Package: MEIGOR (via r-universe)

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Type Package

Title MEIGOR - MEtaheuristics for bIoinformatics Global Optimization

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Description MEIGOR provides a comprehensive environment for performing global optimization tasks in bioinformatics and systems biology. It leverages advanced metaheuristic algorithms to efficiently search the solution space and is specifically tailored to handle the complexity and high-dimensionality of biological datasets. This package supports various optimization routines and is integrated with Bioconductor's infrastructure for a seamless analysis workflow.

License GPL-3

Encoding UTF-8

LazyData false

biocViews SystemsBiology, Optimization, Software

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VignetteBuilder knitr

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essR-package *Global optimization algorithm for MINLPs based on Scatter Search*

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
Date:	2012-02-04
License:	GPL-3
LazyLoad:	yes

Author(s)

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References

Egea, J.A., Maria, R., Banga, J.R. (2010) An evolutionary method for complex-process optimization. Computers & Operations Research 37(2): 315-324.

Egea, J.A., Balsa-Canto, E., Garcia, M.S.G., Banga, J.R. (2009) Dynamic optimization of nonlinear processes with an enhanced scatter search method. Industrial & Engineering Chemistry Research 49(9): 4388-4401.

See Also

essR

MEIGOR-package *Global optimization Toolbox*

Description

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

Details

Package:	MEIGOR
Type:	Package
Version:	0.99.0
Date:	2012-09-10
License:	GPLv3
LazyLoad:	yes

Author(s)

Jose Egea David Henriques Thomas Cokelaer Alejandro F. Villaverde Julio R. Banga Julio Saez-Rodriguez

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References

Egea, J.A., Maria, R., Banga, J.R. (2010) An evolutionary method for complex-process optimization. Computers & Operations Research 37(2): 315-324.

Egea, J.A., Balsa-Canto, E., Garcia, M.S.G., Banga, J.R. (2009) Dynamic optimization of nonlinear processes with an enhanced scatter search method. Industrial & Engineering Chemistry Research 49(9): 4388-4401.

See Also

essR essR

BayesFit *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:

$minf(x, p_1, p_2, ..., p_n)$

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

problem	List containing problem settings.
opts	A list of n_threads lists containing options for each cooperative instance of essR.
max_eval	Maximum bumber 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.
...	Additional variables.

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 eSSR 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

```
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;

sfStop()

problem<-list(f=rosen10, 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")
sfStop()
```

CeVNSR *Global optimization algorithm for MINLPs based on VNS using a Co-operative Strategy*

Description

Solves optimization problems with intenger 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 bumber 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.
...	Additional variables.

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$iteration_res[[iteration+1]][[thread_number]].
numeval	Vector with size of n_iter+1 containing the number objective function evaluations at the end of each iteration.
time	Vector with size of n_iter+1 containing the time spent at the end of an iteration.
x_sd	A list containing the standard deviation of decision each variable at the end of an iteration. It follows the format: results$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

rvnds_hamming MEIGO

---

cnolist *A CNOlist from CellNOptR paclage*

Description

A CNOlist from CellNoptR to use with provided examples

---

cnolist_cellnopt *A CNOlist from CellNOptR paclage*

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.

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. 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 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$sig_value' while annealing to meet 'accept_rate_target'. Defaults to a reasonable value. anneal_length: int, optional. Length of initial "burn-in" annealing period. Defaults to 10 'nsteps', or if 'use_hessian' is TRUE, to 'hessian_period' (i.e. anneal until first hessian is calculated) T_init: float, optional. Initial temperature for annealing. Defaults to a resonable value. accept_rate_target: float, optional. Desired acceptance rate during annealing. Defaults to a reasonable value. See also 'sigma_adj_interval' above. sigma_max: float, optional. Maximum value for 'output$sig_value'. Defaults to a resonable value. sigma_min: float, optional. Minimum value for 'output$sig_value'. Defaults to a resonable value. sigma_step: float, optional. Increment for 'output$sig_value' adjustments. Defaults to a resonable 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.

`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 mmove. 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' setps. sig_value: float. Current value of sigma, the scaling factor for the proposal distribution. The MCMC algorithm dynamically tunes this to maintain the aaceptance 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'. positions: array of float. Trace of all proposed moves. Size is 'num_estimate' x 'nsteps'. priors: array of float. Trace of all priors corresponding to 'positions'. Length is 'nsteps'. likelihoods: array of float. Trace of all likelihoods corresponding to 'positions'. Length is 'nsteps'. posteriors: array of float. Trace of all posteriors corresponding to 'positions'. Length is 'nsteps'. alphas: array of float. Trace of 'alpha' parameter and calculated values. Length is 'nsteps'. sigmas: array of float. Trace of 'sigma' parameter and calculated values. Length is 'nsteps'. delta_posteriors: array of float. Trace of 'delta_posterior' parameter and calculated values. Length is 'nsteps'. ts: array of float. Trace of 'T' parameter and calculated values. Length is 'nsteps'. accepts: logical array. Trace of wheter each proposed move was accepted or not. Length is 'nsteps'. rejects: logical array. Trace of wheter each proposed move was rejected or not. Length is 'nsteps'. hessians: array of float. Trace of all hessians. Size is 'num_estimate' x 'num_estimate' x 'num_hessians' where 'num_hessians' is the actual number of hessians to be calculated.

`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

```
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)
```

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:

$minf(x, p_1, p_2, ..., p_n)$

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).
opts$combination: Type of combination of Refset elements (Default 1);1: hyper-rectangles; 2: linear combinations.

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$local_iterprint: Print each iteration of local solver on screen (Binary; default = 0).
opts$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`	Best objective function value found after the optimization
`xbest`	Vector providing the best function value
`cpu_time`	Time in seconds consumed in the optimization
`f`	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
`local_solutions`	Local solutions found by the local solver (in rows)
`local_solutions_values`	Function values of the local solutions
`end_crit`	Criterion to finish the optimization:

1 Maximal number of function evaluations achieved
2 Maximum allowed CPU Time achieved
3 Value to reach achieved

Note

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:

Egea, J.A., Maria, R., Banga, J.R. (2010) An evolutionary method for complex-process optimization. Computers & Operations Research 37(2): 315-324.

Egea, J.A., Balsa-Canto, E., Garcia, M.S.G., Banga, J.R. (2009) Dynamic optimization of nonlinear processes with an enhanced scatter search method. Industrial & Engineering Chemistry Research 49(9): 4388-4401.

Examples

```
#1 Unconstrained problem

ex1 <- function(x){
 y<-4*x[1]*x[1]-2.1*x[1]^4+1/3*x[1]^6+x[1]*x[2]-4*x[2]*x[2]+4*x[2]^4;
 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);
 g[1]<-x[2]-2*x[1]^4+8*x[1]^3-8*x[1]^2;
 g[2]<-x[2]-4*x[1]^4+32*x[1]^3-88*x[1]^2+96*x[1];
 return(list(F=F,g=g))
}

# global optimum
#x*=[2.32952, 3.17849];
#f(x*)=-5.50801

#========================= PROBLEM SPECIFICATIONS ===========================
problem<-list(f="ex2",x_L=rep(0,2),x_U=c(3,4), c_L=rep(-Inf,2), c_U=c(2,36))
opts<-list(maxeval=750, local_solver="solnp", local_n2=1)
```

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

Results<-essR(problem,opts);



#3 Constrained problem with equality constraints

ex3<-function(x,k1,k2,k3,k4){
 f=-x[4];
#Equality constraints
 g<-rep(0,5);
 g[1]=x[4]-x[3]+x[2]-x[1]+k4*x[4]*x[6];
 g[2]=x[1]-1+k1*x[1]*x[5];
 g[3]=x[2]-x[1]+k2*x[2]*x[6];
 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
#x*=[0.77152
#  0.516994
#  0.204189
#  0.388811
#  3.0355
#  5.0973];
#
#f(x*)= -0.388811;

#========================= PROBLEM SPECIFICATIONS ===========================
problem<-list(f="ex3",x_L=rep(0,6),x_U=c(rep(1,4),16,16), neq=4, c_L=-Inf, c_U=4)
opts<-list(maxtime=7, local_solver="solnp", local_n2=10)
#========================= END OF PROBLEM SPECIFICATIONS =====================

k1=0.09755988;
k3=0.0391908;
k2=0.99*k1;
k4=0.9*k3;
Results<-essR(problem,opts,k1,k2,k3,k4);



#4 Mixed integer problem

ex4<-function(x){
 F = x[2]^2 + x[3]^2 + 2.0*x[1]^2 + x[4]^2 - 5.0*x[2] - 5.0*x[3] - 21.0*x[1] + 7.0*x[4];
 g<-rep(0,3);
 g[1] = x[2]^2 + x[3]^2 + x[1]^2 + x[4]^2 + x[2] - x[3] + x[1] - x[4];
```

```
 g[2] = x[2]^2 + 2.0*x[3]^2 + x[1]^2 + 2.0*x[4]^2 - x[2] - x[4];
 g[3] = 2.0*x[2]^2 + x[3]^2 + x[1]^2 + 2.0*x[2] - x[3] - x[4];
 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 *Multistart function for eSS*

Description

Multistart function for eSS

Note

For internal use of CNORode.

---

eucl_dist *Computes the euclidean distance between the rows of two different matrices*

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 *Auxiliary function to perform parallel runs*

Description

Auxiliary function to perform parallel runs

Note

For internal use of MEIGOR.

ith_VNSR *Auxiliary function to perform parallel runs*

Description

Auxiliary function to perform parallel runs

Note

For internal use of MEIGOR.

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

```
#global optimum

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

ex1 <- function(x){
 y<-4*x[1]*x[1]-2.1*x[1]^4+1/3*x[1]^6+x[1]*x[2]-4*x[2]*x[2]+4*x[2]^4;
 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

`model_cellnopt` *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 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$sig_value' while annealing to meet 'accept_rate_target'. Defaults to a reasonable value. anneal_length: int, optional. Length of initial "burn-in" annealing period. Defaults to 10 'nsteps', or if 'use_hessian' is TRUE, to 'hessian_period' (i.e. anneal until first hessian is calculated) T_init: float, optional. Initial temperature for annealing. Defaults to a resonable value. accept_rate_target: float, optional. Desired acceptance rate during annealing. Defaults to a reasonable value. See also 'sigma_adj_interval' above. sigma_max: float, optional. Maximum value for 'output$sig_value'. Defaults to a resonable value. sigma_min: float, optional. Minimum value for 'output$sig_value'. Defaults to a resonable value. sigma_step: float, optional. Increment for 'output$sig_value' adjustments. Defaults to a resonable 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$maxdist: Percentage of the problem dimension which will be perturbed in the furthest neighborhood (varies between 0 and1, default is 0.5).
opts$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

```
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<-10;

problem<-list(f="rosen10", x_L=rep(-5,nvar), x_U=rep(1,nvar))

opts<-list(maxeval=2000, maxtime=3600*69, use_local=1, aggr=0, local_search_type=1, decomp=1, maxdist=0.5)

algorithm<-"VNS";

Results<-MEIGO(problem,opts,algorithm);
```

rvnds_local — *Local search in VNS*

Description

Local search in VNS

Note

For internal use of MEIGOR.

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 functions 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 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.

`ssm_isdif2` *Calculates relative errors between two vectors*

Description

This function is used internally by essR to calculate relative errors between two vectors

Note

For internal use of MEIGOR.

`ssm_localsolver` *Configure local solver*

Description

Sets the different options and parameters for the local solvers invoked by essR

Note

For internal use of MEIGOR.

`ssm_optset` *Assigns values to the options defined by the user*

Description

This function is used internally by essR for assigning values to the options defined by the user

Note

For internal use of MEIGOR.

ssm_penalty_function *Calculates the penalized objective function in constrained problems*

Description

This function is used internally by essR to calculate the penalized objective function in constrained problems

Note

For internal use of MEIGOR.

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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