

Package: OSFD (via r-universe)

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Type Package

Title Output Space-Filling Design

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Description A method to generate a design in the input space that sequentially fills the output space of a black-box function. The output space-filling design will be helpful in inverse design or feature-based modeling problem. Please see Wang et al.(2023) <[DOI:10.48550/arXiv.2305.07202](https://doi.org/10.48550/arXiv.2305.07202)> for details. This work is supported by U.S. National Foundation grant CMMI-1921646.

License GPL (>= 2)

Depends Rcpp (>= 1.0.8), lhs, twinning, dplyr

LinkingTo Rcpp, RcppArmadillo, twinning

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OSFD-package

*A sequential algorithm to generate designs that fill the output space***Description**

A sequential method to generate a design that produces points filling the output space. The underlying mapping f from input space to output space is assumed to be a black-box function that can be evaluated in the forward direction. Please see Wang et al. (2023) for details.

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References

Wang, Shangkun, Adam P. Generale, Surya R. Kalidindi, and V. Roshan Joseph. "Sequential Designs for Filling Output Spaces." *Technometrics*, to appear (2023).

ball_unif

*(Quasi) uniform points in a p-dimensional ball***Description**

ball_unif generate random or quasi-random uniform points in a p-dimensional ball.

Usage

```
ball_unif(cen, rad, n, rand = TRUE)
```

Arguments

cen	a vector specifying the center of the ball.
rad	radius of the ball.
n	number of points.
rand	whether to generate random or quasi random points. Default value is TRUE.

Details

ball_unif generate random uniform points or quasi uniform points by twinning algorithm in a p-dimensional ball.

Value

a matrix of the generated points.

References

Vakayil, Akhil, and V. Roshan Joseph. "Data twinning." *Statistical Analysis and Data Mining: The ASA Data Science Journal* 15.5 (2022): 598-610.

Wang, Shangkun, Adam P. Generale, Surya R. Kalidindi, and V. Roshan Joseph. "Sequential Designs for Filling Output Spaces." *Technometrics*, to appear (2023).

Examples

```
x = ball_unif(c(0,0),1,10,rand=FALSE)
plot(x,type='p')
```

mMdist

Minimax distance

Description

mMdist computes the minimax distance of a design in a specified region. A large uniform sample from the specified region is needed to compute the minimax distance.

Usage

```
mMdist(X, X_space)
```

Arguments

X a matrix specifying the design.

X_space a large sample of uniform points in the space of interest.

Details

mMdist approximates the minimax distance of a set of points X by the large sample X_space in the space of interest.

Value

the minimax distance.

References

Johnson, Mark E., Leslie M. Moore, and Donald Ylvisaker. "Minimax and maximin distance designs." *Journal of statistical planning and inference* 26.2 (1990): 131-148.

Wang, Shangkun, Adam P. Generale, Surya R. Kalidindi, and V. Roshan Joseph. "Sequential Designs for Filling Output Spaces." *Technometrics*, to appear (2023).

Examples

```
# the minimax distance of a random Latin hypercube design
D = randomLHS(5,2)
mMdist(D,replicate(2,runif(1e5)))
```

OSFD

Output space-filling design

Description

This function is for producing designs that fill the output space.

Usage

```
OSFD(
  D = NULL,
  f,
  p,
  q,
  n_ini = NA,
  n,
  scale = TRUE,
  method = "EI",
  CAND = NULL,
  rand_out = FALSE,
  rand_in = FALSE
)
```

Arguments

D	a matrix of the initial design. If not specified, a random Latin hypercube design of size <code>n_ini</code> and dimension <code>p</code> will be generated as initial design.
f	black-box function.
p	input dimension.
q	output dimension.
n_ini	the size of initial design. This initial size must be specified if D is not provided.
n	the size of the final design.
scale	whether to scale the output points to 0 to 1 for each dimension.
method	two choices: 'EI' or 'Greedy'; the default is 'EI'.
CAND	the candidate points in the input space. If Null, it will be automatically generated.

rand_out	whether to use random uniform points or quasi random points by twinning algorithm for generating points in spheres for output space approximation. The default value is FALSE.
rand_in	whether to use random uniform points or quasi random points by twinning algorithm for generating points in spheres for input space candidate sets. The default value is FALSE.

Details

OSFD produces a design that fills the output space using the sequential algorithm by Wang et al. (2023).

Value

D	the final design points in the input space
Y	the output points

References

Wang, Shangkun, Adam P. Generale, Surya R. Kalidindi, and V. Roshan Joseph. "Sequential Designs for Filling Output Spaces." *Technometrics*, to appear (2023).

Examples

```
# test function: inverse-radius function (Wang et.al 2023)
inverse_r = function(x){
  epsilon = 0.1
  y1=1/(x[1]^2+x[2]^2+epsilon^2)^(1/2)
  if (x[2]==0){
    y2 = 0
  }else if (x[1]==0) {
    y2 = pi/2}else{
    y2 = atan(x[2]/x[1])
  }
  return (c(y1=y1,y2=y2))
}

set.seed(2022)
p = 2
q = 2
f = inverse_r
n_ini = 10
n = 50
osfd = OSFD(f=f,p=p,q=q,n_ini=n_ini,n=n)
D = osfd$D
Y = osfd$Y
```

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