobol index estimates.
  - ci: a matrix giving the confidence intervals of the Sobol index estimates according to conf.
  - varPG: a matrix giving the variance of the Sobol index estimates due to the Gaussian process approximation.
  - varMC: a matrix giving the variance of the Sobol index estimates due to the Monte-Carlo integrations.
  - xnew: if sequential=TRUE, a matrix giving the point in candidate which is the best to simulate.
  - xnewi: if sequential=TRUE, an integer giving the index of the point in candidate which is the best to simulate.

• T: a list containing the results of the kriging-based sensitivity analysis for the TOTAL effects:
  - mean: a matrix giving the mean of the Sobol index estimates.
  - var: a matrix giving the variance of the Sobol index estimates.
  - ci: a matrix giving the confidence intervals of the Sobol index estimates according to conf.
  - varPG: a matrix giving the variance of the Sobol index estimates due to the Gaussian process approximation.
  - varMC: a matrix giving the variance of the Sobol index estimates due to the Monte-Carlo integrations.
  - xnew: if sequential.tot=TRUE, a matrix giving the point in candidate which is the best to simulate.
  - xnewi: if sequential.tot=TRUE, an integer giving the index of the point in candidate which is the best to simulate.

Author(s)

Loic Le Gratiet, EDF R&D - CNRS, I3S

References


See Also

sobol, sobol2002, sobol2007, sobolEff, soboljansen, sobolMultOut, km
Examples

```
## Not run:
library(DiceKriging)

#-----------------------------#
# kriging model building
#-----------------------------#

d <- 2; n <- 16
design.fact <- expand.grid(x1=seq(0,1,length=4), x2=seq(0,1,length=4))
y <- apply(design.fact, 1, branin)

m <- km(design=design.fact, response=y)

#-----------------------------#
# sobol samples & candidate points
#-----------------------------#

n <- 1000
X1 <- data.frame(matrix(runif(d * n), nrow = n))
X2 <- data.frame(matrix(runif(d * n), nrow = n))
candidate <- data.frame(matrix(runif(d * 100), nrow = 100))

#----------------------------
# Kriging-based Sobol
#----------------------------

res <- sobolGP(
  model = m,
  type="UK",
  MCMmethod="sobol",
  X1,
  X2,
  nsim = 100,
  conf = 0.95,
  nboot=100,
  sequential = TRUE,
  candidate,
  sequential.tot=FALSE,
  max.iter = 1000
)

res
plot(res)
x <- ask(res)
y <- branin(x)
res.new <- tell(res,y,x)
res.new

## End(Not run)
```
soboljansen

Monte Carlo Estimation of Sobol’ Indices (improved formulas of
Jansen (1999) and Saltelli et al. (2010))

Description

soboljansen implements the Monte Carlo estimation of the Sobol’ indices for both first-order and
total indices at the same time (alltogether $2p$ indices), at a total cost of $(p+2) \times n$ model evaluations.
These are called the Jansen estimators.

Usage

soboljansen(model = NULL, X1, X2, nboot = 0, conf = 0.95, ...)
## S3 method for class 'soboljansen'
tell(x, y = NULL, return.var = NULL, ...)
## S3 method for class 'soboljansen'
print(x, ...)
## S3 method for class 'soboljansen'
plot(x, ylim = c(0, 1), y_col = NULL, y_dim3 = NULL, ...)

Arguments

model a function, or a model with a predict method, defining the model to analyze.
X1 the first random sample.
X2 the second random sample.
nboot the number of bootstrap replicates.
conf the confidence level for bootstrap confidence intervals.
x a list of class "sobol" storing the state of the sensitivity study (parameters, data, estimates).
y a vector of model responses.
return.var a vector of character strings giving further internal variables names to store in
the output object x.
ylim y-coordinate plotting limits.
y_col an integer defining the index of the column of x$y$ to be used for plotting the corresponding sensitivity indices (only applies if x$y$ is a matrix or an array). If set to NULL (as per default) and x$y$ is a matrix or an array, the first column (respectively the first element in the second dimension) of x$y$ is used (i.e. y_col = 1).
y_dim3 an integer defining the index in the third dimension of x$y$ to be used for plotting the corresponding sensitivity indices (only applies if x$y$ is an array). If set to NULL (as per default) and x$y$ is a three-dimentional array, the first element in the third dimension of x$y$ is used (i.e. y_dim3 = 1).
... for soboljansen: any other arguments for model which are passed unchanged each time it is called.
**Details**

This estimator is good for large first-order indices, and (large and small) total indices.

This version of `soboljansen` also supports matrices and three-dimensional arrays as output of `model`. If the model output is a matrix or an array, \( V, S \) and \( T \) are matrices or arrays as well (depending on the type of \( y \) and the value of `nboot`).

The bootstrap outputs \( V.\text{boot}, S.\text{boot} \) and \( T.\text{boot} \) can only be returned if the model output is a vector (using argument `return.var`). For matrix or array output, these objects can’t be returned.

**Value**

`soboljansen` returns a list of class "soboljansen", containing all the input arguments detailed before, plus the following components:

- `call`: the matched call.
- `x`: a `data.frame` containing the design of experiments.
- `y`: either a vector, a matrix or a three-dimensional array of model responses (depends on the output of `model`).
- `V`: the estimations of Variances of the Conditional Expectations (VCE) with respect to each factor and also with respect to the complementary set of each factor ("all but \( X_i \)).
- `S`: the estimations of the Sobol’ first-order indices.
- `T`: the estimations of the Sobol’ total sensitivity indices.

Users can ask more output variables with the argument `return.var` (for example, bootstrap outputs \( V.\text{boot}, S.\text{boot} \) and \( T.\text{boot} \)).

**Author(s)**

Bertrand Iooss, with contributions from Frank Weber (2016)

**References**


**See Also**

`sobol, sobol2002, sobol2007, sobolmartinez, sobolEff, sobolmarasobolMultOut`
Examples

# Test case: the non-monotonic Sobol g-function

# The method of sobol requires 2 samples
# There are 8 factors, all following the uniform distribution
# on [0,1]

library(boot)
n <- 1000
X1 <- data.frame(matrix(runif(8 * n), nrow = n))
X2 <- data.frame(matrix(runif(8 * n), nrow = n))

# sensitivity analysis
x <- soboljansen(model = sobol.fun, X1, X2, nboot = 100)
print(x)
plot(x)

# Only for demonstration purposes: a model function returning a matrix
sobol.fun_matrix <- function(x){
  res_vector <- sobol.fun(x)
  cbind(res_vector, 2 * res_vector)
}
x_matrix <- soboljansen(model = sobol.fun_matrix, X1, X2)
plot(x_matrix, y.col = 2)
title(main = "y.col = 2")

# Also only for demonstration purposes: a model function returning a
# three-dimensional array
sobol.fun_array <- function(x){
  res_vector <- sobol.fun(x)
  res_matrix <- cbind(res_vector, 2 * res_vector)
  array(data = c(res_matrix, 5 * res_matrix),
        dim = c(length(res_vector), 2, 2))
}
x_array <- soboljansen(model = sobol.fun_array, X1, X2)
plot(x_array, y.col = 2, y_dim3 = 2)
title(main = "y.col = 2, y_dim3 = 2")

---

sobolmara

*Monte Carlo Estimation of Sobol’ Indices via matrix permutations*

Description

sobolmara implements the Monte Carlo estimation of the first-order Sobol’ sensitivity indices using the formula of Mara and Joseph (2008), called the Mara estimator. This method allows the estimation of all first-order p indices at a cost of 2N model calls (the random sample size), then independently of p (the number of inputs).
Usage

sobolmara(model = NULL, X1, ...)
## S3 method for class 'sobolmara'
tell(x, y = NULL, return.var = NULL, ...)
## S3 method for class 'sobolmara'
print(x, ...)
## S3 method for class 'sobolmara'
plot(x, ylim = c(0, 1), ...)

Arguments

model a function, or a model with a predict method, defining the model to analyze.
X1 the random sample.
x a list of class "soboleff" storing the state of the sensitivity study (parameters, data, estimates).
y a vector of model responses.
return.var a vector of character strings giving further internal variables names to store in the output object x.
ylim y-coordinate plotting limits.
... any other arguments for model which are passed unchanged each time it is called.

Details

The estimator used by sobolmara is based on rearrangement of a unique matrix via random permuta-
tions (see Mara and Joseph, 2008). Bootstrap confidence intervals are not available.

Value

sobolmara returns a list of class "sobolmara", containing all the input arguments detailed before, plus the following components:

call the matched call.
X a data.frame containing the design of experiments.
y a vector of model responses.
S the estimations of the Sobol’ sensitivity indices.

Author(s)

Bertrand Iooss

References

# Test case: the non-monotonic Sobol g-function

# The method of sobolmara requires 1 sample
# (there are 8 factors, all following the uniform distribution on [0,1])
n <- 1000
X1 <- data.frame(matrix(runif(8 * n), nrow = n))

# sensitivity analysis
x <- sobolmara(model = sobol.fun, X1 = X1)
print(x)
plot(x)

sobolmartinez

**Monte Carlo Estimation of Sobol’ Indices (formulas of Martinez (2011))**

### Description

sobolmartinez implements the Monte Carlo estimation of the Sobol’ indices for both first-order and total indices using correlation coefficients-based formulas, at a total cost of \((p + 2) \times n\) model evaluations. These are called the Martinez estimators.

### Usage

sobolmartinez(model = NULL, X1, X2, nboot = 0, conf = 0.95, ...)

### Arguments

- **model**: a function, or a model with a predict method, defining the model to analyze.
- **X1**: the first random sample.
- **X2**: the second random sample.
- **nboot**: the number of bootstrap replicates, or zero to use theoretical formulas based on confidence interfaces of correlation coefficient (Martinez, 2011).
- **conf**: the confidence level for bootstrap confidence intervals.
- **x**: a list of class "sobol" storing the state of the sensitivity study (parameters, data, estimates).
y a vector of model responses.
return.var a vector of character strings giving further internal variables names to store in the output object x.
ylim y-coordinate plotting limits.
y_col an integer defining the index of the column of x$y to be used for plotting the corresponding sensitivity indices (only applies if x$y is a matrix or an array). If set to NULL (as per default) and x$y is a matrix or an array, the first column (respectively the first element in the second dimension) of x$y is used (i.e. y_col = 1).
y_dim3 an integer defining the index in the third dimension of x$y to be used for plotting the corresponding sensitivity indices (only applies if x$y is a matrix or an array). If set to NULL (as per default) and x$y is a three-dimensional array, the first element in the third dimension of x$y is used (i.e. y_dim3 = 1).

for sobolmartinez: any other arguments for model which are passed unchanged each time it is called

Details

This estimator supports missing values (NA or NaN) which can occur during the simulation of the model on the design of experiments (due to code failure) even if Sobol' indices are no more rigorous variance-based sensitivity indices if missing values are present. In this case, a warning is displayed. This version of sobolmartinez also supports matrices and three-dimensional arrays as output of model. Bootstrapping (including bootstrap confidence intervals) is also supported for matrix or array output. However, theoretical confidence intervals (for nboot = 0) are only supported for vector output. If the model output is a matrix or an array, V, S and T are matrices or arrays as well (depending on the type of y and the value of nboot).

The bootstrap outputs V.boot, S.boot and T.boot can only be returned if the model output is a vector (using argument return.var). For matrix or array output, these objects can’t be returned.

Value

sobolmartinez returns a list of class "sobolmartinez", containing all the input arguments detailed before, plus the following components:
call the matched call.
X a data.frame containing the design of experiments.
y either a vector, a matrix or a three-dimensional array of model responses (depends on the output of model).
V the estimations of normalized variances of the Conditional Expectations (VCE) with respect to each factor and also with respect to the complementary set of each factor ("all but X_i").
S the estimations of the Sobol’ first-order indices.
T the estimations of the Sobol’ total sensitivity indices.

Users can ask more output variables with the argument return.var (for example, bootstrap outputs V.boot, S.boot and T.boot).
Author(s)

Bertrand Iooss, with contributions from Frank Weber (2016)

References


See Also

sobol, sobol2002, sobol2007, soboljansen, soboltouati, sobolEff, sobolmara, sobolMultOut

Examples

# Test case : the non-monotonic Sobol g-function

# The method of sobol requires 2 samples
# There are 8 factors, all following the uniform distribution
# on [0,1]

library(boot)
n <- 1000
X1 <- data.frame(matrix(runif(8 * n), nrow = n))
X2 <- data.frame(matrix(runif(8 * n), nrow = n))

# sensitivity analysis

x <- sobolmartinez(model = sobol.fun, X1, X2, nboot = 0)
print(x)
plot(x)

# Only for demonstration purposes: a model function returning a matrix
sobol.fun_matrix <- function(X){
  res_vector <- sobol.fun(X)
  cbind(res_vector, 2 * res_vector)
}
x_matrix <- sobolmartinez(model = sobol.fun_matrix, X1, X2)
plot(x_matrix, y_col = 2)
title(main = "y_col = 2")

# Also only for demonstration purposes: a model function returning a
# three-dimensional array
sobol.fun_array <- function(X){
  res_vector <- sobol.fun(X)
  res_matrix <- cbind(res_vector, 2 * res_vector)
  array(data = c(res_matrix, 5 * res_matrix),
       dim = c(length(res_vector), 2, 2))
}
x_array <- sobolmartinez(model = sobol.fun_array, X1, X2)
plot(x_array, y_col = 2, y_dim3 = 2)
title(main = "y_col = 2, y_dim3 = 2")
sobolMultOut

Monte Carlo Estimation of Aggregated Sobol’ Indices for multiple and functional outputs

Description

sobolMultOut implements the aggregated Sobol’ indices for multiple outputs. It consists in averaging all the Sobol indices weighted by the variance of their corresponding output. Moreover, this function plots the functional (unidimensional) Sobol’ indices for functional (unidimensional) model output. Sobol’ indices for both first-order and total indices are estimated by Monte Carlo formulas.

Usage

sobolMultOut(model = NULL, q = 1, X1, X2, MCMETHOD = "sobol",
plotFCT=FALSE, ...)
## S3 method for class 'sobolMultOut'
print(x, ...)
## S3 method for class 'sobolMultOut'
plot(x, ylim = c(0, 1), ...)

Arguments

model a function, or a model with a predict method, defining the model to analyze.
q dimension of the model output vector.
X1 the first random sample.
X2 the second random sample.
MCMETHOD a character string specifying the Monte-Carlo procedure used to estimate the Sobol indices. The available methods are: "sobol", "sobol2002", "sobol2007", "soboljansen", sobolmara, "sobolmartinez" and sobolGP.
plotFCT if TRUE, 1D functional Sobol indices are plotted in an external window (default=FALSE).
x a list of class MCMETHOD storing the state of the sensitivity study (parameters, data, estimates).
ylim y-coordinate plotting limits.
... any other arguments for model which are passed unchanged each time it is called

Details

For this function, there are several gaps: the bootstrap estimation of confidence intervals is not available and the tell function does not work.
Value

`sobolMultOut` returns a list of class `MCmethod`, containing all its input arguments, plus the following components:

- `call`: the matched call.
- `X`: a data.frame containing the design of experiments.
- `y`: the response used.
- `V`: the estimations of the aggregated Variances of the Conditional Expectations (VCE) with respect to each factor and also with respect to the complementary set of each factor ("all but X").
- `S`: the estimations of the aggregated Sobol' first-order indices.
- `T`: the estimations of the aggregated Sobol' total sensitivity indices.

Author(s)

Bertrand Iooss

References


See Also

`sobol`, `sobol2002`, `sobol2007`, `soboljansen`, `sobolmara`, `sobolmartinez`, `sobolGP`

Examples

```r
# Not run:
# Functional toy function: Arctangent temporal function (Auder, 2011)
# X: input matrix (in [-7,7]^2)
# q: number of discretization steps of [0,2pi] interval
# output: vector of q values
atantemp <- function(X, q = 100){
  n <- dim(X)[[1]]
  t <- (0:(q-1)) * (2*pi) / (q-1)
  res <- matrix(0, ncol=q, nrow=n)
  for (i in 1:n) res[i,] <- atan(X[i,1]) * cos(t) + atan(X[i,2]) * sin(t)
  return(res)
}
# Tests functional toy fct
```
sobolowen

Monte Carlo Estimation of Sobol’ Indices (improved formulas of Owen (2013))

Description

sobolowen implements the Monte Carlo estimation of the Sobol’ indices for both first-order and total indices at the same time (alltogether \(2^p\) indices). Take as input 3 independent matrices. These are called the Owen estimators.

Usage

sobolowen(model = NULL, X1, X2, X3, nboot = 0, conf = 0.95, varest = 2, ...)
## S3 method for class 'sobolowen'
tell(x, y = NULL, return.var = NULL, varest = 2, ...)
## S3 method for class 'sobolowen'
print(x, ...)
## S3 method for class 'sobolowen'
plot(x, ylim = c(0, 1), ...)
Arguments

- `model`: a function, or a model with a `predict` method, defining the model to analyze.
- `x1`: the first random sample.
- `x2`: the second random sample.
- `x3`: the third random sample.
- `nboot`: the number of bootstrap replicates.
- `conf`: the confidence level for bootstrap confidence intervals.
- `varest`: choice for the variance estimator for the denominator of the Sobol’ indices. `varest=1` is for a classical estimator. `varest=2` (default) is for the estimator proposed in Janon et al. (2012).
- `x`: a list of class "sobol" storing the state of the sensitivity study (parameters, data, estimates).
- `y`: a vector of model responses.
- `return.var`: a vector of character strings giving further internal variables names to store in the output object `x`.
- `ylim`: y-coordinate plotting limits.
- `...`: any other arguments for `model` which are passed unchanged each time it is called.

Value

`sobolowen` returns a list of class "sobolowen", containing all the input arguments detailed before, plus the following components:

- `call`: the matched call.
- `X`: a data.frame containing the design of experiments.
- `y`: the response used.
- `V`: the estimations of Variances of the Conditional Expectations (VCE) with respect to each factor and also with respect to the complementary set of each factor ("all but \(X_i\)).
- `S`: the estimations of the Sobol’ first-order indices.
- `T`: the estimations of the Sobol’ total sensitivity indices.

Users can ask more output variables with the argument `return.var` (for example, bootstrap outputs `V.boot`, `S.boot` and `T.boot`).

Author(s)

Taieb Touati and Bernardo Ramos

References


sobolroalhs

See Also

sobol, sobol2002, sobol2007, soboljansen, sobolmartinez, soboleff, sobolmara, sobolGP

Examples

# Test case: the non-monotonic Sobol g-function

# The method of sobolowen requires 3 samples
# There are 8 factors, all following the uniform distribution
# on [0,1]

library(boot)

n <- 1000

X1 <- data.frame(matrix(runif(8 * n), nrow = n))

X2 <- data.frame(matrix(runif(8 * n), nrow = n))

X3 <- data.frame(matrix(runif(8 * n), nrow = n))

# sensitivity analysis

## Not run:
x <- sobolowen(model = sobol.fun, X1, X2, X3, nboot = 100)
print(x)
plot(x)

## End(Not run)

---

sobolroalhs  

**Sobol' Indices Estimation Using Replicated OA-based LHS**

Description

sobolroalhs implements the estimation of the Sobol' sensitivity indices introduced by Tissot & Prieur (2012) using two Orthogonal Array-based Latin Hypercubes. This function allows the estimation of all first-order indices or all closed second-order indices (containing the sum of the second-order effect between two inputs and the individual effects of each input) at a total cost of $2 \times N$. For closed second-order indices $N = q^2$ where $q \geq d - 1$ is a prime number denoting the number of levels of the orthogonal array, and where $d$ is the number of factors.

Usage

sobolroalhs(model = NULL, factors, runs, order, conf=0.95, tail=TRUE, na.rm=FALSE, ...)

## S3 method for class 'sobolroalhs'
tell(x, y = NULL, ...)

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

## S3 method for class 'sobolroalhs'
plot(x, ylim = c(0,1), type="standard", ...)

---
**Arguments**

- `model` a function, or a model with a `predict` method, defining the model to analyze.
- `factors` an integer specifying the number of factors, or a vector of character strings giving their names.
- `runs` an integer specifying the number $N$ of model runs.
- `order` an integer specifying the order of the indices (1 or 2).
- `conf` the confidence level for confidence intervals.
- `tail` a boolean specifying the method used to choose the number of levels of the orthogonal array (see first Warning messages).
- `na.rm` a boolean specifying if the response of the model contains NA values.
- `x` a list of class "sobolroalhs" storing the state of the sensitivity study (parameters, data, estimates).
- `y` a vector of model responses.
- `ylim` coordinate plotting limits for the indices values.
- `type` a character specifying the type of estimator to plot (standard for the basic estimator or monod for the Janon-Monod estimator.)
- `...` any other arguments for `model` which are passed unchanged each time it is called.

**Details**

The method used by `sobolroalhs` only considers models whose inputs follow uniform distributions on $[0,1]$. The transformations of each input (between its initial distribution and a U$[0,1]$ distribution) have therefore to be realized before the call to `sobolroalhs()`.

Bootstrap confidence intervals are not available with this method; the given confidence intervals come from asymptotical formula.

**Value**

`sobolroalhs` returns a list of class "sobolroalhs", containing all the input arguments detailed before, plus the following components:

- `call` the matched call.
- `X` a matrix containing the design of experiments.
- `OA` the orthogonal array constructed (NULL if `order`=1).
- `levels` the number of levels of the orthogonal array constructed (NULL if `order`=1).
- `y` a vector of model responses.
- `V` a data.frame containing the estimations of the variance (Vs for the standard variance and Veff for the Janon-Monod variance).
- `S` a data.frame containing the estimations of the Sobol’ sensitivity indices (S for the standard estimator and Seff for the Janon-Monod estimator).
Warning messages

"The number of model evaluations (runs) you entered is not the square of a prime number. It has been replaced by :
when order = 2, the number of levels of the orthogonal array must be a prime number. If the number of runs specified is not a square of a prime number then this warning message indicates that the number of runs was replaced depending on the value of tail. If tail = TRUE (resp. tail = FALSE) the new number of runs is equals to the square of the prime number preceding (resp. following) the square root of runs.

"The number of model evaluations (runs) you entered is not satisfying the constraint \( n \geq (d - 1)^2 \). It has been replaced by :
when order = 2, the number of runs must satisfied the constraint \( N \geq (d - 1)^2 \) where \( d \) is the number of factors. This warning message indicates that the number of runs was replaced by the square of the prime number following (or equals to) \( d - 1 \).

References


See Also

sobolmara

Examples

library(numbers)

# Test case : the non-monotonic Sobol g-function

# The method of sobol requires 2 samples
# (there are 8 factors, all following the uniform distribution on [0,1])

# first-order sensitivity indices
x <- sobolrhoalhs(model = sobol.fun, factors = 8, runs = 1000, order = 1)
print(x)
plot(x)

# closed second-order sensitivity indices
x <- sobolrhoalhs(model = sobol.fun, factors = 8, runs = 1000, order = 2)
print(x)
plot(x)

# Test case : the Ishigami function

# New function because sobolrhoalhs() works with U[0,1] inputs
ishigami1.fun=function(x) ishigami.fun(x*2*pi-pi)

# first-order sensitivity indices
x <- sobolrhoalhs(model = ishigami1.fun, factors = 3, runs = 100000, order = 1)
print(x)
plot(x)
# closed second-order sensitivity indices
x <- sobolroalhs(model = ishigami1.fun, factors = 3, runs = 100000, order = 2)
print(x)
plot(x)

# dealing with NA values
x <- sobolroalhs(model = NULL, factors = 3, runs = 100000, order = 1, na.rm = TRUE)
y <- ishigami1.fun(x$x)
# we randomly insert NA values in y
pos <- sample(length(y), 100)
y[pos] <- NA
tell(x, y)
print(x)
plot(x)

sobolTIIlo

Liu and Owen Estimation of Total Interaction Indices

Description

sobolTIIlo implements the asymptotically efficient formula of Liu and Owen (2006) for the estimation of total interaction indices as described e.g. in Section 3.4 of Fruth et al. (2014). Total interaction indices (TII) are superset indices of pairs of variables, thus give the total influence of each second-order interaction. The total cost of the method is \(\left(\frac{1}{N} + 1\right) \times n\) where \(N\) is the number of indices to estimate. Asymptotic confidence intervals are provided. Via plotFG (which uses functions of the package igraph), the TII can be visualized in a so-called FANOVA graph as described in section 2.2 of Muehlenstaedt et al. (2012).

Usage

sobolTIIlo(model = NULL, X1, X2, conf = 0.95, ...)

## S3 method for class 'sobolTIIlo'
tell(x, y = NULL, ...)

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

## S3 method for class 'sobolTIIlo'
plot(x, ylim = NULL, ...)

## S3 method for class 'sobolTIIlo'
plotFG(x)

Arguments

model a function, or a model with a predict method, defining the model to analyze.
X1 the first random sample.
X2 the second random sample.
conf the confidence level for asymptotic confidence intervals, defaults to 0.95.
sobolTIIlo

x a list of class "sobolTIIlo" storing the state of the sensitivity study (parameters, data, estimates).

y a vector of model responses.

... any other arguments for model which are passed unchanged each time it is called.

ylim optional, the y limits of the plot.

Value

sobolTIIlo returns a list of class "sobolTIIlo", containing all the input arguments detailed before, plus the following components:

call the matched call.

X a data.frame containing the design of experiments.

y a vector of model responses.

V the estimation of the overall variance.

tii.unscaled the unscaled estimations of the TII.

tii.scaled the scaled estimations of the TII together with asymptotic confidence intervals.

Author(s)

Jana Fruth

References


See Also

sobolTIIpf

Examples

# Test case : the Ishigami function

# The method requires 2 samples
n <- 1000
X1 <- data.frame(matrix(runif(3 * n, -pi, pi), nrow = n))
X2 <- data.frame(matrix(runif(3 * n, -pi, pi), nrow = n))

# sensitivity analysis (the true values of the scaled TII are 0, 0.244, 0)
x <- sobolTIIlo(model = ishigami.fun, X1 = X1, X2 = X2)
sobolTIIpf

Pick-freeze Estimation of Total Interaction Indices

Description
sobolTIIpf implements the pick-freeze estimation of total interaction indices as described in Section 3.3 of Fruth et al. (2014). Total interaction indices (TII) are superset indices of pairs of variables, thus give the total influence of each second-order interaction. The pick-freeze estimation enables the strategy to reuse evaluations of Saltelli (2002). The total costs are $(1 + N) \times n$ where $N$ is the number of indices to estimate. Via plotFG, the TIIs can be visualized in a so-called FANOVA graph as described in section 2.2 of Muehlenstaedt et al. (2012).

Usage
sobolTIIpf(model = NULL, X1, X2, ...) # S3 method for class 'sobolTIIpf'
tell(x, y = NULL, ...) # S3 method for class 'sobolTIIpf'
print(x, ...) # S3 method for class 'sobolTIIpf'
plot(x, ylim = NULL, ...) # S3 method for class 'sobolTIIpf'
plotFG(x)

Arguments
model a function, or a model with a predict method, defining the model to analyze.
X1 the first random sample.
X2 the second random sample.
x a list of class "sobolTIIpf" storing the state of the sensitivity study (parameters, data, estimates).
y a vector of model responses.
... any other arguments for model which are passed unchanged each time it is called.
ylim optional, the y limits of the plot.
sobolTIIf returns a list of class "sobolTIIf", containing all the input arguments detailed before, plus the following components:

- **call**: the matched call.
- **X**: a `data.frame` containing the design of experiments.
- **y**: a vector of model responses.
- **V**: the estimation of the overall variance.
- **tii.unscaled**: the unscaled estimations of the TIIs together.
- **tii.scaled**: the scaled estimations of the TIIs.

**Author(s)**

Jana Fruth

**References**


**See Also**

`sobolTIIf0`

**Examples**

```r
# Test case: the Ishigami function

# The method requires 2 samples
n <- 1000
X1 <- data.frame(matrix(runif(3 * n, -pi, pi), nrow = n))
X2 <- data.frame(matrix(runif(3 * n, -pi, pi), nrow = n))

# sensitivity analysis (the true values are 0, 0.244, 0)
x <- sobolTIIf(model = ishigami.fun, X1 = X1, X2 = X2)
print(x)

# plot of tiis and FANOVA graph
plot(x)

## Not run:
library(igraph)
plotFG(x)

## End(Not run)
```
soboltouati

Monte Carlo Estimation of Sobol’ Indices (formulas of Martinez (2011) and Touati (2016))

Description

soboltouati implements the Monte Carlo estimation of the Sobol’ indices for both first-order and total indices using correlation coefficients-based formulas, at a total cost of \((p + 2) \times n\) model evaluations. These are called the Martinez estimators. It also computes their confidence intervals based on asymptotic properties of empirical correlation coefficients.

Usage

soboltouati(model = NULL, X1, X2, conf = 0.95, ...)
## S3 method for class 'soboltouati'
tell(x, y = NULL, return.var = NULL, ...)
## S3 method for class 'soboltouati'
print(x, ...)
## S3 method for class 'soboltouati'
plot(x, ylim = c(0, 1), ...)

Arguments

- `model`: a function, or a model with a `predict` method, defining the model to analyze.
- `X1`: the first random sample.
- `X2`: the second random sample.
- `conf`: the confidence level for confidence intervals, or zero to avoid their computation if they are not needed.
- `x`: a list of class "sobol" storing the state of the sensitivity study (parameters, data, estimates).
- `y`: a vector of model responses.
- `return.var`: a vector of character strings giving further internal variables names to store in the output object `x`.
- `ylim`: y-coordinate plotting limits.
- `...`: any other arguments for `model` which are passed unchanged each time it is called.

Details

This estimator supports missing values (NA or NaN) which can occur during the simulation of the model on the design of experiments (due to code failure) even if Sobol’ indices are no more rigorous variance-based sensitivity indices if missing values are present. In this case, a warning is displayed.
Value

`soboltouati` returns a list of class "soboltouati", containing all the input arguments detailed before, plus the following components:

- **call**: the matched call.
- **X**: a `data.frame` containing the design of experiments.
- **y**: the response used.
- **V**: the estimations of normalized variances of the Conditional Expectations (VCE) with respect to each factor and also with respect to the complementary set of each factor ("all but \( X_i \)).
- **S**: the estimations of the Sobol' first-order indices.
- **T**: the estimations of the Sobol' total sensitivity indices.

Author(s)

Taieb Touati, Khalid Boumhaout

References


See Also

`sobol`, `sobol2002`, `sobol2007`, `soboljansen`, `sobolEff`, `sobolmara`, `sobolmartinez`

Examples

```r
# Test case : the non-monotonic Sobol g-function

# The method of sobol requires 2 samples
# There are 8 factors, all following the uniform distribution
# on [0,1]

library(boot)
n <- 1000
X1 <- data.frame(matrix(runif(8 * n), nrow = n))
X2 <- data.frame(matrix(runif(8 * n), nrow = n))

# sensitivity analysis

x <- soboltouati(model = sobol.fun, X1, X2)
print(x)
plot(x)
```
**Description**

`src` computes the Standardized Regression Coefficients (SRC), or the Standardized Rank Regression Coefficients (SRRC), which are sensitivity indices based on linear or monotonic assumptions in the case of independent factors.

**Usage**

```r
src(X, y, rank = FALSE, nboot = 0, conf = 0.95)
## S3 method for class 'src'
print(x, ...)
## S3 method for class 'src'
plot(x, ylim = c(-1,1), ...)
```

**Arguments**

- `X` a data frame (or object coercible by `as.data.frame`) containing the design of experiments (model input variables).
- `y` a vector containing the responses corresponding to the design of experiments (model output variables).
- `rank` logical. If `TRUE`, the analysis is done on the ranks.
- `nboot` the number of bootstrap replicates.
- `conf` the confidence level of the bootstrap confidence intervals.
- `x` the object returned by `src`.
- `ylim` the y-coordinate limits of the plot.
- `...` arguments to be passed to methods, such as graphical parameters (see `par`).

**Value**

`src` returns a list of class "src", containing the following components:

- `call` the matched call.
- `SRC` a data frame containing the estimations of the SRC indices, bias and confidence intervals (if `rank = FALSE`).
- `SRRC` a data frame containing the estimations of the SRRC indices, bias and confidence intervals (if `rank = TRUE`).

**Author(s)**

Gilles Pujol
References

See Also
pcc

Examples

```r
# a 100-sample with X1 ~ U(0.5, 1.5)
# X2 ~ U(1.5, 4.5)
# X3 ~ U(4.5, 13.5)

library(boot)
n <- 100
X <- data.frame(X1 = runif(n, 0.5, 1.5),
                 X2 = runif(n, 1.5, 4.5),
                 X3 = runif(n, 4.5, 13.5))

# linear model : Y = X1 + X2 + X3
y <- with(X, X1 + X2 + X3)

# sensitivity analysis
x <- src(X, y, nboot = 100)
print(x)
plot(x)
```

Support indices: Measuring the effect of input variables over their support

Description
Function to estimate and plot the support index functions (first order and total) for one variable (Fruth et al., 2016) `xi`

Usage
```
support(fun, d, xi = 1, h = 0.01, n = 5000, n.points = 50, q, q.arg, ...)
```

Arguments
- `fun` a function defining the model to analyze.
- `d` number of input variables of the model.
- `xi` the number of the studied input variable.
support

h  small over which to approximate the derivative.
n  number of Monte Carlo estimates.
n.points  number of equally spread points over the domain to evaluate the function.
q  a vector of quantile functions names corresponding to wanted factors distributions (see details below).
q.arg  a list of quantile functions parameters (see details below).
...  any other arguments for the plot of the support indices which are passed unchanged each time it is called.

Details

If the arguments q and q.arg are not given, the factors are taken uniformly distributed on \([0, 1]\). The argument q must be list of character strings, giving the names of the quantile functions (one for each factor), such as `qunif`, `qnorm`... It can also be a single character string, meaning same distribution for all. The argument q.arg must be a list of lists, each one being additional parameters for the corresponding quantile function. For example, the parameters of the quantile function `qunif` could be `list(min=1, max=2)`, giving an uniform distribution on \([1, 2]\). If q is a single character string, then q.arg must be a single list (rather than a list of one list).

Value

`support` returns a list, containing the first order support indices and the total support indices. Note that the function returns plot and values at the same time.

Author(s)

Jana Fruth

References


Examples

col1 <- "lightskyblue1"
colT <- "lightskyblue4"
ylim <- c(0,75)
n.points <- 50

#X1
a <- support(fun=ishigami.fun, d=3, xi=1, h=0.01, n=5000, n.points=n.points,
  q="qunif", q.arg=list(min=-pi, max=pi), ylim=ylim, xaxt="n", ylab="$X1$")
legend("topleft", legend=c("first-order support index", "total support index"),
  fill=c(col1,colT), bty="n")

#x2
support(fun=ishigami.fun, d=3, xi=2, h=0.01, n=5000, n.points=n.points,
template.replace

Replace Values in a Template Text

Description
template.replace replaces keys within special markups with values in a so-called template file. Pieces of R code can be put into the markups of the template file, and are evaluated during the replacement.

Usage

```r
template.replace(text, replacement, eval = FALSE,
                 key.pattern = NULL, code.pattern = NULL)
```

Arguments
text vector of character strings, the template text.
replacement the list values to replace in text.
eval boolean, TRUE if the code within code.pattern has to be evaluated, FALSE otherwise.
key.pattern custom pattern for key replacement (see below)
code.pattern custom pattern for code replacement (see below)

Details

In most cases, a computational code reads its inputs from a text file. A template file is like an input file, but where some missing values, identified with generic keys, will be replaced by specific values.

By default, the keys are enclosed into markups of the form `$\{KEY\}`.

Code to be interpreted with R can be put in the template text. Pieces of code must be enclosed into markups of the form `@\{CODE\}`. This is useful for example for formating the key values (see example). For interpreting the code, set eval = TRUE.

Users can define custom patterns. These patterns must be perl-compatible regular expressions (see `regexp`). The default ones are:

```r
key.pattern = "\$\{(KEY)\}"
code.pattern = "@\{(CODE)\}"
```

Note that special characters have to be escaped both (one for perl, one for R).
Author(s)

Gilles Pujol

Examples

txt <- c("Hello $(name)!", "$(a) + $(b) = @(a)+@$(b))", "pi = @(format(pi,digits=5))")
replacement <- list(name = "world", a = 1, b = 2)
# 1. without code evaluation:
txt.rpl1 <- template.replace(txt, replacement)
print(txt.rpl1)
# 2. with code evaluation:
txt.rpl2 <- template.replace(txt, replacement, eval = TRUE)
print(txt.rpl2)

Description

These functions are standard testcase for sensitivity analysis benchmarks. For a scalar output (see Saltelli et al. 2000, section 2.9):

• the g-function of Sobol’ with 8 inputs, X ~ U[0,1];
• the function of Ishigami with 3 inputs, X ~ U[-pi,pi];
• the function of Morris with 20 inputs, X ~ U[0,1].

For functional output cases:

• the Arctangent temporal function with 2 inputs, X ~ U[-7,7] (Auder, 2011). The functional support is on [0,2pi];
• the Cambell1D function with 4 inputs, X ~U[-1,5] (Campbell et al. 2006). The functional support is on [-90,90].

Usage

sobol.fun(X)
ishigami.fun(X)
morris.fun(X)
atantemp.fun(X, q = 100)
campbell1D.fun(X, theta = -90:90)

Arguments

X a matrix (or data.frame) containing the input sample.
q for the atantemp() function: the number of discretization steps of the functional output
theta for the campbell1D() function: the discretization steps (angles in degrees)
Value

A vector of function responses.

Author(s)

Gilles Pujol

References


Examples

```r
## Not run:

# Examples for the functional toy functions

# atantemp function

y0 <- atantemp.fun(matrix(c(-7,0,7,-7,0,7),ncol=2))
plot(y0[1,1,type="l"])
apply(y0,1,lines)

n <- 100
X <- matrix(c(runif(2*n,-7,7)),ncol=2)
y <- atantemp.fun(X)
x11()
plot(y0[2,],ylim=c(-2,2),type="l")
apply(y,1,lines)

# campbell1d function

N1=100  # nombre de simulations pour courbes 1D
min=-1 ; max=5
nominal=(max+min)/2

X1 = NULL ; y1 = NULL
Xnom=matrix(nominal,nr=1,nc=4)
ynom=campbell1D.fun(Xnom,theta=-90:90)
x11()
plot(ynom,ylim=c(8,30),type="l",col="red")
for (i in 1:N1){
  X=matrix(runif(4,min=min,max=max),nr=1,nc=4)
  rbind(X1,X)
y=campbell1D.fun(X,theta=-90:90)
  rbind(y1,y)
  lines(y)
}

## End(Not run)
```
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