Package 'simplexdesign'

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Type Package

Title Simplex Design for Stochastic Simulations and Agent Based Models

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Description Design statistical experiments on agent based models, including a coordinate exchange algorithm for homogeneous agents, and more generally any simplex. There is also an optimization algorithm for the case with multiple classes of homogeneous agents. See our paper ``Uncertainty Quantification for Models of Homogeneous Agents'' for more details when it is published.

Depends R (>= 3.6.0)

Imports ggplot2 (>= 3.2.1), GGally (>= 1.4.0), Rfast (>= 1.9.5),
progress (>= 1.2.2), DiceDesign (>= 1.8.1), stats

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`MmSimplex` *Maxmin Simplex Design*

Description

Constructs a Maximin space-filling design on a k-dimensional simplex.

Usage

```
MmSimplex(k,N,l,cords = 1, randst = 1, phival = 50, tol = 0.0001)
```

Arguments

`k`	Number of factors in the design
`N`	Number of experimental runs
`l`	Number of levels for the search grid
`cords`	Number of coordinates to exchange simultaneously using an exchange algorithm
`randst`	Number of random starts to the design
`phival`	Value of p in the PhiP criterion
`tol`	Tolerance of the optimization, the value for which an improvement smaller than this ends the optimization

Details

This function applies a coordinate-exchange algorithm to optimize the Maximin distance criterion for a simplex. A maximin design maximizes the minimum interpoint distance and is one commonly used space-filling criterion. We do not optimize this criterion directly, but rather optimizes

$$\phi_p = (\sum\sum d_{ij}^{-p})^{1/p}$$

This is done for optimization purposes since it is a smoother criteria.

Value

D1 The optimal design among the random starts standardized to [0,1]

phival The phiP value of the design

phistore A vector of phiP values from each random start

References

- Johnson, M. E., L. M. Moore, and D. Ylvisaker (1990). Minimax and maximin distance designs. Journal of statistical planning and inference 26 (2). 131-148.
- Meyer, R. K., and C.J. Nachtsheim (1995). The coordinate-exchange algorithm for constructing exact optimal experimental designs. Technometrics 37 (1). 60-69.

Examples

```
## Generate Design
time1 <- Sys.time()
D1 <- MmSimplex(5,40,10,cords = 1,randst = 2,phival = 50)
Sys.time() - time1

##View best design scaled to [0,1]^5
D1[[1]]

##View PhiP criterion for best design among 2 random starts
D1[[2]]
```

`paircormin` *Minimize Pairwise Correlation*

Description

Optimizes run order within classes of homogeneous agents to minimize pairwise correlation using Simulated Annealing.

Usage

```
paircormin(Design, kvec, ti = 10, tf = 0.0001, alph = 0.99, iter = 2000)
```

Arguments

`Design`	The unoptimized design
`kvec`	A vector containing the number of columns in each block of the design
`ti`	Initial temperature value for SA
`tf`	Final temperature value for SA
`alph`	Decay parameter for SA (should be less than 1)
`iter`	Number of iterations at each temperature value, should increase with design size

Details

This function optimizes run order within each block of a design made of multiple simplexes to minimize pairwise correlations using a Simulated Annealing algorithm. The criterion of interest is the sum of squared cor(xi,xj) for all pairs of columns between classes. It is recommended that the parameters (such as ti, tf, and iter) are scaled with the size of the design size, and that the criterion values should settle to some local optimal value.

Value

Design The design optimized to minimize pairwise correlations between input classes.

CritVals The pairwise correlations at each temperature change, useful for checking if the SA algorithm has converged.

Examples

```
# Generate Unoptimized Design
D1 <- MmSimplex(3,30,10,cords = 1,randst = 1,phival = 50)
D2 <- MmSimplex(3,30,10,cords = 1,randst = 1,phival = 50)
D3 <- MmSimplex(3,30,10,cords = 1,randst = 1,phival = 50)
D <- cbind(D1[[1]],D2[[1]],D3[[1]])
c1 <- sum(cor(D1[[1]])[upper.tri(cor(D1[[1]]))]^2)
c2 <- sum(cor(D2[[1]])[upper.tri(cor(D2[[1]]))]^2)
c3 <- sum(cor(D3[[1]])[upper.tri(cor(D3[[1]]))]^2)
## Sum all pariwise correlations and
sum(cor(D)[upper.tri(cor(D))]^2) - (c1 + c2 + c3)
## Optimize run order
Dopt <- paircormin(D, c(3,3,3), ti = 0.01, tf = 0.0005, iter = 25)
sum(cor(Dopt[[1]])[upper.tri(cor(Dopt[[1]]))]^2) - (c1 + c2 + c3)
```

PairPlot *Design Projection Plot*

Description

Plots the projection of all pairs of inputs from a design from MmSimplex. Can actually be used for any design on a Simplex.

Usage

```
PairPlot(Design, greys = TRUE)
```

Arguments

Design	List object from MmSimplex, also works with a matrix input
greys	Draws grey boxes to indicate the region of valid design points

Value

A ggplot object

Examples

```
## Generate Design
D1 <- MmSimplex(3,75,10,cords = 1,randst = 1,phival = 50)

##Plot Design
PairPlot(D1)
```

simplexdesign *simplexdesign*

Description

simplexdesign is a small collection of tools for the design of statistical experiments on Agent Based Models. It includes a coordinate exchange algorithm for homogeneous agents, and more generally any simplex. There is also an optimization algorithm for the case with multiple classes of homogeneous agents. See our paper "Uncertainty Quantification for Models of Homogeneous Agents" for more details when it is published.

simplexdesign functions

- MmSimplex : Constructs a Maximin space-filling design on a k-dimensional simplex.
- paircormin : Optimizes run order within classes of homogeneous agents to minimize pairwise correlation using Simulated Annealing.
- PairPlot : Plots the projection of all pairs of inputs from a design from MmSimplex. Can actually be used for any design on a Simplex.

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