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Description Implements several ABC algorithms for

performing parameter estimation, model selection, and goodness-of-fit. Cross-validation tools are also available for measuring the accuracy of ABC estimates, and to calculate the misclassification probabilities of different models.

Repository CRAN

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NeedsCompilation no

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abc

Parameter estimation with Approximate Bayesian Computation (ABC)

Description

This function performs multivariate parameter estimation based on summary statistics using an ABC algorithm. The algorithms implemented are rejection sampling, and local linear or non-linear (neural network) regression. A conditional heteroscedastic model is available for the latter two algorithms.

Usage

```
abc(target, param, sumstat, tol, method, hcorr = TRUE, transf = "none",
logit.bounds, subset = NULL, kernel = "epanechnikov", numnet =
10, sizenet = 5, lambda = c(0.0001,0.001,0.01), trace = FALSE, maxit =
500, ...)
```

| target | a vector of the observed summary statistics. |
|--------------|---|
| param | a vector, matrix or data frame of the simulated parameter values, i.e. the depen- dent variable(s) when method is "loclinear", "neuralnet" or "ridge". |
| sumstat | a vector, matrix or data frame of the simulated summary statistics, i.e. the independent variables when method is "loclinear", "neuralnet" or "ridge". |
| tol | tolerance, the required proportion of points accepted nearest the target values. |
| method | a character string indicating the type of ABC algorithm to be applied. Possible values are "rejection", "loclinear", "neuralnet" and "ridge". See also Details. |
| hcorr | logical, the conditional heteroscedastic model is applied if TRUE (default). |
| transf | a vector of character strings indicating the kind of transformation to be applied to the parameter values. The possible values are "log", "logit", and "none" (default), when no is transformation applied. See also Details. |
| logit.bounds | a matrix of bounds if transf is "logit". The matrix has as many lines as parameters (including the ones that are not "logit" transformed) and 2 columns. First column is the minimum bound and second column is the maximum bound. |

| subset | a logical expression indicating elements or rows to keep. Missing values in param and/or sumstat are taken as FALSE. | | | | | | |
|---------|---|--|--|--|--|--|--|
| kernel | a character string specifying the kernel to be used when method is "loclinear", "neuralnet" or "ridge". Defaults to "epanechnikov". See density for de- tails. | | | | | | |
| numnet | the number of neural networks when method is "neuralnet". Defaults to 10. It indicates the number of times the function nnet is called. | | | | | | |
| sizenet | the number of units in the hidden layer. Defaults to 5. Can be zero if there are no skip-layer units. See nnet for more details. | | | | | | |
| lambda | a numeric vector or a single value indicating the weight decay when method is "neuralnet". See nnet for more details. By default, 0.0001, 0.001, or 0.01 is randomly chosen for each of the networks. | | | | | | |
| trace | logical, if TRUE switches on tracing the optimization of nnet. Applies only when method is "neuralnet". | | | | | | |
| maxit | numeric, the maximum number of iterations. Defaults to 500. Applies only when method is "neuralnet". See also nnet. | | | | | | |
| | other arguments passed to nnet. | | | | | | |
| | | | | | | | |

These ABC algorithms generate random samples from the posterior distributions of one or more parameters of interest, $\theta_1, \theta_2, \ldots, \theta_n$. To apply any of these algorithms, (i) data sets have to be simulated based on random draws from the prior distributions of the θ_i 's, (ii) from these data sets, a set of summary statistics have to be calculated, S(y), (iii) the same summary statistics have to be calculated from the observed data, $S(y_0)$, and (iv) a tolerance rate must be chosen (tol). See cv4abc for a cross-validation tool that may help in choosing the tolerance rate.

When method is "rejection", the simple rejection algorithm is used. Parameter values are accepted if the Euclidean distance between S(y) and $S(y_0)$ is sufficiently small. The percentage of accepted simulations is determined by tol. When method is "loclinear", a local linear regression method corrects for the imperfect match between S(y) and $S(y_0)$. The accepted parameter values are weighted by a smooth function (kernel) of the distance between S(y) and $S(y_0)$, and corrected according to a linear transform: $\theta^* = \theta - b(S(y) - S(y_0))$. θ^* 's represent samples form the posterior distribution. This method calls the function lsfit from the stats library. When using the "loclinear" method, a warning about the collinearity of the design matrix of the regression might be issued. In that situation, we recommend to rather use the related "ridge" method that performs local-linear ridge regression and deals with the collinearity issue. The non-linear regression correction method ("neuralnet") uses a non-linear regression to minimize the departure from non-linearity using the function nnet. The posterior samples of parameters based on the rejection algorithm are returned as well, even when one of the regression algorithms is used.

Several additional arguments can be specified when method is "neuralnet". The method is based on the function nnet from the library nnet, which fits single-hidden-layer neural networks. numnet defines the number of neural networks, thus the function nnet is called numnet number of times. Predictions from different neural networks can be rather different, so the median of the predictions from all neural networks is used to provide a global prediction. The choice of the number of neural networks is a trade-off between speed and accuracy. The default is set to 10 networks. The number of units in the hidden layer can be specified via sizenet. Selecting the number of hidden units is similar to selecting the independent variables in a linear or non-linear regression. Thus, it corresponds to the complexity of the network. There is several rule of thumb to choose the number of hidden units, but they are often unreliable. Generally speaking, the optimal choice of sizenet depends on the dimensionality, thus the number of statistics in sumstat. It can be zero when there are no skip-layer units. See also nnet for more details. The method "neuralnet" is recommended when dealing with a large number of summary statistics.

If method is "loclinear", "neuralnet" or "ridge", a correction for heteroscedasticity is applied by default (hcorr = TRUE).

Parameters maybe transformed priori to estimation. The type of transformation is defined by transf. The length of transf is normally the same as the number of parameters. If only one value is given, that same transformation is applied to all parameters and the user is warned. When a parameter transformation used, the parameters are back-transformed to their original scale after the regression estimation. No transformations can be applied when method is "rejection".

Using names for the parameters and summary statistics is strongly recommended. Names can be supplied as names or colnames to param and sumstat (and target). If no names are supplied, P1, P2, ... is assigned to parameters and S1, S2, ... to summary statistics and the user is warned.

Value

The returned value is an object of class "abc", containing the following components:

| adj.values | The regression adjusted values, when method is "loclinear", "neuralnet" or "ridge". |
|--------------|--|
| unadj.values | The unadjusted values that correspond to "rejection" method. |
| SS | The summary statistics for the accepted simulations. |
| weights | The regression weights, when method is "loclinear", "neuralnet" or "ridge". |
| residuals | The residuals from the regression when method is "loclinear", "neuralnet" or "ridge". These are the "raw" residuals from lsfit or nnet, respectively, thus they are not on the original scale of the parameter(s). |
| dist | The Euclidean distances for the accepted simulations. |
| call | The original call. |
| na.action | A logical vector indicating the elements or rows that were excluded, including both NA/NaN's and elements/rows selected by subset. |
| region | A logical expression indicting the elements or rows that were accepted. |
| transf | The parameter transformations that have been used. |
| logit.bounds | The bounds, if transformation was "logit". |
| kernel | The kernel used. |
| method | Character string indicating the method, i.e. "rejection", "loclinear", or "neuralnet". |
| lambda | A numeric vector of length numnet. The actual values of the decay parame- ters used in each of the neural networks, when method is "neuralnet". These values are selected randomly from the supplied vector of values. |
| numparam | Number of parameters used. |

| abc | |
|-----|--|
| auc | |

| numstat | Number of summary statistics used. |
|---------|---|
| aic | The sum of the AIC of the numparam regression. Returned only if method is "loclinear". It is used for selecting informative summary statistics. |
| bic | The same but with the BIC. |
| names | A list with two elements: parameter.names and statistics.names. Both contain a vector of character strings with the parameter and statistics names, respectively. |

Author(s)

Katalin Csillery, Olivier Francois and Michael Blum with some initial code from Mark Beaumont.

References

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Blum, M.G.B. and Francois, O. (2010) Non-linear regression models for Approximate Bayesian Computation. *Statistics and Computing* **20**, 63-73.

Csillery, K., M.G.B. Blum, O.E. Gaggiotti and O. Francois (2010) Approximate Bayesian Computation (ABC) in practice. *Trends in Ecology and Evolution*, **25**, 410-418.

See Also

summary.abc, hist.abc, plot.abc, lsfit, nnet, cv4abc

Examples

```
require(abc.data)
data(musigma2)
?musigma2
## The rejection algorithm
##
rej <- abc(target=stat.obs, param=par.sim, sumstat=stat.sim, tol=.1, method =
"rejection")
## ABC with local linear regression correction without/with correction
## for heteroscedasticity
##
lin <- abc(target=stat.obs, param=par.sim, sumstat=stat.sim, tol=.1, hcorr =</pre>
FALSE, method = "loclinear", transf=c("none","log"))
linhc <- abc(target=stat.obs, param=par.sim, sumstat=stat.sim, tol=.1, method =
"loclinear", transf=c("none","log"))
## posterior summaries
##
```

```
linsum <- summary(linhc, intvl = .9)</pre>
linsum
## compare with the rejection sampling
summary(linhc, unadj = TRUE, intvl = .9)
## posterior histograms
##
hist(linhc, breaks=30, caption=c(expression(mu),
expression(sigma^2)))
## or send histograms to a pdf file
## Not run:
hist(linhc, file="linhc", breaks=30, caption=c(expression(mu),
expression(sigma^2)))
## End(Not run)
## diagnostic plots: compare the 2 'abc' objects: "loclinear",
## "loclinear" with correction for heteroscedasticity
##
plot(lin, param=par.sim)
plot(linhc, param=par.sim)
## example illustrates how to add "true" parameter values to a plot
##
postmod <- c(post.mu[match(max(post.mu[,2]), post.mu[,2]),1],</pre>
             post.sigma2[match(max(post.sigma2[,2]), post.sigma2[,2]),1])
plot(linhc, param=par.sim, true=postmod)
## artificial example to show how to use the logit tranformations
##
myp <- data.frame(par1=runif(1000,-1,1),par2=rnorm(1000),par3=runif(1000,0,2))</pre>
mys <- myp+rnorm(1000,sd=.1)</pre>
myt <- c(0,0,1.5)
lin2 <- abc(target=myt, param=myp, sumstat=mys, tol=.1, method =</pre>
"loclinear", transf=c("logit", "none", "logit"), logit.bounds = rbind(c(-1,
1), c(NA, NA), c(0, 2)))
summary(lin2)
```

cv4abc

Cross validation for Approximate Bayesian Computation (ABC)

Description

This function performs a leave-one-out cross validation for ABC via subsequent calls to the function abc. A potential use of this function is to evaluate the effect of the choice of the tolerance rate on the quality of the estimation with ABC.

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cv4abc

Usage

```
cv4abc(param, sumstat, abc.out = NULL, nval, tols, statistic = "median",
prior.range = NULL, method, hcorr = TRUE, transf = "none", logit.bounds
= c(0,0), subset = NULL, kernel = "epanechnikov", numnet = 10, sizenet =
5, lambda = c(0.0001,0.001,0.01), trace = FALSE, maxit = 500, ...)
```

| param | a vector, matrix or data frame of the simulated parameter values. |
|--------------|---|
| sumstat | a vector, matrix or data frame of the simulated summary statistics. |
| abc.out | an object of class "abc", optional. If supplied, all arguments passed to abc are extracted from this object, except for sumstat, param, and tol, which always have to be supplied as arguments. |
| nval | size of the cross-validation sample. |
| tols | a single tolerance rate or a vector of tolerance rates. |
| statistic | a character string specifying the statistic to calculate a point estimate from the posterior distribution of the parameter(s). Possible values are "median" (default), "mean", or "mode". |
| prior.range | a range to truncate the prior range. |
| method | a character string indicating the type of ABC algorithm to be applied. Possible values are "rejection", "loclinear", and "neuralnet". See also abc. |
| hcorr | logical, if TRUE (default) the conditional heteroscedastic model is applied. |
| transf | a vector of character strings indicating the kind of transformation to be applied to the parameter values. The possible values are "log", "logit", and "none" (default), when no is transformation applied. See also abc. |
| logit.bounds | a vector of bounds if transf is "logit". These bounds are applied to all parameters that are to be logit transformed. |
| subset | a logical expression indicating elements or rows to keep. Missing values in param and/or sumstat are taken as FALSE. |
| kernel | a character string specifying the kernel to be used when method is "loclinear" or "neuralnet". Defaults to "epanechnikov". See density for details. |
| numnet | the number of neural networks when method is "neuralnet". Defaults to 10. It indicates the number of times the function nnet is called. |
| sizenet | the number of units in the hidden layer. Defaults to 5. Can be zero if there are no skip-layer units. See nnet for more details. |
| lambda | a numeric vector or a single value indicating the weight decay when method is "neuralnet". See nnet for more details. By default, 0.0001, 0.001, or 0.01 is randomly chosen for each of the networks. |
| trace | logical, TRUE switches on tracing the optimization of nnet. Applies only when method is "neuralnet". |
| maxit | numeric, the maximum number of iterations. Defaults to 500. Applies only when method is "neuralnet". See also nnet. |
| | other arguments passed to nnet. |

A simulation is selected repeatedly to be a validation simulation, while the other simulations are used as training simulations. Each time the function abc is called to estimate the parameter(s). A total of nval validation simulations are selected.

The arguments of the function abc can be supplied in two ways. First, simply give them as arguments when calling this function, in which case abc.out can be NULL. Second, via an existing object of class "abc", here abc.out. WARNING: when abc.out is supplied, the same sumstat and param objects have to be used as in the original call to abc. Column names of sumstat and param are checked for match.

See summary.cv4abc for calculating the prediction error from an object of class "cv4abc".

Value

An object of class "cv4abc", which is a list with the following elements

| call | The original calls to abc for each tolerance rates. |
|-----------|---|
| cvsamples | Numeric vector of length nval, indicating which rows of the param and sumstat matrices were used as validation values. |
| tols | The tolerance rates. |
| true | The parameter values that served as validation values. |
| estim | The estimated parameter values. |
| names | A list with two elements: parameter.names and statistics.names. Both contain a vector of character strings with the parameter and statistics names, respectively. |
| seed | The value of .Random.seed when cv4abc is called. |

See Also

abc, plot.cv4abc, summary.cv4abc

Examples

```
require(abc.data)
data(musigma2)
## this data set contains five R objects, see ?musigma2 for
## details
## cv4abc() calls abc(). Here we show two ways for the supplying
## arguments of abc(). 1st way: passing arguments directly. In this
## example only 'param', 'sumstat', 'tol', and 'method', while default
## values are used for the other arguments.
## Number of eval. should be much more greater in realistic settings
cv.rej <- cv4abc(param=par.sim, sumstat=stat.sim, nval=5,
tols=c(.1,.2,.3), method="rejection")
## 2nd way: first creating an object of class 'abc', and then using it
## to pass its arguments to abc().</pre>
```

cv4postpr

```
lin <- abc(target=stat.obs, param=par.sim, sumstat=stat.sim, tol=.2,</pre>
method="loclinear", transf=c("none","log"))
cv.lin <- cv4abc(param=par.sim, sumstat=stat.sim, abc.out=lin, nval=5,</pre>
tols=c(.1,.2,.3))
## using the plot method. Different tolerance levels are plotted with
## different heat.colors. Smaller the tolerance levels correspond to
## "more red" points.
## !!! consider using the argument 'exclude' (plot.cv4abc) to supress
## the plotting of any outliers that mask readibility !!!
plot(cv.lin, log=c("xy", "xy"), caption=c(expression(mu),
expression(sigma^2)))
## comparing with the rejection sampling
plot(cv.rej, log=c("", "xy"), caption=c(expression(mu), expression(sigma^2)))
## or printing results directly to a postscript file...
## Not run:
plot(cv.lin, log=c("xy", "xy"), caption=c(expression(mu),
expression(sigma^2)), file="CVrej", postscript=TRUE)
## End(Not run)
## using the summary method to calculate the prediction error
summary(cv.lin)
## compare with rejection sampling
summary(cv.rej)
```

cv4postpr

Leave-one-our cross validation for model selection ABC

Description

This function performs a leave-one-out cross validation for model selection with ABC via subsequent calls to the function postpr.

Usage

```
cv4postpr(index, sumstat, postpr.out = NULL, nval, tols, method,
subset = NULL, kernel = "epanechnikov", numnet = 10, sizenet = 5, lambda
= c(0.0001,0.001,0.01), trace = FALSE, maxit = 500, ...)
```

| index | a vector of model indices. It can be character or numeric and will be coerced |
|---------|---|
| | to factor. It must have the same length as the number of rows in sumstat to |
| | indicate which row of sumstat belong to which model. |
| sumstat | a vector, matrix or data frame of the simulated summary statistics. |

| postpr.out | an object of class "postpr", optional. If supplied, all arguments passed to postpr are extracted from this object, except for sumstat, index, and tols, which always have to be supplied as arguments. |
|------------|--|
| nval | the size of the cross-validation sample for each model. |
| tols | a single tolerance rate or a vector of tolerance rates. |
| method | a character string indicating the type of simulation required. Possible values are "rejection", "mnlogistic", "neuralnet". See postpr for details. |
| subset | a logical expression indicating elements or rows to keep. Missing values in index and/or sumstat are taken as FALSE. |
| kernel | a character string specifying the kernel to be used when method is "loclinear" or "neuralnet". Defaults to "epanechnikov". See density for details. |
| numnet | the number of neural networks when method is "neuralnet". Defaults to 10. It indicates the number of times the function nnet is called. |
| sizenet | the number of units in the hidden layer. Defaults to 5. Can be zero if there are no skip-layer units. See nnet for more details. |
| lambda | a numeric vector or a single value indicating the weight decay when method is "neuralnet". See nnet for more details. By default, 0.0001, 0.001, or 0.01 is randomly chosen for each of the networks. |
| trace | logical, TRUE switches on tracing the optimization of ${\tt nnet}.$ Applies only when method is "neuralnet". |
| maxit | numeric, the maximum number of iterations. Defaults to 500. Applies only when method is "neuralnet". See also nnet. |
| | other arguments passed to nnet. |
| | |

For each model, a simulation is selected repeatedly to be a validation simulation, while the other simulations are used as training simulations. Each time the function postpr is called to estimate the parameter(s).

Ideally, we want nval to be equal to the number of simulations for each model, however, this might take too much time. Users are warned not to choose a too large number of simulations (especially when the neural networks are used). Beware that the actual number of cross-validation estimation steps that need to be performed is nval*the number of models.

The arguments for the function postpr can be supplied in two ways. First, simply give them as arguments when calling this function, in which case postpr.out can be NULL. Second, via an existing object of class "postpr", here postpr.out. WARNING: when postpr.out is supplied, the same sumstat and param objects have to be used as in the original call to postpr. Column names of sumstat and param are checked for match.

See summary.cv4postpr for calculating the prediction error from an object of class "cv4postpr" and plot.cv4postpr for visualizing the misclassification of the models using barplots.

Value

An object of class "cv4postpr", which is a list with the following elements

| call | The original calls to postpr for each tolerance rates. |
|-----------|--|
| cvsamples | Numeric vector of length nval*the number of models, indicating which rows of sumstat were used as validation values. |
| tols | The tolerance rates. |
| true | The true models. |
| estim | The estimated model probabilities. |
| method | The method used. |
| names | A list of two elements: model contains the model names, and statistics.names the names of the summary statistics. |
| seed | The value of .Random.seed when cv4postpr is called. |

See Also

postpr, summary.cv4postpr, plot.cv4postpr

Examples

```
require(abc.data)
data(human)
###Reduce the sample size of the simulations to reduce the running time.
###Do not do that with your own data!
ss<-c(1:1000,50001:51000,100001:101000)
cv.modsel <- cv4postpr(models[ss], stat.3pops.sim[ss,], nval=5, tols=c(.05,.1), method="rejection")
summary(cv.modsel)
plot(cv.modsel, names.arg=c("Bottleneck", "Constant", "Exponential"))</pre>
```

expected.deviance Expected deviance

Description

Model selection criterion based on posterior predictive distributions and approximations of the expected deviance.

Usage

```
expected.deviance(target, postsumstat, kernel = "gaussian", subset=NULL,
print=TRUE)
```

| target | a vector of the observed summary statistics. |
|-------------|---|
| postsumstat | a vector, matrix or data frame of summary statistics simulated a posteriori. |
| kernel | a character string specifying the kernel to be used when. Defaults to "gaussian". See density for details. |
| subset | a logical expression indicating elements or rows to keep. Missing values in postsumstat are taken as FALSE. |
| print | prints out what percent of the distances have been zero. |

This function implements an approximation for the expected deviance based on simulation performed a posteriori. Thus, after the posterior distribution of parameters or the posterior model probabilities have been determined, users need to re-simulate data using the posterior. The Monte-Carlo estimate of the expected deviance is computed from the simulated data as follows: $D = -\frac{2}{n} \sum_{j=1}^{n} \log(K_{\epsilon}(|| s^j - s_0 ||)))$, where n is number of simulations, K is the statistical kernel, ϵ is the error, i.e. difference between the observed and simulated summary statistics below which simulations were accepted in the original call to postpr, the s^j 's are the summary statistics obtained from the posterior predictive simulations, and s_0 are the observed values of the summary statistics. The expected devaince averaged over the posterior distribution to compute a deviance information criterion (DIC).

Value

A list with the following components:

expected.deviance

| | The approximate expected deviance. |
|------|--|
| dist | The Euclidean distances for summary statistics simulated a posteriori. |

References

Francois O, Laval G (2011) Deviance information criteria for model selection in approximate Bayesian computation *arXiv*:0240377.

Examples

```
## Function definitions
skewness <- function(x) {</pre>
sk <- mean((x-mean(x))^3)/(sd(x)^3)</pre>
return(sk)
}
kurtosis <- function(x) {</pre>
k \le mean((x-mean(x))^4)/(sd(x)^4) - 3
return(k)
}
## Observed summary statistics
obs.sumstat <- c(2.004821, 3.110915, -0.7831861, 0.1440266)
## Model 1 (Gaussian)
## ####################
## Simulate data
theta <- rnorm(10000, 2, 10)
zeta <- 1/rexp(10000, 1)</pre>
param <- cbind(theta, zeta)</pre>
y <- matrix(rnorm(200000, rep(theta, each = 20), sd = rep(sqrt(zeta),</pre>
each = 20)), nrow = 20, ncol = 10000)
## Calculate summary statistics
s <- cbind(apply(y, 2, mean), apply(y, 2, sd), apply(y, 2, skewness),</pre>
```

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```
apply(y, 2, kurtosis))
## ABC inference
gaus <- abc(target=obs.sumstat, param = param, sumstat=s, tol=.1, hcorr =</pre>
FALSE, method = "loclinear")
param.post <- gaus$adj.values</pre>
## Posterior predictive simulations
postpred.gaus <- matrix(rnorm(20000, rep(param.post[,1], each = 20), sd</pre>
= rep(sqrt(param.post[,2]), each = 20)), nrow = 20, ncol = 1000)
statpost.gaus <- cbind(apply(postpred.gaus, 2,</pre>
mean),apply(postpred.gaus, 2, sd),apply(postpred.gaus,
2,skewness),apply(postpred.gaus, 2,kurtosis))
# Computation of the expected deviance
expected.deviance(obs.sumstat, statpost.gaus)$expected.deviance
expected.deviance(obs.sumstat, statpost.gaus, kernel =
"epanechnikov") $ expected. deviance
## Modele 2 (Laplace)
## Simulate data
zeta <- rexp(10000)</pre>
param <- cbind(theta, zeta)</pre>
y <- matrix(theta + sample(c(-1,1),200000, replace = TRUE)*rexp(200000,</pre>
rep(zeta, each = 20)), nrow = 20, ncol = 10000)
## Calculate summary statistics
s <- cbind( apply(y, 2, mean), apply(y, 2, sd), apply(y, 2, skewness),</pre>
apply(y, 2, kurtosis))
## ABC inference
lapl <- abc(target=obs.sumstat, param = param, sumstat=s, tol=.1, hcorr =</pre>
FALSE, method = "loclinear")
param.post <- lapl$adj.values</pre>
## Posterior predictive simulations
postpred.lapl <- matrix(param.post[,1] + sample(c(-1,1),20000, replace =</pre>
TRUE)*rexp(20000, rep(param.post[,2], each = 20)), nrow = 20, ncol =
1000)
statpost.lapl <- cbind(apply(postpred.lapl, 2,</pre>
mean),apply(postpred.lapl, 2, sd),apply(postpred.lapl,
2,skewness),apply(postpred.lapl, 2,kurtosis))
## Computation of the expected deviance
expected.deviance(obs.sumstat, statpost.lapl)$expected.deviance
expected.deviance(obs.sumstat, statpost.lapl, kernel =
"epanechnikov") $ expected. deviance
```

Description

gfit

Perform a test for goodness-of-fit.

Usage

```
gfit(target, sumstat, nb.replicate, tol=.01, statistic=mean, subset=NULL,
trace=FALSE)
```

Arguments

| target | a data frame or vector of the observed summary statistic. |
|--------------|--|
| sumstat | a vector, matrix or data frame of the simulated summary statistics. |
| nb.replicate | number of replicates used to estimate the null distribution of the goodness-of-fit statistic. |
| tol | a tolerance rate. Defaults to 0.01 |
| statistic | define the goodness-of-fit statistic. Typical values are median (default), mean, or max. When using median fo instance, the g.o.f. statistic is the median of the distance between observed and accepted summary statistics. |
| subset | optional. A logical expression indicating elements or rows to keep. Missing values in sumstat are taken as FALSE. |
| trace | a boolean indicating if a trace should be displayed when calling the function. Default to FALSE. |

Details

The null distribution is estimated using already performed simulations contained in sumstat as pseudo-observed datasets. For each pseudo-observed dataset, the rejection algorithm is performed to obtain a value of the goodness-of-fit statistic. A better estimate of the P-value is obtained for larger nb.replicate but the running time of the function is increased.

Value

An object of class "gfit", which is a list with the following elements

| dist.obs | the value of the goodness-of-fit statistic for the data. |
|----------|---|
| dist.sim | a vector of size nb.replicate. It is a sample of the null distribution of the test statistic. |

Author(s)

Louisiane Lemaire and Michael Blum.

gfit

gfitpca

See Also

abc, plot.gfit, summary.gfit, gfitpca

Examples

```
## human demographic history
require(abc.data)
data(human)
## Perform a test of goodness-of-fit.
## The data are the European data and we test the fit of the bottleneck
## model (good fit) and of the constant-size population model (poor fit)
## Use larger values of \code{nb.replicate} (e.g. 1000)
## for real applications
res.gfit.bott=gfit(target=stat.voight["italian",],
sumstat=stat.3pops.sim[models=="bott",], statistic=mean, nb.replicate=10)
res.gfit.const=gfit(target=stat.voight["italian",],
sumstat=stat.3pops.sim[models=="const",], statistic=mean, nb.replicate=10)
```

```
## Plot the distribution of the null statistic and indicate where is the
## observed value.
plot(res.gfit.bott, main="Histogram under H0")
## Call the function \code{summary}
## It computes the P-value, call \code{summary} on the vector
## \code{dist.sim} and returns the value of the observed statistic
summary(res.gfit.bott)
```

gfitpca

Goodness of fit with principal component analysis

Description

Perform a priori goodness of fit using the two first components obtained with PCA.

Usage

```
gfitpca(target, sumstat, index, cprob=0.1, xlim=NULL, ylim=NULL, ...)
```

| target | a data frame or vector of the observed summary statistic. |
|-----------|--|
| sumstat | a matrix or data frame of the simulated summary statistics. |
| index | a vector of models names. It must be character and have the same length as the number of row in sumstat to indicate which row belong to which model. |
| cprob | cprob is the proportion of points outside the displayed envelope. Default to 0.1 which corresponds to a 90% envelope. |
| xlim,ylim | optional, numeric vectors of length 2, giving the x and y coordinates ranges. |
| | other parameters passed to plot. |

The function performs PCA using the a priori simulated summary statistics. It displays envelopes containing 1-hprob percent of the simulations. The projection of the observed summary statistics is displayed in order to check if they are contained or not in the envelopes. If the projection lies outside the envelope of a given model, it is an indication of poor fit.

Author(s)

Louisiane Lemaire and Michael Blum

See Also

abc, plot.gfit, summary.gfit, gfit

Examples

```
## human demographic history
require(abc.data)
data(human)
## five R objects are loaded. See ?human and vignette("abc") for details.
## Perform a priori goodness of fit for 3 different demographic models
## The envelopes containing 90% of the simulations are displayed.
## For the European data, a reasonable fit is only provided by the
## bottleneck model.
## The number of simulations is reduced to improve speed (do not do that
## with your own data)
index<-c(1:5000,50001:55000,100001:105000)
gfitpca(target=stat.voight["italian",], sumstat=stat.3pops.sim[index,],
index=models[index], cprob=0.1)</pre>
```

hist.abc

Posterior histograms

Description

Histograms of posterior samples from objects of class "abc".

Usage

```
## S3 method for class 'abc'
hist(x, unadj = FALSE, true = NULL, file = NULL,
postscript = FALSE, onefile = TRUE, ask =
!is.null(deviceIsInteractive()), col.hist = "grey", col.true = "red",
caption = NULL, ...)
```

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hist.abc

Arguments

| x | an object of class "abc". |
|------------|---|
| unadj | logical, if TRUE the unadjusted values are plotted even if method is "loclinear" or "neuralnet". |
| true | the true parameter value(s), if known. Vertical bar(s) are drawn at the true value(s). If more than one parameters were estimated, a vector of the true values have to be supplied. |
| file | a character string giving the name of the file. See postscript for details on accepted file names. If NULL (the default) histograms are printed to the null device (e.g. X11). If not NULL histograms are printed on a pdf device. See also postscript. |
| postscript | logical; if FALSE (default) histograms are printed on a pdf device, if TRUE on a postscript device. |
| onefile | logical, if TRUE (the default) allow multiple figures in one file. If FALSE, generate a file name containing the page number for each page. See postscript for further details. |
| ask | logical; if TRUE (the default), the user is asked before each plot, see par(ask=.). |
| col.hist | the colour of the histograms. |
| col.true | the colour of the vertical bar at the true value. |
| caption | captions to appear above the histogram(s); character vector of valid graphics annotations, see as graphicsAnnot for details. When NULL (default), parnames are used, which are extracted from x (see abc). Can be set to NA to suppress all captions. |
| | other parameters passed to hist. |

Value

A list of length equal to the number of parameters, the elements of which are objects of class "histogram". See hist for details.

See Also

abc, plot.abc

Examples

see ?abc for examples

plot.abc

Description

A plotting utile for quick visualization of the quality of an ABC analysis from an object of class "abc" generated with methods "loclinear" or "neuralnet" (see abc for details). Four plots are currently available: a density plot of the prior distribution, a density plot of the posterior distribution, a scatter plot of the Euclidean distances as a function of the parameter values, and a Normal Q-Q plot of the residuals from the regression.

Usage

```
## S3 method for class 'abc'
plot(x, param, subsample = 1000, true = NULL, file = NULL,
postscript = FALSE, onefile = TRUE, ask =
!is.null(deviceIsInteractive()), ...)
```

Arguments

| x | an object of class "abc" generated with methods "loclinear" or "neuralnet" (see abc for details). |
|------------|---|
| param | a vector or matrix of parameter values from the simulations that were used in the original call to abc. |
| subsample | the number of rows (simulations) to be plotted. Rows are randomly selected from param. |
| true | a vector of true parameter values, if known. Vertical lines are drawn at these values. |
| file | a character string giving the name of the file. See postscript for details on accepted file names. If NULL (the default) plots are printed to the null device (e.g. X11). If not NULL plots are printed on a pdf device. See also postscript. |
| postscript | logical; if FALSE (default) plots are printed on a pdf device, if TRUE on a postscript device. |
| onefile | logical, if TRUE (the default) allow multiple figures in one file. If FALSE, generate a file name containing the page number for each page. See postscript for further details. |
| ask | logical; if TRUE (the default), the user is asked before each plot, see par(ask=.). |
| | other parameters passed to plot. |

Details

In order to use this function, one of the regression correction methods had to be used in the original call to abc, i.e. "loclinear" or "neuralnet" (see abc for details). Four plots are printed for each parameter. (i) A density plot of the prior distribution. (ii) A density plot of the posterior distribution using the regression correction (red thick lines) and, for reference, using the simple

plot.cv4abc

rejection method (black fine lines). The prior distribution (in the posterior distributions' range) is also displayed (dashed lines). (iii) A scatter plot of the log Euclidean distances as a function of the true parameter values. Points corresponding to the accepted simulations are displayed in red. (iv) A Normal Q-Q plot of the residuals from the regression, thus from lsfit when method was "loclinear", and from nnet when method was "neuralnet" in the original abc.

For plots (i) and (iii) not the whole data but a subsample is used, the size of which can be is given by subsample. This is to avoid plots that may take too much time to print.

If a parameter transformation was applied in the original call to abc, the same transformations are applied to the parameters for plotting (on plots (i)-(iii)).

See Also

abc, hist.abc, summary.abc

Examples

see ?abc for examples

plot.cv4abc

Cross-validation plots for ABC

Description

Plotting method for cross-validation ABC objects. Helps to visually evaluate the quality of the estimation and/or the effect of the tolerance level.

Usage

```
## S3 method for class 'cv4abc'
plot(x, exclude = NULL, log = NULL, file = NULL,
postscript = FALSE, onefile = TRUE, ask =
!is.null(deviceIsInteractive()), caption = NULL, ...)
```

| х | an object of class "cv4abc". |
|---------|---|
| exclude | a vector of row indices indicating which rows should be excluded from plotting. Useful when the prior distribution has a long tail. |
| log | character vector of the same length as the number of parameters in the "cv4abc" object. Allows plotting on a log scale. Possible values are "" (normal scale) and "xy" (log scale for both the x and y axis). "x" and "y" are possible as well, but not of any interest here. Negative values are set to NA and there is a warning. |
| file | a character string giving the name of the file. See postscript for details on accepted file names. If NULL (the default) plots are printed to the null device (e.g. X11). If not NULL plots are printed on a pdf device. See also postscript. |

| postscript | logical; if FALSE (default) plots are printed on a pdf device, if TRUE on a postscript device. |
|------------|---|
| onefile | logical, if TRUE (the default) allow multiple figures in one file. If FALSE, generate a file name containing the page number for each page. See postscript for further details. |
| ask | logical; if TRUE (the default), the user is asked before each plot, see par(ask=.). |
| caption | captions to appear above the plot(s); character vector of valid graphics annota- tions, see as.graphicsAnnot. By default, parnames from x are extracted (see abc). Can be set to "" or NA to suppress all captions. |
| | other parameters passed to plot. |
| | |

Different tolerance levels are plotted with heat.colors. Thus, the colors correspond to different levels of the tolerance rate in an increasing order from red to yellow.

See Also

cv4abc, abc

Examples

see ?cv4abc for examples

plot.cv4postpr Barplot of model misclassification

Description

Displays a barplot of either the proportion of simulations classified to any of the models or the mean misclassification probabilities of models for all tolerance levels in the "cv4postpr" object.

Usage

```
## S3 method for class 'cv4postpr'
plot(x, probs = FALSE, file = NULL, postscript
= FALSE, onefile = TRUE, ask = !is.null(deviceIsInteractive()), caption
= NULL, ...)
```

| х | an object of class "cv4postpr". |
|-------|---|
| probs | logical, if TRUE the mean posterior model probabilities are plotted. If FALSE the frequencies of the simulations classified to the different models (default). |
| file | a character string giving the name of the file. See postscript for details on accepted file names. If NULL (the default) plots are printed to the null device (e.g. X11). If not NULL plots are printed on a pdf device. See also postscript. |

plot.gfit

| postscript | logical; if FALSE (default) plots are printed on a pdf device, if TRUE on a postscript device. |
|------------|---|
| onefile | logical, if TRUE (the default) allow multiple figures in one file. If FALSE, generate a file name containing the page number for each page. See postscript for further details. |
| ask | logical; if TRUE (the default), the user is asked before each plot, see par(ask=.). |
| caption | captions to appear above the plot(s); character vector of valid graphics anno- tations, see as.graphicsAnnot. Can be set to "" or NA to suppress all captions. |
| | other parameters passed to barplot. |

Details

Model are distinguised with different intensities of the gray colour. The first model in alphabetic order has the darkest colour. If the classification of models is perfect (so that the frequency (or probability) of each model is zero for all but the correct model) each bar has a single colour of its corresponding model.

See Also

cv4postpr, summary.cv4postpr

Examples

see ?cv4postpr for examples

plot.gfit Goodness-of-fit plot for ABC

Description

Plotting method for goodness-of-fit ABC objects.

Usage

```
## S3 method for class 'gfit'
plot(x, breaks="Freedman-Diaconis", main, ...)
```

| Х | an object of class "gfit". |
|--------|---|
| breaks | number of cells for the histogram. Defaults to "Freedman-Diaconis". |
| main | title for the plot |
| | other parameters passed to plot. |

Plot the distribution of the statistic under the null hypothesis and indicate where is the observed value.

See Also

gfit, abc, summary.gfit, hist

Examples

see ?gfit for examples

postpr

Estimating posterior model probabilities

Description

Model selection with Approximate Bayesian Computation (ABC).

Usage

```
postpr(target, index, sumstat, tol, subset = NULL, method, corr=TRUE,
kernel="epanechnikov", numnet = 10, sizenet = 5, lambda =
c(0.0001,0.001,0.01), trace = TRUE, maxit = 500, ...)
```

| target | a vector of the observed summary statistics. |
|---------|---|
| index | a vector of model indices. It can be character or numeric and will be coerced to factor. It must have the same length as sumstat to indicate which row of sumstat belong to which model. |
| sumstat | a vector, matrix or data frame of the simulated summary statistics. |
| tol | numeric, the required proportion of points nearest the target values (tolerance), or a vector of the desired tolerance values. If a vector is given |
| subset | a logical expression indicating elements or rows to keep. Missing values in index and/or sumstat are taken as FALSE. |
| method | a character string indicating the type of simulation required. Possible values are "rejection", "mnlogistic", "neuralnet". See Details. |
| corr | logical, if TRUE (default) posterior model probabilities are corrected for the num- ber of simulations performed for each model. If equal number of simulations are available for all models, corr has no effect. |
| kernel | a character string specifying the kernel to be used when method is "mnlogistic" or "neuralnet". Defaults to "epanechnikov". See density for details. |
| numnet | the number of neural networks when method is "neuralnet". It corresponds to the number of times the function nnet is called. |

postpr

| sizenet | the number of units in the hidden layer. Can be zero if there are no skip-layer units. |
|---------|---|
| lambda | a numeric vector or a single value indicating the weight decay when method is "neuralnet". By default, 0.0001, 0.001, or 0.01 is randomly chosen for the each of the networks. See nnet for more details. |
| trace | logical, TRUE switches on tracing the optimization of nnet (applies when method is "neuralnet"). |

| maxit | numeric, the maximum number of iterations. Defaults to 500. See also nnet. |
|-------|--|
| | |

other arguments passed on from nnet. . . .

Details

The function computes the posterior model probabilities. Simulations have to be performed with at least two distinct models. When method is "rejection", the posterior probability of a given model is approximated by the proportion of accepted simulations given this model. This approximation holds when the different models are a priori equally likely, and the same number of simulations is performed for each model. When method is "mnlogistic" the posterior model probabilities are estimated using a multinomial logistic regression as implemented in the function multinom from the package nnet. When method is "neuralnet", neural networks are used to predict the probabilities of models based on the observed statistics using nnet. This method can be useful if many summary statistics are used.

Names for the summary statistics are strongly recommended. Names can be supplied as colnames to sumstat (and target). If no names are supplied S1, S2, ... to summary statistics will be assigned to parameters and the user will be warned.

Value

An object of class "postpr", containing the following components:

| pred | a vector of model probabilities when method is "mnlogistic" or "neuralnet". |
|-----------|---|
| values | the vector of model indices in the accepted region using the rejection method. |
| weights | vector of regression weights when method is "mnlogistic" or "neuralnet". |
| SS | summary statistics in the accepted region. |
| call | the original call. |
| na.action | a logical vector indicating the elements or rows that were excluded, including both NA/NaN's and elements/rows selected by subset |
| method | a character string indicating the method used, i.e. "rejection", "mnlogistic" or "neuralnet". |
| corr | logical, if TRUE the posterior model probabilities are corrected for the number of simulations performed for each model. |
| nmodels | the number of simulations performed for each model a priori. |
| models | a character vector of model names (a priori). |
| numstat | the number of summary statistics used. |
| names | a list of two elements: model contains the model names, and statistics.names the names of the summary statistics. |

Author(s)

Katalin Csillery, Olivier Francois and Michael Blum with some initial code from Mark Beaumont.

References

Beaumont, M.A. (2008) Joint determination of topology, divergence time, and immigration in population trees. In *Simulation, Genetics, and Human Prehistory* (Matsumura, S., Forster, P. and Renfrew, C., eds) McDonald Institute for Archaeological Research

See Also

summary.postpr

Examples

```
## an artifical example
ss <- cbind(runif(1000),rt(1000,df=20))
postpr(target=c(3), index=c(rep("norm",500),rep("t",500)),
sumstat=ss[,1], tol=.1, method="rejection")
## human demographic history
require(abc.data)
data(human)
## five R objects are loaded. See ?human and vignette("abc") for details.
## illustrate the informativeness of two summary statistics: mean and
## variance of Tajima's D
par(mfcol = c(1,3))
boxplot(stat.3pops.sim[,"pi"]~models, main="Mean nucleotide diversity")
boxplot(stat.3pops.sim[,"TajD.m"]~models, main="Wean Tajima's D")
boxplot(stat.3pops.sim[,"TajD.v"]~models, main="Var in Tajima's D")
```

```
## model selection with ABC for the European population
```

```
modsel.it <- postpr(stat.voight["italian",], models, stat.3pops.sim, tol=.05, method="mnlogistic")
summary(modsel.it)</pre>
```

```
## In Europe, the most supported model
## is a population bottleneck
## Check that in Africa, population expansion is the most supported model, while in
## Asia, it is a population bottleneck
##modsel.ha <- postpr(stat.voight["hausa",], models, stat.3pops.sim,
##tol=.05, method="mnlogistic")
##modsel.ch <- postpr(stat.voight["chinese",], models, stat.3pops.sim,
## tol=.05, method="mnlogistic")
```

summary.abc

Description

Calculates simple summaries of posterior samples: the minimum and maximum, the weighted mean, median, mode, and credible intervals.

Usage

```
## S3 method for class 'abc'
summary(object, unadj = FALSE, intvl = .95, print = TRUE,
digits = max(3, getOption("digits")-3), ...)
```

Arguments

| object | an object of class "abc". |
|--------|--|
| unadj | logical, if TRUE it forces to plot the unadjusted values when method is "loclinear" or "neuralnet". |
| intvl | size of the symmetric credible interval. |
| print | logical, if TRUE prints messages. Mainly for internal use. |
| digits | the digits to be rounded to. Can be a vector of the same length as the number of parameters, when each parameter is rounded to its corresponding digits. |
| | other arguments passed to density. |

Details

If method is "rejection" in the original call to abc, posterior means, medians, modes and percentiles defined by intvl, 95 by default (credible intervals) are calculated. If a regression correction was used (i.e. method is "loclinear" or "neuralnet" in the original call to abc) the weighted posterior means, medians, modes and percentiles are calculated.

To calculate the mode, parameters are passed on from density.default. Note that the posterior mode can be rather different depending on the parameters to estimate the density.

Value

The returned value is an object of class "table". The rows are,

| Min. | minimun |
|-------------|--------------------|
| Lower perc. | lower percentile |
| Median | or weighted median |
| Mean | or weighted mean |
| Mode | or weighted mode |
| Upper perc. | upper percentile |
| Max. | maximum |
| | |

See Also

abc, hist.abc, plot.abc

Examples

see ?abc for examples

summary.cv4abc Calculates the cross-validation prediction error

Description

This function calculates the prediction error from an object of class "cv4abc" for each parameter and tolerance level.

Usage

```
## S3 method for class 'cv4abc'
summary(object, print = TRUE, digits = max(3,
getOption("digits")-3), ...)
```

Arguments

| object | an object of class "abc". |
|--------|--|
| print | logical, if TRUE prints messages. Mainly for internal use. |
| digits | the digits to be rounded to. Can be a vector of the same length as the number of parameters, when each parameter is rounded to its corresponding digits. |
| | other arguments passed to density. |

Details

The prediction error is calculated as $\frac{\sum((\theta^*-\theta)^2)}{nval \times Var(\theta)}$, where θ is the true parameter value, θ^* is the predicted parameter value, and nval is the number of points where true and predicted values are compared.

Value

The returned value is an object of class "table", where the columns correspond to the parameters and the rows to the different tolerance levels.

See Also

cv4abc,plot.cv4abc

Examples

see ?cv4abc for examples

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summary.cv4postpr Confusion matrix and misclassification probabilities of models

Description

This function calculates the confusion matrix and the mean misclassification probabilities of models from an object of class "cv4postpr".

Usage

```
## S3 method for class 'cv4postpr'
summary(object, probs = TRUE, print = TRUE, digits =
max(3, getOption("digits")-3), ...)
```

Arguments

| | other arguments. |
|--------|--|
| digits | the digits to be rounded to. |
| print | logical, if TRUE prints the mean models probabilities. |
| probs | logical, if TRUE (default), mean posterior model probabilities are returned. |
| object | an object of class "cv4postpr". |

Value

If probs=FALSE a matrix with the frequencies of the simulations classified to the different models (the confusion matrix). If probs=TRUE, a list with two components:

| conf.matrix | The confusion matrix. |
|-------------|---|
| probs | The mean model misclassification probabilities. |

See Also

cv4postpr,plot.cv4postpr

Examples

see ?cv4postpr for examples

summary.gfit

Description

This function calculates the p-value of the goodness-of-fit test from an object of class "gfit".

Usage

S3 method for class 'gfit'
summary(object, ...)

Arguments

| object | an object of class "gfit". |
|--------|-------------------------------------|
| | other parameters passed to summary. |

Details

It computes the P-value, call summary on the vector of statistics simulated under the null and returns the value of the observed statistic.

Value

A list of the following elements

| pvalue | P-value for goodness-of-fit. |
|------------|--|
| s.dist.sim | the result of a call to the function summary. Provides a summary of the distribu- tion of the goodness-of-fit statistic simulated under the null. |
| dist.obs | the observed value goodness-of-fit statistic. |

See Also

gfit, abc, plot.gfit

Examples

see ?gfit for exemples

summary.postpr

Description

This function extracts the posterior model probabilities and calculates the Bayes factors from an object of class "postpr".

Usage

```
## S3 method for class 'postpr'
summary(object, rejection = TRUE, print = TRUE, digits
= max(3, getOption("digits")-3), ...)
```

Arguments

| object | an object of class "postpr". |
|-----------|---|
| rejection | logical, if method is "mnlogistic" or "neuralnet", should the approximate model probabilities based on the rejection method returned. |
| print | logical, if TRUE prints the mean models probabilities. |
| digits | the digits to be rounded to. |
| | other arguments. |

Value

A list with the following components if method="rejection":

| Prob | an object of class table of the posterior model probabilities. |
|--|--|
| BayesF | an object of class table with the Bayes factors between pairs of models. |
| A list with the following components if method is "mnlogistic" or "neuralnet" and rejection is TRUE: | |
| rejection | a list with the same components as above |
| mnlogistic | a list with the same components as above |

See Also

postpr

Examples

see ?postpr for examples

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