Package ‘LatticeDesign’

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Version 3.0-1

Title Lattice-Based Space-Filling Designs

Description Lattice-based space-filling designs with fill or separation distance properties including interleaved lattice-based minimax distance designs proposed in Xu He (2017) <doi:10.1093/biomet/asx036>, interleaved lattice-based maximin distance designs proposed in Xu He (2018) <doi:10.1093/biomet/asy069>, interleaved lattice-based designs with low fill and high separation distance properties proposed in Xu He (2024) <doi:10.1137/23M156940X>, rotated sphere packing designs proposed in Xu He (2017) <doi:10.1080/01621459.2016.1222289>, sliced rotated sphere packing designs proposed in Xu He (2019) <doi:10.1080/00401706.2018.1458655>, and densest packing-based maximum projections designs proposed in Xu He (2021) <doi:10.1093/biomet/asaa057> and Xu He (2018) <doi:10.48550/arXiv.1709.02062>.

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Contents

`LatticeDesign-package` *LatticeDesign package*

Description

Generate lattice-based space-filling designs with fill or separation distance properties. These include interleaved lattice-based minimax distance designs, interleaved lattice-based maximin distance designs, interleaved lattice-based designs with both fill and separation distance properties, (sliced) rotated sphere packing designs, and densest packing-based maximum projections designs.

Details

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Important functions in this package are: `InterleavedMinimaxD` generates an interleaved lattice-based minimax distance design. `InterleavedMaximinD` generates an interleaved lattice-based maximin distance design. `InterleavedFillSepD` generates an interleaved lattice-based design with both fill and separation distance properties. `DPMPD` generates a densest packing-based maximum projection design. `RSPD` generates a rotated sphere packing design. `SlicedRSPD` generates a sliced rotated sphere packing design by partitioning one rotated sphere packing design. `AdaptiveRSPD` generates a sliced rotated sphere packing design by enlarging one rotated sphere packing design.

All those functions generate space-filling designs with fill or separation distance properties. Such designs are useful for accurate emulation of computer experiments, fitting nonparametric models and resource allocation. They are constructed from lattices, i.e., sets of points with group structures.

`RSPD` and `DPMPD` generate designs in two to eight dimensions with both unprojected and projective distance properties. Such designs are desirable when possibly the output value is insensitive to some variables. `DPMPD` can be seen as an upgrade of `RSPD` using new magic rotation matrices. Another distinction is that `RSPD` generates designs with better unprojected fill distance for nonboundary regions while `DPMPD` generates designs with better unprojected separation distance. `RSPD` and `DPMPD` construct designs by rescaling, rotating, translating and extracting the points of the lattice with asymptotically optimal fill and separation distance, respectively.

`SlicedRSPD` and `AdaptiveRSPD` generate sliced rotated sphere packing designs, i.e., a rotated sphere packing design that can be partitioned into several smaller rotated sphere packing designs. `SlicedRSPD` partitions one rotated sphere packing design. The generated designs are useful for computer experiments with a categorical variable, computer experiments from multiply resources and model validation. Alternatively, `AdaptiveRSPD` enlarges a smaller rotated sphere packing design, which is useful for adaptive design of computer experiments.

`InterleavedMinimaxD` generates designs in two to eight dimensions with low fill distance. `InterleavedMaximinD` generates designs with high separation distance. `InterleavedFillSepD` generates designs with both properties. `InterleavedMaximinD` and `InterleavedFillSepD` allow users to specify the relative importance of variables and is applicable to problems with any number of variables. These designs are useful for accurate emulation of computer experiments when the variables are almost equally important in predicting the output value or relatively accurate a priori guess on the variable importance is available. On the other hand, these designs are poor in projective distance properties and are thus not recommended when the output value is insensitive to many unknown variables.

Author(s)

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References

He, Xu (2017). "Rotated sphere packing designs", *Journal of the American Statistical Association*, 112(520): 1612-1622.

He, Xu (2017). "Interleaved lattice-based minimax distance designs", *Biometrika*, 104(3): 713-725.

He, Xu (2018). "Lattice-based designs with quasi-uniform projections", arXiv:1709.02062v2.

He, Xu (2019). "Interleaved lattice-based maximin distance designs", *Biometrika*, 106(2): 453-464.

He, Xu (2019). "Sliced rotated sphere packing designs", *Technometrics*, 61(1): 66-76.

He, Xu (2021). "Lattice-based designs possessing quasi-optimal separation distance on all projections", *Biometrika*, 108(2): 443-454.

He, Xu (2024). "Efficient Kriging using interleaved lattice-based designs with low fill and high separation distance properties", *SIAM/ASA Journal on Uncertainty Quantification*, 12(4): 1113-1134.

`AdaptiveRSPD` *Sliced rotated sphere packing designs by enlarging a design*

Description

Generates a sliced rotated sphere packing design by enlarging one rotated sphere packing design.

Usage

```
AdaptiveRSPD(p=2,n,w=100)
```

Arguments

`p`	Number of dimensions, must be an integer greater than one.
`n`	Number of points of the small design, must be a positive integer.
`w`	Number of rotation matrices to try.

Details

This function generates a small rotated sphere packing design and the candidate points for enlarging it.

Value

The value returned from the function is a list containing the following components:

`Design`	The generated design.
`candidates`	The candidate points to add.
`generator`	The generator matrix.
`rotation`	The rotation matrix.
`delta`	The value of parameter delta.
`Theta`	The value of parameter Theta.
`l`	The value of parameter l.
`FillDistance`	The fill distance of the design for the nonboundary region.

References

He, Xu (2018). "Sliced rotated sphere packing designs", *Technometrics*, 61(1): 66-76.

Examples

```
AdaptiveRSPD(p=2,n=50,w=100)
```

`CCs` *Continuous choices*

Description

These data sets give the solutions found from the continuous optimization algorithm. Data sets CCs2, CCs3, CCs4, CCs5, CCs6, CCs7, and CCs8 give the choices in 2, 3, 4, 5, 6, 7, and 8 dimensions, respectively.

Usage

```
data(CCs2);
data(CCs3);
data(CCs4);
data(CCs5);
data(CCs6);
data(CCs7);
data(CCs8);
```

Format

Matrices containing the choices.

References

He, Xu (2024). "Efficient Kriging using interleaved lattice-based designs with low fill and high separation distance properties", *SIAM/ASA Journal on Uncertainty Quantification*, 12(4): 1113-1134.

DPMPD — *Densest packing-based maximum projection designs*

Description

Generates a densest packing-based maximum projection design.

Usage

```
DPMPD(p,n,rotation="magic",w=100)
```

Arguments

`p`	Number of dimensions, must be an integer greater than one and no higher than eight.
`n`	Number of points, must be an integer greater than one.
`rotation`	Optional, whether to use magic rotation matrices (for p=2,3,4,6,8, recommended) or random rotation matrices.
`w`	Number of rotation matrices to try.

Details

This function generates a densest packing-based maximum projection design in two to eight dimensions. For p=2,4,8 with rotation="magic", the designs are generated following the Biometrika paper "Lattice-based designs possessing quasi-optimal separation distance on all projections". For p=3,6 with rotation="magic", the designs are generated following the arXiv paper "Lattice-based designs with quasi-uniform projections". For other p or rotation!="magic", the designs are generated from random rotations.

Value

The value returned from the function is a list containing the following components:

`Design`	The generated design.
`ProjectiveSeparationDistance`	The projective separation distance of the generated design, from one-dimensional projections to the unprojected design.

References

He, Xu (2021). "Lattice-based designs possessing quasi-optimal separation distance on all projections", *Biometrika*, 108(2): 443-454.

He, Xu (2018). "Lattice-based designs with quasi-uniform projections", arXiv:1709.02062v2.

Examples

```
DPMPD(p=4,n=200,w=100)
```

GeneratorMatrices — *Generator matrices of standard interleaved lattices, treating dimension permuted lattices as different lattices*

Description

These data sets give the generator matrices of standard interleaved lattices, treating dimension permuted lattices as different lattices. Data sets GeneratorMatrices2, GeneratorMatrices3, GeneratorMatrices4, and GeneratorMatrices5 give the matrices in 2, 3, 4, and 5, dimensions, respectively.

Usage

```
data(GeneratorMatrices2);
data(GeneratorMatrices3);
data(GeneratorMatrices4);
data(GeneratorMatrices5);
```

Format

Matrices containing generator matrices.

References

He, Xu (2019). "Interleaved lattice-based maximin distance designs", *Biometrika*, 106(2): 453-464.

GMs — *Generator matrices of standard interleaved lattices, treating dimension permuted lattices as the same lattice*

Description

These data sets give the generator matrices of standard interleaved lattices, treating dimension permuted lattices as the same lattice. Data sets GMs2, GMs3, GMs4, GMs5, GMs6, GMs7, and GMs8 give the matrices in 2, 3, 4, 5, 6, 7, and 8 dimensions, respectively.

Usage

```
data(GMs2);
data(GMs3);
data(GMs4);
data(GMs5);
data(GMs6);
data(GMs7);
data(GMs8);
```

Format

Matrices containing generator matrices.

References

He, Xu (2017). "Interleaved lattice-based minimax distance designs", *Biometrika*, 104(3): 713-725.

InterleavedFillSepD *Interleaved lattice-based fill and separation distance designs*

Description

Generates an interleaved lattice-based design with low fill and high separation distance properties.

Usage

```
InterleavedFillSepD(p,n,w=rep(1,p),pfrom=p,a=1/2,nmin=floor(n*.8),nmax=ceiling(n*1.2),
coefF=-4,coefS=1,msC=0,NL=10,NP=100,NJ=10,NS=100);
```

Arguments

p	Number of dimensions.
n	Targeted number of points, must be an integer greater than one.
w	Optional, weights of the dimensions.
pfrom	Optional, number of dimensions designs are generated and supplemented from, no more than p and no more than 8.
a	Optional, translation parameter with a=0 for uniform design and a=1 for pushing the points to the boundary.
nmin	Optional, minimal acceptable number of points, no less than n.
nmax	Optional, maximal acceptable number of points, no greater than n.
coefF	Optional, coefficient of r_F in the criterion.
coefS	Optional, coefficient of r_S in the criterion.
msC	Optional, maximal allowed sum of projuct weights for pairs of binary aliased dimensions.

NL	Optional, maximum number of lattices to try.
NP	Optional, maximum number of dimension permutations to try.
NJ	Optional, maximum number of discretization choices for each lattice and s vector combination.
NS	Optional, maximum number of choices to supplement from.

Details

This function generates an interleaved lattice-based design with low fill and high separation distance properties in p dimensions and around n points, following the algorithm provided in the paper "Efficient Kriging using interleaved lattice-based designs with low fill and high separation distance properties".

Value

The value returned from the function is a matrix containing the generated design. Remark that no qualified design might be found if (a) both nmax and nmin are to close to n, (b) both n and msC are small, or (c) both pfrom and msC are small while p is much bigger than pfrom.

References

He, Xu (2024). "Efficient Kriging using interleaved lattice-based designs with low fill and high separation distance properties", *SIAM/ASA Journal on Uncertainty Quantification*, 12(4): 1113-1134.

Examples

```
InterleavedFillSepD(p=2,n=20);
```

`InterleavedMaximinD` *Interleaved lattice-based maximin distance designs*

Description

Generates an interleaved lattice-based maximin distance design.

Usage

```
InterleavedMaximinD(p,n,weight=rep(1,p));
InterleavedMaximinDAlg1(p,n,weight=rep(1,p));
InterleavedMaximinDAlg2(p,n,weight=rep(1,p));
InterleavedMaximinDAlg3(p,n,weight=rep(1,p));
```

Arguments

p	Number of dimensions, must be an integer greater than one.
n	Targeted number of points, must be an integer greater than one.
weight	Optional, the weights used in the distance measure, higher for more important variable.

Details

This function generates an interleaved lattice-based maximin distance design in p dimensions and at least n points, following the algorithms provided in the paper "Interleaved lattice-based maximin distance designs". Function InterleavedMaximinD uses the recommended algorithm provided in the paper. Functions InterleavedMaximinDAlg1, InterleavedMaximinDAlg2, and InterleavedMaximinDAlg3 use Algorithm 1, 2, and 3, respectively. For InterleavedMaximinDAlg1, p must be no greater than 5. For InterleavedMaximinDAlg3, p must be greater than 8.

Value

The value returned from the function is a list containing the following components:

`Design` The generated design.

`SeparationDistance` The separation distance of the generated design.

`m` The actual number of points of the generated design.

`DesignTransformed` The generated design that is transformed to the rectangular design space given the weights.

`weight` The weight used in the distance measure, higher for more important variable.

`s_vector` The numbers of distinct levels of the generated design.

`L01` The base design.

References

He, Xu (2019). "Interleaved lattice-based maximin distance designs", *Biometrika*, 106(2): 453-464.

Examples

```
InterleavedMaximinD(p=3,n=10,weight=rep(1,3));
InterleavedMaximinDAlg1(p=3,n=10);
InterleavedMaximinDAlg2(p=6,n=10);
InterleavedMaximinDAlg3(p=9,n=257);
```

`InterleavedMinimaxD` *Interleaved lattice-based minimax distance designs*

Description

Generates an interleaved lattice-based minimax distance design.

Usage

```
InterleavedMinimaxD(p,n,maxdissimilarity=2*p);
```

Arguments

p	Number of dimensions, must be an integer between 2 and 8.
n	Targeted number of points, must be an integer greater than one.
maxdissimilarity	Optional, the maximum dissimilarity allowed for the number of levels.

Details

These functions generate an interleaved lattice-based minimax distance design in p dimensions and at most n points, following the algorithm provided in the paper "Interleaved lattice-based minimax distance designs".

Value

The value returned from the function is a list containing the following components:

Design	The generated design.
TargetFillDistance	The target fill distance, an estimate of the fill distance.
ActualSize	The actual number of points of the generated design.
s_vector	The numbers of distinct levels of the generated design.
L01	The base design.

References

He, Xu (2017). "Interleaved lattice-based minimax distance designs", *Biometrika*, 104(3): 713-725.

Examples

```
InterleavedMinimaxD(p=2,n=20);
```

LRS — *Vertexes of a polytope giving halfspace definition*

Description

Computes the radius, widths, and vertexes of a polytope giving halfspace definition. The program is a R shell of LRS (v.5.1a with lrsmp.h), a reverse search vertex enumeration program/CH package in C which is developed by David Avis. Consider the problem of Ax<=b, where A is an n*p matrix, x is a p-vector, and b is an n-vector. Please make sure that the solution of x is nonempty and bounded. Then the nonequalities give the halfspace definition of a polytope. Also make sure that A and b are rational numbers.

Usage

```
LRS(numerator,denominator);
```

Arguments

`numerator`	The numerators of cbind(b,A), an n*(p+1) matrix of integer numbers.
`denominator`	The denominators of cbind(b,A), an n*(p+1) matrix of integer numbers.

Details

This function computes the radius, widths, and vertexes of a polytope giving halfspace definition. It is used in constructing interleaved lattice-based minimax distance designs. Currently only tested when the maximum values of numerators and denominators are below 2^20. If the nonequalities are not defined by rational numbers, round-up to small rational numbers is needed before calling the function. The computation is slow for large p but very fast for slow p. Avoid redundant nonequalities may accelerate the calculation.

Value

The value returned from the function is a list containing the following components:

`Radius`	The maximum L2 distance of vertexes to the origin.
`MaxValue`	The maximum k-dimensional value of the vertexes, for k from 1 to p.
`Vertexes`	The vertexes of the polytope.

References

He, Xu (2017). "Interleaved lattice-based minimax distance designs", *Biometrika*, 104(3): 713-725.

See Also

`InterleavedMinimaxD`.

Examples

```
num = matrix(0,5,3)
den = matrix(1,5,3)
num[1,2] = -1;  den[1,2] = 2;
num[1,1] = 1;   den[1,1] = 8;
num[2,3] = -1;
num[2,1] = 1;   den[2,1] = 2;
num[3,2] = -1;  den[3,2] = 4;
num[3,3] = -1;  den[3,3] = 2;
num[3,1] = 5;   den[3,1] = 32;
num[4,2] = 1;
num[4,1] = 0;
num[5,3] = 1;
num[5,1] = 0;
LRS(num,den)
```

`ProjSepD` *Projective separation distance of a design*

Description

Computes the projective separation distance of a design.

Usage

```
ProjSepD(design);
```

Arguments

`design`	The experimental design, must be a matrix whose rows indicate experimental runs.

Details

This function computes the squared projective separation distance of a design.

Value

The value returned from the function gives the squared one-dimensional, two-dimensional, ..., (p-1)-dimensional projective separation distances, and the unprojected separation distance, where p is the number of dimensions of the design.

References

He, Xu (2021). "Lattice-based designs possessing quasi-optimal separation distance on all projections", *Biometrika*, 108(2): 443-454.

Examples

```
design = rbind(1:3,c(41,1.2,1.3),c(5.4,5.48,5.7),c(4.3,2.3,2));
ProjSepD(design);
```

`RSPD` *Rotated sphere packing designs*

Description

Generates a rotated sphere packing design.

Usage

```
RSPD(p=2,n,rotation="magic",w=100)
```

Arguments

p	Number of dimensions, must be an integer greater than one.
n	Number of points, must be a positive integer.
rotation	Optional, whether to use the magic rotation matrix (for p=2, recommended) or random rotation matrices.
w	Number of rotation matrices to try, fixed to 1 when p=2 and rotation="magic".

Details

This function generates a rotated sphere packing design.

Value

The value returned from the function is a list containing the following components:

Design	The generated design.
generator	The generator matrix.
rotation	The rotation matrix.
delta	The value of parameter delta.
Theta	The value of parameter Theta.
l	The value of parameter l.
FillDistance	The fill distance of the design for the nonboundary region.

References

He, Xu (2017). "Rotated sphere packing designs", *Journal of the American Statistical Association*, 112(520): 1612-1622.

Examples

```
RSPD(p=2,n=50,rotation="magic",w=100)
```

SlicedRSPD *Sliced rotated sphere packing designs by partitioning a design*

Description

Generates a sliced rotated sphere packing design by partitioning one rotated sphere packing design.

Usage

```
SlicedRSPD(p=2,n,rotation="magic",w=100)
```

Arguments

p	Number of dimensions, must be an integer greater than one.
n	Number of points, must be a positive integer.
rotation	Optional, whether to use magic rotation matrices (for p=2, recommended) or random rotation matrices.
w	Number of rotation matrices to try.

Details

This function generates a rotated sphere packing design and the slice indexes of points.

Value

The value returned from the function is a list containing the following components:

Design	The generated design.
slices	The slice indexes of design points.
generator	The generator matrix.
rotation	The rotation matrix.
delta	The value of parameter delta.
Theta	The value of parameter Theta.
l	The value of parameter l.
FillDistance	The fill distance of the design for the nonboundary region.

References

He, Xu (2019). "Sliced rotated sphere packing designs", *Technometrics*, 61(1): 66-76.

Examples

```
SlicedRSPD(p=2,n=50,rotation="magic",w=100)
```

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