Package ‘propagate’

February 20, 2015

Type Package
LazyLoad no
LazyData no
Title Propagation of Uncertainty
Version 1.0-4
Date 2014-04-04
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Description Propagation of uncertainty using higher-order Taylor expansion and Monte Carlo simulation.
License GPL (>= 2)
Depends R (>= 2.13.0), MASS, tmvtnorm, Rcpp (>= 0.10.1), ff, minpack.lm
LinkingTo Rcpp
NeedsCompilation yes
Repository CRAN
Date/Publication 2014-09-27 12:26:57

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bigcor

Creating very large correlation/covariance matrices

Description

The storage of a value in double format needs 8 bytes. When creating large correlation matrices, the amount of RAM might not suffice, giving rise to the dreaded "cannot allocate vector of size ..." error. For example, an input matrix with 50000 columns/100 rows will result in a correlation matrix with a size of 50000 x 50000 x 8 Byte / (1024 x 1024 x 1024) = 18.63 GByte, which is still more than most standard PCs. bigcor uses the framework of the 'ff' package to store the correlation/covariance matrix in a file. The complete matrix is created by filling a large preallocated empty matrix with sub-matrices at the corresponding positions. See 'Details'. Calculation time is ~ 20s for an input matrix of 10000 x 100 (cols x rows).

Usage

bigcor(x, fun = c("cor", "cov"), size = 2000, verbose = TRUE, ...)

Arguments

x
the input matrix.

fun
create either a correlation or covariance matrix.

size
the n x n block size of the submatrices. 2000 has shown to be time-effective.

verbose
logical. If TRUE, information is printed in the console when running.

... other parameters to be passed to cor or cov.

Details

Calculates a correlation matrix \( C \) or covariance matrix \( \Sigma \) using the following steps:
1) An input matrix \( x \) with \( N \) columns is split into equal size blocks (+ a possible remainder block) of size \( n: A_1, \ldots, A_n; B_1, \ldots, B_n \) etc. The block size can be defined by the user, size = 2000 is a good value because cor can handle this quite quickly (~ 400 ms). If the matrix has 13796 columns, the split will be 2000; 2000; 2000; 2000; 2000; 2000; 1796.
2) For all combinations of blocks, the \( n \times n \) correlation sub-matrix is calculated, so \( A/A, A/B, B/B \) etc.
3) The sub-matrices are transferred into a preallocated \( N \times N \) empty matrix at the corresponding position (where the correlations would usually reside). To ensure symmetry around the diagonal, this is done twice in the upper and lower triangle.

Since the resulting matrix is in 'ff' format, one has to subset to extract regions into normal matrix-like objects. See 'Examples'.

Value

The corresponding correlation/covariance matrix in 'ff' format.

Author(s)

Andrej-Nikolai Spiess

References

http://rmazing.wordpress.com/2013/02/22/bigcor-large-correlation-matrices-in-r/

Examples

```r
# Small example to prove similarity
# to standard 'cor'. We create a matrix
# by subsetting the complete 'ff' matrix.
MAT <- matrix(rnorm(70000), ncol = 700)
COR <- bigcor(MAT, size = 2000, fun = "cor")
COR <- COR[1:nrow(COR), 1:ncol(COR)]
all.equal(COR, cor(MAT)) # => TRUE

# Not run:
# Create large matrix.
MAT <- matrix(rnorm(137500), ncol = 13750)
COR <- bigcor(MAT, size = 2000, fun = "cor")

# Extract submatrix.
SUB <- COR[1:3000, 1:3000]

# End(Not run)
```

contribution

Contribution to propagated uncertainty for each variable

Description

Calculates the relative "contribution" \( C_i \) of each variable \( x_i \) to the propagated uncertainty, as defined in the Expression of the Uncertainty of Measurement in Calibration, Eqn 4.2, page 9 (see 'References'). In the implementation here, the contributions are rescaled to sum up to 1.
contribution

Usage

contribution(object, plot = TRUE, ...)

Arguments

object an object obtained from propagate.
plot logical. If TRUE, a barplot with the contributions is plotted.
... other parameters for barplot.

Details

\[ C_i = \frac{\partial f}{\partial x_i} \sigma_i \]

with \( C_i \) = the "contribution", which is calculated by \( \text{object}\$evalGrad \times \text{sqrt(diag(object}\$\text{covMat})\).

Value

A named vector with relative contributions for each variable and a barplot of the values, if \( \text{plot} = \text{TRUE} \).

Author(s)

Andrej-Nikolai Spiess

References


Examples

EXPR1 <- expression(x*y)
x <- c(5, 0.2)
y <- c(1, 0.1)
DF1 <- cbind(x, y)
RES1 <- propagate(expr = EXPR1, data = DF1, type = "stat",
                  do.sim = TRUE, verbose = TRUE)
contribution(RES1)
Cor2Cov

Converting a correlation matrix into a covariance matrix

Description

Converts a correlation matrix into a covariance matrix using variance information. It is therefore the opposite of cov2cor.

Usage

cor2cov(C, var)

Arguments

C a symmetric numeric correlation matrix C.
var a vector of variances \( \sigma_n^2 \).

Details

Calculates the covariance matrix \( \Sigma \) using a correlation matrix \( C \) and outer products of the standard deviations \( \sigma_n \):

\[
\Sigma = C \cdot \sqrt{\sigma_n^2} \otimes \sqrt{\sigma_n^2}
\]

Value

The corresponding covariance matrix.

Author(s)

Andrej-Nikolai Spiess

Examples

```r
## Example in Annex H.2 from the GUM 2008 manual
## (see 'References'), simultaneous resistance
## and reactance measurement.
data(H.2)
attach(H.2)

## Original covariance matrix.
COV <- cov(H.2)
## extract variances
VAR <- diag(COV)

## cor2cov covariance matrix.
COV2 <- cor2cov(cor(H.2), VAR)

## Equal to original covariance matrix.
all.equal(COV2, COV)
```
**Datasets**

Datasets from the GUM "Guide to the expression of uncertainties in measurement" (2008)

**Description**

Several datasets found in "Annex H" of the GUM that are used in illustrating the different approaches to quantifying measurement uncertainty.

**Usage**

H. 2  
H. 3  
H. 4

**Details**

**H.2: Simultaneous resistance and reactance measurement, Table H.2**

This example demonstrates the treatment of multiple measurands or output quantities determined simultaneously in the same measurement and the correlation of their estimates. It considers only the random variations of the observations; in actual practice, the uncertainties of corrections for systematic effects would also contribute to the uncertainty of the measurement results. The data are analysed in two different ways with each yielding essentially the same numerical values.

H.2.1 The measurement problem:

The resistance $R$ and the reactance $X$ of a circuit element are determined by measuring the amplitude $V$ of a sinusoidally-alternating potential difference across its terminals, the amplitude $I$ of the alternating current passing through it, and the phase-shift angle $\phi$ of the alternating potential difference relative to the alternating current. Thus the three input quantities are $V$, $I$, and $\phi$ and the three output quantities - the measurands - are the three impedance components $R$, $X$, and $Z$. Since $Z^2 = R^2 + X^2$, there are only two independent output quantities.

H.2.2 Mathematical model and data:

The measurands are related to the input quantities by Ohm’s law:

$$R = \frac{V}{I} \cos \phi; \quad X = \frac{V}{I} \sin \phi; \quad Z = \frac{V}{I} \quad (H.7)$$

**H.3: Calibration of a thermometer, Table H.6**

This example illustrates the use of the method of least squares to obtain a linear calibration curve and how the parameters of the fit, the intercept and slope, and their estimated variances and covariance, are used to obtain from the curve the value and standard uncertainty of a predicted correction.

H.3.1 The measurement problem:

A thermometer is calibrated by comparing $n = 11$ temperature readings $t_k$ of the thermometer, each having negligible uncertainty, with corresponding known reference temperatures $t_{R,k}$ in the temperature range 21°C to 27°C to obtain the corrections $b_k = t_{R,k} - t_k$ to the readings. The measured corrections $b_k$ and measured temperatures $t_k$ are the input quantities of the evaluation. A linear calibration curve

$$b(t) = y_1 + y_2(t - t_0) \quad (H.12)$$
is fitted to the measured corrections and temperatures by the method of least squares. The parameters \( y_1 \) and \( y_2 \), which are respectively the intercept and slope of the calibration curve, are the two measurands or output quantities to be determined. The temperature \( t_0 \) is a conveniently chosen exact reference temperature; it is not an independent parameter to be determined by the least-squares fit. Once \( y_1 \) and \( y_2 \) are found, along with their estimated variances and covariance, Equation (H.12) can be used to predict the value and standard uncertainty of the correction to be applied to the thermometer for any value \( t \) of the temperature.

**H.4: Measurement of activity, Table H.7**

This example is similar to example H.2, the simultaneous measurement of resistance and reactance, in that the data can be analysed in two different ways but each yields essentially the same numerical result. The first approach illustrates once again the need to take the observed correlations between input quantities into account.

**H.4.1 The measurement problem:**

The unknown radon \( ^{222}\text{Rn} \) activity concentration in a water sample is determined by liquid-scintillation counting against a radon-in-water standard sample having a known activity concentration. The unknown activity concentration is obtained by measuring three counting sources consisting of approximately 5g of water and 12g of organic emulsion scintillator in vials of volume 22ml:

- Source (a) a *standard* consisting of a mass \( m_S \) of the standard solution with a known activity concentration;
- Source (b) a matched *blank* water sample containing no radioactive material, used to obtain the background counting rate;
- Source (c) the *sample* consisting of an aliquot of mass \( m_x \) with unknown activity concentration.

Six cycles of measurement of the three counting sources are made in the order standard - blank - sample; and each dead-time-corrected counting interval \( T_0 \) for each source during all six cycles is 60 minutes. Although the background counting rate cannot be assumed to be constant over the entire counting interval (65 hours), it is assumed that the number of counts obtained for each blank may be used as representative of the background counting rate during the measurements of the standard and sample in the same cycle. The data are given in Table H.7, where \( t_S, t_B, t_x \) are the times from the reference time \( t = 0 \) to the midpoint of the dead-time-corrected counting intervals \( T_0 = 60 \) min for the standard, blank, and sample vials, respectively; although \( t_B \) is given for completeness, it is not needed in the analysis;

\( C_S, C_B, C_x \) are the number of counts recorded in the dead-time-corrected counting intervals \( T_0 = 60 \) min for the standard, blank, and sample vials, respectively.

The observed counts may be expressed as

\[
C_S = C_B + \epsilon A_S T_0 m_S e^{-\lambda t_S} \quad (H.18a)
\]
\[
C_x = C_B + \epsilon A_x T_0 m_x e^{-\lambda t_x} \quad (H.18b)
\]

where

- \( \epsilon \) is the liquid scintillation detection efficiency for \( ^{222}\text{Rn} \) for a given source composition, assumed to be independent of the activity level;
- \( A_S \) is the activity concentration of the standard at the reference time \( t = 0 \);
- \( A_x \) is the measurand and is defined as the unknown activity concentration of the sample at the reference time \( t = 0 \);
- \( m_S \) is the mass of the standard solution;
- \( m_x \) is the mass of the sample aliquot;
- \( \lambda \) is the decay constant for \( ^{222}\text{Rn} \): \( \lambda = (\ln 2)/T_{1/2} = 1.25894 \cdot 10^{-4} \) min\(^{-1}\)(\( T_{1/2} = 5505.8 \) min).
(...) This suggests combining Equations (H.18a) and (H.18b) to obtain the following expression for the unknown concentration in terms of the known quantities:

\[ ... = A_S \frac{m_S}{m_x} \frac{C_x - C_B}{C_S - C_B} e^{\lambda(t_x - t_S)} \] (H.19)

where \((C_x - C_B)e^{\lambda t_x}\) and \((C_S - C_B)e^{\lambda t_S}\) are, respectively, the background-corrected counts of the sample and the standard at the reference time \(t = 0\) and for the time interval \(T_0 = 60\) min.

Author(s)
Andrej-Nikolai Spiess, taken mainly from the GUM 2008 manual.

References

Evaluation of measurement data - Supplement 1 to the Guide to the expression of uncertainty in measurement - Propagation of distributions using a Monte Carlo Method.

Examples
```r
## See "Examples" in 'propagate'.
```

---

**fitDistr**

*Fitting distributions to observations/Monte Carlo simulations*

**Description**

This function fits 21 different continuous distributions by (weighted) NLS to the histogram or kernel density of the Monte Carlo simulation results as obtained by `propagate` or any other vector containing large-scale observations. Finally, the fits are sorted by ascending AIC.

**Usage**

```r
fitDistr(object, type = c("hist", "dens"), nbin = 100,
          weights = NULL, verbose = TRUE, plot = TRUE, ...)
```

**Arguments**

- `object` an object of class 'propagate' or a vector containing observations.
- `type` probability density functions are fitted to either the density values of the "hist"ogram or of the kernel "dens"ity estimates.
- `nbin` in case of `type = "hist"`, the number of bins in the histogram.
weights numeric or logical. Either a numeric vector of weights, or if TRUE, the distributions are fitted with weights = 1/(counts per bin).

verbose logical. If TRUE, steps of the analysis are printed to the console.

plot logical. If TRUE, a plot with the "best" distribution (in terms of lowest AIC) on top of the histogram or kernel density curve is displayed.

... other parameters to be passed to density or histogram.

Details

Fits the following 21 distributions using residual sum-of-squares as the minimization criterion for optim:

2) Skewed-normal distribution (propagate::dsn) => http://en.wikipedia.org/wiki/Skew_normal_distribution
4) Log-normal distribution (dlnorm) => http://en.wikipedia.org/wiki/Log-normal_distribution
5) Scaled and shifted t-distribution (propagate::dst) => GUM 2008, Chapter 6.4.9.2.
8) Triangular distribution (propagate::dtriang) => http://link.springer.com/article/10.1007%2Fs001840200230
9) Trapezoidal distribution (propagate::dtrap) => http://link.springer.com/article/10.1007%2Fs001840200230
10) Curvilinear Trapezoidal distribution (propagate::dctrap) => GUM 2008, Chapter 6.4.3.1
14) Laplace distribution (propagate::dlaplace) => http://en.wikipedia.org/wiki/Laplace_distribution
15) Gumbel distribution (propagate::dgumbel) => http://en.wikipedia.org/wiki/Gumbel_distribution
16) Johnson SU distribution (propagate::dJSU) => http://en.wikipedia.org/wiki/Johnson_SU_distribution
17) Johnson SB distribution (propagate::dJSB) => http://www.mathwave.com/articles/johnson_sb_distribution.html
18) Three-parameter Weibull distribution (propagate::dweibull2) => http://en.wikipedia.org/wiki/Weibull_distribution
19) Four-parameter beta distribution (propagate::dbeta2) => http://en.wikipedia.org/wiki/Beta_distribution#Four_parameters_2
20) Arcsine distribution (propagate::darcsin) => http://en.wikipedia.org/wiki/Arcsine_distribution
Distributions 3) and 16) - 19) are sometimes hard to fit because the start parameters are not readily deducible from the kernel density estimates or some parameters are highly sensitive to shape changes. For these five cases, a grid of starting values with different magnitudes is used to obtain the best parameter combination with respect to lowest residual sum-of-squares ("brute force" approach).

The goodness-of-fit (GOF) is calculated with AIC from the (weighted) log-likelihood of the fit:

\[
\ln(L) = 0.5 \cdot \left( -N \cdot \left( \ln(2\pi) + 1 + \ln(N) - \sum_{i=1}^{n} \log(w_i) + \ln \left( \sum_{i=1}^{n} w_i \cdot x_i^2 \right) \right) \right), \quad \text{AIC} = 2k - 2\ln(L)
\]

with \( x_i \) = the residuals from the NLS fit, \( N \) = the length of the residual vector, \( k \) = the number of parameters of the fitted model and \( w_i \) = the weights.

In contrast to some other distribution fitting softwares (i.e. Easyfit, Mathwave) that use residual sum-of-squares/Anderson-Darling/Kolmogorov-Smirnov statistics as GOF measures, the application of AIC accounts for increasing number of parameters in the distribution fit and therefore compensates for overfitting. Hence, this approach is more similar to ModelRisk (Vose Software) and as employed in fitdist of the 'MASS' package. Another application is to identify a possible distribution for the raw data prior to using Monte Carlo simulations from this distribution. However, a decent number of observations should be at hand in order to obtain a realistic estimate of the proper distribution. See 'Examples'.

The code for the density functions is in file "distr-densities.R".

IMPORTANT: It can be feasible to set weights = TRUE in order to give more weight to bins with low counts. See 'Examples'.

ALSO: Distribution fitting is highly sensitive to the number of defined histogram bins, so it is advisable to change this parameter and inspect if the order of fitted distributions remains stable!

Value

A list with the following items:

aic: the ascendingly sorted AIC dataframe.
fit: a list of the results from nls.lm for each distribution model.
bestfit: the best model in terms of lowest AIC.
fitted: the fitted values from the best model.
residuals: the residuals from the best model.

Author(s)

Andrej-Nikolai Spiess

References

Continuous univariate distributions, Volume 1.
Johnson NL, Kotz S and Balakrishnan N.
A guide on probability distributions.
R-forge distributions core team.
Univariate distribution relationships.
Leemis LM and McQueston JT.

Examples

```r
## Not run:
## Linear example, small error
## => family of normal distributions.
EXPR1 <- expression(x + 2 * y)
x <- c(5, 0.01)
y <- c(1, 0.01)
DF1 <- cbind(x, y)
RES1 <- propagate(expr = EXPR1, data = DF1, type = "stat",
    do.sim = TRUE, verbose = TRUE)
fitDistr(RES1)$aic

## Ratio example, larger error
## => family of skewed distributions.
EXPR2 <- expression(x/2 * y)
x <- c(5, 0.1)
y <- c(1, 0.02)
DF2 <- cbind(x, y)
RES2 <- propagate(expr = EXPR2, data = DF2, type = "stat",
    do.sim = TRUE, verbose = TRUE)
fitDistr(RES2)$aic

## Exponential example, large error
## => family of log-normal distributions.
EXPR3 <- expression(x*(2 * y))
x <- c(5, 0.1)
y <- c(1, 0.1)
DF3 <- cbind(x, y)
RES3 <- propagate(expr = EXPR3, data = DF3, type = "stat",
    do.sim = TRUE, verbose = TRUE)
fitDistr(RES3)$aic

## Rectangular input distributions result
## in trapezoidal output distribution.
A <- runif(100000, 20, 25)
B <- runif(100000, 3, 3.5)
DF4 <- cbind(A, B)
EXPR4 <- expression(A + B)
RES4 <- propagate(EXPR4, data = DF4, type = "sim",
    use.cov = FALSE, do.sim = TRUE)
fitDistr(RES4)$aic

## Fitting with 1/counts as weights.
EXPR5 <- expression(x + 2 * y)
x <- c(5, 0.05)
y <- c(1, 0.05)
DF5 <- cbind(x, y)
RES5 <- propagate(expr = EXPR5, data = DF5, type = "stat",
    do.sim = TRUE, verbose = TRUE)
```
**Description**

Calculates the uncertainty of a model by using interval arithmetics based on a "combinatorial sequence grid evaluation" approach, thereby avoiding the classical dependency problem that inflates the result interval.

**Usage**

`interval(df, expr, seq = 10, plot = TRUE)`

**Arguments**

- **df**: a 2-row dataframe/matrix with lower border values `A_i` in the first row and upper border values `B_i` in the second row. Column names must correspond to the variable names in `expr`.
- **expr**: an expression, such as `expression(x/y)`.
- **seq**: the sequence length from `A_i` to `B_i` in `[A_i, B_i]`.
- **plot**: logical. If `true`, plots the evaluations and min/max values as blue border lines.

**Details**

For two variables `x`, `y` with intervals `[x_1, x_2]` and `[y_1, y_2]`, the four basic arithmetic operations `(op) ∈ \{+,-,\cdot,/\}` are

\[
[x_1, x_2] \langle op \rangle [y_1, y_2] = 
\begin{align*}
&\min(x_1 \langle op \rangle y_1, x_1 \langle op \rangle y_2, x_2 \langle op \rangle y_1, x_2 \langle op \rangle y_2), \\
&\max(x_1 \langle op \rangle y_1, x_1 \langle op \rangle y_2, x_2 \langle op \rangle y_1, x_2 \langle op \rangle y_2)
\end{align*}
\]

So for a function `f([x_1, x_2], [y_1, y_2], [z_1, z_2], ...)` with `k` variables, we have to create all combinations `C_i = \{(x_1, x_2), (y_1, y_2), (z_1, z_2), ...\}`, evaluate their function values `R_i = f(C_i)` and select `R = [\min R_i, \max R_i]`.

The so-called **dependency problem** is a major obstacle to the application of interval arithmetic and arises when the same variable exists in several terms of a complicated and often nonlinear function. In these cases, over-estimation can cover a range that is significantly larger, i.e. `\min R_i \ll \min f(x, y, z, ...), \max R_i \gg \max f(x, y, z, ...)`. For an example, see [http://en.wikipedia.org/wiki/index.php?title=Interval_arithmetic](http://en.wikipedia.org/wiki/index.php?title=Interval_arithmetic) under "Dependency problem". A partial solution to this problem is to refine `R_i` by dividing `[x_1, x_2]` into `i` smaller subranges to obtain sequence `(x_1, x_{1.1}, x_{1.2}, x_{1.i}, x_2)`. Again, all combinations are evaluated as described above, resulting in a larger number of `R_i` in which `\min R_i` and `\max R_i` may be closer to `\min f(x, y, z, ...)` and `\max f(x, y, z, ...)`, respectively. This is the "combinatorial sequence grid evaluation" approach.
which works quite well in scenarios where monotonicity changes direction (see 'Examples'), obvi-
ating the need to create multivariate derivatives (Hessians) or use some multivariate minimization
algorithm.
If intervals are of type \([- x_1, x_2] \), a zero is included into the middle of the sequence to avoid
wrong results in case of even powers, i.e. \([-1, 1]^2 = [-1, 1][-1, 1] = [-1, 1]\) when actually the
right interval is \([0, 1]\), see curve\((x^2, -1, 1)\).

Value

A 2-element vector with the resulting interval and an (optional) plot of all evaluations.

Author(s)

Andrej-Nikolai Spiess

Examples

```
## Example 1: even squaring of negative interval.
EXPR1 <- expression(x^2)
DAT1 <- data.frame(x = c(-1, 1))
interval(DAT1, EXPR1)

## Example 2: A complicated nonlinear model.
## Reduce sequence length to 2 => original interval
## for quicker evaluation.
EXPR2 <- expression(C * sqrt((520 * H * P)/(M * (t + 60))))
H <- c(64, 65)
M <- c(16, 16.2)
P <- c(361, 365)
t <- c(165, 170)
C <- c(38.4, 38.5)
DAT2 <- makedat(EXPR2)
interval(DAT2, EXPR2, seq = 2)

## Example 3: Body Mass Index taken from
EXPR3 <- expression(m/h^2)
m <- c(79.5, 80.5)
h <- c(1.795, 1.805)
DAT3 <- makedat(EXPR3)
interval(DAT3, EXPR3)

## Example 4: Linear model.
EXPR4 <- expression(a * x + b)
a <- c(1, 2)
b <- c(5, 7)
x <- c(2, 3)
DAT4 <- makedat(EXPR4)
interval(DAT4, EXPR4)

## Example 5: Overestimation from dependency problem.
# Original interval with seq = 2 => [1, 7]
```
EXP5 <- expression(x^2 - x + 1)
x <- c(-2, 1)
DAT5 <- makeDat(EXPR5)
interval(DAT5, EXPR5, seq = 2)

# Refine with large sequence => [0.75, 7]
interval(DAT5, EXPR5, seq = 100)
# Tallies with curve function.
curve(x^2 - x + 1, -2, 1)

## Example 6: Underestimation from dependency problem.
## Original interval with seq = 2 => [0, 0]
EXPR6 <- expression(x - x^2)
x <- c(0, 1)
DAT6 <- makeDat(EXPR6)
interval(DAT6, EXPR6, seq = 2)

# Refine with large sequence => [0, 0.25]
interval(DAT6, EXPR6, seq = 100)
# Tallies with curve function.
curve(x - x^2, 0, 1)

---

**makeDat**  
*Create a dataframe from the variables defined in an expression*

**Description**

Creates a dataframe from the variables defined in an expression by *cbinding* the corresponding data found in the workspace. This is a convenience function for creating a dataframe to be passed to *propagate*, when starting with data which was simulated from distributions, i.e. when *type* = "sim". Will throw an error if a variable is defined in the expression but is not available from the workspace.

**Usage**

```r
makeDat(expr)
```

**Arguments**

- `expr` an expression to be use for *propagate*.

**Value**

A dataframe containing the data defined in `expr` in columns.

**Author(s)**

Andrej-Nikolai Spiess
Examples

```r
## Simulating from uniform
## and normal distribution,
## run 'propagate'.
EXPR1 <- expression(a + b*c)
a <- rnorm(100000, 12, 1)
b <- rnorm(100000, 5, 0.1)
c <- runif(100000, 6, 7)

DAT1 <- makeDat(EXPR1)
propagate(EXPR1, DAT1, type = "sim", cov = FALSE)
```

makeDerivs

*Utility functions for creating Gradient- and Hessian-like matrices with symbolic derivatives and evaluating them in an environment*

Description

These are three different utility functions that create matrices containing the symbolic partial derivatives of first (`makeGrad`) and second (`makeHess`) order and a function for evaluating these matrices in an environment. The evaluations of the symbolic derivatives are used within the `propagate` function to calculate the propagated uncertainty, but these functions may also be useful for other applications.

Usage

```r
makeGrad(expr, order = NULL)
makeHess(expr, order = NULL)
evalDerivs(deriv, envir)
```

Arguments

- `expr` an expression, such as `expression(x/y)`.
- `order` order of creating partial derivatives, i.e. c(2, 1). See 'Examples'.
- `deriv` a matrix returned from `makeGrad` or `makeHess`.
- `envir` an environment to evaluate in. By default the workspace.

Details

Given a function \( f(x_1, x_2, \ldots, x_n) \), the following matrices containing symbolic derivatives of \( f \) are returned:

**makeGrad:**

\[
\nabla(f) = \left[ \frac{\partial f}{\partial x_1}, \ldots, \frac{\partial f}{\partial x_n} \right]
\]
makeHess:

\[ H(f) = \begin{bmatrix}
\frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\
\frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2}
\end{bmatrix} \]

Value
The symbolic or evaluated Gradient/Hessian matrices.

Author(s)
Andrej-Nikolai Spiess

References
Petersen KB & Pedersen MS.

Examples
EXPR <- expression(a^b + sin(c))
ENVIR <- list(a = 2, b = 3, c = 4)

## First-order partial derivatives: Gradient.
GRAD <- makeGrad(EXPR)

## This will evaluate the Gradient.
evalDerivs(GRAD, ENVIR)

## Second-order partial derivatives: Hessian.
HESS <- makeHess(EXPR)

## This will evaluate the Hessian.
evalDerivs(HESS, ENVIR)

## Change derivatives order.
GRAD <- makeGrad(EXPR, order = c(2,1,3))
evalDerivs(GRAD, ENVIR)
Description

These two functions are fast C++ versions for column- and row-wise variance calculation on matrices/data.frames and are meant to substitute the classical apply(mat, 1, var) approach.

Usage

```r
colVarsC(x)
rowVarsC(x)
```

Arguments

- `x` a matrix or data.frame

Details

They are coded in a way that they automatically remove NA values, so they behave like na.rm = TRUE.

Value

A vector with the variance values.

Author(s)

Andrej-Nikolai Spiess

Examples

```r
## Speed comparison on large matrix.
## ~110x speed increase!
## Not run:
MAT <- matrix(rnorm(10 * 500000), ncol = 10)
system.time(RES1 <- apply(MAT, 1, var))

system.time(RES2 <- rowVarsC(MAT))
all.equal(RES1, RES2)

## End(Not run)
```
mixcov

Mixing covariances matrices, raw data, summary data or error values into a single covariance matrix.

Description

This function 'mixes' (aggregates) data from covariances matrices, raw and summary (mu, error) data or single error values into one final covariance matrix suitable for use in `propagate`.

Usage

```r
mixcov(..., use = "everything", method = "pearson")
```

Arguments

- `...`: either covariance matrices, raw data, summary data or error values to be aggregated into a single covariance matrix.
- `use`: see `cov`.
- `method`: see `cov`.

Details

'Mixes' (aggregates) data of the following types into a final covariance matrix:

1) matrix/dataframe `A` of raw data with \( A_1, A_2, \ldots, A_m \) variables and at least two observations per variable. This will be transformed into a covariance matrix.

2) vectors of summary data of type `c(mu, sigma)`.

3) covariance matrices `V` that are already available.

4) single error values `sigma`.

This is accomplished by filling a \( m_1 + m_2 + \ldots + m_n \) sized square matrix `C` successively with elements 1 \( \ldots m_1, m_1 + 1 \ldots m_1 + m_2, \ldots, m_n + 1 \ldots m_n + m_{n+1} \) with either covariance matrices at \( C_{m_n+1 \ldots m_n+m_{n+1}, m_n+1 \ldots m_n+m_{n+1}} \) or single variance values on the diagonals at \( C_{m_n, m_n} \).

Value

The 'mixed' (aggregated) covariance matrix.

Author(s)

Andrej-Nikolai Spiess
References

Evaluation of measurement data - Guide to the expression of uncertainty in measurement.

Evaluation of measurement data - Supplement 1 to the Guide to the expression of uncertainty in measurement - Propagation of distributions using a Monte Carlo Method.

Examples

########################################################################
## Example in Annex H.4 from the GUM 2008 manual
## (see 'References'), measurement of activity.
## This will give exactly the same values as Table H.8.
data(H.4)
attach(H.4)
T0 <- 60
lambda <- 1.25894E-4
Rx <- ((Cx - Cb)/60) * exp(lambda * tx)
Rs <- ((Cs - Cb)/60) * exp(lambda * ts)

mRx <- mean(Rx)
sRx <- sd(Rx)/sqrt(6)
mRx
sRx

mRs <- mean(Rs)
sRs <- sd(Rs)/sqrt(6)
mRs
sRs

R <- Rx/Rs
mR <- mean(R)
sR <- sd(R)/sqrt(6)
mR
sR

cor(Rx, Rs)

## Definition as in H.4.3.
As <- c(0.1368, 0.0018)
ms <- c(5.0192, 0.005)
mx <- c(5.0571, 0.001)

## We have to scale Rs/Rx by sqrt(6) to get the
## corresponding covariances.
Rs <- Rs/sqrt(6)
Rx <- Rx/sqrt(6)

## Here we mix the raw data in matrix format
moments

Skewness and (excess) Kurtosis of a vector of values

Description

These functions calculate skewness and excess kurtosis of a vector of values. They were taken from the package 'moments'.

Usage

skewness(x, na.rm = FALSE)
kurtosis(x, na.rm = FALSE)

Arguments

x          a numeric vector, matrix or data frame.
na.rm      logical. Should missing values be removed?

Details

Skewness:
\[
\frac{1}{n} \sum_{i=1}^{n} (x_i - \bar{x})^3 \left( \frac{1}{n} \sum_{i=1}^{n} (x_i - \bar{x})^2 \right)^{3/2}
\]

(Excess) Kurtosis:
\[
\frac{1}{n} \sum_{i=1}^{n} (x_i - \bar{x})^4 \left( \frac{1}{n} \sum_{i=1}^{n} (x_i - \bar{x})^2 \right)^2 - 3
\]
**Value**

The skewness/kurtosis values.

**Author(s)**

Andrej-Nikolai Spiess

**Examples**

```r
X <- rnorm(100, 20, 2)
skewness(X)
kurtosis(X)
```

---

**numDerivs**

*Functions for creating Gradient and Hessian matrices by numerical differentiation (Richardson’s method) of the partial derivatives*

**Description**

These two functions create Gradient and Hessian matrices by Richardson’s central finite difference method of the partial derivatives for any expression.

**Usage**

```r
numGrad(expr, envir = .GlobalEnv)
numHess(expr, envir = .GlobalEnv)
```

**Arguments**

- `expr`: an expression, such as `expression(x/y)`.
- `envir`: the `environment` to evaluate in.

**Details**

Calculates first- and second-order numerical approximation using Richardson’s **central difference** formula:

\[
\begin{align*}
    f'_i(x) & \approx \frac{f(x_1, \ldots, x_i + d, \ldots, x_n) - f(x_1, \ldots, x_i - d, \ldots, x_n)}{2d} \\
    f''_i(x) & \approx \frac{f(x_1, \ldots, x_i + d, \ldots, x_n) - 2f(x_1, \ldots, x_n) + f(x_1, \ldots, x_i - d, \ldots, x_n)}{d^2}
\end{align*}
\]

**Value**

The numeric Gradient/Hessian matrices.
Note

The two functions are modified versions of the `gend` function in the `numDeriv` package, but a bit more easy to handle because they use expressions and the function's x value must not be defined as splitted scalar values x[1], x[2], ... in the body of the function.

Author(s)

Andrej-Nikolai Spiess

Examples

```r
## Check for equality of symbolic
## and numerical derivatives.
EXPR <- expression(2*x + sin(2 * y) - cos(z))
x <- 5
y <- 10
z <- 20

symGRAD <- evalDerivs(makeGrad(EXPR))
numGRAD <- numGrad(EXPR)
all.equal(symGRAD, numGRAD)

symHES <- evalDerivs(makeHess(EXPR))
numHES <- numHess(EXPR)
all.equal(symHES, numHES)
```

Description

Creates two different plots from `propagate` objects:
i) a histogram of the evaluated results from the multivariate simulated data, along with a density curve and 95% confidence intervals.
ii) a boxplot of the evaluated results from the multivariate simulated data, along with first- and second-order mean/s.d. and 95% confidence intervals.

Usage

```r
## S3 method for class 'propagate'
plot(x, logx = FALSE, ...)
```

Arguments

- `x` an object returned from `propagate`.
- `logx` logical. Should the data be displayed on a logarithmic abscissa?
- `...` other parameters to `hist` or `boxplot`.
Value

A plot as described above.

Author(s)

Andrej-Nikolai Spiess

Examples

```r
EXPR1 <- expression(x^2 * sin(y))
x <- c(5, 0.01)
y <- c(1, 0.01)
DF1 <- cbind(x, y)
RES1 <- propagate(expr = EXPR1, data = DF1, type = "stat",
                 do.sim = TRUE, verbose = TRUE)
plot(RES1)
```

Description

A function for calculating confidence intervals for the fitted values of nonlinear models by using first-/second-order Taylor expansion and Monte Carlo simulation. This approach can be used to construct more realistic error estimates and confidence/prediction intervals for nonlinear models than what is possible with only a simple linearization (first-order Taylor expansion) approach. Another application is when there is an "error in x" setup with uncertainties in the predictor variable (See 'Examples'). This function will also work in the presence of multiple predictors with/without errors.

Usage

```r
predictNLS(model, newdata, interval = c("confidence", "prediction", "none"),
            alpha = 0.05, ...)
```

Arguments

- **model**: a model obtained from `nls` or `nlsLM` (package 'minpack.lm').
- **newdata**: A named list or data frame in which to look for variables with which to predict. The first \( n \) columns must contain the predictor values, the following \( n \) columns can contain errors. See `predict.nls` and 'Examples'.
- **interval**: A character string indicating if confidence/prediction intervals on the mean responses are to be calculated or not.
- **alpha**: the 1 - confidence level.
- ... other parameters to be supplied to `propagate`. 
**Details**

Calculation of the propagated uncertainty $\sigma_y^2$ using $\nabla_x C_x \nabla_x^T$ is called the "Delta Method" and is widely applied in NLS fitting. However, this method is based on first-order Taylor expansion and thus assumes linearity around $f(x)$. The second-order approach as implemented in the `propagate` function can partially correct for this restriction by using a second-order polynomial around $f(x)$.

Confidence/prediction intervals are calculated in a usual way using $t(1 - \frac{\alpha}{2}, \nu) \cdot \sigma_{prop}$ or $t(1 - \frac{\alpha}{2}, \nu) \cdot \sqrt{\sigma_{prop}^2 + rv}$, respectively, where $rv$ is the residual variance $\sum_{i=1}^{n} (y_i - \hat{y}_i)^2 / (n - \nu)$. If errors are supplied to the predictor values in `newdata`, for $n$ predictor values they have to be in the next $n$ columns, i.e. predictors in $[, 1:3]$, and errors in $[, 4:6]$.

**Value**

A list with the following items:

- summary: The mean/error estimates obtained from first-/second-order Taylor expansion and Monte Carlo simulation, together with calculated confidence/prediction intervals based on asymptotic normality.
- prop: the complete output from `propagate` for each value in `newdata`.

**Author(s)**

Andrej-Nikolai Spiess

**References**

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Bates DM & Watts DG.

Statistical Error Propagation.
Tellinghuisen J.

Least-squares analysis of data with uncertainty in x and y: A Monte Carlo methods comparison.
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From the author’s blog:
http://rmazing.wordpress.com/2013/08/14/predictnls-part-1-monte-carlo-simulation-confidence-intervals-for-nls-models/

**Examples**

```r
## Example from ?nls.
DNasel <- subset(DNase, Run == 1)
```
predictNLS

```r
fm3DNase1 <- nls(density ~ Asym/(1 + exp((xmid - log(conc))/scal)),
                 data = DNase1, start = list(Asym = 3, xmid = 0, scal = 1))

## Using a single predictor value without error.
PROP1 <- predictNLS(fm3DNase1, newdata = data.frame(conc = 2))
PRED1 <- predict(fm3DNase1, newdata = data.frame(conc = 2))
PROP1$summary
PRED1
## => Prop.Mean.1 equal to PRED1

## Not run:
## Using a sequence of predictor values without error.
CONC <- seq(1, 12, by = 1)
PROP2 <- predictNLS(fm3DNase1, newdata = data.frame(conc = CONC))
PRED2 <- predict(fm3DNase1, newdata = data.frame(conc = CONC))
PROP2$summary
PRED2
## => Prop.Mean.1 equal to PRED2

## Using a sequence of predictor values with error.
DAT <- data.frame(conc = CONC, error = rnorm(12, 0, 0.1))
PROP3 <- predictNLS(fm3DNase1, newdata = DAT)
PRED3 <- predict(fm3DNase1, newdata = DAT)
PROP3$summary
PRED3
## => Prop.Mean.1 equal to PRED3

## Plot predicted and confidence values from
## first-/second-order Taylor expansion
## and Monte Carlo simulation.
plot(DNase1$conc, DNase1$density)
lines(DNase1$conc, fitted(fm3DNase1), lwd = 2, col = 1)
points(CONC, PROP2$summary[, 1], col = 2, pch = 16)
lines(CONC, PROP2$summary[, 5], col = 2)
lines(CONC, PROP2$summary[, 6], col = 2)

## End(Not run)

## Using multiple predictor values
## 1: Setup of response values
## with gaussian error of 10%.
x <- seq(1, 10, by = 0.01)
y <- seq(10, 1, by = -0.01)
a <- 2
b <- 5
c <- 10
z <- a * exp(b * x)^sin(y/c)
z <- z + sapply(z, function(x) rnorm(1, x, 0.1 * x))

## 2: Fit 'nls' model.
MOD <- nls(z ~ a * exp(b * x)^sin(y/c),
          start = list(a = 2, b = 5, c = 10))

## 3: Newdata without errors and prediction.
DAT1 <- data.frame(x = 4, y = 3)
```
print.propagate

Printing function for 'propagate' objects

Description

Prints the statistical results obtained from `propagate`.

Usage

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

Arguments

- `x` an object returned from `propagate`.
- `...` other parameters for future methods.

Value

A printed summary containing the results from error propagation and Monte Carlo simulation.

Author(s)

Andrej-Nikolai Spiess

Examples

```r
EXPR1 <- expression(x^2 * sin(y))
x <- c(5, 0.01)
y <- c(1, 0.01)
DF1 <- cbind(x, y)
RES1 <- propagate(expr = EXPR1, data = DF1, type = "stat",
                  do.sim = TRUE, verbose = TRUE)
RES1
```
propagate

Description

A general function for the calculation of uncertainty propagation by first-/second-order Taylor expansion and Monte Carlo simulation including covariances. Input data can be any symbolic/numeric differentiable expression and data based on replicates, summaries (mean & s.d.) or sampled from a distribution. Uncertainty propagation is based completely on matrix calculus accounting for full covariance structure. Monte Carlo simulation is conducted using multivariate normal or t-distributions with covariance structure.

Usage

propagate(expr, data, type = c("stat", "raw", "sim"), second.order = TRUE,
  do.sim = TRUE, dist.sim = c("norm", "t"), df.t = NULL,
  use.cov = TRUE, nsim = 100000, alpha = 0.05, ...)

Arguments

expr
  an expression, such as expression(x+y).

data
  a dataframe or matrix containing either a) the replicates in columns when using type = "raw", b) the means in first and standard deviations in second rows when using type = "stat" or c) sampled data generated from any of R’s distributions or those implemented in this package (rdistr), if type = "sim". Column names must match the variable names.

type
  either "stat" if means and standard deviations are supplied, "raw" if raw replicates are given or "sim" in case of simulated data.

second.order
  logical. If TRUE, error propagation will be calculated with first- and second-order Taylor expansion. See 'Details'.

do.sim
  logical. Should Monte Carlo simulation be applied?

dist.sim
  "norm" will use a multivariate normal distribution for Monte Carlo simulation, "t" a multivariate t-distribution. See 'Details'.

df.t
  degrees of freedom when using dist.sim = "t" and no raw observations are supplied (i.e. type = "stat" or type = "sim"). See 'Details'.

use.cov
  logical or variance-covariance matrix with the same column descriptions as data. See 'Details'.

nsim
  the number of Monte Carlo simulations to be performed, minimum is 10000.

alpha
  the 1 - confidence level.

... other parameters to be supplied to future methods.
Details

The implemented methods are:

1) Monte Carlo simulation:
For each variable $m$ in data, simulated data $x = [X_1, X_2, \ldots, X_n]$ with $n = n_{\text{sim}}$ samples is generated from a multivariate normal distribution $x_{m,n} \sim \mathcal{N}(\mu, \Sigma)$ or multivariate t-distribution $x_{m,n} \sim t(\mu, \Sigma, \nu)$ using means $\mu_m$ and covariance matrix $\Sigma$ constructed from the standard deviations $\sigma_m$ of each variable. All data is coerced into a new dataframe that has the same covariance structure as the initial data: $\Sigma(\text{data}) = \Sigma(x_{m,n})$. Each row $i = 1, \ldots, n$ of the simulated dataset $x_{m,n}$ is evaluated with expr. $y_i = f(x_{m,i})$, and summary statistics (mean, sd, median, mad, confidence interval based on alpha) are calculated on $y$. If sample sizes for raw replicated data when setting type = "raw" are small, simulation from a multivariate t-distribution is advocated (Possolo, 2010). If this is done, the resulting distribution can have very heavy tails resulting in less stringent estimates of $\sigma_y$ and larger confidence intervals. In this case, the degrees of freedom used are $n - 1$. However, when setting type = "stat" or type = "sim", the degrees of freedom have to be supplied by the user in df.t.

2) Error propagation:
The propagated error is calculated by first-/second-order Taylor expansion accounting for full covariance structure using matrix algebra.

The following transformations based on two variables $x_1, x_2$ illustrate the equivalence of the matrix-based approach with well-known classical notations:

**First-order mean:** $E[y] = f(\bar{x})$

**First-order variance:** $\sigma_y^2 = \nabla_x C_x \nabla_x^T$:

$$
\begin{bmatrix}
  j_1 j_2 \\
  j_1 \\
  j_2 
\end{bmatrix}
\begin{bmatrix}
  \sigma_1^2 \\
  \sigma_2 \sigma_1 \\
  \sigma_2 
\end{bmatrix}
\begin{bmatrix}
  j_1 j_2 \\
  j_1 \\
  j_2 
\end{bmatrix} =
\begin{array}{c}
  j_1 j_2 \sigma_1^2 + 2 j_1 j_2 \sigma_1 \sigma_2 + (j_2^2 \sigma_2^2) \\
  \sum_{i=1}^{2} j_i^2 \sigma_i^2 + \sum_{i=1}^{2} \sum_{j=1}^{2} j_i j_k \sigma_{i,j} \\
  \sum_{i=1}^{2} \sum_{j=1}^{2} j_i j_k \sigma_{i,j}
\end{array}
$$

Classical notation

**Second-order mean:** $E[y] = f(\bar{x}) + \frac{1}{2} \text{tr}(H_{xx} C_n)$:

$$
\begin{bmatrix}
  h_1 & h_2 \\
  h_3 & h_4 
\end{bmatrix}
\begin{bmatrix}
  \sigma_1^2 \\
  \sigma_2 \sigma_1 \\
  \sigma_2 
\end{bmatrix}
\begin{bmatrix}
  h_1 & h_2 \\
  h_3 & h_4 
\end{bmatrix} =
\begin{array}{c}
  \sigma_1^2 + h_1 \sigma_2 \sigma_1 + h_2 \sigma_2^2 \\
  h_1 \sigma_2 \sigma_1 + h_2 \sigma_2^2 \\
  h_1 \sigma_2 \sigma_1 + h_2 \sigma_2^2
\end{array}
$$

$$
= \frac{1}{2} \left( \sum_{i=1}^{2} \frac{\partial f}{\partial x_i} \right)^2 f
$$

**Second-order variance:** $\sigma_y^2 = \nabla_x C_x \nabla_x^T + \frac{1}{2} \text{tr}(H_{xx} C_n H_{xx} C_n)$:

$$
\begin{bmatrix}
  \sigma_1^2 & \sigma_1 \sigma_2 \\
  \sigma_2 \sigma_1 & \sigma_2 
\end{bmatrix}
\begin{bmatrix}
  \sigma_1^2 & \sigma_1 \sigma_2 \\
  \sigma_2 \sigma_1 & \sigma_2 
\end{bmatrix} =
\begin{array}{c}
  \sigma_1^2 \sigma_1^2 + 2 \sigma_1 \sigma_2 \sigma_1 \sigma_2 + \sigma_2^2 \sigma_2^2 \\
  \sum_{i=1}^{2} \sum_{j=1}^{2} j_i j_k \sigma_{i,j}
\end{array}
$$

$$
= \frac{1}{2} \left( \sum_{i=1}^{2} \frac{\partial f}{\partial x_i} \right)^2 f
$$
\[
= \frac{1}{2!} \left( \sum_{i=1}^{2} \partial_{x_i} \sigma_i \right)^2 f \right)^2
\]

with \( E(y) \) = expectation of \( y \), \( \sigma^2_y \) = variance of \( y \), \( \nabla_x \) = the \( p \times n \) gradient matrix with all partial first derivatives \( \partial_j \), \( C_x \) = the \( p \times p \) covariance matrix, \( H_{xx} \) the Hessian matrix with all partial second derivatives \( h_i \), \( \sigma_i \) = the uncertainties and \( \text{tr}(\cdot) \) = the trace (sum of diagonal) of a matrix. Note that because the hessian matrices are symmetric matrices, \( h_2 = h_3 \). For a detailed derivation, see 'References'.

The second-order Taylor expansion corrects for bias in nonlinear expressions as the first-order Taylor expansion assumes linearity around \( \bar{x}_i \). There is also a Python library available for second-order error propagation ('soerp', https://pypi.python.org/pypi/soerp). The 'propagate' package gives exactly the same results, see last example under "Examples".

Depending on the input expression, the error propagation may result in an error that is not normally distributed. The Monte Carlo simulation, starting with normal distributions of the variables, can clarify this. For instance, a high tendency from deviation of normality is encountered in formulas in which the error of the denominator is relatively large or in exponential models with a large error in the exponent.

For setups in which there is no symbolic derivation possible (i.e. \( e < expression(abs(x)) => \) "Function 'abs' is not in the derivatives table") the function automatically switches from symbolic (using makeGrad or makeHess) to numeric (numGrad or numHess) differentiation.

The function will try to evaluate the expression in an environment using eval which results in a significant speed enhancement (~ 10-fold). If that fails, evaluation is done over the rows of the simulated data using apply.

Value

A list with the following components:

- \( \text{datSIM} \) a vector containing the \( n_{sim} \) simulated multivariate values for each variable in column format.
- \( \text{resSIM} \) a vector containing the \( n_{sim} \) values obtained from the row-wise expression evaluations \( f(x_{m,i}) \) of the simulated data in \( \text{datSIM} \).
- \( \text{datPROP} \) \( n_{sim} \) values generated from a normal distribution with \( \mu \) and \( \sigma \) as calculated from the propagated error.
- \( \text{gradient} \) the symbolic gradient vector \( \nabla_x \) of partial first-order derivatives.
- \( \text{evalGrad} \) the evaluated gradient vector \( \nabla_x \) of partial first-order derivatives.
- \( \text{covMat} \) the covariance matrix \( C_x \) used for Monte Carlo simulation and error propagation.
- \( \text{hessian} \) the symbolic hessian matrix \( H_{xx} \) of partial second-order derivatives.
- \( \text{evalHess} \) the evaluated hessian matrix \( H_{xx} \) of partial second-order derivatives.
- \( \text{prop} \) a summary vector containing first-/second-order expectations and uncertainties as well as the confidence interval based on \( \alpha \) from \( \text{datPROP} \).
- \( \text{sim} \) a summary vector containing the mean, standard deviation, median, MAD as well as the confidence interval based on \( \alpha \) from \( \text{datSIM} \).
Author(s)
Andrej-Nikolai Spiess

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Royston P.
*Stat Comp* (1992), **2**: 117-119.

**Examples**

```r
## From summary data:
EXPR1 <- expression(x/y)
x <- c(5, 0.01)
y <- c(1, 0.01)
DF1 <- cbind(x, y)
RES1 <- propagate(expr = EXPR1, data = DF1, type = "stat",
                  do.sim = TRUE, verbose = TRUE)
RES1$prop
RES1$sim

## From raw data:
EXPR2 <- expression(x/y)
x <- c(2, 2.1, 2.2, 2, 2.3, 2.1)
y <- c(4, 4.1, 3.8, 4.1, 3.1, NA)
DF2 <- cbind(x, y)
RES2 <- propagate(expr = EXPR2, data = DF2, type = "raw",
                  do.sim = TRUE, verbose = TRUE)
RES2$prop
RES2$sim

## Compare to using a multivariate t-distribution
## because of low sample size => larger confidence
## intervals.
RES2b <- propagate(expr = EXPR2, data = DF2, type = "raw",
                   do.sim = TRUE, verbose = TRUE, dist.sim = "t")
RES2b$sim

## Example using a recursive function:
## no Taylor expansion possible, only Monte-Carlo.
a <- c(5, 0.1)
b <- c(100, 2)
DAT <- cbind(a, b)
```

```
propagate(f, DAT, nsim = 100000)

# Example in Annex H.1 from the GUM 2008 manual
# (see 'References'), an end gauge calibration study. At first, we will only use the first-order Taylor expansion.
EXPR3 <- expression(ls + d - ls * (da * the + as * dt))
ls <- c(50000023, 25)
d <- c(215, 9.7)
da <- c(0, 0.58E-6)
the <- c(-0.1, 0.41)
as <- c(11.5E-6, 1.2E-6)
dt <- c(0, 0.029)
DF3 <- cbind(ls, d, da, the, as, dt)
RES3 <- propagate(expr = EXPR3, data = DF3, type = "stat",
do.sim = TRUE, verbose = TRUE,
second.order = FALSE)
RES3$prop
RES3$sim

# Proof that covariance of Monte-Carlo simulated dataset is the same as from initial data.
RES3$covMat
cov(RES3$datSIM)
all.equal(RES3$covMat, cov(RES3$datSIM))

# Expanded uncertainty GUM H.1.6
# with 16 degrees of freedom.
qt(0.005, 16, lower.tail = FALSE) * 31.71
# propagate: 92.62
# GUM H.1.6: 93

# Second-order terms GUM H.1.7.
RES4 <- propagate(expr = EXPR3, data = DF3, type = "stat",
do.sim = TRUE, verbose = TRUE,
second.order = TRUE)
RES4$prop
RES4$sim

# Also similar to the non-matrix-based approach
## in Wang et al. (2005, page 408): u1 = 33.91115.
## NOTE: After second-order correction, uncertainty is more
## similar to the value obtained from Monte Carlo simulation!

### Example in Annex H.2 from the GUM 2008 manual
### (see 'References'), simultaneous resistance
### and reactance measurement.

data(H.2)

## This gives exactly the means, uncertainties and
## correlations as given in Table H.2:
colMeans(H.2)
sqrt(colVarsC(H.2))/sqrt(5)
cor(H.2)

### H.2.3 Approach 1 using mean values and
### standard uncertainties:
EXPR6a <- expression((V/I) * cos(phi)) ## R
EXPR6b <- expression((V/I) * sin(phi)) ## X
EXPR6c <- expression(V/I) ## Z
MEAN6 <- colMeans(H.2)
SD6 <- sqrt(colVarsC(H.2))
DF6 <- rbind(MEAN6, SD6)

COV6ab <- cov(H.2) ## covariance matrix of V, I, phi
COV6c <- cov(H.2[, 1:2]) ## covariance matrix of V, I

RES6a <- propagate(expr = EXPR6a, data = DF6, type = "stat",
do.sim = TRUE, verbose = TRUE, use.cov = COV6ab,
second.order = TRUE)

RES6b <- propagate(expr = EXPR6b, data = DF6, type = "stat",
do.sim = TRUE, verbose = TRUE, use.cov = COV6ab,
second.order = TRUE)

RES6c <- propagate(expr = EXPR6c, data = DF6[, 1:2], type = "stat",
do.sim = TRUE, verbose = TRUE, use.cov = COV6c,
second.order = TRUE)

## This gives exactly the same values of mean and sd/sqrt(5)
## as given in Table H.4.
RES6a$prop
RES6b$prop
RES6c$prop

### Example in Annex H.3 from the GUM 2008 manual
### (see 'References'), calibration of a thermometer.
### For this example, we can use the predict.lm function
### of R directly to return the error of predicted values.
data(H.3)
LM <- lm(bk ~ I(tk - 20), data = H.3)
## This will give exactly the same values as in H.3.3.
summary(LM)

## This will give exactly the same values as the
## fourth column ("Predicted correction") of Table H.6.
predict(LM)

## This will give exactly the same values as the
## fifth column ("Difference...") of Table H.6.
H.3$b_k - predict(LM)

## Uncertainty in a predicted value. This will give
## exactly the values in H.3.4.
predict(LM, newdata = data.frame(tk = 30), se.fit = TRUE)

################################ GUM 2008 Supplement 1 (1) ################################
## Example from 9.2.2 of the GUM 2008 Supplement 1
## (see 'References'), normally distributed input
## quantities. Assign values as in 9.2.2.1.
EXPR7 <- expression(X1 + X2 + X3 + X4)
X1 <- c(0, 1)
X2 <- c(0, 1)
X3 <- c(0, 1)
X4 <- c(0, 1)
DF7 <- cbind(X1, X2, X3, X4)
RES7 <- propagate(expr = EXPR7, data = DF7, type = "stat",
                  do.sim = TRUE, verbose = TRUE, nsim = 1E5)
## This will give exactly the same results as in
## 9.2.2.6, Table 2.
RES7$prop
RES7$sim

################################ GUM 2008 Supplement 1 (2) ################################
## Example from 9.3 of the GUM 2008 Supplement 1
## (see 'References'), mass calibration.
## Formula 24 in 9.3.1.3 and values as in 9.3.1.4, Table 5.
EXPR8 <- expression((Mrc + dMrc) * (1 + (Pa - Pa0) * ((1/Pw) - (1/Pr))) - Mnom)
Mrc <- rnorm(1E5, 100000, 0.050)
dMrc <- rnorm(1E5, 1.234, 0.020)
Pa <- runif(1E5, 1.10, 1.30) ## E(Pa) = 1.2, (b_a)/2 = 0.1
Pw <- runif(1E5, 7000, 9000) ## E(Pw) = 8000, (b_a)/2 = 1000
Pr <- runif(1E5, 7950, 8050) ## E(Pr) = 8000, (b_a)/2 = 50
Pa0 <- 1.2
Mnom <- 100000
DF8 <- cbind(Mrc, dMrc, Pa, Pw, Pr, Pa0, Mnom)
RES8 <- propagate(expr = EXPR8, data = DF8, type = "sim",
                   do.sim = TRUE, verbose = TRUE, nsim = 1E5)
## This will give exactly the same results as in
## 9.3.2.3, Table 6
RES8$prop
RES8$sim

################################ GUM 2008 Supplement 1 (3) ################################
## Example from 9.4 of the GUM 2008 Supplement 1
## (see 'References'), comparison loss in microwave
## power meter calibration, zero covariance.
## Formula 28 in 9.4.1.5 and values as in 9.4.1.7.
EXPR9 <- expression(X1^2 - X2^2)
X1 <- c(0.050, 0.005)
X2 <- c(0, 0.005)
DF9 <- cbind(X1, X2)
RES9a <- propagate(expr = EXPR9, data = DF9, type = "stat",
do.sim = TRUE, verbose = TRUE, nsim = 1e5)
## This will give exactly the same results as in
## 9.4.2.2.7, Table 8, x1 = 0.050.
RES9a$prop
RES9a$sim

## Using covariance matrix with r(x1, x2) = 0.9
## We convert to covariances using cor2cov.
COR9 <- matrix(c(1, 0.9, 0.9, 1), nrow = 2)
COV9 <- cor2cov(COR9, c(0.005^2, 0.005^2))
colnames(COV9) <- c("X1", "X2")
rownames(COV9) <- c("X1", "X2")
RES9b <- propagate(expr = EXPR9, data = DF9, type = "stat",
use.cov = COV9, do.sim = TRUE,
verbose = TRUE, nsim = 1e5)
## This will give exactly the same results as in
## 9.4.3.2.1, Table 9, x1 = 0.050.
RES9b$prop
RES9b$sim

########## GUM 2008 Supplement 1 (4) ###########
## Example from 9.5 of the GUM 2008 Supplement 1
## Assignment of PDF's as in Table 10 of 9.5.2.1.
EXPR10 <- expression(Ls + D + d1 + d2 - Ls*(da*(t0 + Delta) + as * dt) - Lnom)
Lnom <- 50000000
Ls <- propagate::rstd(100000, mean = 50000623, sd = 25, df = 18)
D <- propagate::rstd(100000, mean = 215, sd = 6, df = 25)
d1 <- propagate::rstd(100000, mean = 0, sd = 4, df = 5)
d2 <- propagate::rstd(100000, mean = 0, sd = 7, df = 8)
as <- runif(100000, 9.5E-6, 13.5E-6)
t0 <- rnorm(100000, -0.1, 0.2)
Delta <- propagate::rarcsin(100000, -0.5, 0.5)
da <- propagate::rctrap(100000, -1E-6, 1E-6, 0.1E-6)
dt <- propagate::rctrap(100000, -0.050, 0.050, 0.025)
DF10 <- cbind(Ls, D, d1, d2, as, t0, Delta, da, dt, Lnom)
RES10 <- propagate(expr = EXPR10, data = DF10, type = "sim",
use.cov = FALSE, verbose = TRUE,
alpha = 0.01)
RES10
## This gives the same results as in 9.5.4.2, Table 11.
## However: results are exacter than in the GUM 2008
## manual, especially when comparing sd(Monte Carlo)
## sd(second-order Taylor expansion)
## GUM 2008 gives 32 and 36, respectively.
rDistr

Creating random samples from a variety of useful distributions

Description

These are random sample generators for 15 different continuous distributions which are not readily available as other distributions in R. Some of them are implemented in other specialized packages (i.e. `rsn` in package ‘sn’ or `rtrapezoid` in package ‘trapezoid’), but here they are collated in a way that makes them easily accessible for Monte Carlo-based uncertainty propagation.

Details

Random samples can be drawn from the following distributions:

1) Skewed-normal distribution: `propagate::rsn(n, location = 0, scale = 1, shape = 0)`
2) Generalized normal distribution: `propagate::rgnorm(n, alpha = 1, xi = 1, kappa = -0.1)`
3) Scaled and shifted t-distribution: `propagate::rst(n, mean = 0, sd = 1, df = 2)`
4) Gumbel distribution: `propagate::rgumbel(n, location = 0, scale = 1)`
5) Johnson SU distribution: `propagate::rjsu(n, xi = 0, lambda = 1, gamma = 1, delta = 1)`
6) Johnson SB distribution: `propagate::rjsb(n, xi = 0, lambda = 1, gamma = 1, delta = 1)`
7) 3P Weibull distribution: `propagate::rweibull2(n, location = 0, shape = 1, scale = 1)`
8) 4P Beta distribution: `propagate::rbeta2(n, alpha1 = 1, alpha2 = 1, a = 0, b = 0)`
9) Triangular distribution: `propagate::rtriang(n, a = 0, b = 1, c = 0.5)`
10) Trapezoidal distribution: `propagate::rtrap(n, a = 0, b = 1, c = 2, d = 3)`
11) Curvilinear Trapezoidal distribution: `propagate::rctrap(n, a = 0, b = 1, d = 0.1)`
12) Generalized trapezoidal distribution: `propagate::rgtrap(n, min = 0, model = 1/3, mode2 = 2/3, max = 1, n1 = 2, n3 = 2, alpha = 1)`
13) Laplacian distribution: `propagate::rlaplace(n, mean = 0, sigma = 1)`
14) Arcsine distribution: `propagate::rarcsin(n, a = 2, b = 1)`
15) von Mises distribution: `propagate::rmises(n, mu = 1, kappa = 3)`

with \( n \) = number of samples.
1) - 10) and 13) - 14) use the inverse cumulative distribution function as mapping functions for runif (Inverse Transform Method):

1) \( U \sim \mathcal{U}(0, 1) \)
2) \( Y = F^{-1}(U, \beta) \)

11), 12) and 15) employ "Rejection Sampling" using a uniform envelope distribution (Acceptance Rejection Method):

1) Find \( F_{max} = \max(F([x_{min}, x_{max}], \beta) \)
2) \( U_{max} = 1/(x_{max} - x_{min}) \)
3) \( A = F_{max}/U_{max} \)
4) \( U \sim \mathcal{U}(0, 1) \)
5) \( X \sim \mathcal{U}(x_{min}, x_{max}) \)
6) \( Y \iff U \leq A \cdot U(X, x_{min}, x_{max})/F(X, \beta) \)

These three distributions are coded in a vectorized approach and are hence not much slower than implementations in C/C++ (0.2 - 0.5 sec for 100000 samples; 3 GHz Quadcore processor, 4 GByte RAM).

The code for the random generators is in file "distr-samplers.R".

**Value**

A vector with \( n \) samples from the corresponding distribution.

**Author(s)**

Andrej-Nikolai Spiess

**References**

Inverse CDFs were taken from:
"The Ultimate Univariate Probability Distribution Explorer"

Rejection Sampling in R:
Playing with R: Rejection Sampling.

An example of rejection sampling.
http://www.mas.ncl.ac.uk/~ndjw1/teaching/sim/reject/circ.html.

Rejection Sampling in general:
Non-uniform random variate generation.
Devroye L.

Distributions:
Continuous univariate distributions, Volume 1.
Johnson NL, Kotz S and Balakrishnan N.
See Also

See also `propagate`, in which GUM 2008 Supplement 1 examples use these distributions.

Examples

```r
## Not run:
## First we create random samples from the
## von Mises distribution.
X <- propagate::rmises(100000, mu = 10, kappa = 3)

## then we fit all available distributions
## with 'fitDistr'.
fitDistr(X)$aic
## => von Mises wins! (lowest AIC)

## End(Not run)
```

statVec

Transform an input vector into one with defined mean and standard deviation

Description

Transforms an input vector into one with defined \( \mu \) and \( \sigma \) by using a scaled-and-shifted Z-transformation.

Usage

```r
statVec(x, mean, sd)
```

Arguments

- **x**: the input vector to be transformed.
- **mean**: the desired mean of the created vector.
- **sd**: the desired standard deviation of the created vector.

Details

Calculates vector \( V \) using a Z-transformation of the input vector \( X \) and subsequent scaling by \( sd \) and shifting by \( mean \):

\[
V = \frac{X - \mu_X}{\sigma_X} \cdot sd + mean
\]

Value

A vector with defined \( \mu \) and \( \sigma \).

Author(s)

Andrej-Nikolai Spiess
Examples

```r
## Create a 10-sized vector with mean = 10 and s.d. = 1.
X <- rnorm(10, 5, 2)
mean(X) # => mean is not 5!
sd(X) # => s.d. is not 2!

Z <- statVec(X, 5, 2)
mean(Z) # => mean is 5!
sd(Z) # => s.d. is 2!
```

summary.propagate  
Summary function for 'propagate' objects

Description

Provides a printed summary of the results obtained by `propagate`, such as statistics of the first/second-order uncertainty propagation, Monte Carlo simulation, the covariance matrix and symbolic as well as evaluated versions of the Gradient and Hessian matrices. If `do.sim = TRUE` had been set in `propagate`, skewness/kurtosis and Shapiro-Wilk/Kolmogorov-Smirnov tests for normality are calculated on the Monte-Carlo evaluations.

Usage

```r
## S3 method for class 'propagate'
summary(object, ...)
```

Arguments

- `object`:
  - an object returned from `propagate`.
- `...`:
  - other parameters for future methods.

Value

A printed summary as described above.

Author(s)

Andrej-Nikolai Spiess

Examples

```r
EXPR1 <- expression(x^2 * sin(y))
x <- c(5, 0.01)
y <- c(1, 0.01)
DF1 <- cbind(x, y)
RES1 <- propagate(expr = EXPR1, data = DF1, type = "stat",
                   do.sim = TRUE, verbose = TRUE)
summary(RES1)
```
Description

Calculates the Welch-Satterthwaite approximation to the 'effective degrees of freedom' by using the samples' uncertainties and degrees of freedoms, as described in Welch (1947) and Satterthwaite (1946).

Usage

WelchSatter(ufinal, usamp, df, alpha = 0.05)

Arguments

ufinal the propagated uncertainty of \( y \).
usamp the uncertainties of the samples, \( x_i \).
df the degrees of freedom of the samples, \( \nu_i \).
alpha the significance level for the t-statistic. See 'Details'.

Details

\[
\nu_{\text{eff}} \approx \frac{u(y)^4}{\sum_{i=1}^{n} \frac{u(x_i)^4}{\nu_i}}, \quad k = t(1 - \frac{\alpha}{2}, \nu_{\text{eff}}), \quad u_{\text{exp}} = k \cdot u(y)
\]

Value

A list with the following items:

ws.df the 'effective degrees of freedom'.
k the coverage factor for calculating the expanded uncertainty.
u.exp the expanded uncertainty.

Author(s)

Andrej-Nikolai Spiess

References

The generalization of "Student's" problem when several different population variances are involved. Welch BL. Biometrika (1947), 34: 28-35.
Examples

## Taken from GUM H.1.6, 4).

WelchSatter(32, c(25, 9.7, 2.9, 16.6), c(18, 25.6, 50, 2), alpha = 0.01)
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