

Package ‘maximin’

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Title Space-Filling Design under Maximin Distance

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Suggests lhs

Description Constructs a space-filling design under the criterion of maximum-minimum distance. Both discrete and continuous searches are provided.

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lola_kn	<i>spatial locations of 1535 weather stations</i>
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Description

The dataset contains spatial locations of 1535 weather stations for measuring solar irradiance across the continental United States.

Usage

```
data(lola_kn)
```

Format

A data frame containing 1535 observations and 2 variables

Source

<https://onlinelibrary.wiley.com/doi/abs/10.1002/sam.11414>

References

F. Sun, R.B. Gramacy, B. Haaland, S.Y. Lu, and Y. Hwang (2019) *Synthesizing Simulation and Field Data of Solar Irradiance*, *Statistical Analysis and Data Mining*, 12(4), 311-324; preprint on arXiv:1806.05131.

maximin

Space-filling design under the criterion of maximin distance

Description

Generates a space-filling design under the criterion of maximum-minimum distance; both discrete and continuous searches are provided.

Usage

```
maximin.cand(n, Xcand, Tmax, Xorig=NULL, init=NULL, verb=FALSE, tempfile=NULL)
maximin(n, p, T, Xorig=NULL, Xinit=NULL, verb=FALSE, plot=FALSE, boundary=FALSE)
```

Arguments

n	the number of space-filling locations
Xcand	the candidate set, from which each space-filling location is selected
Tmax	the number of iterations; $T_{\max} \leq \text{nrow}(X_{\text{cand}})$; to be safe, set $T_{\max} = \text{nrow}(X_{\text{cand}})$.
Xorig	the existing design; $\text{ncol}(X_{\text{orig}}) = \text{ncol}(X_{\text{cand}})$
init	the initial indices of X; it can be randomly selected from Xcand or introduced from a previous experiment.
verb	progress indicator — every tenth iteration is printed out; by default verb = FALSE.
tempfile	the name of a temporary file given the progress is saved with each iteration; by default tempfile = NULL
p	the dimensionality of input space
T	the number of iterations; $T > n$; setting $T = 10 * n$ is a good starting point.

Xinit	the (initial) design introduced from a previous experiment
plot	if plot = TRUE, then the search space and the "start location → new location" with each iteration is plotted; if $p > 2$, then TWO input coordinates are RANDOMLY chosen for plotting; it is worth noticing that the search space only VISUALLY makes sense when $p = 2$.
boundary	if boundary = TRUE, then for each iteration, the "to-be-swapped-in" location will be away from the boundary in addition to being away from other X locations and Xorig; how far is it? $\min(d, 4 * d.bound)$, where d is the Euclidean distance between the "to-be-swapped-in" location and other X locations as well as Xorig, while d.bound is the minimum Euclidean distance between the "to-be-swapped-in" location and the boundaries.

Details

Constructing a space-filling design under the criterion of maximum-minimum distance is quite useful in computer experiments and related fields. Previously, researchers would construct such a design in a random accept-reject way, i.e., randomly propose a location within the study region to replace a randomly selected row from the initial design. If such a proposal increases the minimum pairwise Euclidean distance, then accept the replacement; otherwise keep the original design location. By repeatedly proposing (and accept-rejecting) in this way one is able to construct an (approximately) space-filling design. However the algorithm is inefficient computationally. The reason is that the proposals are not optimized in any way.

In this package, we provide an alternative to build up a well-defined space-filling design more efficiently. There are two versions, one is with discrete search, while the other is with continuous search. For the former, each iteration proposes to swap out a row from the initial design with the minimum distance, and swap in one location from a candidate set to increase the minimum distance. For the latter, the core idea is the same, but instead of working with a candidate set, `optim` is used to maximize the distance between the "to-be-swapped-in" location and other design locations as well as to any existing design, Xorig. Several heuristics are deployed for situations where the search becomes stuck in a local mode. One involves moving to a location with non-minimum distance, and the other is to jump to a location which has the maximum minimum distance.

For a visualization of applying `maximin.cand` in a real-life problem on solar irradiance, see Sun et al. (2019).

`maximin.cand` returns the indices of Xcand, which makes the final space-filling design, and the minimum pairwise Euclidean distance with each iteration

`maximin` returns the combined existing design and the space-filling design, together with the minimum pairwise Euclidean distance with each iteration

Value

`maximin.cand` returns

inds	the indices of Xcand, which makes the final space-filling design
mis	the minimum distance with each iteration; $\text{length}(\text{mis}) = T_{\max} + 1$

`maximin` returns

Xf	$\text{dim}(Xf) = (\text{nrow}(Xorig) + n) * p$
mi	the minimum distance with each iteration; $\text{length}(mi) = T + 1$

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References

F. Sun, R.B. Gramacy, B. Haaland, S.Y. Lu, and Y. Hwang (2019) *Synthesizing Simulation and Field Data of Solar Irradiance*, *Statistical Analysis and Data Mining*, 12(4), 311-324; preprint on arXiv:1806.05131.

M.H.Y. Tan (2013) *Minimax Designs for Finite Design Regions*, *Technometrics*, 55(3), 346-358.

M.E. Johnson, L.M. Moore, and D. Yivisaker (1990) *Minimax and Maximin Distance Designs*, *Journal of Statistical Planning and Inference*, 26(2), 131-148.

Examples

```
## Not run:
## maximin.cand
# generate the design
library("lhs")
n <- 100
p <- 2
Xorig <- randomLHS(10, p)
x1 <- seq(0, 1, length.out=n)
Xcand <- expand.grid(replicate(p, x1, simplify=FALSE))
names(Xcand) <- paste0("x", 1:2)
T <- nrow(Xcand)
Xsparse <- maximin.cand(n=n, Xcand=Xcand, Tmax=T, Xorig=Xorig,
                       init=NULL, verb=FALSE, tempfile=NULL)

maxmd <- as.numeric(format(round(max(na.omit(Xsparse$mis)), 5), nsmall=5))

# visualization
par(mfrow=c(1, 2))
X <- Xcand[Xsparse$inds,]
plot(X$x1, X$x2, xlab=expression(x[1]), ylab=expression(x[2]),
      xlim=c(0, 1), ylim=c(0, 1),
      main=paste0("n=", n, "_p=", p, "_maximin=", maxmd))
points(Xorig, col=2, pch=20)
abline(h=c(0, 1), v=c(0, 1), lty=2, col=2)
if(!is.null(Xorig))
{
  legend("topright", "Xorig", xpd=TRUE, horiz=TRUE,
        inset=c(-0.03, -0.05), pch=20, col=2, bty="n")
}
plot(log(na.omit(Xsparse$mis)), type="b",
      xlab="iteration", ylab="log(minimum distance)",
      main="progress on minimum distance")
abline(v=n, lty=2)
mtext(paste0("design size=", n), at=n, cex=0.6)

## End(Not run)
```

```
## maximin
# generate the design
library("lhs")
n <- 10
p <- 2
T <- 10*n
Xorig <- randomLHS(10, p)
Xsparse <- maximin(n=n, p=p, T=T, Xorig=Xorig, Xinit=NULL,
  verb=FALSE, plot=FALSE, boundary=FALSE)
maxmd <- as.numeric(format(round(Xsparse$mi[T+1], 5), nsmall=5))

# visualization
par(mfrow=c(1,2))
plot(Xsparse$Xf[,1], Xsparse$Xf[,2], xlab=expression(x[1]), ylab=expression(x[2]),
  xlim=c(0, 1), ylim=c(0, 1),
  main=paste0("n=", n, " p=", p, " T=", T, " maximin=", maxmd))
points(Xorig, col=2, pch=20)
abline(h=c(0,1), v=c(0,1), lty=2, col=2)
if(!is.null(Xorig)) legend("topright", "Xorig", xpd=TRUE, horiz=TRUE,
  inset=c(-0.03, -0.05), pch=20, col=2, bty="n")
plot(log(Xsparse$mi), type="b", xlab="iteration", ylab="log(minimum distance)",
  main="progress on minimum distance")
abline(v=n, lty=2)
mtext(paste0("design size=", n), at=n, cex=0.6)
abline(v=T, lty=2)
mtext(paste0("max.md=", maxmd), at=T, cex=0.6)
```

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