Package ‘MOLHD’

May 6, 2018

Type Package
Title Multiple Objective Latin Hypercube Design
Version 0.2
Author Ruizhe Hou, Lu Lu
Maintainer Ruizhe Hou <houruizhe1210@gmail.com>
Depends R (>= 3.4.0)
Imports fields, arrangements
License LGPL
NeedsCompilation yes
Repository CRAN
Date 2018-5-6
RoxygenNote 6.0.1
Date/Publication 2018-05-06 16:49:25 UTC

R topics documented:

MOLHD-package .................................................... 2
cp2 ................................................................. 3
cp3 ................................................................. 4
LHD ................................................................. 5
md ................................................................. 5
miM ................................................................. 6
miMLHD ............................................................ 7
Description

The MOLHD package provides useful and efficient functions for generating the optimal Maximin distance, Maximum Projection and miniMax distance (only for low dimensions) designs within the class of Latin hypercube designs for computer experiments. Ant it provides functions generating Pareto front optimal designs for each two of the three criteria and all the three criteria within the class of Latin hypercube designs. It also provides functions to compute the criteria for a given design.

Details

Package: MOLHD
Type: Package
Version: 0.2
Date: 2018-5-6
Lisense: LGPL

This package contains functions for generating the optimal maximin distance designs, maximum projection designs and minimax distance designs for low dimensions within the class of Latin hypercube designs (LHDs). This packages also contains functions for generating designs on the Pareto front of each two of the three criteria as maximin distance criterion, minimax distance criterion, and maximum projection criterion. This package also contains functions to compute each criterion for a random Latin hypercube design.

Since minimax distance design is computational expensive, it is only approximately estimated when the design is at low dimension.

Author(s)

Ruizhe Hou, Lu Lu

Maintainer: Ruizhe Hou<houruii1210@gmail.com>
cpf2

Combine Pareto front designs of 2 criteria

Description

Combine Pareto front designs of 2 criteria

Usage

cpf2(newdes, newpfval, curdes, curpfval)

Arguments

newdes a matrix which is a column bind of new designs
newpfval a matrix each row is 2 criteria corresponding to each design
curdes a matrix which is a column bind of current designs on Pareto front
curpfval a matrix each row is 2 criteria corresponding to each Pareto front design

Details

This function is used to combine 2 criteria Pareto front designs

Value

pfdes The column bind of Pareto front designs
pfvals The Pareto front values corresponding to the Pareto front designs

Examples

# Combine Pareto fronts each with 5 random starts for Mm and mp criteria
## Not run:
pf1 = pfMp(20,2,crlim = cbind(c(4.5,6.5),c(26,36)),nstarts = 5)
pf2 = pfMp(20,2,crlim = cbind(c(4.5,6.5),c(26,36)),nstarts = 5)
pfnew = cpf2(pf1$pfdes, pf1$pfvals, pf2$pfdes, pf2$pfvals)
pfnew$pfdes
pfnew$pfvals
## End(Not run)
cpf3

Combine Pareto front designs of 3 criteria

Description
Combine Pareto front designs of 3 criteria

Usage

cpf3(newdes, newpfval, curdes, curpfval)

Arguments

newdes a matrix which is a column bind of new designs
newpfval a matrix each row is 3 criteria corresponding to each design
curdes a matrix which is a column bind of current designs on Pareto front
curpfval a matrix each row is 3 criteria corresponding to each Pareto front design

Details
This function is used to combine 3 criteria Pareto front designs

Value

pfdes The column bind of Pareto front designs
pfvals The Pareto front values corresponding to the Pareto front designs

Examples

# Combine Pareto fronts each with 1 random start for Mm, mp and mM criteria
## Not run:
pf1=pfMpm(20,2,crlim = cbind(c(4.5,6.5),c(26,36),c(0.12,0.62)),num = 15,nstarts = 1)
pf2=pfMpm(20,2,crlim = cbind(c(4.5,6.5),c(26,36),c(0.12,0.62)),num = 15,nstarts = 1)
pfnew=cpf3(pf1$pfdes,pf1$pfvals,pf2$pfdes,pf2$pfvals)
pfnew$pfdes
pfnew$pfvals

## End(Not run)
**LHD**

*Generate a random Latin Hypercube design*

**Description**

Generate a random Latin Hypercube design

**Usage**

\[ \text{LHD}(n, p) \]

**Arguments**

- \( n \) \hspace{1cm} \text{number of runs desired}
- \( p \) \hspace{1cm} \text{number of design factors}

**Value**

- **design** \hspace{1cm} a Latin Hypercube Design that is not scaled (i.e. the grid point locations are integers)
- **standDesign** \hspace{1cm} a standard Latin Hypercube Design that is scaled to (0,1); design locations are placed at the centers of selected grids.

**Examples**

```r
# Generate a random Latin hypercube design with 20 runs and 2 variables
D <- LHD(n = 20, p = 2)
D$design
D$standDesign
```

**md**

*Minimum distance between any two points in the design*

**Description**

Minimum distance between any two points in the design

**Usage**

\[ \text{md}(\mathbf{D}) \]

**Arguments**

- \( \mathbf{D} \) \hspace{1cm} a design matrix, rows are design locations, columns are design factors
Value

MinimumDistance
Minimum distance between any two points in the design

number
number of pairs in the design achieve the minimum distance

Examples

```r
#compute the minimum distance between any two points in design D
d = md(D = cbind(c(0.875, 0.375, 0.125, 0.625), c(0.375, 0.125, 0.625, 0.875)))
d$MinimumDistance
d$number
```

miM

The miniMax criterion based on an approximate fill distance measure

Description

The miniMax criterion based on an approximate fill distance measure

Usage

```r
miM(D, num = 50)
```

Arguments

- `D`: a design matrix, rows are design locations, columns are design factors
- `num`: Optional, default is "50". The fineness of the gridded points to divide the design space. Each dimension is evenly divided by num+1 points. Lower this parameter when dimension is high to reduce computing time.

Details

This function calculates the approximate fill distance for the design by using a set of gridded points, the maximum error of the value can be computed.

Value

fill distance with 4 decimals

Examples

```r
#Compute the approximate fill distance of a design D
d = miM(D = cbind(c(0.875, 0.375, 0.125, 0.625), c(0.375, 0.125, 0.625, 0.875)), num = 20)
```
miMLHD

Generate the optimal Latin Hypercube Design based on the miniMax criterion.

Description

Generate the optimal Latin Hypercube Design based on the miniMax criterion.

Usage

miMLHD(n, p, num = 50, temp0 = 0, nstarts = 1, times = 300,
maxiter = 1e+06)

Arguments

n         number of runs desired
p         number of variables desired
num       Optional, default is "50". The fineness of the gridded points to divide the
design space. Each dimension is evenly divided by num+1 points. Lower this parameter
when dimension is high to reduce computing time.
temp0     Initial temperature for simulated annealing
nstarts   Optional, default is "1". The number of random starts
times     Optional, default is "300". The maximum number of non-improving searches
allowed before terminating the search.
maxiter   Optional, default is "1e+06". The maximum total number of iterations for each
random start. Lower this number if the design is prohibitively large and you
want to terminate the algorithm prematurely to report the best design found

Details

This function is to search the optimal Latin Hypercube design based on the miniMax criterion using
the columnwise exchange algorithm coupled with the simulated annealing algorithm, and several
computational shortcuts to improve efficiency. The approximate miniMax criterion is computed by
using a set of gridded points to approximate the continuous design space, the maximum error of the
value can be computed. (Can only work in relatively low dimensions)

Value

design    The optimal miniMax design matrix
criterion The approximate miniMax criterion for the chosen fineness of the grids
iterations The total iterations
time_rec   Time to complete the search
Examples

```r
# Generate the optimal minimax distance LHD(20,2)
## Not run:
D = mlR2LHD(n = 20, p = 2)
D$design
D$criterion

## End(Not run)
```

---

**Mm**

*Computer the approximate Maximin Criterion for a design.*

**Description**

Computer the approximate Maximin Criterion for a design.

**Usage**

```r
Mm(D, power = 100)
```

**Arguments**

- **D**
  - A design matrix
- **power**
  - Optional, default is "100". The power parameter $r$ in the average reciprocal inter-point distance measure. When $r$ is approaching infinity, minimizing the average reciprocal inter-point distance measure is equivalent to maximizing the minimum distance among the design points.

**Value**

The approximate Maximin criterion with 4 decimals

**Examples**

```r
# Compute the maximin criterion of a random LHD(20,2)
des = LHD(n = 20, p = 2)$standDesign
Mm(D = des, power = 150)
```
Generate the optimal Maximin Latin Hypercube Design.

**Description**
Generate the optimal Maximin Latin Hypercube Design.

**Usage**
```
MmLHD(n, p, power = 100, temp0 = 0, nstarts = 1, times = 300, maxiter = 1e+06)
```

**Arguments**
- `n`: number of runs desired
- `p`: number of variables desired
- `power`: Optional, default is "100". The power parameter r in the average reciprocal inter-point distance measure. When r turns to infinity, minimizing the average reciprocal inter-point distance measure is equivalent to maximizing the minimum distance among the design points.
- `temp0`: Initial temperature
- `nstarts`: Optional, default is "1". The number of random starts
- `times`: Optional, default is "300". The maximum number of non-improving searches allowed. Lower this parameter if you expect the search to converge faster.
- `maxiter`: Optional, default is "1e+06". The maximum total number of iterations for each random start. Lower this number if the design is prohibitively large and you want to terminate the algorithm prematurely to report the best design found.

**Details**
This function is to search the optimal Maximin design using columnwise exchange algorithm coupled with the simulated annealing algorithm and several computational shortcuts to improve efficiency.

**Value**
- `design`: The optimal Maximin design matrix
- `criterion`: The approximate Maximin criterion of the design under chosen "power" parameter
- `iterations`: The total iterations
- `time_rec`: Time to complete the search
Examples

# Generate the optimal maximin distance LHD(20,2)
D=mlHD(n=20,p=2)
D$design
D$criterion

\[
mp(D)
\]

Computer the MaxPro Criterion for a design.

Description

Computer the MaxPro Criterion for a design.

Usage

\[
mp(D)
\]

Arguments

\[
D \quad \text{a design matrix}
\]

Details

This function is to compute the MaxPro criterion for measuring projection characteristic of a computer experiment.

Value

The MaxPro Criterion with 4 decimals

Examples

# Compute the \(mp\) criterion of a random LHD(20,2)
D=LHD(20,2)$standDesign
mp(D)
Generate the optimal MaxPro Latin Hypercube Design.

Usage

\texttt{mplhd(n, p, temp0 = 0, nstarts = 1, times = 300, maxiter = 1e+06)}

Arguments

- \texttt{n}: number of runs desired
- \texttt{p}: number of design factors desired
- \texttt{temp0}: Initial temperature for simulated annealing
- \texttt{nstarts}: Optional, default is "1". The number of random starts
- \texttt{times}: Optional, default is "300". The maximum number of non-improving searches allowed. Lower this parameter if you expect the search to converge faster.
- \texttt{maxiter}: Optional, default is "1e+06". The maximum total number of iterations. Lower this number if the design is prohibitively large and you want to terminate the search prematurely to report the best design found.

Details

This function is to search the optimal Latin Hypercube Design based on the MaxPro criterion using the columnwise exchange algorithm coupled with the simulated annealing algorithm, and several computational shortcuts to improve efficiency.

Value

- \texttt{design}: The optimal LHD design matrix based on the MaxPro criterion
- \texttt{criterion}: The MaxPro criterion of the selected optimal LHD design
- \texttt{iterations}: The total iterations
- \texttt{time_rec}: Time to complete the search

Examples

\begin{verbatim}
#Generate a optimal maximum projection LHD(20,2) design
D=mpLHD(n=20,p=2)
D$design
D$criterion
\end{verbatim}
pfMm

Generate the Pareto front for the optimal Latin Hypercube Designs based on both the Maximin and miniMax criteria.

Description

Generate the Pareto front for the optimal Latin Hypercube Designs based on both the Maximin and miniMax criteria.

Usage

pfMm(n, p, crlim, num, nstarts = 1, times = 300, maxiter = 1e+06, 
    temp0 = 0, wtset = cbind(c(1, 0), c(0.8, 0.2), c(0.6, 0.4), c(0.4, 0.6),
    c(0.2, 0.8), c(0, 1)))

Arguments

n  
number of runs desired

p  
number of design factors desired

crlim  
a matrix saving the best and worst values for each criterion to be used for defining the scaling choices for converting the natural criteria values onto a desirability scale between 0 and 1. Each column corresponds to one criterion. The best and worst values are recommended based on the values from each single criterion search. It is recommended that slightly wider range is used for defining the scaling choice for the Pareto front search.

num  
The fineness of the grids to approximate the approximate the continuous design space. Lower this parameter when dimension is high to reduce computing time.

nstarts  
Optional, default is "1". The number of random starts

times  
Optional, default is "300". The maximum number of non-improving searches allowed before terminating the search. Lower this parameter if you expect the search to converge faster.

maxiter  
Optional, default is "1e+06". The maximum total number of iterations. Lower this parameter if the design is prohibitively large.

temp0  
Initial temperature for simulated annealing

wtset  
Optional, default is "cbind(c(1,0),c(0.8,0.2),c(0.6,0.4),c(0.4,0.6),c(0.2,0.8),c(0,1))". The set of weight combinations to guide the search in varied directions. Each column is a weight vector that guides the search in a certain direction.

Details

This function is to search for the Pareto front and the Pareto set of LHDs based on the Maximin and miniMax criteria. Each design on Pareto front is not dominated by any other design. This function utilizes a version of simulated annealing algorithm and several computational shortcuts to efficiently generate the optimal Latin hypercube designs. Choose a lower maximum limit of the criteria but high enough for Pareto front designs will save the computing time.
Value

- `pfdes`: The column bind of Pareto front designs whose criteria values are on the Pareto front.
- `pfvals`: The Pareto front of criteria values based on the Maximin and miniMax criteria. Columns are the optimization criteria.
- `time_rec`: Time to complete the search

Examples

```r
# Generate the Pareto front designs of maximin and minimax distance criterion for LHD(10,2)
D1 = mlhd(n=10, p=2, nstarts=30)
D2 = miMLHD(n=10, p=2, num=15, nstarts=30)
Mmlim = c(D1$criterion-0.2, D1$criterion-0.2+2)
mMlim = c(D2$criterion-0.05, D2$criterion-0.05+0.5)
crlim = cbind(Mmlim, mMlim)
pf = pfm(10, 2, crlim, num = 15, nstarts = 30)
pf$pvals
pf$pfdes
pf$time_rec
```

Description

Generate the Pareto front for optimal Latin Hypercube Designs based on both the Maximin and the MaxPro criteria.

Usage

```r
pfmp(n, p, crlim, nstarts = 1, times = 300, maxiter = 1e+06, temp0 = 0,
wtset = cbind(c(1, 0), c(0.8, 0.2), c(0.6, 0.4), c(0.4, 0.6), c(0.2, 0.8), c(0, 1)))
```

Arguments

- `n`: number of runs desired
- `p`: number of design factors desired
- `crlim`: a matrix saving the best and worst values for each criterion to be used for defining the scaling choices for converting the natural criteria values onto a desirability scale between 0 and 1. Each column corresponds to one criterion. The best
and worst values are recommended based on the values from each single criterion search. It is recommended that slightly wider range is used for defining the scaling choice for the Pareto front search.

- **nstarts**: Optional, default is "1". The number of random starts.
- **times**: Optional, default is "300". The maximum number of non-improving searches allowed before terminating the search. Lower this parameter if you expect the search to converge faster.
- **maxiter**: Optional, default is "1e+06". The maximum total number of iterations. Lower this number if the design is prohibitively large and you want to terminate the search earlier to report the best design found.
- **temp0**: Initial temperature for simulated annealing.
- **wtset**: Optional, default is "cbind(c(1,0),c(0.8,0.2),c(0.6,0.4),c(0.4,0.6),c(0.2,0.8),c(0,1))". The set of weight combinations to guide the search in varied directions. Each column is a weight vector that guides the search in a certain direction.

**Details**

This function is to search the Pareto front and the Pareto set of designs based on the Maximin and Maxpro criteria. Each design on Pareto front is not dominated by any other design. This function utilizes a version of simulated annealing algorithm and several computational shortcuts to efficiently generate the optimal Latin hypercube designs. Choose a lower maximum limit of the criteria but high enough for Pareto front designs will save the computing time.

**Value**

- **pfdes**: The column bind of Pareto front designs whose criteria values are on the Pareto front.
- **pfvals**: The Pareto front of criteria values based on the Maximin and MaxPro criteria. Columns are the optimization criteria.
- **time_rec**: Time to complete the search.

**Examples**

```r
# Generate the Pareto designs of maximin distance and maximum projection for LHD(10,5)
## Not run:
D1=mmlhd(n=10,p=5,nstarts=30)
D2=mplhd(n=10,p=5,nstarts=30)
Mmlim=c(D1$criterion-0.2,D1$criterion-0.2+2)
mplim=c(D2$criterion-2,D2$criterion-2+10)
crlim=cbind(Mmlim,mplim)
pf=pfmp(10,5,crlim,nstarts = 30)
pf$pfvals
pf$pfdes
pf$time_rec
## End(Not run)
```
pfMpm

Generate the Pareto front for the optimal Latin Hypercube Designs based on the Maximin, MaxPro and miniMax criteria.

Description

Generate the Pareto front for the optimal Latin Hypercube Designs based on the Maximin, MaxPro and miniMax criteria.

Usage

pfMpm(n, p, crlim, num, nstarts = 1, times = 300, maxiter = 1e+06,
       temp0 = 0, wtset = cbind(c(1, 0, 0), c(0.5, 0.5, 0), c(0.5, 0, 0.5), c(0,
                                0.5, 0.5), c(0, 1, 0), c(0, 0, 1), c(1/3, 1/3, 1/3)))

Arguments

- **n**: number of runs desired
- **p**: number of design factors desired
- **crlim**: a matrix saving the best and worst values for each criterion to be used for defining the scaling choices for converting the natural criteria values onto a desirability scale between 0 and 1. Each column corresponds to one criterion. The best and worst values are recommended based on the values from each single criterion search. It is recommended that slightly wider range is used for defining the scaling choice for the Pareto front search.
- **num**: The fineness of the grids to approximate the approximate the continuous design space. Lower this parameter when dimension is high to reduce computing time.
- **nstarts**: Optional, default is "1". The number of random starts
- **times**: Optional, default is "300". The maximum number of non-improving searches allowed before terminating the search. Lower this parameter if you expect the search to converge faster.
- **maxiter**: Optional, default is "1e+06". The maximum total number of iterations. Lower this number if the design is prohibitively large.
- **temp0**: Initial temperature for simulated annealing
- **wtset**: Optional, default is "cbind(c(1,0,0),c(0.5,0.5,0),c(0.5,0,0.5),c(0,0.5,0.5),c(0,1,0),
                                         c(0,0,1),c(1/3,1/3,1/3))". The set of weight combinations to guide the search in varied directions. Each column is a weight vector that guides the search in a certain direction.

Details

This function is to search for the Pareto front and the Pareto set of LHDs based on the Maximin, Maxpro and miniMax criteria. Each design on Pareto front is not dominated by any other design. This function utilizes a version of simulated annealing algorithm and several computational shortcuts to efficiently generate the optimal Latin hypercube designs. Choose a lower maximum limit of the criteria but high enough for Pareto front designs will save the computing time.
pfpm

Generate the Pareto front for the optimal Latin Hypercube Designs based on both the MaxPro and miniMax criteria.

Description

Generate the Pareto front for the optimal Latin Hypercube Designs based on both the MaxPro and miniMax criteria.

Usage

pfpm(n, p, crlim, num, nstarts = 1, times = 300, maxiter = 1e+06, temp0 = 0, wtset = cbind(c(1, 0), c(0.8, 0.2), c(0.6, 0.4), c(0.4, 0.6), c(0.2, 0.8), c(0, 1)))

Arguments

n number of runs desired
p number of design factors desired

Examples

# Not run:
D1=mmlhd(n=10,p=2,nstarts=30)
D2=mlhd(n=10,p=2,nstarts=30)
D3=miMLHD(n=10,p=2,num=15,nstarts=30)
Mmlim=c(D1$criterion-0.2,D1$criterion-0.2+2)
Mplim=c(D2$criterion-2,D2$criterion-2+10)
MMlim=c(D3$criterion-0.05,D3$criterion-0.05+0.5)
crlim=cbind(Mmlim,Mplim,MMlim)
pf=pfpm(10,2,crlim,num = 15,nstarts = 30)
pf$pvals
pf$pfdes
pf$time_rec

## End(Not run)
pfpm

crlim a matrix saving the best and worst values for each criterion to be used for defining the scaling choices for converting the natural criteria values onto a desirability scale between 0 and 1. Each column corresponds to one criterion. The best and worst values are recommended based on the values from each single criterion search. It is recommended that slightly wider range is used for defining the scaling choice for the Pareto front search.

num The fineness of the grids to approximate the approximate the continuous design space. Lower this parameter when dimension is high to reduce computing time.

nstarts Optional, default is "1". The number of random starts.

times Optional, default is "300". The maximum number of non-improving searches allowed before terminating the search. Lower this parameter if you expect the search to converge faster.

maxiter Optional, default is "1e+06". The maximum total number of iterations. Lower this number if you expect the search to converge faster.

temp0 Initial temperature for simulated annealing.

wtset Optional, default is "cbind(c(1,0),c(0.8,0.2),c(0.6,0.4),c(0.4,0.6),c(0.2,0.8),c(0,1))". The set of weight combinations to guide the search in varied directions. Each column is a weight vector that guides the search in a certain direction.

Details

This function is to search for the Pareto front and the Pareto set of LHDs based on the MaxPro and miniMax criteria. Each design on Pareto front is not dominated by any other design. This function utilizes a version of simulated annealing algorithm and several computational shortcuts to efficiently generate the optimal Latin hypercube designs. Choose a lower maximum limit of the criteria but high enough for Pareto front designs will save the computing time.

Value

pfdes The column bind of Pareto front designs whose criteria values are on the Pareto front.

pfvals The Pareto front of criteria values based on the Maximin and miniMax criteria. Columns are the optimization criteria.

time_rec Time to complete the search

Examples

# Generate the Pareto front designs of maximum projection and minimax distance criteria for LHD(10,2)
## Not run:
D1=mplHD(n=10,p=2,times=1000,nstarts=30)
D2=mimlHD(n=10,p=2,num=15,nstarts=30)
mplim=c(D1$criterion-2,D1$criterion+2+20)
mmlim=c(D2$criterion-0.05,D2$criterion-0.05+0.5)
crlim=cbind(mplied,mmlim)
$pf=pfpm(10,2,crlim,num = 15,nstarts = 30)
pf$pfvals
pf$pfdes
pf$time_rec

## End(Not run)
Index

*Topic Computer Experiments Criteria

md, 5
miM, 6
Mm, 8
mp, 10

*Topic Computer Experiments

LHD, 5
miMLHD, 7
MmLHD, 9
mplHD, 11
pfMm, 12
pfMp, 13
pfMpm, 15
pfpm, 16

*Topic Design of Experiments

LHD, 5
miMLHD, 7
MmLHD, 9
mplHD, 11
pfMm, 12
pfMp, 13
pfMpm, 15
pfpm, 16

*Topic Pareto front

cpf2, 3
cpf3, 4

*Topic package

MOLHD-package, 2

cpf2, 3
cpf3, 4

LHD, 5

md, 5
miM, 6
miMLHD, 7
Mm, 8
MmLHD, 9

MOLHD (MOLHD-package), 2
MOLHD-package, 2
mp, 10
mplHD, 11
pfMm, 12
pfMp, 13
pfMpm, 15
pfpm, 16