Package 'DiceDesign'

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Description

Space-Filling Designs (SFD) and space-filling criteria (distance-based and uniformity-based).

Details

Package: DiceDesign
Type: Package
Version: 1.2
Date: 2013-26-12
License: GPL-3

This package provides tools to create some specific Space-Filling Design (SFD) and to test their quality:

- Latin Hypercube Design (randomized or centered)
- Strauss SFD and Maximum entropy SFD, WSP design
- Optimal (low-discrepancy and maximin) Latin Hypercube Design by simulated annealing and genetic algorithms,
- Discrepancies criteria, distance measures,
- Minimal spanning tree criteria,
- Radial scanning statistic

Note

Part of this work was conducted within the frame of the DICE (Deep Inside Computer Experiments) Consortium between ARMINES, Renault, EDF, IRSN, ONERA and TOTAL S.A. (http://dice.emse.fr/).

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In this package only Faure's sequence is implemented. Note that the **randtoolbox** package provides the following quasi random sequences: the Sobol sequence, the Halton (hence Van Der Corput) sequence and the Torus sequence (also known as Kronecker sequence). Note also that the **lhs** package provides other types of algorithms to compute optimized LHS.

Author(s)

J. Franco, D. Dupuy, O. Roustant, G. Damblin and B. Iooss. Thanks to A. Jourdan for discussions about OA131.

```
(maintainer: Celine Helbert <Celine.Helbert@ec-lyon.fr>)
```

References

Damblin G., Couplet M., and Iooss B. (2013). Numerical studies of space filling designs: optimization of Latin Hypercube Samples and subprojection properties, *Journal of Simulation*, 7:276-289, 2013. http://www.gdr-mascotnum.fr/doku.php?id=iooss1

Fang K.-T., Li R. and Sudjianto A. (2006) Design and Modeling for Computer Experiments, *Chapman & Hall*.

Santner T.J., Williams B.J. and Notz W.I. (2003) The Design and Analysis of Computer Experiments, *Springer*, 121-161.

Roustant O., Franco J., Carraro L., Jourdan A. (2010), A radial scanning statistic for selecting space-filling designs in computer experiments, MODA-9 proceedings, http://www.emse.fr/~roustant

```
# ******
# Designs of experiments
# ******
# A maximum entropy design with 20 points in [0,1]^2
p <- dmaxDesign(20,2,0.9,200)
plot(p$design,xlim=c(0,1),ylim=c(0,1))
# *******
# Criteria: L2-discrepancy
# *******
dp <- discrepancyCriteria(p$design,type=c('L2','C2'))</pre>
# Coverage measure
covp <- coverage(p$design)</pre>
# *********
# Criteria: Minimal Spanning Tree
# *********
mstCriteria(p$design,plot2d=TRUE)
# *******************
# Radial scanning statistic: Detection of defects of Sobol designs
# ********************
# requires randtoolbox package
```

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```
# in 2D
rss <- rss2d(design=sobol(n=20, dim=2), lower=c(0,0), upper=c(1,1),
type="l", col="red")
# in 8D. All pairs of dimensions are tried to detect the worst defect
# (according to the specified goodness-of-fit statistic).
d <- 8
n <- 10*d
rss <- rss2d(design=sobol(n=n, dim=d), lower=rep(0,d), upper=rep(1,d),
type="l", col="red")
# avoid this defect with scrambling ?
    1. Faure-Tezuka scrambling (type "?sobol" for more details and options)
rss <- rss2d(design=sobol(n=n, dim=d, scrambling=2), lower=rep(0,d),</pre>
upper=rep(1,d), type="l", col="red")
     2. Owen scrambling
rss <- rss2d(design=sobol(n=n, dim=d, scrambling=1), lower=rep(0,d),
upper=rep(1,d), type="l", col="red")
```

coverage

Coverage

Description

Compute the coverage measure

Usage

coverage(design)

library(randtoolbox)

Arguments

design

a matrix (or a data.frame) representing the design of experiments representing the design of experiments in the unit cube $[0,1]^d$. If this last condition is not fulfilled, a transformation into $[0,1]^d$ is applied before the computation of the criteria.

Details

The coverage criterion is defined by

$$coverage = \frac{1}{\bar{\gamma}} \left[\frac{1}{n} \sum_{i=1}^{n} (\gamma_i - \bar{\gamma})^2 \right]^{1/2}$$

where γ_i is the minimal distance between the point x_i and the other points of the design and $\bar{\gamma}$ is the mean of the γ_i .

Note that for a regular mesh, cov=0. Then, a small value of cov means that the design is close to a regular grid.

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Value

A real number equal to the value of the coverage criterion for the design.

Author(s)

J. Franco

References

Gunzburer M., Burkdart J. (2004) *Uniformity measures for point samples in hypercubes* http://people.sc.fsu.edu/~burkardt/pdf/ptmeas.pdf.

See Also

```
other distance criteria like meshRatio, phiP and mindist. discrepancy measures provided by discrepancyCriteria.
```

Examples

```
dimension <- 2
n <- 40
X <- matrix(runif(n*dimension),n,dimension)
coverage(X)</pre>
```

discrepancyCriteria

Discrepancy measure

Description

Compute discrepancy criteria.

Usage

```
discrepancyCriteria(design,type='all')
```

Arguments

design a matrix (or a data.frame) corresponding to the design of experiments. The

discrepancy criteria are computed for a design in the unit cube $[0,1]^d$. If this

condition is not satisfied the design is automatically rescaled.

type type of discrepancies (single value or vector) to be computed:

```
'all' all type of discrepancies (default)
'C2' centered L2-discrepancy
'L2' L2-discrepancy
'L2star' L2star-discrepancy
'M2' modified L2-discrepancy
```

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'S2' symmetric L2-discrepancy wrap-around L2-discrepancy

Details

The discrepancy measures how far a given distribution of points deviates from a perfectly uniform one. Different L2 discrepancies are available in DiceDesign. For example, if we denote by Vol(J) the volume of a subset J of $[0;1]^d$ and A(X;J) the number of points of X falling in J, the L2 discrepancy is:

$$D_{L2}(X) = \left[\int_{[0,1]^{2d}} \left(\frac{A(X, J_{a,b})}{n} - Vol(J_{a,b}) \right)^2 dadb \right]^{1/2}$$

where $a = (a_1; ...; a_d)'$, $b = (b_1; ...; b_d)'$ and $J_{a,b} = [a_1; b_1) \times ... \times [a_d; b_d)$. The other L2-discrepancies are defined according to the same principle with different form from the subset J. Among all the possibilities, discrepancyCriteria implements only the L2 discrepancies because it can be expressed analytically even for high dimension.

Centered L2-discrepancy is computed using the analytical expression done by Hickernell (1998). The user will refer to Pleming and Manteufel (2005) to have more details about the wrap around discrepancy.

Value

A list containing the L2-discrepancies of the design.

Author(s)

J. Franco, D. Dupuy & B. Iooss

References

Fang K.T, Li R. and Sudjianto A. (2006) Design and Modeling for Computer Experiments, *Chapman & Hall*.

Franco J. (2008) Planification d'experiences numerique en phase exploratoire pour la simulation des phenomenes complexes, *PhD thesis, Ecole Nationale Superieure des Mines de Saint Etienne*.

Hickernell F.J. (1998) A generalized discrepancy and quadrature error bound. *Mathematics of Computation*, **67**, 299-322.

Pleming J.B. and Manteufel R.D. (2005) *Replicated Latin Hypercube Sampling*, 46th Structures, Structural Dynamics & Materials Conference, 16-21 April 2005, Austin (Texas) – AIAA 2005-1819.

See Also

distance criteria (coverage, meshRatio, mindist and phiP)

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Examples

```
dimension <- 2
n <- 40
X <- matrix(runif(n*dimension),n,dimension)
discrepancyCriteria(X)</pre>
```

discrepESE_LHS

Enhanced Stochastic Evolutionnary (ESE) algorithm for Latin Hypercube Sample (LHS) optimization via L2-discrepancy criteria

Description

The objective is to produce low-discrepancy LHS. ESE is a powerful genetic algorithm to produce space-filling designs. It has been adapted here to main discrepancy criteria.

Usage

```
discrepESE_LHS(design,T0=0.005*discrepancyCriteria(design,type='C2')[[1]],
inner_it=100,J=50,it=2,criterion="C2")
```

Arguments

design a matrix (or a data.frame) corresponding to the design of experiments.

The initial temperature of the ESE algorithm

inner_it The number of iterations for inner loop

J The number of new proposed LHS inside the inner loop

it The number of iterations for outer loop

criterion The criterion to be optimized. One can choose three different L2-discrepancies:

the C2 (centered) discrepancy ("C2"), the L2-star discrepancy ("L2star") and the

W2 (wrap-around) discrepancy ("W2")

Details

This function implements a stochastic algorithm (ESE) to produce optimized LHS. It is based on Jin et al works (2005). Here, it has been adapted to some discrepancy criteria taking into account new ideas about the revaluations of discrepancy value after a LHS elementary perturbation (in order to avoid computing all terms in the discrepancy formulas).

Value

A list containing:

InitialDesign the starting design

T0 the initial temperature of the ESE algorithm inner_it the number of iterations for inner loop

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J	the number of new proposed LHS inside the inner loop
it	the number of iterations for outer loop
criterion	the criterion to be optimized
design	the matrix of the final design (low-discrepancy LHS)
critValues	vector of criterion values along the iterations
tempValues	vector of temperature values along the iterations
probaValues	vector of acceptation probability values along the iterations

Author(s)

G.Damblin & B. Iooss

References

Damblin G., Couplet M., and Iooss B. (2013). Numerical studies of space filling designs: optimization of Latin Hypercube Samples and subprojection properties, *Journal of Simulation*, 7:276-289, 2013. http://www.gdr-mascotnum.fr/doku.php?id=iooss1

M. Morris and J. Mitchell (1995) Exploratory designs for computational experiments. Journal of Statistical Planning and Inference, 43:381-402.

R. Jin, W. Chen and A. Sudjianto (2005) An efficient algorithm for constructing optimal design of computer experiments. Journal of Statistical Planning and Inference, 134:268-287.

See Also

Latin Hypercube Sample(lhsDesign),discrepancy criteria(discrepancyCriteria), geometric criterion (mindistphiP), optimization (maximinSA_LHS,maximinESE_LHS,discrepSA_LHS)

```
## Not run:
dimension <- 2
n <- 10
X <- lhsDesign(n,dimension)$design
Xopt <- discrepESE_LHS(X,T0=0.005*discrepancyCriteria(X,type='C2')[[1]],inner_it=100,J=50,it=2)
plot(Xopt$design)
plot(Xopt$critValues,type="1")
## End(Not run)</pre>
```

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Description

The objective is to produce low-discrepancy LHS. SA is an efficient algorithm to produce space-filling designs. It has been adapted here to main discrepancy criteria.

Usage

```
discrepSA_LHS(design,T0=10,c=0.95,it=2000,criterion="C2",
profile="GEOM",Imax=100)
```

Arguments

design	a matrix (or a data.frame) corresponding to the design of experiments
Т0	The initial temperature
С	A constant parameter regulating how the temperature goes down
it	The number of iterations
criterion	The criterion to be optimized. One can choose three different L2-discrepancies: the C2 (centered) discrepancy ("C2"), the L2-star discrepancy ("L2star") and the W2 (wrap-around) discrepancy ("W2")
profile	The temperature down-profile, purely geometric called "GEOM", geometrical according to the Morris algorithm called "GEOM_MORRIS" or purely linear called "LINEAR"
Imax	A parameter given only if you choose the Morris down-profile. It adjusts the number of iterations without improvement before a new elementary perturbation

Details

This function implements a classical routine to produce optimized LHS. It is based on the work of Morris and Mitchell (1995). They have proposed a SA version for LHS optimization according to mindist criterion. Here, it has been adapted to some discrepancy criteria taking in account new ideas about the reevaluations of a discrepancy value after a LHS elementary perturbation (in order to avoid computing all terms in the discrepancy formulas).

Value

A list containing:

InitialDesign	the starting design
Т0	the initial temperature of the SA algorithm
С	the constant parameter regulating how the temperature goes down
it	the number of iterations

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the matrix of the final design (low-discrepancy LHS)

criterion	the criterion to be optimized
profile	the temperature down-profile
Imax	The parameter given in the Morris down-profile

critValues vector of criterion values along the iterations

tempValues vector of temperature values along the iterations

probaValues vector of acceptation probability values along the iterations

Author(s)

design

G.Damblin & B. Iooss

References

Damblin G., Couplet M., and Iooss B. (2013). Numerical studies of space filling designs: optimization of Latin Hypercube Samples and subprojection properties, *Journal of Simulation*, 7:276-289, 2013. http://www.gdr-mascotnum.fr/doku.php?id=iooss1

M. Morris and J. Mitchell (1995) Exploratory designs for computationnal experiments. Journal of Statistical Planning and Inference, 43:381-402.

R. Jin, W. Chen and A. Sudjianto (2005) An efficient algorithm for constructing optimal design of computer experiments. Journal of Statistical Planning and Inference, 134:268-287.

See Also

Latin Hypercube Sample(lhsDesign),discrepancy criteria(discrepancyCriteria), geometric criterion (mindistphiP), optimization (maximinSA_LHS,maximinESE_LHS,discrepESE_LHS)

```
dimension <- 2
n <- 10
X <- lhsDesign(n,dimension)$design
Xopt <- discrepSA_LHS(X,T0=10,c=0.99,it=2000,criterion="C2")
plot(Xopt$design)
plot(Xopt$critValues,type="1")
## Not run:
    Xopt <- discrepSA_LHS(X,T0=10,c=0.99,it=1000,criterion="C2",profile="GEOM_MORRIS")
## End(Not run)</pre>
```

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dmaxDesign	Maximum Entropy Designs	

Description

Space-Filling Designs with n experiments based on covariance matrix in $[0,1]^d$.

Usage

```
dmaxDesign(n, dimension, range, niter_max=1000, seed=NULL)
```

Arguments

n number of experiments
dimension number of variables
range range of variogram
niter_max number of iterations

seed used to generate uniform design

Details

Maximum entropy design is a kind of optimal design based on Shannon's definition of entropy as the amount of information. Originally, maximum entropy sampling was proposed by Shewry and Wynn (1987). The goal of the design is to maximize the entropy defined as the determinant of the correlation matrix using a Fedorov-Mitchell exchange algorithm.

The spatial correlation matrix is defined by $C = (\rho_{ij})$:

$$\rho_{ij} = 1 - \gamma (h_{ij}) \quad \text{if } h_{ij} \le a, \\ \rho_{ij} = 0 \quad \text{if } h_{ij} > a,$$

where h_{ij} is the distance between x_i and x_j , a denotes the range of the variogram and γ is a spherical variogram:

$$\gamma(h) = 1.5 \frac{h}{a} - 0.5 \left(\frac{h}{a}\right)^3 \text{ for } h \le a$$

Value

A list with components:

n the number of points

design the design of experiments

dimension the number of variables

range the range of the variogram

niter_mx the number of iterations

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design_init the initial distribution

det_init the value of the determinant for the initial distribution det_end the value of the determinant at the end of the procedure

seed the value of the seed

Author(s)

J. Franco

References

Currin C., Mitchell T., Morris M. and Ylvisaker D. (1991) *Bayesian Prediction of Deterministic Functions With Applications to the Design and Analysis of Computer Experiments*, American Statistical Association, **86**, 416, 953-963.

Shewry, M. C. and Wynn and H. P. (1987) *Maximum entropy sampling*, Journal of Applied Statistics 14, 165-170.

Examples

```
n <- 20
dimension <- 2
range <-0.9
niter_max <- 200
out <- dmaxDesign(n,dimension,range,niter_max)</pre>
```

factDesign

Full Factorial Designs

Description

Create a factorial design with n = pow(levels, dimension) experiments in $[0,1]^d$.

Usage

```
factDesign(dimension, levels)
```

Arguments

dimension an integer given the number of input variables

levels an integer given the number of levels

Details

It is possible to take a different number of levels for any factor. In this case, the argument levels should be a vector.

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Value

factDesign returns a list containing all the input arguments detailed before, plus the following components:

n the number of experiments design the design of experiments

Author(s)

G. Pujol and J. Franco

Examples

```
## First example
g <- factDesign(2,7)
plot(g$design,xlim=c(0,1),ylim=c(0,1))
## Second example
g <- factDesign(2,c(2,7))
plot(g$design,xlim=c(0,1),ylim=c(0,1))</pre>
```

lhsDesign

Latin Hypercube Designs

Description

Simple (random) Latin Hypercube Design (randomized or centered) with n experiments in $[0,1]^d$.

Usage

```
lhsDesign(n, dimension, randomized=TRUE, seed=NULL)
```

Arguments

n number of experiments dimension number of variables

randomized TRUE for randomized LHS; FALSE for centered LHS

seed seed used to generate the random permutations and perturbations

Details

This program builds a Latin Hypercube Design (LHD), also called a Latin Hypercube Sample (LHS), on the space $[0,1]^d$ (with uniform probability measures). LHD aims at ensuring that each variable has its whole range well scanned: the range of each variable is divided into n equally probable stratas. Each stratum of each variable contains only one point of the LHD. Centered LHD is obtained by choosing for each point the center of the corresponding case, while randomized LHD is obtained by adding random perturbations inside each point case.

Once the sample is generated, the uniform sample from a column can be transformed to any distribution by using the quantile functions.

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Value

A list with components:

n the number of points
dimension the number of variables
design the design of experiments

randomized the type of LHD seed the value of the seed

Author(s)

B. Iooss

References

McKay M., Conover W. and Beckman R. (1979) A comparison of three methods for selecting values of input variables in the analysis of output from a computer code, Technometrics, **21**, 2, 239-245.

Stein M. (1987) Large sample properties of simulations using Latin hypercube sampling, Technometrics, **29**, 143-151.

See Also

LHD optimization (maximinSA_LHS,discrepSA_LHS,maximinESE_LHS,discrepESE_LHS)

Examples

```
n <- 20
dimension <- 2
out <- lhsDesign(n,dimension)</pre>
```

maximinESE_LHS Enhanced Stochastic Evolutionnary (ESE) algorithm for Latin Hyper-

cube Sample (LHS) optimization via phiP criteria

Description

The objective is to produce maximin LHS. ESE is a powerful genetic algorithm allowing to produce space-filling designs.

Usage

```
maximinESE_LHS(design,T0=0.005*phiP(design,p=50),inner_it=100,J=50,it=1,p=50)
```

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Arguments

design a matrix (or a data.frame) corresponding to the design of experiments.

To The initial temperature of the ESE algorithm inner_it The number of iterations for inner loop

J The number of new proposed LHS inside the inner loop

it The number of iterations for outer loop

p power required in phiP criterion

Details

This function implements a stochastic algorithm (ESE) to produce optimized LHS. It is based on Jin et al works (2005).

Value

A list containing:

InitialDesign the starting design

T0 the initial temperature of the ESE algorithm inner_it the number of iterations for inner loop

J the number of new proposed LHS inside the inner loop

it the number of iterations for outer loop

p power required in phiP criterion

design the matrix of the final design (maximin LHS)

critValues vector of criterion values along the iterations

tempValues vector of temperature values along the iterations

probaValues vector of acceptation probability values along the iterations

Author(s)

G.Damblin & B. Iooss

References

Damblin G., Couplet M., and Iooss B. (2013). Numerical studies of space filling designs: optimization of Latin Hypercube Samples and subprojection properties, *Journal of Simulation*, 7:276-289, 2013. http://www.gdr-mascotnum.fr/doku.php?id=iooss1

M. Morris and J. Mitchell (1995) Exploratory designs for computationnal experiments. Journal of Statistical Planning and Inference, 43:381-402.

R. Jin, W. Chen and A. Sudjianto (2005) An efficient algorithm for constructing optimal design of computer experiments. Journal of Statistical Planning and Inference, 134:268-287.

Pronzato, L. and Muller, W. (2012). Design of computer experiments: space filling and beyond, *Statistics and Computing*, 22:681-701.

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See Also

Latin Hypercube Sample(lhsDesign),discrepancy criteria(discrepancyCriteria), geometric criterion (mindistphiP), optimization (maximinSA_LHS,discrepESE_LHS,discrepSA_LHS)

Examples

```
dimension <- 2
n <- 10
X <- lhsDesign(n,dimension)$design
Xopt <- maximinESE_LHS(X,T0=0.005*phiP(X),inner_it=100,J=50,it=2)
plot(Xopt$design)
plot(Xopt$critValues,type="l")</pre>
```

maximinSA_LHS

Simulated annealing (SA) routine for Latin Hypercube Sample (LHS) optimization via phiP criteria

Description

The objective is to produce maximin LHS. SA is an efficient algorithm to produce space-filling designs.

Usage

```
maximinSA_LHS(design, T0=10, c=0.95, it=2000, p=50, profile="GEOM", Imax=100)
```

Arguments

design	a matrix (or a data.frame) corresponding to the design of experiments
TØ	The initial temperature of the SA algorithm
С	A constant parameter regulating how the temperature goes down
it	The number of iterations
р	power required in phiP criterion
profile	The temperature down-profile, purely geometric called "GEOM", geometrical according to the Morris algorithm called "GEOM_MORRIS" or purely linear called "LINEAR"
Imax	A parameter given only if you choose the Morris down-profile. It adjusts the number of iterations without improvement before a new elementary perturbation

Details

This function implements a classical routine to produce optimized LHS. It is based on the work of Morris and Mitchell (1995). They have proposed a SA version for LHS optimization according to mindist criterion. Here, it has been adapted to the phiP criterion. It has been shown (Pronzato and Muller, 2012, Damblin et al., 2013) that optimizing phiP is more efficient to produce maximin designs than optimizing mindist. When p tends to infinity, optimizing a design with phi_p is equivalent to optimizing a design with mindist.

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Value

A list containing:

InitialDesign the starting design

To the initial temperature of the SA algorithm

c the constant parameter regulating how the temperature goes down

it the number of iterations

p power required in phiP criterion profile the temperature down-profile

Imax The parameter given in the Morris down-profile design the matrix of the final design (maximin LHS) vector of criterion values along the iterations tempValues vector of temperature values along the iterations

probaValues vector of acceptation probability values along the iterations

Author(s)

G.Damblin & B. Iooss

References

Damblin G., Couplet M., and Iooss B. (2013). Numerical studies of space filling designs: optimization of Latin Hypercube Samples and subprojection properties, *Journal of Simulation*, 7:276-289, 2013. http://www.gdr-mascotnum.fr/doku.php?id=iooss1

M. Morris and J. Mitchell (1995) Exploratory designs for computationnal experiments. Journal of Statistical Planning and Inference, 43:381-402.

R. Jin, W. Chen and A. Sudjianto (2005) An efficient algorithm for constructing optimal design of computer experiments. Journal of Statistical Planning and Inference, 134:268-287.

Pronzato, L. and Muller, W. (2012). Design of computer experiments: space filling and beyond, *Statistics and Computing*, 22:681-701.

See Also

Latin Hypercube Sample(lhsDesign),discrepancy criteria(discrepancyCriteria), geometric criterion (mindistphiP), optimization (discrepSA_LHS,maximinESE_LHS,discrepESE_LHS)

```
dimension <- 2
n <- 10
X <- lhsDesign(n,dimension)$design
Xopt <- maximinSA_LHS(X,T0=10,c=0.99,it=2000)
plot(Xopt$design)
plot(Xopt$critValues,type="1")
plot(Xopt$tempValues,type="1")
## Not run:</pre>
```

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```
Xopt <- maximinSA_LHS(X,T0=10,c=0.99,it=1000,profile="GEOM_MORRIS")
## End(Not run)</pre>
```

meshRatio

MeshRatio measure

Description

The meshRatio criterion is the ratio between the maximimum and the minimum distance between two points of the experimental design.

Usage

```
meshRatio(design)
```

Arguments

design

a matrix (or a data.frame) representing the design of experiments in the unit cube $[0,1]^d$. If this last condition is not fulfilled, a transformation into $[0,1]^d$ is applied before the computation of the criteria.

Details

The meshRatio criterion is defined by

$$meshRatio = \frac{\max_{1 \le i \le n} \gamma_i}{\min_{1 \le i \le n} \gamma_i}$$

where γ_i denotes the minimal distance between the point x_i and the other points of the design. Note that for a regular mesh, meshRatio=1.

Value

A real number equal to the value of the meshRatio criterion for the design.

Author(s)

J. Franco

References

Gunzburer M. and Burkdart J. (2004) *Uniformity measures for point samples in hypercubes* http://people.sc.fsu.edu/~burkardt/pdf/ptmeas.pdf.

See Also

other distance criteria like meshRatio, phiP and mindist. discrepancy measures provided by discrepancyCriteria.

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Examples

```
dimension <- 2
n <- 40
X <- matrix(runif(n*dimension),n,dimension)
meshRatio(X)</pre>
```

mindist

Mindist measure

Description

Compute the mindist criterion (also called maximin)

Usage

```
mindist(design)
```

Arguments

design

a matrix (or a data.frame) representing the design of experiments in the unit cube $[0,1]^d$. If this last condition is not fulfilled, a transformation into $[0,1]^d$ is applied before the computation of the criteria.

Details

The mindist criterion is defined by

$$mindist = \min_{x_i \in X} (\gamma_i)$$

where γ_i is the minimal distance between the point x_i and the other points x_k of the design.

A higher value corresponds to a more regular scaterring of design points.

Value

A real number equal to the value of the mindist criterion for the design.

Author(s)

J. Franco

References

Gunzburer M., Burkdart J. (2004) *Uniformity measures for point samples in hypercubes* http://people.sc.fsu.edu/~burkardt/pdf/ptmeas.pdf.

Jonshon M.E., Moore L.M. and Ylvisaker D. (1990) *Minmax and maximin distance designs*, J. of Statis. Planning and Inference, 26, 131-148.

Chen V.C.P., Tsui K.L., Barton R.R. and Allen J.K. (2003) A review of design and modeling in computer experiments, Handbook of Statistics, 22, 231-261.

20 mstCriteria

See Also

other distance criteria like meshRatio and phiP, discrepancy measures provided by discrepancyCriteria.

Examples

```
dimension <- 2
n <- 40
X <- matrix(runif(n*dimension),n,dimension)
mindist(X)</pre>
```

mstCriteria

Deriving the MST criteria

Description

Compute both the mean and the standard deviation of the Minimal Spanning Tree (MST)

Usage

```
mstCriteria(design,plot2d="FALSE")
```

Arguments

design a matrix (or a data.frame) corresponding to the design of experiments.

plot2d an argument for visualizing the mst of a 2d design

Details

In our context, a MST is a tree whose the sum of the lengthes of the edges is minimal. Even if unicity does not hold, the overall length is stable. The mean and the standard deviation of the lengthes of the edges are usually derived to analyze the geometric profile of the design. A large mean and a small standard deviation characterize a so-called quasi-periodic design.

Value

A list containing two components:

tree a list containing the MST: each component of it contains a vector with all ver-

tices which are connected with the experiment corresponding to the number of

the components

stats vector with both the mean and the standard deviation values of the lengthes of

the edges

Author(s)

G.Damblin & B.Iooss

OA131 21

References

Damblin G., Couplet M., and Iooss B. (2013). Numerical studies of space filling designs: optimization of Latin hypercube samples and subprojection properties, *Journal of Simulation*, 7:276-289, 2013. http://www.gdr-mascotnum.fr/doku.php?id=iooss1

Dussert, C., Rasigni, G., Rasigni, M., and Palmari, J. (1986). Minimal spanning tree: A new approach for studying order and disorder. Physical Review B, 34(5):3528-3531.

Franco J. (2008). Planification d'experiences numerique en phase exploratoire pour la simulation des phenomenes complexes, *PhD thesis*, *Ecole Nationale Superieure des Mines de Saint Etienne*.

Franco, J., Vasseur, O., Corre, B., and Sergent, M. (2009). Minimum spanning tree: A new approach to assess the quality of the design of computer experiments. Chemometrics and Intelligent Laboratory Systems, 97:164-169.

Prim, R.C. (1957). Shortest connection networks and some generalizations, in *Bell System Technical Journal* 36:1389-1401.

Examples

```
dimension <- 2
n <- 40
X <- matrix(runif(n*dimension),n,dimension)
mstCriteria(X,plot2d=TRUE)</pre>
```

0A131

A 3D orthogonal array of strength 2

Description

A 3-dimensional linear orthogonal array (OA) of strength 2 with 49 points. The design points are equally spaced into 2 dimensional coordinate planes. However by construction, such OAs satisfy a linear relation, here: $x1 + 3*x2 + x3 = 0 \pmod{7}$. As a consequence, the design points are contained in parallel planes orthogonal to (1,3,1). Actually, they are also contained in parallel planes orthogonal to other directions, as (2,-1,2) or (3,2,3), since the congruence relation leads to $2*x1 - x2 + 2*x3 = 0 \pmod{7}$ or $3*x1 + 2*x2 + 3*x3 = 0 \pmod{7}$. For instance, they are contained in 4 parallel planes orthogonal to (2,-1,2).

Usage

```
data(0A131)
```

Format

A data frame with 49 observations on the following 3 variables.

- x1 first coordinate
- x2 second coordinate
- x3 third coordinate

OA131_scrambled

Source

Roustant O., Franco J., Carraro L., Jourdan A. (2010), A radial scanning statistic for selecting space-filling designs in computer experiments, MODA-9 proceedings, www.emse.fr/~roustant

Examples

OA131_scrambled

A scrambled 3D orthogonal array of strength 2

Description

This design is obtained by adding a uniform noise to each coordinate of the orthogonal array OA131.

Usage

```
data(OA131_scrambled)
```

Format

A data frame with 49 observations on the following 3 variables.

- x1 first coordinate
- x2 second coordinate
- x3 third coordinate

Source

Roustant O., Franco J., Carraro L., Jourdan A. (2010), A radial scanning statistic for selecting space-filling designs in computer experiments, MODA-9 proceedings, www.emse.fr/~roustant

```
data(OA131)
data(OA131_scrambled)

pairs(OA131, xlim=c(0,1), ylim=c(0,1))
pairs(OA131_scrambled, xlim=c(0,1), ylim=c(0,1))
```

phiP 23

phiP phiP criterion

Description

Compute the ϕ_p criterion (strongly linked to mindist criterion)

Usage

```
phiP(design,p=50)
```

Arguments

design a matrix (or a data.frame) corresponding to the design of experiments.

p the "p" in the Lp norm which is taken

Details

The ϕ_p criterion is defined by the L_p norm of the sum of the inverses of the design inter-point euclidean distances:

$$\phi_p = \left[\sum_{i,j=1\dots N, i < j} d_{ij}^{-p} \right]^{\frac{1}{p}}$$

A higher value corresponds to a more regular scaterring of design points.

When p tends to infinity, optimizing a design with ϕ_p is equivalent to optimizing a design with mindist.

Value

A real number equal to the value of the ϕ_p criterion for the design.

Author(s)

G.Damblin & B.Iooss

References

Damblin G., Couplet M., and Iooss B. (2013). Numerical studies of sapce filling designs: optimization of Latin Hypercube Samples and subprojection properties, *Journal of Simulation*, 7:276-289, 2013. http://www.gdr-mascotnum.fr/doku.php?id=iooss1

Fang K.-T., Li R. and Sudjianto A. (2006). Design and Modeling for Computer Experiments, *Chapman & Hall*.

Pronzato, L. and Muller, W. (2012). Design of computer experiments: space filling and beyond, *Statistics and Computing*, 22:681-701.

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See Also

```
geometric criterion (mindist)
```

Examples

```
dimension <- 2
n <- 40
X <- matrix(runif(n*dimension),n,dimension)
phiP(X)</pre>
```

rss2d

2D graphical tool for defect detection of Space-Filling Designs.

Description

For a 2-dimensional design, the 2D radial scanning statistic (RSS) scans angularly the domain. In each direction, it compares the distribution of projected points to their theoretical distribution under the assumption that all design points are drawn from uniform distribution. For a d-dimensional design, all pairs of dimensions are scanned. The RSS detects the defects of low discrepancy sequences or orthogonal arrays, and can be used for selecting space-filling designs.

Usage

```
rss2d(design, lower, upper, gof.test.type="greenwood",
   gof.test.stat=NULL, transform=NULL, n.angle=360, graphics=1,
   trace=TRUE, lines.lwd = 1, lines.lty = "dotted", ...)
```

Arguments

gof.test.stat

design a matrix or data.frame containing the d-dimensional design of experiments. The

row no. i contains the values of the d input variables corresponding to simulation

no. i

lower the domain lower boundaries.
upper the domain upper boundaries.

gof.test.type an optional character indicating the kind of statistical test to be used to test the

goodness-of-fit of the design projections to their theoretical distribution. Several tests are available, see unif.test.statistic. Default is "greenwood".

tests are available, see all 1. tests. Set act 15 feel wood.

an optional number equal to the goodness-of-fit statistic at level 5%. Default is the modified test statistic for fully specified distribution (see details below).

the modified test statistic for fully specified distribution (see details selow).

transform an optional character indicating what type of transformation should be applied

before testing uniformity. Only one choice available "spacings", that lead to

over-detection. Default - and recommended - is NULL.

n.angle an optional number indicating the number of angles used. Default is 360 corre-

sponding to a 0.5-degree discretization step. Note that the RSS curve is contin-

uous.

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graphics	an optional integer indicating whether a graph should be produced. If negative, no graph is produced. If superior to 2, the RSS curve only is plotted in the worst 2D coordinate subspace (corr. to the worst value of statistic). If 1 (default), the design is also added, with its projections onto the worst (oblique) axis.
trace	an optional boolean. Turn it to FALSE if you want no verbosity.
lines.lwd	optional number specifying the width of the straight lines involved in the graphical outputs (axis and projections)
lines.lty	optional character string specifying the type of the straight lines involved in the graphical outputs (axis and projections)
• • •	optional graphical parameters of plot function, to draw the RSS curve.

Value

a list with components:

global.stat	a matrix containing the values of the global statistic (equal to the maximum of statistic values over the RSS curve) for all pairs of dimensions.
worst.case	the worst pair of dimensions, that is the one that gives the worst value of ${\tt global}$. ${\tt stat}$.
worst.dir	the worst direction, that is the one that gives the worst value of the global statistic in the coordinate plane defined by worst.case.
stat	a vector of length n.angle containing the statitic values for each angle, in the coordinate plane defined by worst.case.
angle	a vector of length n. angle containing the corresponding angles used.
curve	a (2*n.angle)x2 matrix containing the discretized RSS curve.
<pre>gof.test.stat</pre>	the threshold at significance level 0.05 for the specified goodness-of-fit statistic. It is equal to the radius of the circle superimposed on the RSS figure.

Author(s)

O. Roustant

References

Roustant O., Franco J., Carraro L., Jourdan A. (2010), A radial scanning statistic for selecting space-filling designs in computer experiments, MODA-9 proceedings, www.emse.fr/~roustant

D Agostino R.B., Stephens M.A. (1986), Goodness-of-fit techniques, CRC Press, New York.

See Also

```
unif.test.statistic, unif.test.quantile, rss3d\\
```

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Examples

```
# Detection of defects of Sobol designs
# requires randtoolbox package
library(randtoolbox)
# in 2D
rss < rss2d(design=sobol(n=20, dim=2), lower=c(0,0), upper=c(1,1), type="1",
# in 8D.
# All pairs of dimensions are tried to detect the worst defect
# (according to the specified goodness-of-fit statistic).
d <- 8
n <- 10*d
rss <- rss2d(design=sobol(n=n, dim=d), lower=rep(0,d), upper=rep(1,d), type="1",
  col="red")
# avoid this defect with scrambling ?
     1. Faure-Tezuka scrambling (type "?sobol" for more details and options)
rss <- rss2d(design=sobol(n=n, dim=d, scrambling=2), lower=rep(0,d),
  upper=rep(1,d), type="l", col="red")
     2. Owen scrambling
rss <- rss2d(design=sobol(n=n, dim=d, scrambling=1), lower=rep(0,d),
  upper=rep(1,d), type="l", col="red")
```

rss3d

3D graphical tool for defect detection of Space-Filling Designs.

Description

For a 3-dimensional design, the 3D radial scanning statistic (RSS) scans angularly the domain. In each direction, it compares the distribution of projected points to their theoretical distribution under the assumption that all design points are drawn from uniform distribution. For a d-dimensional design, all triplets of dimensions are scanned. The RSS detects the defects of low discrepancy sequences or orthogonal arrays, and can be used for selecting space-filling designs.

Usage

```
rss3d(design, lower, upper, gof.test.type = "greenwood",
  gof.test.stat = NULL, transform = NULL, n.angle = 60,
  graphics = 1, trace = TRUE)
```

Arguments

design

a matrix or data.frame containing the d-dimensional design of experiments. The row no. i contains the values of the d input variables corresponding to simulation no. i

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the domain lower boundaries. lower the domain upper boundaries. upper gof.test.type an optional character indicating the kind of statistical test to be used to test the goodness-of-fit of the design projections to their theoretical distribution. Several tests are available, see unif.test.statistic. Default is "greenwood". gof.test.stat an optional number equal to the goodness-of-fit statistic at level 5%. Default is the modified test statistic for fully specified distribution (see details below). transform an optional character indicating what type of transformation should be applied before testing uniformity. Only one choice available "spacings", that lead to over-detection. Default - and recommended - is NULL. n.angle an optional number indicating the number of angles used. Default is 60 corresponding to a 3-degree discretization step. Note that the RSS surface is contingraphics an optional integer indicating whether a graph should be produced. If negative, no graph is produced. Otherwise (default), the design is plotted in the worst 3D coordinate subspace (corr. to the worst value of statistic), with its projections onto the worst (oblique) axis. trace an optional boolean. Turn it to FALSE if you want no verbosity.

Details

The RSS surface is continuous. However for computational purposes, a discretization is used. The default discretization step is tunable with n.angle.

Value

a list with components:

global.stat	an array containing the values of the global statistic (equal to the maximum of statistic values over the RSS surface) for all triplets of dimensions.
print.out	the same as global.stat, but with a user-friendly printing.
worst.case	the worst triplet of dimensions, that is the one that gives the worst value of global.stat.
worst.dir	the worst direction, that is the one that gives the worst value of the statistic in the coordinate 3D subspace defined by worst.case.
stat	a matrix of size n.angle*n.angle containing the statistic values for each angles (spherical coordinates).
angle	a matrix of size n.angle*n.angle containing the corresponding angles used (spherical coordinates).
<pre>gof.test.stat</pre>	the threshold at significance level 0.05 for the specified goodness-of-fit statistic.

Author(s)

O. Roustant

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References

Roustant O., Franco J., Carraro L., Jourdan A. (2010), A radial scanning statistic for selecting space-filling designs in computer experiments, MODA-9 proceedings, www.emse.fr/~roustant

D Agostino R.B., Stephens M.A. (1986), Goodness-of-fit techniques, CRC Press, New York.

See Also

```
unif.test.statistic, unif.test.quantile, rss2d
```

```
# An orthogonal array in 3D
data(0A131)
# centering the design points of this 7-levels design
OA <- (OA131 + 0.5)/7
# 2D projections onto coordinate axis
pairs(OA, xlim=c(0,1), ylim=c(0,1))
# Now let us look at the 3D properties with the 3D RSS (requires the rgl package)
rss <- rss3d(OA, lower=c(0,0,0), upper=c(1,1,1))
# The worst direction detected is nearly proportional to (2,-1,2)
# (type "?OA131" for explanations about this linear orthogonal array)
print(rss$worst.dir)
# Now, scramble this design
\# X < - (0A131 + matrix(runif(49*3, 49, 3)))/7
# or load the design obtained this way
data(OA131_scrambled)
OA2 <- OA131_scrambled
# no feature is detected by the 2D RSS:
rss <- rss2d(0A2, lower=c(0,0,0), upper=c(1,1,1))
# 4 clusters are detected by the 3D RSS:
rss <- rss3d(0A2, lower=c(0,0,0), upper=c(1,1,1))
# Defect detection of 8D Sobol sequences
# All triplets of dimensions are tried to detect the worst defect
# (according to the specified goodness-of-fit statistic).
# requires randtoolbox library to generate the Sobol sequence
## Not run:
library(randtoolbox)
d <- 8
n <- 10*d
rss <- rss3d(design=sobol(n=n, dim=d), lower=rep(0,d), upper=rep(1,d))</pre>
## End(Not run)
```

runif.faure 29

runif.faure

Low discrepancy sequence: Faure

Description

Generate a Faure sequence with n experiments in $[0,1]^d$.

Usage

```
runif.faure(n, dimension)
```

Arguments

n the number of experiments dimension the number of variables (<100)

Details

A quasirandom or low discrepancy sequence, such as the Faure, Halton, Hammersley, Niederreiter or Sobol sequences, is "less random" than a pseudorandom number sequence, but more useful for such tasks as approximation of integrals in higher dimensions, and in global optimization. This is because low discrepancy sequences tend to sample space "more uniformly" than random numbers.

see randtoolbox or fOptions packages for other low discrepancy sequences.

Value

runif.halton returns a list containing all the input arguments detailed before, plus the following component:

design

the design of experiments

Author(s)

J. Franco

References

Faure H. (1982) *Discrepance de suites associees a un systeme de numeration (en dimension s)*, Acta Arith. 41, 337-351

```
f <- runif.faure(20,2)
plot(f$design,xlim=c(0,1),ylim=c(0,1))</pre>
```

30 straussDesign

straussDesign Designs based on Strauss process
--

Description

Space-Filling Designs based on Strauss process

Usage

Arguments

n the number of experiments
dimension the number of input variables

RND a real number which represents the radius of interaction

alpha the potential power (default, fixed at 0.5)

repulsion the repulsion parameter in the unit cube (gamma)

NMC the number of McMC iterations (this number must be large to converge)

constraints1D 1 to impose 1D projection constraints, 0 otherwise

repulsion1D the repulsion parameter in 1D

seed seed for the uniform generation of number

Details

Strauss designs are Space-Filling designs initially defined from Strauss process:

$$\pi(X) = k\gamma^{s(X)}$$

where s(X) is is the number of pairs of points (x^i, x^j) of the design $X = (x^1, \dots, x^n)$ that are separated by a distance no greater than the radius of interaction RND, k is the normalizing constant and γ is the repulsion parameter. This distribution corresponds to the particular case alpha=0.

For the general case, a stochastic simulation is used to construct a Markov chain which converges to a spatial density of points $\pi(X)$ described by the Strauss-Gibbs potential. In practice, the Metropolis-Hastings algorithm is implemented to simulate a distribution of points which converges to the stationary law:

$$\pi(X) \propto exp(-U(X))$$

with a potential U defined by:

$$U(X) = \beta \sum_{1 \le i < j \le n} \varphi \left(\|x^i - x^j\| \right)$$

where $\beta = -\ln \gamma$, $\varphi(h) = \left(1 - \frac{h}{RND}\right)^{\alpha}$ if $h \leq \text{RND}$ and 0 otherwise.

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The input parameters of straussDesign function can be interpreted as follows:

- RND is used to compute the number of pairs of points of the design separated by a distance no more than RND. A point is said "in interaction" with another if the spheres of radius RND/2 centered on these points intersect.

- alpha is the potential power α . The case alpha=0 corresponds to Strauss process (0-1 potential).
- repulsion is equal to the γ parameter of the Strauss process. Note that γ belongs to [0,1].
- constraints1D allows to specify some constraints into the margin. If constraints1D==1, two repulsion parameters are needed: one for the all space (repulsion) and the other for the 1D projection (repulsion1D). Default values are repulsion=0.001 and repulsion1D=0.001. Note that the value of the radius of interaction in the one-dimensional axis is not an input parameter and is automatically fixed at 0.75/n.

Value

A list containing:

n the number of experiments dimension the number d of variables

design_init the initial distribution of n points $[0,1]^d$

radius the radius of interaction alpha the potential power alpha repulsion the repulsion parameter γ

NMC the number of iterations McMC

constraints1D an integer indicating if constraints on the factorial axis are imposed. If its value

is different from zero, a component repulsion1D containing the value of the

repulsion parameter γ in dimension 1 is added at the list.

design the design of experiments in $[0,1]^d$ seed the seed corresponding to the design

Author(s)

J. Franco

References

J. Franco, X. Bay, B. Corre and D. Dupuy (2008) *Planification d experiences numeriques a partir du processus ponctuel de Strauss* http://hal.archives-ouvertes.fr/hal-00260701/fr/ (March 06,2008).

```
# Strauss-Gibbs designs in dimension 2 (n=20 points)
S1 <- straussDesign(n=20,dimension=2,RND=0.2)
plot(S1$design,xlim=c(0,1),ylim=c(0,1))
theta <- seq(0,2*pi,by =2*pi/(100 - 1))
for(i in 1:S1$n){</pre>
```

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```
lines(S1$design[i,1]+S1$radius/2*cos(theta),
    S1$design[i,2]+S1$radius/2*sin(theta),col='red')
}
# 2D-Strauss design
S2 <- straussDesign(n=20,dimension=2,RND=0.2,NMC=200,
    constraints1D=0,alpha=0,repulsion=0.01)

plot(S2$design,xlim=c(0,1),ylim=c(0,1))
# 2D-Strauss designs with constraints on the axis
S3 <- straussDesign(n=20,dimension=2,RND=0.18,NMC=200,
    constraints1D=1,alpha=0.5,repulsion=0.1,repulsion1D=0.01)

plot(S3$design,xlim=c(0,1),ylim=c(0,1))
rug(S3$design[,1],side=1)
rug(S3$design[,2],side=2)</pre>
```

unif.test.quantile

Quantile of some uniformity tests

Description

Computes the quantile of a uniformity test at a given significance level (see available tests and levels below).

Usage

```
unif.test.quantile(type, n, alpha)
```

Arguments

type a character indicating which test is used. The choices are the following: "green-wood", "qm" (for Quesenberry-Miller), "ks" (Kolmogorov-Smirnov), "cvm" (Cramer-Von Mises) and "V" (D+ + D- from Kolmogorov-Smirnov).

n an integer equal to the sample size.

alpha a real number equal to significance level. At present stage, only four values are

available: 0.1, 0.05, 0.025 and 0.01.

Details

Modified statistics are used. For alpha = 0.05, the quantile is (see D Agostino and Stephens, 1986, section 4.4.): 1.358/(sqrt(n) + 0.12 + 0.11/sqrt(n)) for Kolmogorov-Smirnov and $0.461/(1+1/n) + 0.4/n - 0.6/n^2$ for Cramer-von Mises. When the design size is < 20, the corrected value seems to be a good approximation, but the non asymptotical value should be preferred.

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Value

A real number equal to the quantile of the specified test at significance level alpha for n observa-

Author(s)

O. Roustant

References

D Agostino R.B., Stephens M.A. (1986), Goodness-of-fit techniques, CRC Press, New York.

See Also

```
unif.test.statistic, rss2d, rss3d
```

unif.test.statistic Statistic of some uniformity tests

Description

Computes the statistic of a uniformity test (see available tests below).

Usage

```
unif.test.statistic(x, type, transform=NULL)
```

Arguments

x a vector containing the sample values.

type a character indicating which test is used. The choices are the following: "green-

wood", "qm" (for Quesenberry-Miller), "ks" (Kolmogorov-Smirnov), "cvm" (Cramer-

Von Mises) and "V" (D+ + D- from Kolmogorov-Smirnov).

transform an optional character indicating what type of transformation should be applied

before testing uniformity. Default is NULL.

Value

A real number equal to the statistic of the specified test.

Author(s)

O. Roustant

References

D Agostino R.B., Stephens M.A. (1986), Goodness-of-fit techniques, CRC Press, New York.

34 wspDesign

See Also

```
unif.test.quantile, rss2d
```

wspDesign

WSP algorithm

Description

The WSP (Wooton, Sergent, Phan-Tan-Luu) algorithm is an iterative algorithm based on suppression of some experiments from an initial design in each step. WSP leads to a space filling design.

Usage

```
wspDesign(design,dmin)
```

Arguments

design a matrix (or a data.frame) corresponding to the design of experiments.

dmin a minimum bound for mindist value of the final design

Details

WSP enables to create a design D which is such that mindist(D)>dmin. However, it cannot assess the number of experiments. Similarly to straussDesign function, WSP is a powerful algorithm to construct space filling designs in high dimension

Value

A list containing:

InitialDesign the starting design

dmin minimum bound for mindist value of the final design

design the matrix of the final design

Author(s)

G.Damblin & B.Iooss

References

J. Santiago, M. Claeys-Bruno, M.Sergent (2012). Construction of space filling designs using WSP algorithm for high dimensional spaces, *Chenometrics and Intelligent Laboratory Systems*, 113:26-31.

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```
dimension <- 2
n <- 100
X <- matrix(runif(n*dimension),n,dimension)
m=wspDesign(X,0.1)
plot(m$design)</pre>
```

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