Package 'DEoptimR'

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Title Differential Evolution Optimization in Pure R

Description Differential Evolution (DE) stochastic algorithms for global optimization of problems with and without constraints. The aim is to curate a collection of its state-of-the-art variants that (1) do not sacrifice simplicity of design,
(2) are essentially tuning-free, and
(3) can be efficiently implemented directly in the R language. Currently, it only provides an implementation of the 'jDE' algorithm by Brest et al. (2006) <doi:10.1109/TEVC.2006.872133>.

Imports stats

Enhances robustbase

License GPL (>= 2)

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JDEoptim

Description

An bespoke implementation of the 'jDE' variant by Brest et al. (2006) doi: 10.1109/TEVC.2006.872133.

Usage

Arguments

lower, upper	numeric vectors of <i>lower</i> or <i>upper</i> bounds, respectively, for the parameters to be optimized over. Must be finite (is.finite) as they bound the hyper rectangle of the initial random population.
fn	(nonlinear) objective function to be <i>minimized</i> . It takes as first argument the vector of parameters over which minimization is to take place. It must return the value of the function at that point.
constr	an optional function for specifying the nonlinear constraints under which we want to minimize fn. Nonlinear equalities should be given first and defined to equal zero $(h_j(X) = 0)$, followed by nonlinear inequalities defined as lesser than zero $(g_i(X) \leq 0)$. This function takes the vector of parameters as its first argument and returns a real vector with the length of the total number of constraints. It defaults to NULL, meaning that <i>bound-constrained</i> minimization is used.
meq	an optional positive integer specifying that the first meq constraints are treated as <i>equality</i> constraints, all the remaining as <i>inequality</i> constraints. Defaults to 0 (inequality constraints only).
eps	maximal admissible constraint violation for equality constraints. An optional real vector of small positive tolerance values with length meq used in the transformation of equalities into inequalities of the form $ h_j(X) - \epsilon \leq 0$. A scalar value is expanded to apply to all equality constraints. Default is 1e-5.
NP	an optional positive integer giving the number of candidate solutions in the ran- domly distributed initial population. Defaults to 10*length(lower).

Fl	an optional scalar which represents the minimum value that the <i>scaling factor</i> F could take. Default is 0.1, which is almost always satisfactory.	
Fu	an optional scalar which represents the maximum value that the <i>scaling factor</i> F could take. Default is 1, which is almost always satisfactory.	
tau_F	an optional scalar which represents the probability that the <i>scaling factor</i> F is updated. Defaults to 0.1, which is almost always satisfactory.	
tau_CR	an optional constant value which represents the probability that the <i>crossover probability</i> CR is updated. Defaults to 0.1, which is almost always satisfactory.	
tau_pF	an optional scalar which represents the probability that the <i>mutation probability</i> p_F in the mutation strategy DE/rand/1/either-or is updated. Defaults to 0.1.	
jitter_factor	an optional tuning constant for <i>jitter</i> . If NULL only <i>dither</i> is used. Defaults to 0.001 .	
tol	an optional positive scalar giving the tolerance for the stopping criterion. Default is 1e-15.	
maxiter	an optional positive integer specifying the maximum number of iterations that may be performed before the algorithm is halted. Defaults to 200*length(lower).	
fnscale	an optional positive scalar specifying the typical magnitude of fn. It is used only in the <i>stopping criterion</i> . Defaults to 1. See 'Details'.	
compare_to	an optional character string controlling which function should be applied to the fn values of the candidate solutions in a generation to be compared with the so-far best one when evaluating the <i>stopping criterion</i> . If "median" the median function is used; else, if "max" the max function is used. It defaults to "median". See 'Details'.	
add_to_init_pop		
	an optional real vector of length length(lower) or matrix with length(lower) rows specifying initial values of the parameters to be optimized which are appended to the randomly generated initial population. It defaults to NULL.	
trace	an optional logical value indicating if a trace of the iteration progress should be printed. Default is FALSE.	
triter	an optional positive integer that controls the frequency of tracing when trace = TRUE. Default is triter = 1, which means that iteration : < value of stopping test > (value of best solution) best solution { index of violated constraints } is printed at every iteration.	
details	an optional logical value. If TRUE the output will contain the parameters in the final population and their respective fn values. Defaults to FALSE.	
	optional additional arguments passed to fn() and constr() if that is not NULL.	

Details

Overview: The setting of the *control parameters* of standard Differential Evolution (DE) is crucial for the algorithm's performance. Unfortunately, when the generally recommended values for these parameters (see, *e.g.*, Storn and Price, 1997) are unsuitable for use, their determination is often difficult and time consuming. The jDE algorithm proposed in Brest *et al.* (2006) employs a simple self-adaptive scheme to perform the automatic setting of control parameters scale factor F and crossover rate CR.

This implementation differs from the original description, most notably in the use of the *DE/rand/1/either-or* mutation strategy (Price *et al.*, 2005), and combination of *jitter with dither* (Storn, 2008).

As done by jDE and its variants (Brest *et al.*, 2021) each worse parent in the current population is *immediately replaced* (asynchronous update) by its newly generated better or equal offspring (Babu and Angira, 2006) instead of updating the current population with all the new solutions at the same time as in classical DE (synchronous update).

As the algorithm subsamples via sample() which from R version 3.6.0 depends on RNGkind(*, sample.kind), exact reproducibility of results from R versions 3.5.3 and earlier requires setting RNGversion("3.5.0"). In any case, do use set.seed() additionally for reproducibility!

Constraint Handling: Constraint handling is done using the approach described in Zhang and Rangaiah (2012), but with a *different reduction updating scheme* for the constraint relaxation value (μ). Instead of doing it once for every generation or iteration, the reduction is triggered for two cases when the *constraints only contain inequalities*. Firstly, every time a feasible solution is selected for replacement in the next generation by a new feasible trial candidate solution with a better objective function value. Secondly, whenever a current infeasible solution gets replaced by a feasible one. If the constraints *include equalities*, then the reduction is not triggered in this last case. This constitutes an original feature of the implementation.

The performance of the constraint handling technique is severely impaired by a small feasible region. Therefore, equality constraints are particularly difficult to handle due to the tiny feasible region they define. So, instead of explicitly including all equality constraints in the formulation of the optimization problem, it might prove advantageous to eliminate some of them. This is done by expressing one variable x_k in terms of the remaining others for an equality constraint $h_j(X) = 0$ where $X = [x_1, \ldots, x_k, \ldots, x_d]$ is the vector of solutions, thereby obtaining a relationship as $x_k = R_{k,j}([x_1, \ldots, x_{k-1}, x_{k+1}, \ldots, x_d])$. But this means that both the variable x_k and the equality constraint $h_j(X) = 0$ can be removed altogether from the original optimization formulation, since the value of x_k can be calculated during the search process by the relationship $R_{k,j}$. Notice, however, that two additional inequalities

$$l_k \leq R_{k,i}([x_1, \ldots, x_{k-1}, x_{k+1}, \ldots, x_d]) \leq u_k$$

where the values l_k and u_k are the lower and upper bounds of x_k , respectively, must be provided in order to obtain an equivalent formulation of the problem. For guidance and examples on applying this approach see Wu *et al.* (2015).

- **Discrete and Integer Variables:** Any DE variant is easily extended to deal with *mixed integer nonlinear programming* problems using a small variation of the technique presented by Lampinen and Zelinka (1999). Integer values are obtained by means of the floor() function *only* for the evaluation of the objective function. This is because DE itself works with continuous variables. Additionally, each upper bound of the integer variables should be added by 1.
 - Notice that the final solution needs to be *converted with* floor() to obtain its *integer* elements.

Stopping Criterion: The algorithm is stopped if

$$\frac{\text{compare_to}\{[\text{fn}(X_1), \dots, \text{fn}(X_{\text{npop}})]\} - \text{fn}(X_{\text{best}})}{\text{fnscale}} \le \text{tol}$$

where the "best" individual X_{best} is the *feasible* solution with the lowest objective function value in the population and the total number of elements in the population, npop, is NP+NCOL(add_to_init_pop). This is a variant of the *Diff* criterion studied by Zielinski and Laur (2008), which was found to yield the best results.

JDEoptim

Value

A list with the following components:

par	The best set of parameters found.	
value	The value of fn corresponding to par.	
iter	Number of iterations taken by the algorithm.	
convergence	An integer code. 0 indicates successful completion. 1 indicates that the iteration limit maxiter has been reached.	
and if details = TRUE:		
poppar	Matrix of dimension (length(lower), npop), with columns corresponding to the parameter vectors remaining in the population.	
popcost	The values of fn associated with poppar, vector of length npop.	

Note

It is possible to perform a warm start, *i.e.*, starting from the previous run and resume optimization, using NP = 0 and the component poppar for the add_to_init_pop argument.

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References

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See Also

Function DEoptim() in the **DEoptim** package has many more options than JDEoptim(), but does not allow constraints in the same flexible manner.

Examples

```
# NOTE: Examples were excluded from testing
        to reduce package check time.
#
# Use a preset seed so test values are reproducible.
set.seed(1234)
# Bound-constrained optimization
   Griewank function
#
#
#
   -600 <= xi <= 600, i = {1, 2, ..., n}
#
   The function has a global minimum located at
   x* = (0, 0, \dots, 0) with f(x*) = 0. Number of local minima
#
   for arbitrary n is unknown, but in the two dimensional case
#
   there are some 500 local minima.
#
#
   Source:
#
     Ali, M. Montaz, Khompatraporn, Charoenchai, and
#
      Zabinsky, Zelda B. (2005).
#
      A numerical evaluation of several stochastic algorithms
#
      on selected continuous global optimization test problems.
#
      Journal of Global Optimization 31, 635-672.
#
griewank <- function(x) {</pre>
    1 + crossprod(x)/4000 - prod( cos(x/sqrt(seq_along(x))) )
}
JDEoptim(rep(-600, 10), rep(600, 10), griewank,
         tol = 1e-7, trace = TRUE, triter = 50)
# Nonlinear constrained optimization
   0 <= x1 <= 34, 0 <= x2 <= 17, 100 <= x3 <= 300
#
   The global optimum is
#
   (x1, x2, x3; f) = (0, 16.666667, 100; 189.311627).
#
#
#
   Source:
#
      Westerberg, Arthur W., and Shah, Jigar V. (1978).
```

JDEoptim

```
#
      Assuring a global optimum by the use of an upper bound
      on the lower (dual) bound.
#
#
      Computers and Chemical Engineering 2, 83-92.
fcn <-
   list(obj = function(x) {
             35*x[1]^0.6 + 35*x[2]^0.6
         },
         eq = 2,
         con = function(x) {
             x1 <- x[1]; x3 <- x[3]
             c(600*x1 - 50*x3 - x1*x3 + 5000,
               600*x[2] + 50*x3 - 15000)
         })
JDEoptim(c(0, 0, 100), c(34, 17, 300),
         fn = fcn$obj, constr = fcn$con, meq = fcn$eq,
         tol = 1e-7, trace = TRUE, triter = 50)
#
   Designing a pressure vessel
#
   Case A: all variables are treated as continuous
#
#
   1.1 <= x1 <= 12.5*, 0.6 <= x2 <= 12.5*,
   0.0 <= x3 <= 240.0*, 0.0 <= x4 <= 240.0
#
   Roughly guessed*
#
   The global optimum is (x1, x2, x3, x4; f) =
#
   (1.100000, 0.600000, 56.99482, 51.00125; 7019.031).
#
#
#
   Source:
#
     Lampinen, Jouni, and Zelinka, Ivan (1999).
#
      Mechanical engineering design optimization
      by differential evolution.
#
#
      In: David Corne, Marco Dorigo and Fred Glover (Editors),
#
      New Ideas in Optimization, McGraw-Hill, pp 127-146
pressure_vessel_A <-</pre>
    list(obj = function(x) {
             x1 <- x[1]; x2 <- x[2]; x3 <- x[3]; x4 <- x[4]
             0.6224*x1*x3*x4 + 1.7781*x2*x3<sup>2</sup> +
             3.1611*x1^2*x4 + 19.84*x1^2*x3
         },
         con = function(x) {
             x1 <- x[1]; x2 <- x[2]; x3 <- x[3]; x4 <- x[4]
             c(0.0193*x3 - x1,
               0.00954 \times x3 - x2,
               750.0*1728.0 - pi*x3^2*x4 - 4/3*pi*x3^3)
         })
JDEoptim(c( 1.1, 0.6, 0.0, 0.0),
         c(12.5, 12.5, 240.0, 240.0),
         fn = pressure_vessel_A$obj,
         constr = pressure_vessel_A$con,
         tol = 1e-7, trace = TRUE, triter = 50)
```

Mixed integer nonlinear programming

```
Designing a pressure vessel
#
#
   Case B: solved according to the original problem statements
            steel plate available in thicknesses multiple
#
            of 0.0625 inch
#
#
   wall thickness of the
#
#
   shell 1.1 [18*0.0625] <= x1 <= 12.5 [200*0.0625]
   heads 0.6 [10*0.0625] <= x2 <= 12.5 [200*0.0625]
#
          0.0 <= x3 <= 240.0, 0.0 <= x4 <= 240.0
#
   The global optimum is (x1, x2, x3, x4; f) =
#
    (1.125 [18*0.0625], 0.625 [10*0.0625],
#
     58.29016, 43.69266; 7197.729).
#
pressure_vessel_B <-</pre>
    list(obj = function(x) {
             x1 <- floor(x[1])*0.0625</pre>
             x2 <- floor(x[2])*0.0625</pre>
             x3 <- x[3]; x4 <- x[4]
             0.6224*x1*x3*x4 + 1.7781*x2*x3<sup>2</sup> +
             3.1611*x1^2*x4 + 19.84*x1^2*x3
         },
         con = function(x) {
             x1 <- floor(x[1])*0.0625</pre>
             x2 <- floor(x[2])*0.0625</pre>
             x3 <- x[3]; x4 <- x[4]
             c(0.0193*x3 - x1,
                0.00954 \times x3 - x2,
                750.0*1728.0 - pi*x3^2*x4 - 4/3*pi*x3^3)
         })
res <- JDEoptim(c( 18,</pre>
                          10,
                                   0.0, 0.0),
                c(200+1, 200+1, 240.0, 240.0),
                fn = pressure_vessel_B$obj,
                 constr = pressure_vessel_B$con,
                 tol = 1e-7, trace = TRUE, triter = 50)
res
# Now convert to integer x1 and x2
c(floor(res$par[1:2]), res$par[3:4])
```

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