# Package 'EasyABC'

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ABC\_emulation

Rejection sampling scheme for ABC using an emulator

#### Description

This function launches a series of nb\_design\_pts model simulations with model parameters drawn in the prior distribution specified in prior\_matrix, build an emulator with these computed design points and then launches a series of nb\_simul emulator simulations.

#### Usage

```
ABC_emulation(
  model,
  prior,
  nb_design_pts,
  nb_simul,
  prior_test = NULL,
  summary_stat_target = NULL,
  emulator_span = 50,
  tol = NULL,
  use_seed = FALSE,
  seed_count = 0,
  n_cluster = 1,
  verbose = FALSE,
  progress_bar = FALSE
)
```

#### **Arguments**

model

a R function implementing the model to be simulated. It must take as arguments a vector of model parameter values and it must return a vector of summary statistics. When using the option use\_seed=TRUE, model must take as arguments a vector containing a seed value and the model parameter values. A tutorial is provided in the package's vignette to dynamically link a binary code to a R function. Users may alternatively wish to wrap their binary executables using the provided functions binary\_model and binary\_model\_cluster. The use of these functions is associated with slightly different constraints on the design of the binary code (see binary\_model and binary\_model\_cluster).

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prior

a list of prior information. Each element of the list corresponds to a model parameter. The list element must be a vector whose first argument determines the type of prior distribution: possible values are "unif" for a uniform distribution on a segment, "normal" for a normal distribution, "lognormal" for a lognormal distribution or "exponential" for an exponential distribution. The following arguments of the list elements contain the characteritiscs of the prior distribution chosen: for "unif", two numbers must be given: the minimum and maximum values of the uniform distribution; for "normal", two numbers must be given: the mean and standard deviation of the normal distribution; for "lognormal", two numbers must be given: the mean and standard deviation on the log scale of the lognormal distribution; for "exponential", one number must be given: the rate of the exponential distribution. User-defined prior distributions can also be provided. See the vignette for additional information on this topic.

nb\_design\_pts

a positive integer equal to the desired number of simulations of the model used to build the emulator.

nb\_simul

a positive integer equal to the desired number of simulations of the emulator.

prior\_test

a string expressing the constraints between model parameters. This expression will be evaluated as a logical expression, you can use all the logical operators including "<", ">", ... Each parameter should be designated with "X1", "X2", ... in the same order as in the prior definition. If not provided, no constraint will be applied.

summary\_stat\_target

a vector containing the targeted (observed) summary statistics. If not provided, ABC\_rejection only launches the simulations and outputs the simulation results.

emulator\_span

a positive number, the number of design points selected for the local regression. 50 by default.

tol

tolerance, a strictly positive number (between 0 and 1) indicating the proportion of simulations retained nearest the targeted summary statistics.

use\_seed

logical. If FALSE (default), ABC\_rejection provides as input to the function model a vector containing the model parameters used for the simulation. If TRUE, ABC\_rejection provides as input to the function model a vector containing an integer seed value and the model parameters used for the simulation. In this last case, the seed value should be used by model to initialize its pseudo-random number generators (if model is stochastic).

seed\_count

a positive integer, the initial seed value provided to the function model (if use\_seed=TRUE). This value is incremented by 1 at each call of the function model.

n\_cluster

a positive integer. If larger than 1 (the default value), ABC\_rejection will launch model simulations in parallel on n\_cluster cores of the computer.

verbose

logical. FALSE by default. If TRUE, ABC\_rejection writes in the current directory intermediary results at the end of each step of the algorithm in the file "output". These outputs have a matrix format, in wich each raw is a different simulation, the first columns are the parameters used for this simulation, and the last columns are the summary statistics of this simulation.

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progress\_bar logical, FALSE by default. If TRUE, ABC\_rejection will output a bar of progres-

sion with the estimated remaining computing time. Option not available with

multiple cores.

#### Value

The returned value is a list containing the following components:

param The model parameters used in the model simulations.

stats The summary statistics obtained at the end of the model simulations.

weights The weights of the different model simulations. In the standard rejection scheme,

all model simulations have the same weights.

stats\_normalization

The standard deviation of the summary statistics across the model simulations.

nsim The number of model simulations performed.

nrec The number of retained simulations (if targeted summary statistics are pro-

vided).

computine The computing time to perform the simulations.

#### Author(s)

Franck Jabot, Thierry Faure and Nicolas Dumoulin

#### References

Jabot, F., Lagarrigues G., Courbaud B., Dumoulin N. (2015). A comparison of emulation methods for Approximate Bayesian Computation. To be published.

#### See Also

```
binary_model, binary_model_cluster, ABC_sequential, ABC_mcmc
```

# Examples

ABC\_mcmc

Coupled to MCMC schemes for ABC

#### **Description**

This function implements three different algorithms to perform coupled to MCMC ABC.

# Usage

```
ABC_mcmc(
  method,
  model,
  prior,
  summary_stat_target,
  prior_test = NULL,
  n_rec = 100,
  n_between_sampling = 10,
  n_cluster = 1,
  use_seed = FALSE,
  verbose = FALSE,
  dist_weights = NULL,
  ...
)
```

#### **Arguments**

method

a character string indicating the ABC-MCMC algorithm to be used. Possible values are "Marjoram\_original", "Marjoram" and "Wegmann". Note that the method "Marjoram\_original" cannot be used with multiple cores.

model

a R function implementing the model to be simulated. It must take as arguments a vector of model parameter values and it must return a vector of summary statistics. When using the option use\_seed=TRUE, model must take as arguments a vector containing a seed value and the model parameter values. A tutorial is provided in the package's vignette to dynamically link a binary code to a R function. Users may alternatively wish to wrap their binary executables using the provided functions binary\_model and binary\_model\_cluster. The use of these functions is associated with slightly different constraints on the design of the binary code (see binary\_model and binary\_model\_cluster).

prior

a list of prior information. Each element of the list corresponds to a model parameter. The list element must be a vector whose first argument determines the type of prior distribution: possible values are "unif" for a uniform distribution on a segment, "normal" for a normal distribution, "lognormal" for a lognormal distribution or "exponential" for an exponential distribution. The following arguments of the list elements contain the characteritiscs of the prior distribution chosen: for "unif", two numbers must be given: the minimum and maximum values of the uniform distribution; for "normal", two numbers must be given: the mean and standard deviation of the normal distribution; for "lognormal", two numbers must be given: the mean and standard deviation on the log scale of the lognormal distribution; for "exponential", one number must be given: the rate of the exponential distribution. User-defined prior distributions can also be provided. See the vignette for additional information on this topic.

summary\_stat\_target

a vector containing the targeted (observed) summary statistics.

prior\_test

a string expressing the constraints between model parameters. This expression will be evaluated as a logical expression, you can use all the logical operators including "<", ">", ... Each parameter should be designated with "X1", "X2", ... in the same order as in the prior definition. If not provided, no constraint will be applied.

n\_rec

a positive integer equal to the desired number of sampled points along the MCMC.

n\_between\_sampling

a positive integer equal to the desired spacing between sampled points along the MCMC.

n\_cluster

a positive integer. If larger than 1 (the default value), ABC\_mcmc will launch model simulations in parallel on n\_cluster cores of the computer.

use\_seed

logical. If FALSE (default), ABC\_mcmc provides as input to the function model a vector containing the model parameters used for the simulation. If TRUE, ABC\_mcmc provides as input to the function model a vector containing an integer seed value and the model parameters used for the simulation. In this last case, the seed value should be used by model to initialize its pseudo-random number generators (if model is stochastic).

verbose

logical. FALSE by default. If TRUE, ABC\_mcmc writes in the current directory intermediary results at the end of each step of the algorithm in the file "output\_mcmc". These outputs have a matrix format, in wich each raw is a different simulation, the first columns are the parameters used for this simulation, the following columns are the summary statistics of this simulation, and the last column is the distance between the simulation and the data.

dist\_weights

a vector containing the weights to apply to the distance between the computed and the targeted statistics. These weights can be used to give more importance to a summary statistisc for example. The weights will be normalized before applying them. If not provided, no weights will be applied.

. . .

Additional arguments can be passed depending on the choosen method (see below)

#### **Details**

See the package's vignette for details on ABC-MCMC.

#### Value

The returned value is a list containing the following components:

param The model parameters used in the model simulations.

stats The summary statistics obtained at the end of the model simulations.

dist The distance of the simulations to the data.

stats\_normalization

The standard deviation of the summary statistics across the model simulations of the initial step. These values are used to normalize the summary statistics before the computation of the Euclidean distance between simulations and data. If method is "Marjoram\_original", this is equal to tab\_normalization. If

method is "Wegmann", this is not provided.

epsilon The final maximal distance between simulations and data in the retained sample

of particles.

nsim The number of model simulations performed.

n\_between\_sampling

The spacing between two sampled points in the MCMC.

computine The computing time to perform the simulations.

min\_stats The minimal values of each summary statistics during the calibration step, given

when method is "Wegmann".

max\_stats The maximal values of each summary statistics during the calibration step, given

when method is "Wegmann".

lambda The lambda values of the Box-Cox transformation, given when method is "Wegmann".

geometric\_mean The geometric means, given when method is "Wegmann".

boxcox\_mean The means of Box-Cox transforms, given when method is "Wegmann".

boxcox\_sd The standard deviations of Box-Cox transforms, given when method is "Wegmann".

pls\_transform The matrix of PLS transformation, given when method is "Wegmann".

numcomp The number of used components for the PLS transformation, given when method

is "Wegmann".

#### Additional parameters

Depending on the choosen method, you can specify the following arguments:

dist\_max a positive number, used when method is "Marjoram\_original". This is the tolerance threshold used during the MCMC. If not provided by the user, it is automatically computed as half the distance between the first simulation and the target summary statistics and a warning is printed.

**tab\_normalization** a vector of the same length as summary\_stat\_target, used when method is "Marjoram\_original". Each element contains a positive number by which each summary statistics must be divided before the computation of the Euclidean distance between simulations and data. If not provided by the user, the simulated summary statistics are divided by the target summary statistics and a warning is printed.

- proposal\_range a vector of the same length as the number of model parameters, used when method is "Marjoram\_original". Each element contains a positive number defining the range of MCMC jumps for each model parameter. If not provided by the user, a default value is used for each parameter and a warning is printed. The default value is 1/50 of the prior range for uniform distributions, 1/20 of the standard deviation of the prior distribution for normal distributions, 1/20 \* exp ( sigma \* sigma for lognormal distributions where sigma is the standard deviation of the prior distribution in the log scale, and 1/20 of the inverse of the rate for exponential distributions.
- **n\_calibration** a positive integer, used when method is "Marjoram" or "Wegmann". This is the number of simulations performed during the calibration step. Default value is 10000.
- **tolerance\_quantile** a positive number between 0 and 1 (strictly), used when method is "Marjoram" or "Wegmann". This is the percentage of simulations retained during the calibration step to determine the tolerance threshold to be used during the MCMC. Default value is 0.01.
- **proposal\_phi** a positive number, used when method is "Marjoram" or "Wegmann". This is a scaling factor defining the range of MCMC jumps. Default value is 1.
- **numcomp** a positive integer, used when method is "Wegmann". This is the number of components to be used for PLS transformations. Default value is 0 which encodes that this number is equal to the number of summary statistics.
- **seed\_count** a positive integer, the initial seed value provided to the function model (if use\_seed=TRUE). This value is incremented by 1 at each call of the function model.
- **progress\_bar** logical, FALSE by default. If TRUE, ABC\_mcmc will output a bar of progression with the estimated remaining computing time. Option not available with multiple cores.
- **max\_pick** a positive number, the max number of fails when moving particle inside the prior. Enabled only if inside\_prior is to TRUE. 10000 by default.

#### Author(s)

Franck Jabot, Thierry Faure and Nicolas Dumoulin

#### References

Marjoram, P., Molitor, J., Plagnol, V. and Tavar\'e, S. (2003) Markov chain Monte Carlo without likelihoods. *PNAS*, **100**, 15324–15328.

Wegmann, D., Leuenberger, C. and Excoffier, L. (2009) Efficient approximate Bayesian computation coupled with Markov chain Monte Carlo without likelihood. *Genetics*, **182**, 1207-1218.

#### See Also

binary\_model, binary\_model\_cluster, ABC\_rejection, ABC\_emulation, ABC\_sequential

#### **Examples**

```
##### EXAMPLE 1 #####
 #######################
 ## the model has two parameters and outputs two summary statistics.
 ## defining a simple toy model:
toy_model<-function(x){ c(x[1] + x[2] + rnorm(1,0,0.1) , x[1] * x[2] + rnorm(1,0,0.1) ) }
 ## define prior information
 toy_prior=list(c("unif",0,1),c("normal",1,2))
# a uniform prior distribution between 0 and 1 for parameter 1, and a normal distribution
 # of mean 1 and standard deviation of 2 for parameter 2.
 ## define the targeted summary statistics
 sum_stat_obs=c(1.5,0.5)
 ## to perform the Marjoram et al. (2003)'s method:
ABC_Marjoram_original<-ABC_mcmc(method="Marjoram_original", model=toy_model, prior=toy_prior,
   summary_stat_target=sum_stat_obs)
 ABC_Marjoram_original
## artificial example to perform the Marjoram et al. (2003)'s method, with modifications
 # drawn from Wegmann et al. (2009) without Box-Cox and PLS transformations.
 ABC_Marjoram<-ABC_mcmc(method="Marjoram", model=toy_model, prior=toy_prior,
   summary_stat_target=sum_stat_obs)
 ABC_Marjoram
 ## artificial example to perform the Wegmann et al. (2009)'s method.
 ##
 ABC_Wegmann<-ABC_mcmc(method="Wegmann", model=toy_model, prior=toy_prior,
   summary_stat_target=sum_stat_obs)
 ABC_Wegmann
 ##### EXAMPLE 2 #####
 #######################
 ## this time, the model is a C++ function packed into a R function -- this time,
 # the option 'use_seed' must be turned to TRUE.
 ## define prior information
trait_prior=list(c("unif",3,5),c("unif",-2.3,1.6),c("unif",-25,125),c("unif",-0.7,3.2))
 trait_prior
 ## define the targeted summary statistics
 sum_stat_obs=c(100,2.5,20,30000)
```

```
## artificial example to perform the Marjoram et al. (2003)'s method.
 ##
n=10
ABC_Marjoram_original<-ABC_mcmc(method="Marjoram_original", model=trait_model,
prior=trait_prior, summary_stat_target=sum_stat_obs, n_rec=n, use_seed=TRUE)
ABC_Marjoram_original
## artificial example to perform the Marjoram et al. (2003)'s method, with modifications
 # drawn from Wegmann et al. (2009) without Box-Cox and PLS transformations.
##
n=10
n_calib=10
 tol_quant=0.2
ABC_Marjoram<-ABC_mcmc(method="Marjoram", model=trait_model, prior=trait_prior,
   summary_stat_target=sum_stat_obs, n_rec=n, n_calibration=n_calib,
   tolerance_quantile=tol_quant, use_seed=TRUE)
ABC_Marjoram
 ## artificial example to perform the Wegmann et al. (2009)'s method.
##
n=10
n_calib=10
 tol_quant=0.2
ABC_Wegmann<-ABC_mcmc(method="Wegmann", model=trait_model, prior=trait_prior,
    summary_stat_target=sum_stat_obs, n_rec=n, n_calibration=n_calib,
    tolerance_quantile=tol_quant, use_seed=TRUE)
ABC_Wegmann
```

ABC\_rejection

Rejection sampling scheme for ABC

#### **Description**

This function launches a series of nb\_simul model simulations with model parameters drawn in the prior distribution specified in prior\_matrix.

#### Usage

```
ABC_rejection(
  model,
  prior,
  nb_simul,
  prior_test = NULL,
  summary_stat_target = NULL,
  tol = NULL,
  use_seed = FALSE,
```

```
seed_count = 0,
n_cluster = 1,
verbose = FALSE,
progress_bar = FALSE
)
```

#### **Arguments**

model

a R function implementing the model to be simulated. It must take as arguments a vector of model parameter values and it must return a vector of summary statistics. When using the option use\_seed=TRUE, model must take as arguments a vector containing a seed value and the model parameter values. A tutorial is provided in the package's vignette to dynamically link a binary code to a R function. Users may alternatively wish to wrap their binary executables using the provided functions binary\_model and binary\_model\_cluster. The use of these functions is associated with slightly different constraints on the design of the binary code (see binary\_model and binary\_model\_cluster).

prior

a list of prior information. Each element of the list corresponds to a model parameter. The list element must be a vector whose first argument determines the type of prior distribution: possible values are "unif" for a uniform distribution on a segment, "normal" for a normal distribution, "lognormal" for a lognormal distribution or "exponential" for an exponential distribution. The following arguments of the list elements contain the characteritiscs of the prior distribution chosen: for "unif", two numbers must be given: the minimum and maximum values of the uniform distribution; for "normal", two numbers must be given: the mean and standard deviation of the normal distribution; for "lognormal", two numbers must be given: the mean and standard deviation on the log scale of the lognormal distribution; for "exponential", one number must be given: the rate of the exponential distribution. User-defined prior distributions can also be provided. See the vignette for additional information on this topic.

nb\_simul

a positive integer equal to the desired number of simulations of the model.

prior\_test

a string expressing the constraints between model parameters. This expression will be evaluated as a logical expression, you can use all the logical operators including "<", ">", ... Each parameter should be designated with "X1", "X2", ... in the same order as in the prior definition. If not provided, no constraint will be applied.

summary\_stat\_target

a vector containing the targeted (observed) summary statistics. If not provided, ABC\_rejection only launches the simulations and outputs the simulation results.

tol

tolerance, a strictly positive number (between 0 and 1) indicating the proportion of simulations retained nearest the targeted summary statistics.

use\_seed

logical. If FALSE (default), ABC\_rejection provides as input to the function model a vector containing the model parameters used for the simulation. If TRUE, ABC\_rejection provides as input to the function model a vector containing an integer seed value and the model parameters used for the simulation. In this last

case, the seed value should be used by model to initialize its pseudo-random

number generators (if model is stochastic).

seed\_count a positive integer, the initial seed value provided to the function model (if use\_seed=TRUE).

This value is incremented by 1 at each call of the function model.

n\_cluster a positive integer. If larger than 1 (the default value), ABC\_rejection will

launch model simulations in parallel on n\_cluster cores of the computer.

verbose logical. FALSE by default. If TRUE, ABC\_rejection writes in the current di-

rectory intermediary results at the end of each step of the algorithm in the file "output". These outputs have a matrix format, in wich each raw is a different simulation, the first columns are the parameters used for this simulation, and the

last columns are the summary statistics of this simulation.

progress\_bar logical, FALSE by default. If TRUE, ABC\_rejection will output a bar of progres-

sion with the estimated remaining computing time. Option not available with

multiple cores.

#### Value

The returned value is a list containing the following components:

param The model parameters used in the model simulations.

stats The summary statistics obtained at the end of the model simulations.

weights The weights of the different model simulations. In the standard rejection scheme,

all model simulations have the same weights.

stats\_normalization

The standard deviation of the summary statistics across the model simulations.

nsim The number of model simulations performed.

nrec The number of retained simulations (if targeted summary statistics are pro-

vided).

computine The computing time to perform the simulations.

#### Author(s)

Franck Jabot, Thierry Faure and Nicolas Dumoulin

#### References

Pritchard, J.K., and M.T. Seielstad and A. Perez-Lezaun and M.W. Feldman (1999) Population growth of human Y chromosomes: a study of Y chromosome microsatellites. *Molecular Biology and Evolution*, **16**, 1791–1798.

#### See Also

binary\_model, binary\_model\_cluster, ABC\_sequential, ABC\_mcmc

#### **Examples**

```
##### EXAMPLE 1 #####
 set.seed(1)
 ## artificial example to show how to use the 'ABC_rejection' function.
 ## defining a simple toy model:
 toy_model<-function(x){ 2 * x + 5 + rnorm(1,0,0.1) }
 ## define prior information
 toy_prior=list(c("unif",0,1)) # a uniform prior distribution between 0 and 1
 ## only launching simulations with parameters drawn in the prior distributions
 set.seed(1)
 n=10
 ABC_sim<-ABC_rejection(model=toy_model, prior=toy_prior, nb_simul=n)
 ABC_sim
 ## launching simulations with parameters drawn in the prior distributions
 # and performing the rejection step
 sum_stat_obs=6.5
 tolerance=0.2
 ABC\_rej < -ABC\_rejection(model = toy\_model, \ prior = toy\_prior, \ nb\_simul = n, \\
   summary_stat_target=sum_stat_obs, tol=tolerance)
## NB: see the package's vignette to see how to pipeline 'ABC_rejection' with the function
 # 'abc' of the package 'abc' to perform other rejection schemes.
 ##### EXAMPLE 2 #####
 ## this time, the model has two parameters and outputs two summary statistics.
 ## defining a simple toy model:
toy_model2<-function(x){ c(x[1] + x[2] + rnorm(1,0,0.1), x[1] * x[2] + rnorm(1,0,0.1)) }
 ## define prior information
 toy_prior2=list(c("unif",0,1),c("normal",1,2))
\# a uniform prior distribution between 0 and 1 for parameter 1, and a normal distribution
 # of mean 1 and standard deviation of 2 for parameter 2.
 ## only launching simulations with parameters drawn in the prior distributions
 set.seed(1)
 n=10
 ABC_sim<-ABC_rejection(model=toy_model2, prior=toy_prior2, nb_simul=n)
 ABC_sim
 ## launching simulations with parameters drawn in the prior distributions
 # and performing the rejection step
 sum_stat_obs2=c(1.5,0.5)
 tolerance=0.2
 ABC_rej<-ABC_rejection(model=toy_model2, prior=toy_prior2, nb_simul=n,
```

summary\_stat\_target=sum\_stat\_obs2, tol=tolerance)

```
## NB: see the package's vignette to see how to pipeline 'ABC_rejection' with the function
   # 'abc' of the package 'abc' to perform other rejection schemes.
   ##### EXAMPLE 3 #####
   #############################
  ## this time, the model is a C++ function packed into a R function -- this time, the option
   # 'use_seed' must be turned to TRUE.
   n=10
  trait_prior=list(c("unif",3,5),c("unif",-2.3,1.6),c("unif",-25,125),c("unif",-0.7,3.2))
   trait_prior
   ## only launching simulations with parameters drawn in the prior distributions
  ABC_sim<-ABC_rejection(model=trait_model, prior=trait_prior, nb_simul=n, use_seed=TRUE)
   ABC_sim
  ## launching simulations with parameters drawn in the prior distributions and performing
   # the rejection step
   sum_stat_obs=c(100,2.5,20,30000)
   tolerance=0.2
   ABC_rej<-ABC_rejection(model=trait_model, prior=trait_prior, nb_simul=n,
     summary_stat_target=sum_stat_obs, tol=tolerance, use_seed=TRUE)
  ## NB: see the package's vignette to see how to pipeline 'ABC_rejection' with the function
   # 'abc' of the package 'abc' to perform other rejection schemes.
   ##### EXAMPLE 4 - Parallel implementations #####
   ## NB: the option use_seed must be turned to TRUE.
   ## For models already running with the option use_seed=TRUE, simply change
   # the value of n_cluster:
   sum_stat_obs=c(100,2.5,20,30000)
   ABC_simb<-ABC_rejection(model=trait_model, prior=trait_prior, nb_simul=n,
     use_seed=TRUE, n_cluster=2)
  ## For other models, change the value of n_cluster and modify the model so that the first
   # parameter becomes a seed information value:
   toy_model_parallel<-function(x){</pre>
set.seed(x[1])
2 * x[2] + 5 + rnorm(1,0,0.1) 
   sum_stat_obs=6.5
   ABC_simb<-ABC_rejection(model=toy_model_parallel, prior=toy_prior, nb_simul=n,
     use_seed=TRUE, n_cluster=2)
```

ABC\_sequential

Sequential sampling schemes for ABC

#### **Description**

This function implements four different algorithms to perform sequential sampling schemes for ABC. Sequential sampling schemes consist in sampling initially model parameters in the prior distribution, just like in a standard rejection-based ABC, in order to obtain a rough posterior distribution of parameter values, and in subsequently sampling close to this rough posterior distribution to refine it. Sequential sampling schemes have been shown to be more efficient than standard rejection-based procedures.

#### Usage

```
ABC_sequential(
  method,
  model,
  prior,
  nb_simul,
  summary_stat_target,
  prior_test = NULL,
  n_cluster = 1,
  use_seed = FALSE,
  verbose = FALSE,
  dist_weights = NULL,
  ...
)
```

#### **Arguments**

method

a character string indicating the sequential algorithm to be used. Possible values are "Beaumont", "Drovandi", "Delmoral", "Lenormand" and "Emulation".

mode1

a R function implementing the model to be simulated. It must take as arguments a vector of model parameter values and it must return a vector of summary statistics. When using the option use\_seed=TRUE, model must take as arguments a vector containing a seed value and the model parameter values. A tutorial is provided in the package's vignette to dynamically link a binary code to a R function. Users may alternatively wish to wrap their binary executables using the provided functions binary\_model and binary\_model\_cluster. The use of these functions is associated with slightly different constraints on the design of the binary code (see binary\_model and binary\_model\_cluster).

prior

a list of prior information. Each element of the list corresponds to a model parameter. The list element must be a vector whose first argument determines the type of prior distribution: possible values are "unif" for a uniform distribution on a segment, "normal" for a normal distribution, "lognormal" for a lognormal distribution or "exponential" for an exponential distribution. The

following arguments of the list elements contain the characteritiscs of the prior distribution chosen: for "unif", two numbers must be given: the minimum and maximum values of the uniform distribution; for "normal", two numbers must be given: the mean and standard deviation of the normal distribution; for "lognormal", two numbers must be given: the mean and standard deviation on the log scale of the lognormal distribution; for "exponential", one number must be given: the rate of the exponential distribution. Note that when using the method "Lenormand", solely uniform prior distributions are supported. User-defined prior distributions can also be provided. See the vignette for additional information on this topic.

nb\_simul

a positive integer equal to the desired number of simulations of the model below the tolerance threshold when method is "Beaumont", "Drovandi" and "Delmoral". When method is "Lenormand", the number of simulations below the tolerance threshold is equal to nb\_simul \* alpha. See the package's vignette and Lenormand et al. (2012) for details.

summary\_stat\_target

a vector containing the targeted (observed) summary statistics.

prior\_test

a string expressing the constraints between model parameters. This expression will be evaluated as a logical expression, you can use all the logical operators including "<", ">", ... Each parameter should be designated with "X1", "X2", ... in the same order as in the prior definition. If not provided, no constraint will be applied.

n\_cluster

a positive integer. If larger than 1 (the default value), ABC\_sequential will launch model simulations in parallel on n\_cluster cores of the computer.

use\_seed

logical. If FALSE (default), ABC\_sequential provides as input to the function model a vector containing the model parameters used for the simulation. If TRUE, ABC\_sequential provides as input to the function model a vector containing an integer seed value and the model parameters used for the simulation. In this last case, the seed value should be used by model to initialize its pseudo-random number generators (if model is stochastic).

verbose

logical. FALSE by default. If TRUE, ABC\_sequential writes in the current directory intermediary results at the end of each step of the algorithm various files. The file "n simul tot step iteration" (where iteration is the step number) contains the total number of simulations performed since the beginning of the algorithm at the end of the step "iteration". The file "R\_step\_iteration" (when using the method "Drovandi") is the parameter R used during the step "iteration" (see Drovandi and Pettitt 2011 for details). The file "p\_acc\_iteration" (when using the method "Lenormand") is the parameter p\_acc computed at the end of the step "iteration" (see Lenormand et al. 2012 for details). The file "tolerance\_step\_iteration" (when using the method "Drovandi", "Delmoral" or "Lenormand") is the tolerance computed at the end of the step "iteration". The file "output\_step\_iteration" gives the simulations kept after each iteration and has a matrix format, in wich each row is a different simulation, the first column is the weight of the simulation, the following columns are the parameters used for this simulation, and the last columns are the summary statistics of this simulation. The file "model\_step\_iteration" gives the simulations performed at each iteration and has a matrix format, in which each row is a different simulation,

the first column is the weight of the simulation, the following columns are the parameters used for this simulation, and the last columns are the summary statistics of this simulation. All these informations are further stored in a list (with the same formats) and are accessible from R - see intermediary in the value section below.

dist\_weights

a vector containing the weights to apply to the distance between the computed and the targeted statistics. These weights can be used to give more importance to a summary statistisc for example. The weights will be normalized before applying them. If not provided, no weights will be applied.

... Additional arguments can be passed depending on the choosen method (see below)

#### Details

See the package's vignette for details on the four algorithms.

#### Value

The returned value is a list containing the following components:

- param The model parameters used in the model simulations.
- stats The summary statistics obtained at the end of the model simulations.
- weights The weights of the different model simulations.
- stats\_normalization The standard deviation of the summary statistics across the model simulations of the initial step. These values are used to normalize the summary statistics before the computation of the Euclidean distance between simulations and data.
- epsilon The final maximal distance between simulations and data in the retained sample of particles.
- 'nsim' The number of model simulations performed.
- computine The computing time to perform the simulations.
- intermediary Intermediary results stored when the option "verbose=TRUE" is chosen. Each element of this list corresponds to a different step. See the argument verbose above for more details on the information stored.

# **Additional parameters**

Depending on the choosen method, you can specify the following arguments:

- seed\_count a positive integer, the initial seed value provided to the function model (if use\_seed=TRUE). This value is incremented by 1 at each call of the function model.
- inside\_prior logical used when methodis "Beaumont", "Lenormand" or "Emulation". TRUE by default. If FALSE, parameter sampling is not restricted to the initial ranges of the prior distribution during the subsequent algorithm steps.
- tolerance\_tab a vector containing the sequence of tolerance thresholds when method is "Beaumont", or the targeted final tolerance threshold when method is "Drovandi".

• alpha a positive number between 0 and 1 (strictly) used when method is "Drovandi", "Delmoral", "Lenormand" or "Emulation". alpha is the proportion of particles rejected at each step in the algorithm "Drovandi". This is the proportion of particles kept at each step in the algorithms "Delmoral", "Lenormand" and "Emulation". Default values are 0.5 when method is "Drovandi", "Lenormand" or "Emulation" and 0.9 for "Delmoral". See the package's vignette for details.

- c a positive number between 0 and 1 (strictly) used when method is "Drovandi". This is the expected proportion of particles which are going to be duplicated at each step. Default value is 0.01. See the package's vignette and Drovandi and Pettitt (2011) for details.
- first\_tolerance\_level\_auto logical used when method is "Drovandi". Default value is TRUE. In this case, the first tolerance threshold is determined by the algorithm, by taking the 1-alpha quantile of the distances between the simulated and targeted summary statistics. If FALSE, the initial tolerance threshold for the first step has to be provided as the first element of the vector tolerance\_tab. In this case, the targeted final tolerance threshold is the second element of tolerance\_tab.
- M a positive integer used when method is "Delmoral". This is the number of model simulations performed for each parameter set. Default value is
- 1. See the package's vignette and Del Moral et al. (2012) for details.
- nb\_threshold a positive integer used when method is "Delmoral". Default value is 0.5\*nb\_simul. This is the minimal effective sample size below which a resampling step is launched. See the package's vignette and Del Moral et al. (2012) for details.
- tolerance\_target a positive number used when method is "Delmoral". This is the targeted final tolerance threshold.
- p\_acc\_min a positive number between 0 and 1 (strictly) used when method is "Lenormand" or "Emulation". This is the stopping criterion of the algorithm: a small number ensures a better convergence of the algorithm, but at a cost in computing time. Default value is 0.05. See the package's vignette and Lenormand et al. (2012) for details.
- n\_step\_emulation a positive integer, the number of times the emulation is repeated. 9 by default.
- emulator\_span a positive number, the number of design points selected for the local regression. 50 by default.
- progress\_bar logical, FALSE by default. If TRUE, ABC\_sequential will output a bar of progression with the estimated remaining computing time. Option not available with multiple cores.
- max\_pick a positive number, the max number of fails when moving particle inside the prior. Enabled only if inside\_prior is to TRUE. 10000 by default.

#### Author(s)

Franck Jabot, Thierry Faure and Nicolas Dumoulin

#### References

Beaumont, M. A., Cornuet, J., Marin, J., and Robert, C. P. (2009) Adaptive approximate Bayesian computation. *Biometrika*, **96**, 983–990.

Del Moral, P., Doucet, A., and Jasra, A. (2012) An adaptive sequential Monte Carlo method for approximate Bayesian computation. *Statistics and Computing*, **22**, 1009–1020.

Drovandi, C. C. and Pettitt, A. N. (2011) Estimation of parameters for macroparasite population evolution using approximate Bayesian computation. *Biometrics*, **67**, 225–233.

Lenormand, M., Jabot, F., Deffuant G. (2012) Adaptive approximate Bayesian computation for complex models. http://arxiv.org/pdf/1111.1308.pdf

Jabot, F., Lagarrigues G., Courbaud B., Dumoulin N. (2015). A comparison of emulation methods for Approximate Bayesian Computation. To be published.

#### See Also

binary\_model, binary\_model\_cluster, ABC\_rejection, ABC\_emulation, ABC\_mcmc

#### **Examples**

```
##### EXAMPLE 1 #####
 #######################
 set.seed(1)
 ## artificial example to show how to use the 'ABC_sequential' function.
 ## defining a simple toy model:
 toy_model<-function(x){ 2 * x + 5 + rnorm(1,0,0.1) }
 ## define prior information
 toy_prior=list(c("unif",0,1)) # a uniform prior distribution between 0 and 1
 ## define the targeted summary statistics
 sum_stat_obs=6.5
 ## to perform the Beaumont et al. (2009)'s method:
 ##
 tolerance=c(1.5,0.5)
 ABC_Beaumont<-ABC_sequential(method="Beaumont", model=toy_model, prior=toy_prior,
 nb_simul=20, summary_stat_target=sum_stat_obs, tolerance_tab=tolerance)
 ABC_Beaumont
 ## to perform the Drovandi and Pettitt (2011)'s method:
 ##
 tolerance=0.5
 c_drov=0.7
 ABC_Drovandi<-ABC_sequential(method="Drovandi", model=toy_model, prior=toy_prior,
 nb_simul=20, summary_stat_target=sum_stat_obs, tolerance_tab=tolerance, c=c_drov)
 ABC_Drovandi
 ## to perform the Del Moral et al. (2012)'s method:
 alpha_delmo=0.5
 tolerance=0.5
 ABC_Delmoral<-ABC_sequential(method="Delmoral", model=toy_model, prior=toy_prior,
nb_simul=20, summary_stat_target=sum_stat_obs, alpha=alpha_delmo, tolerance_target=tolerance)
```

```
ABC_Delmoral
 ## to perform the Lenormand et al. (2012)'s method:
 ##
 pacc=0.4
 ABC_Lenormand<-ABC_sequential(method="Lenormand", model=toy_model, prior=toy_prior,
 nb_simul=20, summary_stat_target=sum_stat_obs, p_acc_min=pacc)
 ABC_Lenormand
 ##### EXAMPLE 2 #####
 ##############################
 ## this time, the model has two parameters and outputs two summary statistics.
 ## defining a simple toy model:
toy_{model} < -function(x) \{ c(x[1] + x[2] + rnorm(1,0,0.1), x[1] * x[2] + rnorm(1,0,0.1)) \}
 ## define prior information
 toy_prior2=list(c("unif",0,1),c("normal",1,2))
# a uniform prior distribution between 0 and 1 for parameter 1, and a normal distribution
 # of mean 1 and standard deviation of 2 for parameter 2.
 ## define the targeted summary statistics
 sum_stat_obs2=c(1.5,0.5)
 ## to perform the Beaumont et al. (2009)'s method:
 tolerance=c(1.5,0.5)
 ABC_Beaumont<-ABC_sequential(method="Beaumont", model=toy_model2, prior=toy_prior2,
 nb_simul=20, summary_stat_target=sum_stat_obs2, tolerance_tab=tolerance)
 ABC_Beaumont
 ## to perform the Drovandi and Pettitt (2011)'s method:
 ##
 tolerance=0.5
 c drov=0.7
 ABC_Drovandi<-ABC_sequential(method="Drovandi", model=toy_model2, prior=toy_prior2,
 nb_simul=20, summary_stat_target=sum_stat_obs2, tolerance_tab=tolerance, c=c_drov)
 ABC_Drovandi
 ## to perform the Del Moral et al. (2012)'s method:
 ##
 alpha_delmo=0.5
 tolerance=0.5
 ABC_Delmoral<-ABC_sequential(method="Delmoral", model=toy_model2, prior=toy_prior2,
nb_simul=20, summary_stat_target=sum_stat_obs2, alpha=alpha_delmo, tolerance_target=tolerance)
 ABC_Delmoral
 ## to perform the Lenormand et al. (2012)'s method:
 ##
pacc=0.4
# Only uniform priors are supported for the method "Lenormand" (since it performs a Latin
 # Hypercube sampling at the beginning):
```

```
toy_prior2=list(c("unif",0,1),c("unif",0.5,1.5))
\# a uniform prior distribution between 0 and 1 for parameter 1, and a normal distribution of
 # mean 1 and standard deviation of 1 for parameter 2.
ABC_Lenormand<-ABC_sequential(method="Lenormand", model=toy_model2, prior=toy_prior2,
 nb_simul=20, summary_stat_target=sum_stat_obs2, p_acc_min=pacc)
 ABC_Lenormand
 ##### EXAMPLE 3 #####
 #############################
## this time, the model is a C++ function packed into a R function -- this time, the option
 # 'use_seed' must be turned to TRUE.
 n=10
 ## define prior information
trait_prior=list(c("unif",3,5),c("unif",-2.3,1.6),c("unif",-25,125),c("unif",-0.7,3.2))
 trait_prior
 ## define the targeted summary statistics
 sum_stat_obs=c(100,2.5,20,30000)
 ## to perform the Beaumont et al. (2009)'s method:
 tolerance=c(8,5)
ABC_Beaumont<-ABC_sequential(method="Beaumont", model=trait_model, prior=trait_prior,
nb_simul=20, summary_stat_target=sum_stat_obs, tolerance_tab=tolerance, use_seed=TRUE)
 ABC_Beaumont
 ## to perform the Drovandi and Pettitt (2011)'s method:
 tolerance=3
 c_drov=0.7
ABC_Drovandi<-ABC_sequential(method="Drovandi", model=trait_model, prior=trait_prior,
   nb_simul=20, summary_stat_target=sum_stat_obs, tolerance_tab=tolerance, c=c_drov,
   use_seed=TRUE)
 ABC_Drovandi
 ## to perform the Del Moral et al. (2012)'s method:
 ##
 alpha_delmo=0.5
 tolerance=3
ABC_Delmoral<-ABC_sequential(method="Delmoral", model=trait_model, prior=trait_prior,
   nb_simul=20, summary_stat_target=sum_stat_obs, alpha=alpha_delmo,
   tolerance_target=tolerance, use_seed=TRUE)
 ABC_Delmoral
 ## to perform the Lenormand et al. (2012)'s method:
 ##
 pacc=0.4
ABC_Lenormand<-ABC_sequential(method="Lenormand", model=trait_model, prior=trait_prior,
   nb_simul=20, summary_stat_target=sum_stat_obs, p_acc_min=pacc, use_seed=TRUE)
 ABC_Lenormand
```

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```
##### EXAMPLE 4 - Parallel implementations #####
   ## NB: the option use_seed must be turned to TRUE.
   ## For models already running with the option use_seed=TRUE, simply change
   # the value of n_cluster:
   sum_stat_obs=c(100,2.5,20,30000)
  ABC_Lenormand<-ABC_sequential(method="Lenormand", model=trait_model, prior=trait_prior,
  nb_simul=20, summary_stat_target=sum_stat_obs, p_acc_min=pacc, use_seed=TRUE, n_cluster=2)
   ABC_Lenormand
   ## For other models, change the value of n_cluster and modify the model so that the
   # first parameter becomes a seed information value:
   toy_model_parallel<-function(x){</pre>
set.seed(x[1])
2 * x[2] + 5 + rnorm(1,0,0.1) }
   sum_stat_obs=6.5
  ABC_Lenormand<-ABC_sequential(method="Lenormand", model=toy_model_parallel, prior=toy_prior,
  nb_simul=20, summary_stat_target=sum_stat_obs, p_acc_min=pacc, use_seed=TRUE, n_cluster=2)
   ABC_Lenormand
```

binary\_model

Wrapper for a binary executable for non-parallel simulations

#### **Description**

This function enables to link a binary executable to a R function.

#### Usage

```
binary_model(command)
```

#### **Arguments**

command

a character string indicating the command to launch the executable on your system.

#### **Details**

A binary executable used with binary\_model has to be placed in the current directory of the R session. It further has to respect several constraints: it has to read the seed for its pseudo-random number generator and the model parameters in a file "input", and it must write the summary statistic in a file "output". The file "input" will be generated by the wrapper binary\_model in the current directory of the R session, and the wrapper will read the file "output" generated by the binary executable. In the file "input", the first line contains the seed, and each subsequent line contains one

binary\_model\_cluster

model parameter value. In the file "output", each summary statistic should be separated by a space or a tab separation. This wrapper should be used for use with a single core of the computer. If the user wishes to use several cores of the computer, the wrapper binary\_model\_cluster should be used. Note that the files "input" and "output" are deleted by the wrapper at the end of the function.

#### Value

A R function wrapping the binary executable, to be used with the EasyABC functions.

#### Author(s)

Franck Jabot, Thierry Faure and Nicolas Dumoulin

#### See Also

```
binary_model_cluster, ABC_rejection, ABC_sequential, ABC_mcmc
```

#### **Examples**

```
## Not run:
    ## artificial example to show how to use the binary_model function with
    # an executable "My_Executable"
ABC_rej<-ABC_rejection(model=binary_model("./My_Executable"), prior=..., n_cluster=1,...)

# NB: on windows, "My_Executable" should be of the form "My_Executable.exe" :
ABC_rej<-ABC_rejection(model=binary_model("./My_Executable.exe"), prior=..., n_cluster=1,...)

## End(Not run)</pre>
```

binary\_model\_cluster Wrapper for a binary executable for parallel simulations

#### **Description**

This function enables to link a binary executable to a R function.

# Usage

```
binary_model_cluster(command)
```

### Arguments

command

a character string indicating the command to launch the executable on your system.

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#### **Details**

A binary executable used with binary\_model\_cluster has to be placed in the current directory of the R session. It further has to respect several constraints: 1- it has to have a single argument: a number k used by the binary executable to know in which files read and write. 2- it has to read the seed for its pseudo-random number generator and the model parameters in a file "inputk" (where k is the argument passed to the executable: input1, input2,...). 3- it has to write the summary statistic in a file "outputk" (where k is the argument passed to the executable: output1, output2,...). The file "inputk" will be generated by the wrapper binary\_model\_cluster in the current directory of the R session, and the wrapper will read the file "outputk" generated by the binary executable. This construction ensures that each core reads and writes in different files. In the file "inputk", the first line contains the seed, and each subsequent line contains one model parameter value. In the file "outputk", each summary statistic should be separated by a space or a tab separation. This wrapper should be used for use with multiple cores of the computer. If the user wishes to use a single core of the computer, the wrapper binary\_model should be used. Note that the files "inputk" and "outputk" are deleted by the wrapper at the end of the function.

#### Value

A R function wrapping the binary executable, to be used with the EasyABC functions.

#### Author(s)

Franck Jabot, Thierry Faure and Nicolas Dumoulin

#### See Also

```
binary_model, ABC_rejection, ABC_sequential, ABC_mcmc
```

#### **Examples**

```
## Not run:
    ## artificial example to show how to use the binary_model function with
    # an executable "My_Executable"
    ABC_rej<-ABC_rejection(model=binary_model_cluster("./My_Executable"),
        prior=..., n_cluster=2,...)
# NB: on windows, "My_Executable" should be of the form "My_Executable.exe" :
    ABC_rej<-ABC_rejection(model=binary_model_cluster("./My_Executable.exe"),
        prior=..., n_cluster=2,...)
## End(Not run)</pre>
```

SABC

Simulated Annealing approach to Approximate Bayesian Computation (SABC)

# Description

Algorithms for the Simulated Annealing approach to Approximate Bayesian Computation (SABC).

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# Usage

```
SABC(
 r.model,
 r.prior,
 d.prior,
 n.sample,
 eps.init,
 iter.max,
 v = ifelse(method == "informative", 0.4, 1.2),
 beta = 0.8,
 delta = 0.1,
 resample = 5 * n.sample,
 verbose = n.sample,
 method = "noninformative",
 adaptjump = TRUE,
 summarystats = FALSE,
 y = NULL,
 f.summarystats = NULL,
)
```

# Arguments

r.model	Function that returns either a random sample from the likelihood or a scalar distance between such a sample and the data. The first argument must be the parameter vector.
r.prior	Function that returns a random sample from the prior.
d.prior	Function that returns the density of the prior distribution.
n.sample	Size of the ensemble.
eps.init	Initial tolerance or temperature.
iter.max	Total number of simulations from the likelihood.
V	Tuning parameter that governs the annealing speed. Defaults to 1.2, for the noninformative algorithm and 0.4, for the informative algorithm.
beta	Tuning parameter that governs the mixing in parameter space. Defaults to 0.8.
delta	Tuning parameter for the resampling steps. Defaults to 0.1.
resample	Number of accepted particle updates after which a resampling step is performed. Defaults to 5*n.sample.
verbose	Shows the iteration progress each verbose simulations from the likelihood. NULL for no output. Defaults to verbose = n.sample.
method	Argument to select algorithm. Accepts noninformative or informative.
adaptjump	Whether to adapt covariance of jump distribution. Default is TRUE.
summarystats	Whether summary statistics shall be calculated (semi-) automatically. Defaults to FALSE.

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y Data vector. Needs to be provided if either summarystats = TRUE or if r.model returns a sample from the likelihood.

f.summarystats If summarystats = TRUE this function is needed for the calculation of the sum-

mary statistics. Defaults to f. summary stats  $(x) = (x, x^2, x^3)$ , where the pow-

ers are to be understood element-wise.

... further arguments passed to r.model

#### **Details**

SABC defines a class of algorithms for particle ABC that are inspired by Simulated Annealing. Unlike other algorithms, this class is not based on importance sampling, and hence does not suffer from a loss of effective sample size due to re-sampling. The approach is presented in detail in Albert, Kuensch, and Scheidegger (2014; see references).

This package implements two versions of SABC algorithms, for the cases of a non-informative or an informative prior. These are described in detail in the paper. The algorithms can be selected using the method argument: method=noninformative or method=informative. In the informative case, the algorithm corrects for the bias caused by an over- or under-representation of the prior.

The argument adapt jump allows a choice of whether to adapt the covariance of the jump distribution. Default is TRUE.

Furthermore, the package allows for three different ways of using the data. If y is not provided, the algorithm expects r.model to return a scalar measuring the distance between a random sample from the likelihood and the data. If y is provided and summarystats = FALSE, the algorithm expects r.model to return a random sample from the likelihood and uses the relative sum of squares to measure the distances between y and random likelihood samples. If summarystats = TRUE the algorithm calculates summary statistics semi-automatically, as described in detail in the paper by Fearnhead et al. (2012; see references). The summary statistics are calculated by means of a linear regression applied to a sample from the prior and the image of f. summarystats of an associated sample from the likelihood.

#### Value

Returns a list with the following components:

E Matrix with ensemble of samples.

P Matrix with prior ensemble of samples.

eps Value of tolerance (temperature) at final iteration.

ESS Effective sample size, due to final bias correction (informative algorithm only).

#### Author(s)

Carlo Albert <u>carlo.albert@eawag.ch</u>, Andreas Scheidegger, Tobia Fasciati. Package initially compiled by Lukas M. Weber.

#### References

C. Albert, H. R. Kuensch and A. Scheidegger, Statistics and Computing 0960-3174 (2014), arXiv:1208.2157, *A Simulated Annealing Approach to Approximate Bayes Computations*.

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P. Fearnhead and D. Prangle, J. R. Statist. Soc. B 74 (2012), Constructing summary statistics for approximate Bayesian computation: semi-automatic approximate Bayesian computation.

# **Examples**

trait\_model

A stochastic individual-based model to demonstrate how the EasyABC functions can be used

#### **Description**

A stochastic individual-based model to demonstrate how the EasyABC functions can be used

#### Usage

```
trait_model(input = c(1, 1, 1, 1, 1, 1))
```

#### **Arguments**

input

the input array variables

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 $\begin{tabular}{ll} trait\_model\_internal & A stochastic individual-based model to demonstrate how the EasyABC \\ functions can be used \\ \end{tabular}$ 

# Description

A stochastic individual-based model to demonstrate how the EasyABC functions can be used

# Usage

trait\_model\_internal(input)

# Arguments

input the input array variables

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