Package 'ROptimus'

December 15, 2022

Title A Parallel General-Purpose Adaptive Optimisation Engine

Version 3.0.0

Description This package is a general purpose optimisation engine.
It supports i) Monte Carlo optimisation with Metropolis criterion
[Chib and Green-
berg (1995) <doi:10.2307/2684568>, Chen and Roux (2015) <doi:10.1063/1.4904889>]
and Acceptance Ratio Simulated Annealing [Ingber (1993 <doi:10.1016/0895-7177(93)90204-
C>)]
on multiple cores, and ii) Acceptance Ratio Replica Exchange Monte
Carlo Optimisation. In each case, the system pseudo-temperature is
dynamically adjusted such that the observed acceptance ratio is kept
near to the desired (fixed or changing) acceptance ratio.

License GPL (>= 3)

Encoding UTF-8

Roxygen list(markdown = TRUE)

RoxygenNote 7.2.3

Imports doParallel (>= 1.0.11), foreach (>= 1.4.4), iterators (>=
1.0.9), parallel (>= 3.4.2)

Depends R (>= 3.1.0)

LazyData true

URL https://github.com/SahakyanLab/ROptimus

NeedsCompilation no

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R topics documented:

`ex.m.fun` *Tutorial 5 m() function*

Description

The m() function supplied to Optimus() for reproducing Tutorial 5. This is for the small executable example.

Usage

```
ex.m.fun
```

Format

Function

`ex.r.fun` *Tutorial 5 r() function*

Description

The r() function supplied to Optimus() for reproducing Tutorial 5. This is for the small executable example.

Usage

```
ex.r.fun
```

Format

Function

`ex.u.fun` *Tutorial 5 u() function*

Description

The u() function supplied to Optimus() for reproducing Tutorial 5. This is for the small executable example.

Usage

```
ex.u.fun
```

Format

Function

IJ_ORIG *Tutorial 5 Genomic Contact Data*

Description

A dataset containing 734 genomic contact pairs for reproducing Tutorial 5. Here, we take a set of 734 pairs of i and j 40-kilobase DNA regions that are known to be in contact inside a cell. Binning the DNA (e.g., a single chromosome) into 40-kb regions, each region is represented as a single integer that is equal to its end position divided by the length of the region, which is 40 kb. For instance, the 1st region, with start and end positions at the 1st and 40000th nucleotides, respectively, is denoted as 1 (40000th base / 40000 bases = 1). This simplifies the notation for a contact between two regions to a pair of positive integers as in used in this dataset.

Usage

```
IJ_ORIG
```

Format

A data frame with 734 rows and 2 variables:

i Integer representing 40-kb contact region partner of j

j Integer representing 40-kb contact region partner of i

Optimus *Acceptance Ratio Simulated Annealing and Acceptance Ratio Replica Exchange Monte Carlo Optimisation Engine*

Description

Acceptance Ratio Simulated Annealing and Acceptance Ratio Replica Exchange Monte Carlo Optimisation Engine

Usage

```
Optimus(
  NUMITER = 1e+06,
  STATWINDOW = 70,
  T.INI = 1e-05,
  T.ADJSTEP = 5e-09,
  TSCLnum = 2,
  T.SCALING = 3,
  T.MIN = 5e-09,
  T.DELTA = 2,
  DUMP.FREQ = 10000,
  LIVEPLOT = TRUE,
  LIVEPLOT.FREQ = 1e+05,
  PDFheight = 29,
  PDFwidth = 20,
```

```
  NCPU = 4,
  LONG = TRUE,
  SEED = 840,
  OPTNAME = "",
  DATA = NULL,
  K.INITIAL = 0,
  rDEF,
  mDEF,
  uDEF,
  EXCHANGE.FREQ = 1000,
  ACCRATIO = c(90, 50, 5, 1),
  CYCLES = 10,
  ACCRATIO.IN = 90,
  ACCRATIO.FIN = 0.5,
  OPT.TYPE = "SA",
  DIR = "./",
  starcore = NULL
)
```

Arguments

NUMITER	Number of model optimisation steps.
STATWINDOW	Number of last ongoing iterations to calculate acceptance ratio for temperature auto-adjustment.
T.INI	Initial temperature (K) for Metropolis criterion.
T.ADJSTEP	Temperature change step-size for temperature auto-adjustment based on the actual acceptance ratio.
TSCLnum	Cutoff for one of the NumofAccRatSMIdeal and NumofAccRatGRIdeal numbers after which the adjustment step is multiplied by T.SCALING.
T.SCALING	See above.
T.MIN	Value to which the pseudo-temperature is set when the
T.DELTA	Minimum value by which acceptance ratio in a STATWINDOW must differ from the ideal acceptance ratio for the temperature control unit to make a temperature adjustment.
DUMP.FREQ	The frequency (in steps) of writing the found ongoing best model.
LIVEPLOT	Plotting the optimisation process in a pdf file.
LIVEPLOT.FREQ	Frequency (in steps) of plotting the results.
PDFheight	Plot height in inches.
PDFwidth	Plot width in inches.
NCPU	Number of CPU cores to use, by running more replicas of the optimisation. The usage of more than 1 cores will attempt to load the foreach and doParallel libraries in the case of SA Optimus
LONG	If TRUE, it means that a long simulation is expected to be done, hence the memory-friendly mode will be activated.
SEED	Setting the seed for the random number generator.
OPTNAME	The name of the optimisation process.
DATA	A list that holds any supplementary data that functions mDEF or uDEF need to access.

K.INITIAL	The initial parameter configuration from which the optimisation process will begin.
rDEF	Function that defines a rule by which the paramters(K) are randomly altered.
mDEF	Model function that operates on the parameters to be optimized (K) and returns an observable object O.
uDEF	Function that evaluates the performance of a given set of parameters K.
EXCHANGE.FREQ	Frequency of exchanges (NUMITER should be divisible by this number, for RE Optimus).
ACCRATIO	Vector of Acceptance Ratios for each replica (length of ACCRATIO must be equal to NCPU, for RE Optimus).
CYCLES	Number of annealing cycles (NUMITER should be divisible by this number, for SA Optimus).
ACCRATIO.IN	Initial acceptance ratio (%) at the beginning of each constituent annealing cycles (for SA Optimus).
ACCRATIO.FIN	Final acceptance ratio (%) at the end of each constituent annealing cycles (for SA Optimus).
OPT.TYPE	String specifying which optimisation protocol to use. Enter "SA" for Simulated Annealing or "RE" for Replica Exchange (default value is "SA")
DIR	String specifying which optimisation protocol to use. (default value is "." i.e. current directory)
starcore	Experimental variable of type list, holding some parameters for in-lab starcore use only.

Value

A probabilistic optimal parameter configuration K.

Examples

```
K <- IJ_ORIG
K$j <- sample(x=K$j, size=nrow(K), replace=FALSE)
out.dir <- tempdir()

Optimus(NCPU=1, OPTNAME="IJ.NEW.OPTI.SA", NUMITER=500, CYCLES=2, DIR=out.dir,
        DUMP.FREQ=10, LONG=FALSE, OPT.TYPE="SA", K.INITIAL=K,
        rDEF=ex.r.fun, mDEF=ex.m.fun, uDEF=ex.u.fun,
        DATA=list(IJ_ORIG=IJ_ORIG, gaplimit=50, numContacts=nrow(IJ_ORIG)))
```

OptimusExamples *Generate script for reproducing a tutorial*

Description

Generate script for reproducing a tutorial

Usage

```
OptimusExamples(
  dir,
  example = 1,
  method = "SA",
  file_name = "example.R",
  mopac = NULL,
  run = FALSE,
  vignette = TRUE
)
```

Arguments

dir	String specifying directory where to save the script and vignette.
example	Integer specifying tutorial or example number based on manual (default value is 1).
method	String specifying which optimisation protocol to use. Enter "SA" for Simulated Annealing or "RE" for Replica Exchange (default value is "SA").
file_name	String specifying file name of script (default value is example.R).
mopac	String specifying the path of the MOPAC (Molecular Orbital PACkage) executable for tutorial 3 (Geometry Optimisation of Vitamin C Molecule) (default value is NULL).
run	If TRUE, automatically run script after generating (default value is FALSE).
vignette	If TRUE, add tutorial vignette to directory (default value is TRUE).

Value

A script (and optionally a vignette) for reproducing a tutorial.

Examples

```
out.dir <- tempdir()
OptimusExamples(dir=out.dir, example=1)
```

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