# Package ‘MEIGOR’

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**License** GPL-3  
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MEIGOR-package

Description

A global optimization package containing several algorithms such as a scatter search implementation and variable neighborhood search (plus cooperative multicore/multimachine implementations of these) and dynamic hill climbing.

Details

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<tr>
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<td>0.99.0</td>
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<td>2012-09-10</td>
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<td>License:</td>
<td>GPLv3</td>
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</table>

Author(s)

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Maintainer: Jose Egea <josea.egea@upct.es>

References

See Also

essR essR

Description

essR attempts to solve problems of the form:
min F(x) subject to:
x
ceq(x) = 0 (equality constraints)
c_L <= c(x) <= c_U (inequality constraints)
x_L <= x <= x_U (bounds on the decision variables)

Constraint functions, if applicable, must be declared in the same script as the objective function as a second output argument, e.g.:

myfunction <- function(x){
calculate fx - scalar containing the objective function value
calculate gx - vector (or empty) containing the constraints values
return(list(fx,gx))
}

Details

Package: MEIGOR
Type: Package
Version: 0.99.6
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LazyLoad: yes

Author(s)

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References


See Also

essR

BayesFit

Description

BayesFit

CeSSR

Global optimization algorithm for MINLPs based on Scatter Search using a Cooperative Strategy

Description

CeSSR attempts to solve problems of the form:

\[
\min f(x, p_1, p_2, \ldots, p_n)
\]

subject to:

\[
c_e = 0
\]

\[
c_L \leq c(x) \leq c_U
\]

\[
x_L \leq x \leq x_U
\]

Usage

CeSSR(problem, opts, max_eval = Inf, max_time = Inf,
      n_iter, is_parallel = TRUE, type = "SOCKS", global_save_list = NULL, ...)

Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>problem</td>
<td>List containing problem settings.</td>
</tr>
<tr>
<td>opts</td>
<td>A list of n_threads lists containing options for each cooperative instance of essR.</td>
</tr>
<tr>
<td>max_eval</td>
<td>Maximum number of evaluations. Default is Inf.</td>
</tr>
<tr>
<td>max_time</td>
<td>Maximum time, default is Inf.</td>
</tr>
<tr>
<td>n_iter</td>
<td>Number of cooperative iterations. Default is 0 which is the same as running multiple single thread (as many as n_cpus) optimization runs.</td>
</tr>
<tr>
<td>is_parallel</td>
<td>Default is TRUE. Sometimes this it is useful to use as FALSE for debugging.</td>
</tr>
<tr>
<td>type</td>
<td>Choose between &quot;SOCKS&quot; and &quot;MPI&quot;. Default is &quot;SOCKS&quot; (socket-connection). If you are using &quot;SOCKS&quot; option and you want to run multiple cpus in different machines you must specify the adress of each machine in hosts. &quot;MPI&quot; mode requires you to have Rmpi installed.</td>
</tr>
<tr>
<td>global_save_list</td>
<td>Specify the names of global variables to be exported.</td>
</tr>
<tr>
<td>...</td>
<td>Additional variables.</td>
</tr>
</tbody>
</table>
CeSSR

Details
Check essR documentation for more information about the input arguments.

Value

- **f_mean**: Vector with size of n_iter+1 containing the mean value of the objective function in each iteration.
- **f_sd**: Vector with size of n_iter+1 containing the standard deviation value of the objective function in each iteration.
- **fbest**: Vector with size of n_iter+1 containing the best value of the objective function in each iteration.
- **iteration_res**: A list containing the results from every CeSSR instance initialized. It follows the format: results$iteration_res[[iteration+1]][[thread_number]]. See also essR
- **numeval**: Vector with size of n_iter+1 containing the number objective function evaluations at the end of each iteration.
- **time**: Vector with size of n_iter+1 containing the time spent at the end of an iteration.
- **x_sd**: A list containing the standard deviation of decision each variable at the end of an iteration. It follows the format: results$iteration_res[[iteration+1]][[thread_number]]
- **xbest**: A list containing the best set of decision variables found and the end of each iteration.

See Also

essR

Examples

```R
two <- function(x){
  f <- 0;
  n = length(x);
  for (i in 1:(n-1)){
    f <- f + 100*(x[i]^2 - x[i+1])^2 + (x[i]-1)^2;
  }
  return(f)
}

nvar = 20;
problem <- list(f=two, x_L=rep(-1000, nvar), x_U=rep(1000, nvar));

# Set 1 nodes and 2 cpu's per node
n_nodes = 1;
n_cpus_per_node = 3;

# Set different values for dim_refset, bal and n2 for each of the 10 cpu's to be used
dim1 = 23;   bal1 = 0;   n2_1 = 0;
dim2 = 33;   bal2 = 0;   n2_2 = 0;
dim3 = 46;   bal3 = 0;   n2_3 = 2;
dim4 = 56;   bal4 = 0;   n2_4 = 4;
dim5 = 72;   bal5 = 0.25; n2_5 = 7;
dim6 = 72;   bal6 = 0.25; n2_6 = 10;
dim7 = 88;   bal7 = 0.25; n2_7 = 15;
dim8 = 101;  bal8 = 0.5;  n2_8 = 20;
```

dim9 = 111; bal9 = 0.25; n2_9 = 50;
dim10 = 123; bal10 = 0.25; n2_10 = 100;

opts_dim = c(dim1, dim2, dim3, dim4, dim5, dim6, dim7, dim8, dim9, dim10);
opts_bal = c(bal1, bal2, bal3, bal4, bal5, bal6, bal7, bal8, bal9, bal10);
opts_n2 = c(n2_1, n2_2, n2_3, n2_4, n2_5, n2_6, n2_7, n2_8, n2_9, n2_10);
D = 10;

# Initialize counter and options
counter = 0;
opts = list();
hosts = c();

for(i in 1:n_nodes){
    for(j in 1:n_cpus_per_node){
        counter = counter + 1;
        # Set the name of every thread
        if(i<10) hosts = c(hosts, paste('node0', i, sep=''));
        if(i>=10 && i<100) hosts = c(hosts, paste('node', i, sep=''));
        opts[[counter]] = list();
        # Set specific options for each thread
        opts[[counter]]$local_balance = opts_bal[counter];
        opts[[counter]]$dim_refset = opts_dim[counter];
        opts[[counter]]$local_n2 = opts_n2[counter];
        # Set common options for each thread
        opts[[counter]]$maxeval = 10000;
        opts[[counter]]$local_solver = "dhc";
        # Options not set will take default values for every thread
    }
}

# Set the address of each machine, defined inside the 'for' loop
opts$hosts = c('localhost', 'localhost', 'localhost');

# Do not define the additional options for cooperative methods (e.g., ce_maxtime, ce_isparallel, etc.)
# They will take their default values
opts$ce_niter = 2;
opts$ce_type = "SOCKS";
opts$ce_isparallel = TRUE;

# Call the solver
Results <- MEIGO(problem, opts, algorithm="CeSSR")
CeVNSR

Description

Solves optimization problems with integer variables. Using several cooperative instances of VNS.

Usage

CeVNSR( problem, opts, max_eval = Inf, max_time = Inf, n_iter = 1, is_parallel = TRUE, type = "SOCKS", global_save_list = NULL, ...)

Arguments

problem          List containing problem settings.
opts             A list of n_threads lists containing options for each cooperative instance of essR.
max_eval         Maximum number of evaluations. Default is Inf.
max_time         Maximum time, default is Inf.
n_iter           Number of cooperative iterations. Default is 0 which is the same as running multiple single thread (as many as n_cpus) optimization runs.
is_parallel      Default is TRUE. Sometimes this it is useful to use as FALSE for debugging.
type             Choose between "SOCKS" and "MPI". Default is "SOCKS" (socket-connection).
                  If you are using "SOCKS" option and you want to run multiple cpus in different machines you must specify the adress of each machine in hosts.
                  "MPI" mode requires you to have Rmpi installed.
global_save_list Specify the names of global variables to be exported.

Details

problem[[ith_thread]]=VNS_problem; opts[[ith_thread]]=VNS_opts;
VNS_problem and VNS_opts correspond to lists as seen in the rvnds_hamming documentation.

Value

f_mean       Vector with size of n_iter+1 containing the mean value of the objective function in each iteration.
f_sd         Vector with size of n_iter+1 containing the standard deviation value of the objective function in each iteration.
fbest        Vector with size of n_iter+1 containing the best value of the objective function in each iteration.
iteration_res A list containing the results from every VNS instance initialized. It follows the format: results$iteration_res[[iteration+1]][[thread_number]].
umeval       Vector with size of n_iter+1 containing the number objective function evaluations at the end of each iteration.
time         Vector with size of n_iter+1 containing the time spent at the end of an iteration.
x_sd         A list containing the standard deviation of decision each variable at the end of an iteration. It follows the format: results$iteration_res[[iteration+1]][[thread_number]]
xbest        A list containing the best set of decision variables found and the end of each iteration.
See Also

rvnds_hamming MEIGO

Examples

```r
rosen10<-function(x){
  f<-0;
  n=length(x);
  for (i in 1:(n-1)){
    f <- f + 100*(x[i]^2 - x[i+1])^2 + (x[i]-1)^2;
  }
  return(f)
}

nvar=20;
problem<-list(f=rosen10, x_L=rep(-1000,nvar), x_U=rep(1000,nvar))

opts=list();
opts[[1]]=list(use_local=1,aggr=1,local_search=1,decomp=1,maxdist=0.8,maxeval=2000);
opts[[2]]=list(use_local=1,aggr=0,local_search=2,decomp=0,maxdist=0.5,maxeval=2000);
opts[[3]]=list(use_local=1,aggr=0,local_search=2,decomp=0,maxdist=0.5,maxeval=2000);
opts[[4]]=list(use_local=1,aggr=0,local_search=2,decomp=0,maxdist=0.5,maxeval=2000);

opts$hosts=c('localhost','localhost','localhost','localhost');

opts$ce_niter=2;
opts$ce_type="SOCKS";
opts$ce_isparallel= TRUE;

Results=MEIGO(problem,opts, algorithm="CeVNSR");
```

### cnolist

**A CNOlist from CellNOptR package**

**Description**

A CNOlist from CellNOptR to use with provided examples

### cur_params

**Current values of all model parameters**

**Description**

For a given set of values for the parameters to be estimated, this method returns an array containing the actual (not log-transformed) values of all model parameters, not just those to be estimated, in the same order as specified in the model. This is helpful when simulating the model at a given position in parameter space.
cur_params

Usage

cur_params(output, options, position = NULL)

Arguments

options

list with entries as explained below. Options set – defines the problem and sets some parameters to control the MCMC algorithm. model: List of model parameters - to estimate. The parameter objects must each have a ‘value’ attribute containing the parameter’s numerical value. estimate_params: list. List of parameters to estimate, all of which must also be listed in ‘options$model$parameters’. initial_values: list of float, optional. Starting values for parameters to estimate. If omitted, will use the nominal values from ‘options$model$parameters’.

step_fn: callable f(output), optional. User callback, called on every MCMC iteration. likelihood_fn: callable f(output, position). User likelihood function. prior_fn: callable f(output, position), optional. User prior function. If omitted, a flat prior will be used. nsteps: int. Number of MCMC iterations to perform. use_hessian: logical, optional. Whether to use the Hessian to guide the walk. Defaults to FALSE. rtol: float or list of float, optional. Relative tolerance for ode solver. atol: float or list of float, optional. Absolute tolerance for ode solver. norm_step_size: float, optional. MCMC step size. Defaults to a reasonable value. hessian_period: int, optional. Number of MCMC steps between Hessian recalculations. Defaults to a reasonable but fairly large value, as Hessian calculation is expensive. hessian_scale: float, optional. Scaling factor used in generating Hessian-guided steps. Defaults to a reasonable value. sigma_adj_interval: int, optional. How often to adjust ‘output$sig_value’ while annealing to meet ‘accept_rate_target’. Defaults to a reasonable value. Length of initial “burn-in” annealing period. Defaults to 10 ’nsteps’, or if ‘use_hessian’ is TRUE, to ‘hessian_period’ (i.e. anneal until first hessian is calculated) T_init: float, optional. Initial temperature for annealing. Defaults to a reasonable value. accept_rate_target: float, optional. Desired acceptance rate during annealing. Defaults to a reasonable value. See also ‘sigma_adj_interval’ above. sigma_max: float, optional. Maximum value for ‘output$sig_value’. Defaults to a reasonable value. sigma_min: float, optional. Minimum value for ‘output$sig_value’. Defaults to a reasonable value. sigma_step: float, optional. Increment for ‘output$sig_value’ adjustments. Defaults to a reasonable value. thermo_temp: float in the range [0,1], optional. Temperature for thermodynamic integration support. Used to scale likelihood when calculating the posterior value. Defaults to 1, i.e. no effect.

output

List of output values with entries as explained below. num_estimate: int. Number of parameters to estimate. estimate_idx: list of int. Indices of parameters to estimate in the model’s full parameter list. initial_values: list of float. Starting values for parameters to estimate, taken from the parameters’ nominal values in the model or explicitly specified in ‘options’. initial_position: list of float. Starting position of the MCMC walk in parameter space (log10 of ‘initial_values’). position: list of float. Current position of MCMC walk in parameter space, i.e. the most recently accepted move. test_position: list of float. Proposed MCMC move. acceptance: int. Number of accepted moves. T: float. Current value of the simulated annealing temperature. T_decay: float. Constant for exponential decay of ‘T’, automatically calculated such that T will decay from ‘options$T_init’ down to 1 over the first ‘options$anneal_length’ steps. sig_value: float. Current value of sigma, the scaling factor for the proposal distribution.
The MCMC algorithm dynamically tunes this to maintain the acceptance rate specified in `options$accept_rate_target`. iter: int. Current MCMC step number. start_iter: int. Starting MCMC step number. ode_options: list. Options for the ODE integrator, currently just 'rtol' for relative tolerance and 'atol' for absolute tolerance. initial_prior: float. Starting prior value, i.e. the value at 'initial_position'. initial_likelihood: float. Starting likelihood value, i.e. the value at 'initial_position'. initial_posterior: float. Starting posterior value, i.e. the value at 'initial_position'. accept_prior: float. Current prior value i.e. the value at 'position'. accept_likelihood: float. Current likelihood value i.e. the value at 'position'. accept_posterior: float. Current posterior value i.e. the value at 'position'. test_prior: float. Prior value at 'test_position'. test_likelihood: float. Likelihood value at 'test_position'. test_posterior: float. Posterior value at 'test_position'. hessian: array of float. Current hessian of the posterior landscape. Size is 'num_estimate' x 'num_estimate'.

position 
list of float, optional. log10 of the values of the parameters being estimated. If omitted, 'output$position' (the most recent accepted output move) will be used. The model’s nominal values will be used for all parameters *not* being estimated, regardless.

Value
A list of the values of all model parameters.

Examples

```r
data("simpleExample", package="MEIGOR")
initial_pars = createLBodeContPars(model, LB_n=1, LB_k=0.1, LB_tau=0.01, UB_n=5, UB_k=0.9, UB_tau=10, random=TRUE)
simData = plotLBodeFitness(cnolist, model, initial_pars, reltol=1e-05, atol=1e-03, maxStepSize=0.01)

f_bayesFit <- function(position, params=initial_pars, exp_var=opts$exp_var) {
  # convert from log
  params$parValues = 10^position
  ysim = getLBodeDataSim(cnolist=cnolist, model=model, ode_parameters=params)
  data_as_vec = unlist(cnolist$valueSignals)
  sim_as_vec = unlist(ysim)
  # set nan (NAs) to 0
  sim_as_vec[is.na(sim_as_vec)] = 0
```
sim_as_vec[is.nan(sim_as_vec)]= 0
return(sum((data_as_vec-sim_as_vec)^2/(2*exp_var^2)))
}
prior_mean = log10(initial_pars$parValues)
prior_var = 10

opts <- list("model"=NULL, "estimate_params"=NULL,"initial_values"=NULL, "tspan"=NULL, "step_fn"=NULL, "likelihood_fn"=NULL, "prior_fn"=NULL, "nsteps"=NULL, "use_hessian"=FALSE, "rtol"=NULL, "atol"=NULL, "norm_step_size"=0.75, "hessian_period"=25000, "hessian_scale"=0.005, "sigma_adj_interval"=NULL, "anneal_length"=NULL, "T_init"=10, "accept_rate_target"=0.3, "sigma_max"=1, "sigma_min"=0.25, "sigma_step"=0.125, "thermo_temp"=1, "seed"=NULL)

opts$nsteps = 2000

opts$likelihood_fn = f_bayesFit
opts$use_hessian = TRUE
opts$hessian_period = opts$nsteps/10

opts$model = list(parameters=list(name=initial_pars$parNames, value=initial_pars$parValues))

opts$estimate_params = initial_pars$parValues

opts$exp_var = 0.01

res = runBayesFit(opts)

initial_pars$parValues = cur_params(output=res, options=opts)

---

dhc Local search algorithm within eSS

Description

Local search algorithm within eSS

Note

For internal use of MEIGOR.

---

essR Global optimization algorithm for MINLPs based on Scatter Search

Description

essR attempts to solve problems of the form:

\[ \min f(x, p_1, p_2, \ldots, p_n) \]

subject to:

\[ c_e = 0 \]
\[ c_L \leq c(x) \leq c_U \]
\[ x_L \leq x \leq x_U \]
Usage

essR(problem, opts = list(maxeval = NULL, maxtime = NULL), ...)

Arguments

problem List containing problem definition.

opts List containing options (if set as opts <- numeric(0) default options will be loaded).

... Additional variables passed to the objective function

Details

Problem definition:

problem$f: Name of the file containing the objective function (String).

problem$x_L: Lower bounds of decision variables (vector).

problem$x_U: Upper bounds of decision variables (vector).

problem$x_0: Initial point(s) (optional; vector or matrix).

problem$f_0: Function values of initial point(s) (optional). These values MUST correspond to feasible points.

NOTE: The dimension of f_0 and x_0 may be different. For example, if we want to introduce 5 initial points but we only know the values for 3 of them, x_0 would have 5 rows whereas f_0 would have only 3 elements. In this example, it is mandatory that the first 3 rows of x_0 correspond to the values of f_0.

Fill the following fields if your problem has non-linear constraints:

problem$neq: Number of equality constraints (Integer; do not define it if there are no equality constraints).

problem$c_L: Lower bounds of nonlinear inequality constraints (vector).

problem$c_U: Upper bounds of nonlinear inequality constraints (vector).

problem$int_var: Number of integer variables (Integer).

problem$bin_var: Number of binary variables (Integer).

problem$vtr: Objective function value to be reached (optional).

User options:

opts$maxeval: Maximum number of function evaluations (Default 1000).

opts$maxtime: Maximum CPU time in seconds (Default 60).

opts$iterprint: Print each iteration on screen: 0-Deactivated; 1-Activated (Default 1).

opts$plot: Plots convergence curves: 0-Deactivated; 1-Plot curves on line; 2-Plot final results (Default 0).

opts$weight: Weight that multiplies the penalty term added to the objective function in constrained problems (Default 1e6).

opts$log_var: Indexes of the variables which will be used to generate diverse solutions in different orders of magnitude (vector).

opts$tolc: Maximum absolute violation of the constraints (Default 1e-5).

opts$prob_bound: Probability (0-1) of biasing the search towards the bounds (Default 0.5).

opts$inter_save: Saves results in a mat file in intermediate iterations. Useful for very long runs (Binary; Default = 0).

Global options:
opts$dim_refset: Number of elements in Refset (Integer; automatically calculated).
opts$ndiverse: Number of solutions generated by the diversificator (Default 10*nvar).

Local options:

opts$local_solver: Choose local solver 0: Local search deactivated (Default), "NM", "BFGS", "CG", "LBFGSB", "SA", "SOLNP".
opts$local_tol: Level of tolerance in local search.
opts$local_iiterprint: Print each iteration of local solver on screen (Binary; default = 0).
opts$local_n1: Number of iterations before applying local search for the 1st time (Default 1).
opts$local_n2: Minimum number of iterations in the global phase between 2 local calls (Default 10).
opts$local_balance: Balances between quality (=0) and diversity (=1) for choosing initial points for the local search (default 0.5).
opts$local_finish: Applies local search to the best solution found once the optimization if finished (same values as opts.local.solver).
opts$local_bestx: When activated (i.e. =1) only applies local search to the best solution found to date, ignoring filters (Default=0).

Value

fbest
xbest
cpu_time
f
x
time
neval
numeval
local_solutions
local_solutions_values
end_crit

R code of the eSS optimization code from: Process Engineering Group IIM-CSIC.
Constraint functions, if applicable, must be declared in the same script as the objective function as a second output argument, e.g.:
myfunction <- function(x){
calculate fx - scalar containing the objective function value
calculate gx - vector (or empty) containing the constraints values
return(list(fx,gx))

Author(s)
Jose Egea

References
If you use essR and publish the results, please cite the following papers:

Examples
#1 Unconstrained problem
ex1 <- function(x){
return(y)
}

#global optimum
#x*=[0.0898, -0.7127];
# or
#x*=[-0.0898, 0.7127];
#
#f(x*)= -1.03163;

#========================= PROBLEM SPECIFICATIONS ===========================
problem<-list(f="ex1",x_L=rep(-1,2),x_U=rep(1,2))
opts<-list(maxeval=500, ndiverse=10, dim_refset=4, local_solver="solnp", local_n2=1)
#========================= END OF PROBLEM SPECIFICATIONS =====================
Results<-essR(problem,opts);

#2 Constrained problem
ex2<-function(x){
F=-x[1]-x[2];
g<=-rep(0,2);
return(list(F=F,g=g))
}

# global optimum
#x*=[2.32952, 3.17849];
#f(x*)=-5.50801
#3 Constrained problem with equality constraints

```r
ex3<-function(x,k1,k2,k3,k4){
  f=-x[4];
  #Equality constraints
  g<-rep(0,5);
  g[2]=x[1]-1+k1*x[1]*x[5];
  g[4]=x[3]+x[1]-1+k3*x[3]*x[5];
  #Inequality constraint
  g[5]=x[5]^0.5+x[6]^0.5;
  return(list(f=f,g=g));
}
```

#global optimum

```r
#x*=[0.77152 0.516994 0.204189 0.388811 3.0355 5.0973];
#f(x*)=-0.388811;
```

#4 Mixed integer problem

```r
ex4<-function(x){
  g<-rep(0,3);
  ```
ith_essR

\[
\]
\[
\]
return(list(F=F, g=g));
}

# global optimum
#x*=[2.23607, 0, 1, 0];
#f(x*)=-40.9575;

#========================= PROBLEM SPECIFICATIONS ===========================

problem<-list(f="ex4", x_L=rep(0,4), x_U=rep(10,4), x_0=c(3,4,5,1), int_var=3, c_L=rep(-Inf,3), c_U=c(8,10,5))

opts<-list(maxtime=2)

#========================= END OF PROBLEM SPECIFICATIONS =====================

Results<-essR(problem,opts);

---

### essR_multistart

**Description**

Multistart function for eSS

**Note**

For internal use of CNORode.

---

### eucl_dist

**Description**

This functions is used internally by essR to compute the euclidean distance between the rows of two different matrices. The matrices must have the same number of columns.

**Note**

For internal use of MEIGOR.

---

### ith_essR

**Description**

Auxiliary function to perform parallel runs

**Note**

For internal use of MEIGOR.
ith_VNSR

**Auxiliary function to perform parallel runs**

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Auxiliary function to perform parallel runs

**Note**

For internal use of MEIGOR.

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**MEIGO**

**MEIGO main function**

**Description**

Wrapper around the different optimisation methods

**Usage**

MEIGO(problem, opts, algorithm, ...)

**Arguments**

- **problem**: List containing problem settings.
- **opts**: A list of n_threads lists containing options for each cooperative instance of essR.
- **algorithm**: One of VNS, ESS, MULTISTART, CESSR, CEVNSR. Check the documentation of each algorithm for more information.
- **...**: Additional input arguments.

**See Also**

essR rvnds_hamming CeVNSR CeSSR

**Examples**

```r
#global optimum
x*=[0.0898, -0.7127];
# or
x*=[-0.0898, 0.7127];
#
fx*= -1.03163;

ex1 <- function(x){
return(y)
}
```

#================================ PROBLEM SPECIFICATIONS =========================
problem <- list(f = ex1, x_L = rep(-1, 2), x_U = rep(1, 2))
opts <- list(maxeval = 500, ndiverse = 40, local_solver = 'DHC', local_finish = 'LBFGSB', local_iterprint = 1)

#========================= END OF PROBLEM SPECIFICATIONS =====================

Results <- MEIGO(problem, opts, algorithm = "ESS");

---

model

_A model from CellNoptR_

Description

A model from CellNoptR to use with provided examples

nls_fobj

_Auxiliary function to evaluate constraints_

Description

Auxiliary function to evaluate constraints

Note

For internal use of MEIGOR.

optim_fobj

_Gateway function to evaluate the objective function when the local solvers are invoked._

Description

This function is used internally by essR to evaluate the objective function when the local solvers are invoked.

Note

For internal use of MEIGOR.

paramsOpt

_Optimal parameters for simulation with CNORode_

Description

Optimal parameters for simulation with CNORode. Use with provided examples
runBayesFit

Running the BayesFit optimisation

Description

"runBayesFit" defines the prior function and runs the BayesFit estimation

Usage

runBayesFit(opts)

Arguments

opts  list with entries as explained below. Options set – defines the problem and sets some parameters to control the MCMC algorithm. model: List of model parameters - to estimate. The parameter objects must each have a 'value' attribute containing the parameter's numerical value. estimate_params: list. List of parameters to estimate, all of which must also be listed in 'options$model$parameters'. initial_values: list of float, optional. Starting values for parameters to estimate. If omitted, will use the nominal values from 'options$model$parameters' step_fn: callable f(output), optional. User callback, called on every MCMC iteration. likelihood_fn: callable f(output, position). User likelihood function. prior_fn: callable f(output, position), optional. User prior function. If omitted, a flat prior will be used. nsteps: int. Number of MCMC iterations to perform. use_hessian: logical, optional. Wheter to use the Hessian to guide the walk. Defaults to FALSE. rtol: float or list of float, optional. Relative tolerance for ode solver. atol: float or list of float, optional. Absolute tolerance for ode solver. norm_step_size: float, optional. MCMC step size. Defaults to a reasonable value. hessian_period: int, optional. Number of MCMC steps between Hessian recalculation. Defaults to a reasonable but fairly large value, as Hessian calculation is expensive. hessian_scale: float, optional. Scaling factor used in generating Hessian-guided steps. Defaults to a reasonable value. sigma_adj_interval: int, optional. How often to adjust ‘output$sig_value’ while annealing to meet ‘accept_rate_target’. Defaults to a reasonable value. anneal_length: int, optional. Length of initial "burn-in" annealing period. Defaults to 10 'nsteps', or if ‘use_hessian’ is TRUE, to 'hessian_period' (i.e. anneal until first hessian is calculated) T_init: float, optional. Initial temperature for annealing. Defaults to a reasonable value. accept_rate_target: float, optional. Desired acceptance rate during annealing. Defaults to a reasonable value. See also 'sigma_adj_interval' above. sigma_max: float, optional. Maximum value for 'output$sig_value'. Defaults to a reasonable value. sigma_min: float, optional. Minimum value for 'output$sig_value'. Defaults to a reasonable value. sigma_step: float, optional. Increment for 'output$sig_value' adjustments. Defaults to a reasonable value. To eliminate adaptive step size, set sigma_step to 1. thermo_temp: float in the range [0,1], optional. Temperature for thermodynamic integration support. Used to scale likelihood when calculating the posterior value. Defaults to 1, i.e. no effect.

Value

The output after the optimisation is finished - a list with entries as explained in 'Arguments'.
Examples

data("simpleExample", package="MEIGOR")
initial_pars = createLBodeContPars(model, LB_n=1, LB_k=0.1, LB_tau=0.01, UB_n=5, UB_k=0.9, UB_tau=10, random=TRUE)
simData = plotLBodeFitness(cnolist, model, initial_pars, reltol=1e-05, atol=1e-03, maxStepSize=0.01)

f_bayesFit <- function(position, params=initial_pars, exp_var=opts$exp_var) {
# convert from log
params$parValues = 10^position
ysim = getLBodeDataSim(cnolist=cnolist, model=model,
ode_parameters=params)
data_as_vec = unlist(cnolist$valueSignals)
sim_as_vec = unlist(ysim)
# set nan (NAs) to 0
sim_as_vec[is.na(sim_as_vec)] = 0
sim_as_vec[is.nan(sim_as_vec)]= 0
return(sum((data_as_vec-sim_as_vec)^2/(2*exp_var^2)))
}
prior_mean = log10(initial_pars$parValues)
prior_var = 10

opts <- list("model"=NULL, "estimate_params"=NULL,"initial_values"=NULL,
"tspan"=NULL, "step_fn"=NULL, "likelihood_fn"=NULL,
"prior_fn"=NULL, "nsteps"=NULL, "use_hessian"=FALSE,
"rtol"=NULL, "atol"=NULL, "norm_step_size"=0.75,
"hessian_period"=25000, "hessian_scale"=0.085,
"sigma_adj_interval"=NULL, "anneal_length"=NULL,
"T_init"=10, "accept_rate_target"=0.3, "sigma_max"=1,
"sigma_min"=0.25, "sigma_step"=0.125, "thermo_temp"=1, "seed"=NULL)

opts$nsteps = 2000
opts$likelihood_fn = f_bayesFit
opts$use_hessian = TRUE
opts$hessian_period = opts$nsteps/10
opts$model = list(parameters=list(name=initial_pars$parNames,
value=initial_pars$parValues))
opts$estimate_params = initial_pars$parValues
opts$exp_var = 0.01

res = runBayesFit(opts)

initial_pars$parValues = cur_params(output=res, options=opts)

-----------------------------------------------------------------------
rvnds_hamming Main VNS function
-----------------------------------------------------------------------

Description
VNS Kernel function

Usage
rvnds_hamming(problem, opts, ...)

Arguments

- **problem**: List containing problem settings definition.
- **opts**: List containing options (if set as opts <- numeric(0) default options will be loaded).
- ... Additional variables passed to the objective function

Details

- `problem$f`: Name of the file containing the objective function (String).
- `problem$x_L`: Lower bounds of decision variables (vector).
- `problem$x_U`: Upper bounds of decision variables (vector).
- `problem$x_0`: Initial point(s) (optional; vector or matrix).
- `problem$f_0`: Function values of initial point(s) (optional). These values MUST correspond to feasible points.

User options:

- `opts$maxeval`: Maximum number of function evaluations (Default 1000).
- `opts$maxtime`: Maximum CPU time in seconds (Default 60).
- `opts$maxdist`: Percentage of the problem dimension which will be perturbed in the furthest neighborhood (varies between 0 and 1, default is 0.5).
- `opts$use_local`: Uses local search (1) or not (0). The default is 1.

The following options only apply when the local search is activated:

- `opts$use_aggr`: Aggressive search. The local search is only applied when the best solution has been improved (1=aggressive search, 0=non-aggressive search, default:0).
- `opts$local search type`: Applies a first (=1) or a best (=2) improvement scheme for the local search (Default: 1).
- `opts$decomp`: Decompose the local search (=1) using only the variables perturbed in the global phase. Default: 1.

Value

- **fbest**: Best objective function value found after the optimization
- **xbest**: Vector providing the best function value
- **cpu_time**: Time in seconds consumed in the optimization
- **func**: Vector containing the best objective function value after each iteration
- **x**: Matrix containing the best vector after each iteration
- **time**: Vector containing the cpu time consumed after each iteration
- **neval**: Vector containing the number of function evaluations after each iteration
- **numeval**: Number of function evaluations

Examples

```r
rosen10<-.function(x){
f<-0;
n=length(x);
for (i in 1:(n-1)){
```
\[ f \leftarrow f + 100 \times (x[i]^2 - x[i+1])^2 + (x[i] - 1)^2; \]
\]
\[ \text{return}(f) \]
\]
\[ nvar \leftarrow 10; \]
\[ \text{problem} \leftarrow \text{list}(f=\text{"rosen10"}, \ x_L=\text{rep}(-5, nvar), \ x_U=\text{rep}(1, nvar)) \]
\[ \text{opts} \leftarrow \text{list}(\text{maxeval}=2000, \ \text{maxtime}=3600 \times 69, \ \text{use_local}=1, \ \text{aggr}=0, \ \text{local_search_type}=1, \ \text{decomp}=1, \ \text{maxdist}=0.5) \]
\[ \text{algorithm} \leftarrow \text{"VNS"}; \]
\[ \text{Results} \leftarrow \text{MEIGO}(\text{problem}, \text{opts}, \text{algorithm}); \]

---

**rvnds_local**  
Local search in VNS  

**Description**  
Local search in VNS

**Note**  
For internal use of MEIGOR.

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**solnp_eq**  
Gateway function to evaluate the equality constraints when solnp is invoked as local solver

**Description**  
This function is used by essR to evaluate the equality constraints when solnp is invoked as local solver

**Note**  
For internal use of MEIGOR.

---

**solnp_fobj**  
Gateway function to evaluate the objective function when solnp is invoked as local solver

**Description**  
This function is used internally by essR to evaluate the objective function when solnp is invoked as local solver

**Note**  
For internal use of MEIGOR.
**solnp_ineq**

*Gateway function to evaluate the inequality constraints when solnp is invoked as local solver*

**Description**

This function is used internally by essR to evaluate the inequality constraints when solnp is invoked as local solver.

**Note**

For internal use of MEIGOR.

**ssm_beyond**

*Function that expands the search direction when a good offspring solution has been found*

**Description**

This function is used internally by essR to expand the search direction when a good offspring solution has been found.

**Note**

For internal use of MEIGOR.

**ssm_defaults**

*Sets the default options for eSSR*

**Description**

This function is used internally by essR to set default options.

**Note**

For internal use of MEIGOR.

**ssm_evalfc**

*Gateway function to evaluate the objective function in essR*

**Description**

This function is used internally by essR to evaluate the objective function.

**Note**

For internal use of MEIGOR.
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<td>For internal use of MEIGOR.</td>
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<tr>
<td></td>
<td>This function is used internally by essR to calculate relative errors between two vectors</td>
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<td><code>ssm_localsolver</code></td>
<td>Configure local solver</td>
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<td>Sets the different options and parameters for the local solvers invoked by essR</td>
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<td>Assigns values to the options defined by the user</td>
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<td>Calculates the penalized objective function in constrained problems</td>
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**ssm_round_int**

*Rounds variables declared as integer of binary*

**Description**

This function is used internally by essR to round variables declared as integer of binary.

**Note**

For internal use of MEIGOR.

**vns_defaults**

*Default options for VNS*

**Description**

Default options for VNS

**Usage**

`vns_defaults(...)`

**Arguments**

`...`

**vns_optset**

*Set VNS options*

**Description**

Set VNS options

**Note**

For internal use of MEIGOR.
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