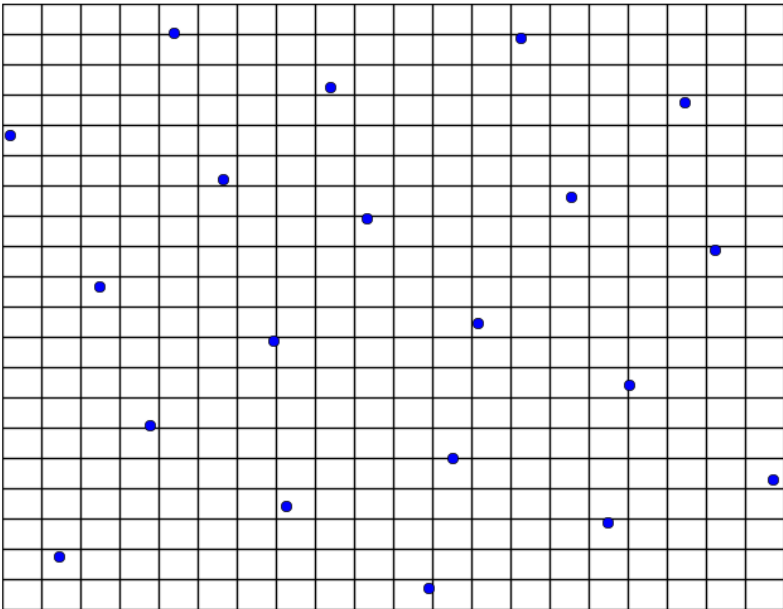


# Documentation of the OTLHS module

Documentation built from package otlhs-1.3

November 18, 2016



*Abstract*

The purpose of this document is to present the OTLHS module.

This document is organized according to the OpenTURNS documentation:

- *Architecture Guide* gives UML diagrams of all implemented classes,
- *Reference Guide* gives some theoretical basis,
- *Use cases Guide* details scripts in Python (the Textual Interface language of OpenTURNS) and helps to learn as quickly as possible the manipulation of the otlhs module,
- *User Manual* details the otlhs objects and gives the list of their methods,
- *Validation Guide* which provides use cases to validate the otlhs module.

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This document makes up the general specification design for the architecture of the OTLHS module. Several classes implement the *pimpl* idiom (pointer to implementation) to hide implementation details.

```

classDiagram
    class SpaceFilling {
        +p_implementation_ SpaceFillingImplementation
        +SpaceFilling()
        +evaluate(in sample): float const
        +perturbLHS(in sample,in crit,in row1,in row2,in column): float const
    }
    class SpaceFillingImplementation {
        +SpaceFillingImplementation()
        +evaluate(in sample): float const
        +perturbLHS(in sample,in crit,in row1,in row2,in column): float const
    }
    class SpaceFillingC2 {
        +SpaceFillingC2()
        +evaluate(in sample): float const
        +perturbLHS(in sample,in crit,in row1,in row2,in column): float const
    }
    class SpaceFillingMinDist {
        +SpaceFillingMinDist()
        +evaluate(in sample): float const
    }
    class SpaceFillingPhiP {
        -P_
        +SpaceFillingPhiP(p:int=50)
        +evaluate(in sample): float const
        +perturbLHS(in sample,in crit,in row1,in row2,in column): float const
    }
    SpaceFilling --|> SpaceFillingImplementation
    SpaceFillingImplementation <|-- SpaceFillingC2
    SpaceFillingImplementation <|-- SpaceFillingMinDist
    SpaceFillingImplementation <|-- SpaceFillingPhiP

```

These classes implement different space filling criteria, which are consumed by `OptimalLHS` algorithms.

```

classDiagram
    class OptimalLHS {
        +OptimalLHS(in lhsDesign)
        +OptimalLHS(in lhsDesign, in spaceFilling)
        +getImplementation()
        +getLHS(): LHSDesign const
        +getSpaceFilling(): SpaceFilling const
        +generate(): LHSResult const
    }
    class OptimalLHSImplementation {
        -lhsDesign_: LHSDesign
        -spaceFilling_: SpaceFilling
        +OptimalLHSImplementation(in lhsDesign)
        +OptimalLHSImplementation(in lhsDesign, in spaceFilling)
        +getLHS(): LHSDesign const
        +getSpaceFilling(): SpaceFilling const
        +generate(): LHSResult const
    }
    class MonteCarloLHS {
        -N_: int
        +MonteCarloLHS(in lhsDesign, in N)
        +MonteCarloLHS(in lhsDesign, in N, in spaceFilling)
        +generate(): LHSResult const
    }
    class SimulatedAnnealingLHS {
        -profile_: TemperatureProfile
        -initialDesign_: NumericalSample
        -bounds_: Interval
        +SimulatedAnnealingLHS(in lhsDesign, in profile, in spaceFilling)
        +SimulatedAnnealingLHS(in initialDesign, in bounds, in profile, in spaceFilling)
        +generate(): LHSResult const
        +generate(nRestart:int): LHSResult const
    }
    class TemperatureProfileImplementation {
        +operator()(in i:int): float const
    }
    class TemperatureProfile {
        -p_implementation_: TemperatureProfileImplementation
        +operator()(in i:int): float const
    }
    class LinearProfile {
        -T0_: float = 10
        -iMax_: int = 2000
        +LinearProfile(in T0, in iMax)
        +operator()(in i:int): float const
    }
    class GeometricProfile {
        -T0_: float = 10
        -c_: float = 0.95
        -iMax_: int = 2000
        +GeometricProfile(T0:float=10, c:float=0.95, iMax:int=2000)
        +operator()(in i:int): float const
    }
    OptimalLHSImplementation <|-- MonteCarloLHS
    OptimalLHSImplementation <|-- SimulatedAnnealingLHS
    OptimalLHSImplementation o--> OptimalLHS
    TemperatureProfileImplementation o--> TemperatureProfile
    TemperatureProfile <|-- LinearProfile
    TemperatureProfile <|-- GeometricProfile

```

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This is the main class hierarchy. The `OptimalLHS` class is an abstract class, inherited by `MonteCarloLHS` and `SimulatedAnnealingLHS`. They implement the `generate` method, which returns an `LHSResult` instance.

### 1.3 LHSResult

LHSResult
<pre> - bounds_: Interval - spaceFilling_: SpaceFilling - restart_: int - optimalCriterion_: float - optimalIndex_: int - collDesigns_: Collection&lt;NumericalSample&gt; - collAlgoHistory_: Collection&lt;NumericalSample&gt; - criteria_: NumericalSample + LHSResult() + LHSResult(in bounds: Interval, in spaceFilling: SpaceFilling) + LHSResult(in bounds: Interval, in spaceFilling: SpaceFilling,             in restart: int) + add(in design: NumericalSample, in criterion: float,       in C2: float, in PhiP: float, in MinDist: float,       in algoHistory: NumericalSample) + getBounds(): Interval const + getNumberOfRestarts(): int const + getOptimalDesign(): NumericalSample const + getOptimalDesign(in restart: int): NumericalSample const + getOptimalValue(): float const + getOptimalValue(in restart: int): float const + getAlgoHistory(): NumericalSample const + getAlgoHistory(in restart: int): NumericalSample const + getC2(): float const + getC2(in restart: int): float const + getPhiP(): float const + getPhiP(in restart: int): float const + getMinDist(): float const + getMinDist(in restart: int): float const + drawHistoryCriterion(in title: String): Graph const + drawHistoryCriterion(in restart: int, in title: String): Graph const + drawHistoryProbability(in title: String): Graph const + drawHistoryProbability(in restart: int, in title: String): Graph const + drawHistoryTemperature(in title: String): Graph const + drawHistoryTemperature(in restart: int, in title: String): Graph const </pre>

LHSDesign
<pre> - bounds_: Interval - size_: int - centeredDesign_: bool = false + LHSDesign(in bounds: Interval, in size: int,             in centeredDesign: bool = false) + getBounds(): Interval const + getSize(): int const + isCenteredDesign(): bool const + generate(): NumericalSample const </pre>

Figure 3: LHSDesign and LHSResult classes

As OpenTURNS already provides an LHS class, we had to rename it into `LHSDesign`. Its constructor takes as arguments variable bounds, the size of the generated sample, and an optional boolean parameter to tell whether randomized (default) or centered LHS have to be generated.

The `LHSResult` class is returned by `OptimalLHS.generate()` and contains algorithm results. The `add` method is called by `OptimalLHS` (once if there is no restart, and one plus one by restart otherwise), and informations can then be extracted by accessors. If no restart argument is specified, informations about global optimum are retrieved. If a restart number is provided, informations about this specific run are retrieved.

## 2 Reference Guide

The OTLHS library provide algorithms to compute optimized Latin Hypercube Sample designs.

### 2.1 Optimized LHS design

#### Mathematical description

##### Goal

Let  $\underline{x}=(x_1, \dots, x_d)$  be a random vector of input parameters. Latin Hypercube Sample (LHS) is a way to distribute  $N$  sample points: each parameter range is divided into  $N$  equal intervals, and sample points are chosen such that any hyperplane in that dimension contains one and only one sample point.

The goal of this module is to improve standard LHS techniques by minimizing a space filling criterion.

##### Principles

We may notice two types of LHS designs:

- Centered design is obtained by choosing for each point the center of the corresponding cell
- Randomized LHS is obtained by adding random perturbations inside each cell

Let us fix the following properties for the input vector  $\underline{x}$ :

- Its marginals are independent
- Its associated probabilistic measure is

$$\mathcal{L}_X(x_1, \dots, x_d) = \mathcal{U}(a_1, b_1) \otimes \mathcal{U}(a_2, b_2) \otimes \dots \otimes \mathcal{U}(a_d, b_d) \quad (1)$$

with  $\mathcal{U}$  the uniform distribution.

In practice, we look for a design in the space  $[0, 1]^d$  and we use an inverse iso-probabilistic transformation to get the result in the original domain.

Let  $\phi : [0, 1]^d \rightarrow \mathbb{R}^+$  be a space filling criterion, which is a measure of “accuracy” of an optimal LHS design. Most of these criteria focus on discrepancy, which measures how far a given distribution of points deviates from a perfectly uniform one.

Two space filling criteria are implemented:

- The centered  $L^2$ -discrepancy, called  $C_2$  and given by:

$$\begin{aligned} C_2(X_d^N)^2 = & \left(\frac{13}{12}\right)^d - \frac{2}{N} \sum_{i=1}^N \prod_{k=1}^d \left(1 + \frac{1}{2}|x_k^{(i)} - 0.5| - \frac{1}{2}|x_k^{(i)} - 0.5|^2\right) \\ & + \frac{1}{N^2} \sum_{i,j=1}^N \prod_{k=1}^d \left(1 + \frac{1}{2}|x_k^{(i)} - 0.5| + \frac{1}{2}|x_k^{(j)} - 0.5| - \frac{1}{2}|x_k^{(i)} - x_k^{(j)}|\right) \end{aligned} \quad (2)$$

This discrepancy is to be minimized to get an optimal design.

- The mindist criterion (minimal distance between two points in the design):

$$\phi(X) = \min ||x^{(i)} - x^{(j)}||_{L^2}, \forall i \neq j = 1, \dots, N \quad (3)$$

This criterion is to be maximized.

- In practice, the  $\phi_p$  criterion is used instead of mindist and writes:

$$\phi_p(X) = \left( \sum_{1 \leq i < j \leq N} ||x^{(i)} - x^{(j)}||_{L^2}^{-p} \right)^{\frac{1}{p}} \quad (4)$$

This is supposed to be more robust. When  $p$  tends to infinity, optimizing a design with  $\phi_p$  is equivalent to optimizing a design with mindist. This criterion is to be minimized to get an optimal design.

The objective is to a LHS design  $X_d^N$  that minimizes a space filling criterion  $\phi$  (or maximizes mindist). For that purpose, two techniques are implemented and presented hereafter.

### Monte Carlo

This problem can be approximated by a Monte Carlo algorithm: a fixed number of designs are generated, and the optimal one is kept. This algorithm is trivial, and described in Algorithm 1.

One of the major drawbacks of Monte Carlo sampling is the CPU time consumption, because the number of generated designs must be high.

### Simulated Annealing

An alternate solution is to use an adapted simulated annealing method, which we will now describe.

Starting from an LHS design, a new design is obtained by permuting one random coordinate of two randomly chosen elements; by construction, this design is also an LHS design. If the new design is better than the previous one, it is kept. If it is worse, it may anyway be kept with some probability, which depends on how these designs compare, but also on a temperature profile  $T$  which decreases over time. This means that jumping away from local extrema becomes less probable over time. This algorithm is detailed in Algorithm 2.

It is important to highlight here that this specific permutation has been chosen in this algorithm because it allows highly efficient computations of criterion during simulated annealing process. The naive criterion evaluation, as is done in Monte Carlo algorithm, has a complexity of  $\mathcal{O}(d \times N^2)$  for  $C_2$  and  $\phi_p$  criteria.

Let us first illustrate with the  $C_2$  criterion. We set  $z_{ik} = x_{ik} - 0.5$ , equation (2) rewrites:

$$C_2(X_d^N)^2 = \left( \frac{13}{12} \right)^d + \sum_{i=1}^N \sum_{j=1}^N c_{ij}$$

with:

$$c_{ij} = \begin{cases} \frac{1}{N^2} \prod_{k=1}^d \frac{1}{2} (2 + |z_{ik}| + |z_{jk}| - |z_{ik} - z_{jk}|) & \text{if } i \neq j \\ \frac{1}{N^2} \prod_{k=1}^d (1 + |z_{ik}|) - \frac{2}{N} \prod_{k=1}^d (1 + \frac{1}{2}|z_{ik}| - \frac{1}{2}z_{ik}^2) & \text{otherwise} \end{cases} \quad (5)$$

We set  $c'$  the elements of a new design  $X_d'^N$  obtained by permuting a coordinate of sample points  $i_1$  and  $i_2$ . We can see that

$$\begin{cases} c'_{ij} = c_{ij} \quad \forall i, j \text{ such that } 1 \leq i, j \leq N, i \notin \{i_1, i_2\}, j \notin \{i_1, i_2\} \\ c'_{i_1 i_2} = c_{i_1 i_2} \\ c_{ij} = c_{ji} \quad \forall 1 \leq i, j \leq N \end{cases} \quad (6)$$

and thus,  $C_2(X')$  becomes:

$$C_2(X_d'^N)^2 = C_2(X_d^N)^2 + c'_{i_1 i_1} + c'_{i_2 i_2} + 2 \sum_{\substack{1 \leq j \leq N \\ j \neq i_1, i_2}} (c'_{i_1 j} + c'_{i_2 j}) - c_{i_1 i_1} - c_{i_2 i_2} - 2 \sum_{\substack{1 \leq j \leq N \\ j \neq i_1, i_2}} (c_{i_1 j} + c_{i_2 j})$$

Updating  $C_2$  criterion can be performed by a  $\mathcal{O}(N)$  algorithm, which has a much better complexity than a naive computation.

The same trick can also be applied on  $\phi_p$  criterion, because we can write

$$\phi_p(X)^p = \sum_{1 \leq i < j \leq N} \|x^{(i)} - x^{(j)}\|_{L^2}^{-p} = \frac{1}{2} \sum_{i=1}^N \sum_{\substack{1 \leq j \leq N \\ j \neq i}} \|x^{(i)} - x^{(j)}\|_{L^2}^{-p} = \sum_{i=1}^N \sum_{j=1}^N f_{ij} \quad (7)$$

with

$$f_{ij} = \begin{cases} \frac{\|x^{(i)} - x^{(j)}\|_{L^2}^{-p}}{2}, & i \neq j \\ 0, & i = j \end{cases} \quad (8)$$

These  $f_{ij}$  coefficients satisfy the same conditions as in (6), so the same computations give:

$$\phi_p(X_d'^N)^p = \phi_p(X_d^N)^p + 2 \sum_{\substack{1 \leq j \leq N \\ j \neq i_1, i_2}} (f'_{i_1 j} + f'_{i_2 j}) - 2 \sum_{\substack{1 \leq j \leq N \\ j \neq i_1, i_2}} (f_{i_1 j} + f_{i_2 j})$$

**Remark** In practice, a marginal transformation is performed to map the initial multivariate distribution into  $[0, 1]^d$ . Optimization is performed in  $[0, 1]^d$  and the inverse transformation maps the design into the initial space.

### Other notations

## Link with OpenTURNS methodology

This method is part of the step C `Propagation of uncertainty` of the global methodology to evaluate a criterion for the output value defined in step A `Specifying the Criteria and the Case Study`. It requires the specification of the joined probability density function of the input variables. The PDF must have an independent copula.

### References and theoretical basics

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**input:** bounds: the bounds of uniform distributions

N: design size

isCentered: boolean (centered if true, random otherwise)

$\phi$ : space filling criterion

MC: number of simulations

**output:** LHS: an optimal design

phi: value of criterion

phi.opt j- 1e308;

**for**  $i \leftarrow 1$  **to** MC **do**

    lhs j- LHSGenerate(bounds,N,isCentered);

    phi j-  $\phi$  (lhs);

**if** phi < phi.opt **then**

        lhs.opt j- lhs;

        phi.optj-phi;

**end**

**end**

**Algorithm 1:** Monte Carlo optimization of LHS design

```

input: bounds: the bounds of uniform distributions
        N: design size
        isCentered: boolean (centered if true, random otherwise)
         $\phi$ : space filling criterion
        nrIter: number of iterations
        T: temperature profile
output: LHS: an optimized design
        phi: value of criterion

lhs.opt  $\leftarrow$  LHSGenerate(bounds, N, isCentered) ;
phi.opt  $\leftarrow \phi$  (lhs.opt);
i  $\leftarrow$  1;
while i  $\leq$  nrIter do
    point1, point2, dim  $\leftarrow$  RandomGenerate (3);
    LHSnew  $\leftarrow$  lhs.opt;
    swap(LHSnew[point1, dim] , lhs.opt[point2, dim]);
    phi  $\leftarrow \phi$  (LHSnew);
    p  $\leftarrow$  min( $\exp(-\frac{\phi - \phi_{\text{opt}}}{T(i)})$ , 1);
    if p == 1 then
        lhs.opt  $\leftarrow$  LHSnew;
        phi.opt  $\leftarrow$  phi;
    else
        dist  $\leftarrow$  Bernoulli(p);
        b  $\leftarrow$  dist.generate();
        if b == 1 then
            lhs.opt  $\leftarrow$  LHSnew;
            phi.opt  $\leftarrow$  phi;
        end
    i  $\leftarrow$  i + 1
end

```

**Algorithm 2:** LHS optimization using Simulated Annealing

## 3 Use Cases Guide

This section presents the main functionalities of the module *otlhs* in their context.

### 3.1 Latin Hypercube Sample

Class `LHSDesign` builds designs of a fixed size, type and bounds. Comparing to the `LHSExperiment` of the `OpenTURNS` library, when regenerating sample, the cells selection changes.

Python script for this use case:

```
import openturns as ot
import otlhs
# Generating a design of size N=100
N = 100
# Considering independent Uniform distributions of dimension 3
# Bounds are (-1,1), (0,2) and (0, 0.5)
bounds = ot.Interval([-1,0,0], [1,2,0.5])
# Random LHS
lhs_random = otlhs.LHSDesign(bounds, N)
randomLHS = lhs_random.generate()
# Centered LHS
lhs_centered = otlhs.LHSDesign(bounds, N, True)
centeredLHS = lhs_centered.generate()
print(centeredLHS)
```

### 3.2 Plot of LHS

Class `PlotDesign` helps to plot a LHS design and draw it in a PDF, PNG, EPS or FIG formats.

Python script for this use case:

```
import openturns as ot
import otlhs
# Generating a design of size N=10
N = 10
# Considering independent Uniform distributions of dimension 3
# Bounds are (-1,1), (0,2) and (0, 0.5)
bounds = ot.Interval([-1,0,0], [1,2,0.5])
# Centered LHS
lhs_centered = otlhs.LHSDesign(bounds, N, True)
centeredLHS = lhs_centered.generate()
# Draw the design + grids
drawable = otlhs.PlotDesign(centeredLHS, bounds, 10, 10)
# This is equivalent to:
# drawable = otlhs.PlotDesign(centeredLHS, bounds)
# Create ot graph
graph = ot.Graph()
```

```
# Add drawable
graph.add(drawable)
# Export into PDF file. Refer to Graph class
graph.draw("design", 640, 480, ot.GraphImplementation.PDF)
```

Notice that there is no `show` method for that class. An alternative is to use the `PyPlotDesign` class. This requires the `matplotlib` module.

Python script for this use case:

```
import openturns as ot
import otlhs
from otlhs.pyplotdesign import PyPlotDesign
import matplotlib.pyplot as plt
# Generating a design of size N=10
N = 10
# Considering independent Uniform distributions of dimension 3
# Bounds are (-1,1), (0,2) and (0, 0.5)
bounds = ot.Interval([-1,0,0], [1,2,0.5])
# Centered LHS
lhs_centered = otlhs.LHSDesign(bounds, N, True)
centeredLHS = lhs_centered.generate()
# Draw design and grid
plot = PyPlotDesign(centeredLHS, bounds, 10, 10)
# Show the graph
plt.show()
# Export the graph
plot.savefig("design.png")
```

### 3.3 LHS and space filling

`SpaceFilling` is an abstract class to compute the criterion value of a given design. `SpaceFillingC2` and `SpaceFillingPhiP` are implemented here. Note that these classes support only the computation of the criterion, and not its optimization.

Python script for this use case:

```
import openturns as ot
import otlhs
# Generating a design of size N=100
N = 100
# Considering independent Uniform distributions of dimension 3
# Bounds are (-1,1), (0,2) and (0, 0.5)
bounds = ot.Interval([-1,0,0], [1,2,0.5])
# Random LHS
lhs = otlhs.LHSDesign(bounds, N)
design = lhs.generate()
# C2
c2 = otlhs.SpaceFillingC2().evaluate(design)
```

```
# PhiP with default p
php = otlhs.SpaceFillingPhiP().evaluate(design)
# mindist
mindist = otlhs.SpaceFillingMinDist().evaluate(design)
# For p->infinity
php_inf = otlhs.SpaceFillingPhiP(100).evaluate(design)
```

### 3.4 Optimized LHS using Monte Carlo

Given a space filling criterion, it is possible to generate many designs and to return the “best” one. This method is trivial to implement but the number of generations may become impractical.

The class `MonteCarloLHS` gives the optimal design using the `LHSDesign` as factory and number of simulations. Default space filling criterion is `SpaceFillingMinDist`.

Python script for this use case:

```
import openturns as ot
import otlhs

# Considering independent Uniform(0,1) distributions of dimension 3
bounds = ot.Interval(3)
designSize = 100
# Random LHS MonteCarlo
lhs = otlhs.LHSDesign(bounds, designSize)
# MonteCarlo, with nSimu=50000 and default space-filling
nSimu = 50000
algo = otlhs.MonteCarloLHS(lhs, nSimu)
result = algo.generate()
# optimal design
design = result.getOptimalDesign()
```

Results may be completed by the fixed criterion value history for all samples, the final criteria values.

Python script for this use case:

```
import openturns as ot
import otlhs
# Generating a design of size N=100
N = 100
# Considering independent Uniform distributions of dimension 3
# Bounds are (-1,1), (0,2) and (0, 0.5)
bounds = ot.Interval([-1,0,0], [1,2,0.5])
# Random LHS MonteCarlo
lhs = otlhs.LHSDesign(bounds, N)
# Fixing C2 crit
space_filling = otlhs.SpaceFillingC2()
# Defining MonteCarlo, with nSimu=50000
nSimu = 50000
algo = otlhs.MonteCarloLHS(lhs, nSimu, space_filling)
result = algo.generate()
```

```
# optimal design
design = result.getOptimalDesign()
history = result.getAlgoHistory()
# Final criteria values
c2 = result.getC2()
phiP = result.getPhiP()
mindist = result.getMinDist()
```

### 3.5 Optimized LHS using simulated annealing

As with Monte Carlo, user decides of a fixed number of iterations, but this time this number is part of the temperature profile. Two profiles are currently provided:

- Linear profile:  $T(i) = T(0) \left(1 - \frac{i}{nrIter}\right)$
- Geometric profile:  $T(i) = T(0)c^i$ ,  $0 < c < 1$ .

Starting from an LHS design, a new design is built by permuting a random coordinate of two randomly chosen sample points; this new design is also an LHS. but not necessary a “more efficient” design. A comparison of criteria of the two designs is done, and the new LHS is accepted with probability

$$\min \left( \exp \left[ -\frac{\phi(\text{LHS}_{\text{new}}) - \phi(\text{LHS})}{T(i)} \right], 1 \right)$$

The simulated annealing algorithm is detailed in Algorithm 2.

Minimal python script for the use case:

```
import openturns as ot
import otlhs
designSize = 100
# Considering independent Uniform(0,1) distributions of dimension 3
bounds = ot.Interval(3)
# Random LHS
lhs = otlhs.LHSDesign(bounds, N)
algo = otlhs.SimulatedAnnealingLHS(lhs)
result = algo.generate()
# Retrieve optimal design
design = result.getOptimalDesign()
```

One could also fix the criterion, the temperature profile and gets more results.

Python script for this use case:

```
import openturns as ot
import otlhs
# Generating a design of size N=100
N = 100
# Considering independent Uniform distributions of dimension 3
# Bounds are (-1,1), (0,2) and (0, 0.5)
bounds = ot.Interval([-1,0,0], [1,2,0.5])
# Random LHS
```

```

lhs = otlhs.LHSDesign(bounds, N)
# Fixing C2 crit
space_filling = otlhs.SpaceFillingC2()
# Defining a temperature profile
# A geometric profile seems accurate with default parameters
# e.g. T0=10, c=0.95, iMax=2000
temperatureProfile = otlhs.GeometricProfile()
algo = otlhs.SimulatedAnnealingLHS(lhs, temperatureProfile, space_filling)
result = algo.generate()
# Retrieve optimal design
design = result.getOptimalDesign()
# Criteria for the optimal design
crit_c2 = result.getC2()
crit_phiP = result.getPhiP()
crit_mindist = result.getMinDist()
# History of the criterion used for optimization
history = result.getAlgoHistory()
criterion_hist = history[:, 0]
# Additional results
temperature_hist = history[:, 1]
probability_hist = history[:, 2]

```

It is also possible to chain several iterations of the whole process with different starting points. Python script for this use case:

```

import openturns as ot
import otlhs
# Generating a design of size N=100
N = 100
# Considering independent Uniform distributions of dimension 3
# Bounds are (-1,1), (0,2) and (0, 0.5)
bounds = ot.Interval([-1,0,0], [1,2,0.5])
# Random LHS
lhs = otlhs.LHSDesign(bounds, N)
# Fixing PhiP crit
space_filling = otlhs.SpaceFillingPhiP()
# Defining a temperature profile
# T0=10, iMax=3000
temperatureProfile = otlhs.LinearProfile(10.0, 3000)
algo = otlhs.SimulatedAnnealingLHS(lhs, temperatureProfile, space_filling)
restart = 50
result = algo.generate(restart)
# Retrieve optimal design
design = result.getOptimalDesign()
# Retrieve all optimal designs
designs = [result.getOptimalDesign(i) for i in xrange(restart)]

```

Finally, we could start the optimization process of LHS using a precomputed LHS design. Python script for this use case:

```

import openturns as ot
import otlhs
# Generating a design of size N=100
N = 100
# Considering independent Uniform distributions of dimension 3
# Bounds are (0,1)^3
bounds = ot.Interval(3)
# Random LHS
lhs = otlhs.LHSDesign(bounds, N)
# Fixing C2 crit for example
space_filling = otlhs.SpaceFillingC2()
# Defining a temperature profile
# T0=10, iMax=3000
temperatureProfile = otlhs.LinearProfile(10.0, 3000)
algo = otlhs.SimulatedAnnealingLHS(lhs, temperatureProfile, space_filling)
result = algo.generate()
# optimal design
design = result.getOptimalDesign()
# check history ==> draw criterion
ot.Show( result.drawHistoryCriterion() )
# Convergence needs to be performed
# New algo starting from this design
algo = otlhs.SimulatedAnnealingLHS(design, bounds, temperatureProfile,
    space_filling)
result = algo.generate()
# New design
design = result.getOptimalDesign()

```

### 3.6 Ishigami test

The following example illustrates the generation of an optimal design for surrogate model learning purposes. The use case proposed here is the Ishigami function. The model requires 3 input parameters, which are known to be uniformly distributed in  $[-\pi, \pi]^3$ .

Python script for a detailed study is proposed hereafter:

```

import openturns as ot
import otlhs
from math import sin, pi
import matplotlib.pyplot as plt
from otlhs.pyplotdesign import PyPlotDesign

# Set seed
ot.RandomGenerator.SetSeed(0)
# Definition of the Ishigami function
dimension = 3
a = 7.0

```



```

b = 0.1

# Create the Ishigami function
input_variables = ["xi1", "xi2", "xi3"]
formula = ["sin(xi1)"+_(" + str(a) + ")"+_("sin(xi2))"+_2+_(" + str(b) + ")"+_xi3^4*_sin(xi1)"]
ishigami_model = ot.NumericalMathFunction(input_variables , formula)
ishigami_model.setName("Ishigami")

# Generating a design of size
N = 150
# Considering independent Uniform distributions of dimension 3
# Bounds are  $(-pi, pi)$ ,  $(-pi, pi)$  and  $(-pi, pi)$ 
bounds = ot.Interval(dimension*[-pi] , dimension*[pi])
# Random LHS
lhs = otlhs.LHSDesign(bounds , N)
# Fixing C2 crit
space_filling = otlhs.SpaceFillingC2()
# Defining a temperature profile
temperatureProfile = otlhs.GeometricProfile()
# Pre conditionning : generate an optimal design with MC
nSimu = 100
algo = otlhs.MonteCarloLHS(lhs , nSimu , space_filling)
result = algo.generate()
initialDesign = result.getOptimalDesign()
print("initial_design_pre-computed. Performing SA optimization...")
# Use of initial design
algo = otlhs.SimulatedAnnealingLHS(initialDesign , bounds ,
    temperatureProfile , space_filling)
result = algo.generate()
print("initial_design_computed")
# Retrieve optimal design
input_database = result.getOptimalDesign()

fig = PyPlotDesign(input_database , bounds , 1 , 1)
fig.set_size_inches(fig.get_size_inches() * 2)
plt.suptitle("Ishigami_design")
plt.savefig("design_ishigami.png")
plt.close(fig)
# Response of the model
print "sampling_size=", N
output_database = ishigami_model(input_database)

# Learning input/output
# Usual chaos meta model
enumerate_function = ot.HyperbolicAnisotropicEnumerateFunction(dimension)
orthogonal_basis =
    ot.OrthogonalProductPolynomialFactory(dimension*[ot.LegendreFactory()]) ,

```

```

        enumerate_function)
basis_size = 100
# Initial chaos algorithm
adaptive_strategy = ot.FixedStrategy(orthogonal_basis, basis_size)
# ProjectionStrategy ==> Sparse
fitting_algorithm = ot.KFold()
approximation_algorithm =
    ot.LeastSquaresMetaModelSelectionFactory(ot.LAR(), fitting_algorithm)
projection_strategy = ot.LeastSquaresStrategy(input_database,
        output_database, approximation_algorithm)
print("Surrogate_model...")
distribution_ishigami = ot.ComposedDistribution(dimension *
        [ot.Uniform(-pi, pi)])
algo_pc = ot.FunctionalChaosAlgorithm(input_database, output_database,
        distribution_ishigami, adaptive_strategy, projection_strategy)
algo_pc.run()
chaos_result = algo_pc.getResult()
print("Surrogate_model_computed")

# Validation
lhs_validation = ot.LHSExperiment(distribution_ishigami, 100)
input_validation = lhs_validation.generate()
output_validation = ishigami_model(input_validation)
# Chaos model evaluation
output_metamodel_sample = chaos_result.getMetaModel()(input_validation)

# Cloud validation ==> change from matplotlib to pure OT
fig = plt.figure()
plt.plot(output_validation, output_validation, 'b-', label='Model')
plt.plot(output_validation, output_metamodel_sample, 'r.', label='SM')
plt.title("Surrogate_model_validation-Ishigami_use_case")
plt.savefig("ishigami_model_validation.png")

```

We illustrate hereafter the design obtained that optimize the  $C_2$  criterion in figure 3.6.

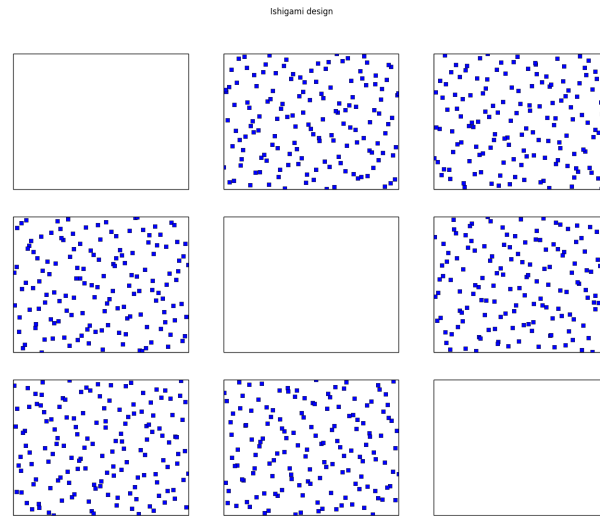


Figure 4: Input design for learning Ishigami model

The design seems accurate. To complete this example, the validation using an independent validation sample is done as illustrated in figure [3.6](#)

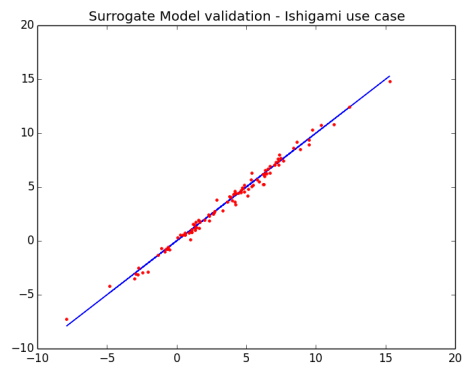


Figure 5: Validation of surrogate model

## 4 User Manual

This section gives an exhaustive presentation of the objects and functions provided by the *otlhs* module, in the alphabetic order.

### 4.1 GeometricProfile

**Usage:**

```
GeometricProfile()
GeometricProfile(T0)
GeometricProfile(T0,c)
GeometricProfile(T0,c,iMax)
```

**Arguments:**

*T0*: a NumericalScalar, initial temperature (10 by default)  
*c*: a NumericalScalar, geometric factor, must be between 0 and 1 exclusive (0.95 by default)  
*iMax*: an UnsignedInteger, number of iterations (2000 by default)

**Value :** a GeometricProfile

**Details :**

GeometricProfile constructor

*operator()*

**Usage :** *operator()(it)*

**Arguments :** an UnsignedInteger, iteration number

**Value :** a NumericalScalar, the value of temperature at the given time

### 4.2 LHSDesign

**Usage:**

```
LHSDesign(bounds, size, randomDesign)
```

**Arguments:**

*bounds*: an Interval, bounds of variables  
*size*: an UnsignedInteger, number of sample points  
*randomDesign*: a Bool, **generate()** method builds a random LHS when true (which is the default), otherwise a centered LHS

**Value :** an LHSDesign

**Details :**

LHSDesign constructor

*getBounds*

**Usage :** *getBounds()*

**Value :** an Interval, which are bounds of variables

*getSize*

**Usage :** *getSize()*

**Value :** an UnsignedInteger, sample size

*isCenteredDesign*

**Usage :** *isCenteredDesign()*

**Value :** a Bool, true if centered designs are generated, false otherwise

*generate*

**Usage :** *generate()*

**Value :** a NumericalSample, new design

### 4.3 LHSResult

**Usage:**

*LHSResult()*

*LHSResult(bounds, spaceFilling)*

*LHSResult(bounds, spaceFilling, restart)*

**Arguments:**

*bounds*: an Interval, specify bounds for each marginal

*spaceFilling*: a SpaceFilling, space filling criterion

*restart*: number of restarts performed during optimization

**Value :** an LHSResult

**Details :**

LHSResult constructor, which is only called by optimization algorithms

*getBounds*

**Usage :** *getBounds()*

**Value :** an Interval, which contains bounds for each marginal

*getNumberOfRestarts*

**Usage :** *getNumberOfRestarts()*

**Value :** an UnsignedInteger, number of restarts performed during optimization

*getOptimalDesign*

**Usage :** *getOptimalDesign()*

**Value :** a NumericalSample, contains the best LHS design

*getOptimalDesign*

**Usage :** *getOptimalDesign(restart)*

**Arguments :** an `UnsignedInteger`, to specify a restart number

**Value :** a `NumericalSample`, contains the best LHS design found during this specific restart

*getOptimalValue*

**Usage :** *getOptimalValue()*

**Value :** a `NumericalScalar`, the criterion value for the optimal LHS design

*getOptimalValue*

**Usage :** *getOptimalValue(restart)*

**Arguments :** an `UnsignedInteger`, to specify a restart number

**Value :** a `NumericalScalar`, the criterion value for the optimal LHS design found during this specific restart

*getAlgoHistory*

**Usage :** *getAlgoHistory()*

**Value :** a `NumericalSample`, contains informations gathered by optimization algorithm

*getAlgoHistory*

**Usage :** *getAlgoHistory(restart)*

**Arguments :** an `UnsignedInteger`, to specify a restart number

**Value :** a `NumericalSample`, contains informations gathered by optimization algorithm during this specific restart

*getC2*

**Usage :** *getC2()*

**Value :** a `NumericalScalar`, the C2 value for the optimal LHS design

*getC2*

**Usage :** *getC2(restart)*

**Arguments :** an `UnsignedInteger`, to specify a restart number

**Value :** a `NumericalScalar`, the C2 value for the optimal LHS design found during this specific restart

*getPhiP*

**Usage :** *getPhiP()*

**Value :** a `NumericalScalar`, the PhiP value for the optimal LHS design

*getPhiP*

**Usage :** *getPhiP(restart)*

**Arguments :** an `UnsignedInteger`, to specify a restart number

**Value :** a NumericalScalar, the PhiP value for the optimal LHS design found during this specific restart

*getMinDist*

**Usage :** *getMinDist()*

**Value :** a NumericalScalar, the mindist value for the optimal LHS design

*getMinDist*

**Usage :** *getMinDist(restart)*

**Arguments :** an UnsignedInteger, to specify a restart number

**Value :** a NumericalScalar, the mindist value for the optimal LHS design found during this specific restart

#### 4.4 LinearProfile

**Usage:**

*LinearProfile()*

*LinearProfile(T0)*

*LinearProfile(T0,iMax)*

**Arguments:**

*T0*: a NumericalScalar, initial temperature (10 by default)

*iMax*: an UnsignedInteger, number of iterations (2000 by default)

**Value :** a LinearProfile

**Details :**

LinearProfile constructor

*operator()*

**Usage :** *operator()(it)*

**Arguments :** an UnsignedInteger, iteration number

**Value :** a NumericalScalar, the value of temperature at the given time

#### 4.5 MonteCarloLHS

**Usage:**

*MonteCarloLHS(LHS, N)*

*MonteCarloLHS(LHS, N, spaceFilling)*

**Arguments:**

*LHS*: an LHS, initial design

*N*: an UnsignedInteger, number of random designs

*spaceFilling*: a SpaceFilling, space filling criterion

**Value :** a MonteCarloLHS

**Details :**

With the first usage, `spaceFilling` is fixed to `SpaceFillingMinDist`

*generate*

**Usage :** *generate()*

**Value :** an LHSResult, this instance contains the best design and some other values

## 4.6 OptimalLHS

**Usage:**

*OptimalLHS(lhs)*

*OptimalLHS(lhs, spaceFilling)*

**Arguments:**

*lhs*: an LHS, initial design

*spaceFilling*: a SpaceFilling, space filling criterion

**Value :** an OptimalLHS

**Details :**

OptimalLHS constructor

*getLHS*

**Usage :** *getLHS()*

**Value :** an LHS, initial design

*getSpaceFilling*

**Usage :** *getSpaceFilling()*

**Value :** a SpaceFilling, space filling criterion

*generate*

**Usage :** *generate()*

**Value :** an LHSResult, this instance contains the best design and some other values

## 4.7 PlotDesign

**Usage:**

*PlotDesign(data, bounds)*

*PlotDesign(data, bounds, Nx, Ny)*

*PlotDesign(data, bounds, Nx, Ny, title)*

*PlotDesign(result)*



*PlotDesign(result, Nx, Ny)*

*PlotDesign(result, Nx, Ny, title)*

#### Arguments:

*data*: a NumericalSample, which represents an LHS design

*bounds*: an Interval, specify bounds for each marginal

*Nx*: an UnsignedInteger, number of grid intervals along X-axis (default value = size of design)

*Ny*: an UnsignedInteger, number of grid intervals along Y-axis (default value = size of design)

*title*: a String, plot title

*result*: an LHSResult, returned by an optimization algorithm

**Value :** a PlotDesign

#### Details :

PlotDesign constructor

## 4.8 SimulatedAnnealingLHS

#### Usage:

*SimulatedAnnealingLHS(lhs)*

*SimulatedAnnealingLHS(lhs, profile)*

*SimulatedAnnealingLHS(lhs, profile, spaceFilling)*

*SimulatedAnnealingLHS(design, bounds)*

*SimulatedAnnealingLHS(design, bounds, profile)*

*SimulatedAnnealingLHS(design, bounds, profile, spaceFilling)*

#### Arguments:

*lhs*: an LHS, initial design factory

*design*: a NumericalSample, an initial design

*bounds*: an Interval, bounds of design

*profile*: a TemperatureProfile, temperature profile

*spaceFilling*: a SpaceFilling, space filling criterion

**Value :** a SimulatedAnnealingLHS

#### Details :

With the first and fourth usages, profile and spaceFilling are respectively setted to default **GeometricProfile** and **SpaceFillingMinDist**

With the second and fifth usages, spaceFilling is setted to **SpaceFillingMinDist**

*generate*

**Usage :** *generate()*

**Value :** an LHSResult, this instance contains the best design and some other values

*generate*

**Usage :** *generate(restart)*

**Arguments :** an UnsignedInteger, the number of restarts

**Value :** an LHSResult, this instance contains the best design and some other values

## 4.9 SpaceFilling

**Usage:**

*SpaceFilling(impl)*

**Arguments:**

*impl*: a SpaceFillingImplementation, a specific implementation of SpaceFilling

**Value :** a SpaceFilling

**Details :**

SpaceFilling constructor

*evaluate*

**Usage :** *evaluate(sample)*

**Arguments :** a NumericalSample

**Value :** a NumericalScalar, value of the criterion evaluated on this sample

## 4.10 SpaceFillingC2

**Usage:**

*SpaceFillingC2()*

**Value :** a SpaceFillingC2

**Details :**

SpaceFillingC2 constructor

*evaluate*

**Usage :** *evaluate(sample)*

**Arguments :** a NumericalSample

**Value :** a NumericalScalar, value of the C2 criterion evaluated on this sample

### 4.11 SpaceFillingMinDist

**Usage:**

*SpaceFillingMinDist()*

**Value :** a SpaceFillingMinDist

**Details :**

SpaceFillingMinDist constructor

*evaluate*

**Usage :** *evaluate(sample)*

**Arguments :** a NumericalSample

**Value :** a NumericalScalar, value of the mindist criterion evaluated on this sample

### 4.12 SpaceFillingPhiP

**Usage:**

*SpaceFillingPhiP(p)*

**Arguments:**

*p*: an UnsignedInteger (by default, 50)

**Value :** a SpaceFillingPhiP

**Details :**

SpaceFillingPhiP constructor

*evaluate*

**Usage :** *evaluate(sample)*

**Arguments :** a NumericalSample

**Value :** a NumericalScalar, value of the PhiP evaluated on this sample

## 5 Validation

This section aims at exposing the methodology used to validate numerical results of the module.

### 5.1 Methodology of validation

This module implements two different algorithms:

- Monte Carlo
- Simulated annealing algorithm; this algorithm is the novelty and requires several steps. It uses also some tips such as the update of criterion after a permutation instead of a complete calculation.

Both algorithms are to be validated.

### 5.2 Preliminary validations

For specific designs, criteria values ( $C_2$ , *mindist* and  $\phi_p$ ) obtained with *otlhs* module are compared with values computed by the **DiceDesign** R package. Those scripts are located in the **validation** folder of this module. Comparisons are very good, absolute error is less than  $10^{-13}$ .

As mentionned previously,  $C_2$  criterion can be computed efficiently when a small perturbation is performed on design. This specific method is compared to the **DiceDesign**'s ones: absolute error is less or equal to  $10^{-10}$ .

Note that for  $\phi_p$  criterion, **DiceDesign** computes the new value after a permutation without taking into account the oldest criterion. In this module, criterion update has been implemented, but is used only when parameter  $p \geq 5$ . Indeed, numerical experiments have shown instability of the update when  $p$  becomes large.

### 5.3 Validation of Monte Carlo algorithm

To get an optimal design using Monte Carlo algorithm, several designs are to be generated and the returned one minimizes the space filling function.

As the evaluation of the criterion does not require any complexity, validation of Monte Carlo algorithm is trivial:

- Fix a criterion to minimize;
- Fix the RandomSeed to a fixed value (0 for example);
- Generate  $N = 100$  designs: get the optimal one and the associated criterion value;
- Fix again the RandomSeed;
- Generate  $N = 10000$  designs: get the optimal one and its associated criterion value;
- Check that the last criterion value is less or equal than to the previous one;

### 5.4 Validation of simulated annealing algorithm

Simulated annealing is compared to Monte Carlo algorithm (with  $N = 10000$ ) and should return better results. Indeed the optimal design is built such as the space filling criterion decreases at each iteration.

Several use cases are proposed for the validation and illustrated hereafter:  
Final criteria should meet requirements.

Test id	Dimension	Size	Temperature profile	Profile parameters	Requirement
1	2	10	Geometric	$T_0 = 10, c = 0.999, iMax = 50000$	$C_2 \leq 0.0664$
2	2	10	Linear	$T_0 = 10, iMax = 50000$	$mindist \geq 0.272$
3	50	100	Geometric	$T_0 = 10, c = 0.999, iMax = 50000$	$C_2 \leq 22.176$
4	50	100	Geometric	$T_0 = 10, c = 0.999, iMax = 50000$	$mindist \geq 2.653$

Table 1: Use cases for the validation &amp; requirements

## 5.5 Results

Designs are generated according to the multivariate distribution  $U[0, 1]^d$ .

### 5.5.1 MonteCarlo results

We first check that Monte Carlo scales linearly with respect to the number of simulations. Random generator seed is reinitialized to the same value when starting Monte Carlo algorithm, this is why criterion always decreases.

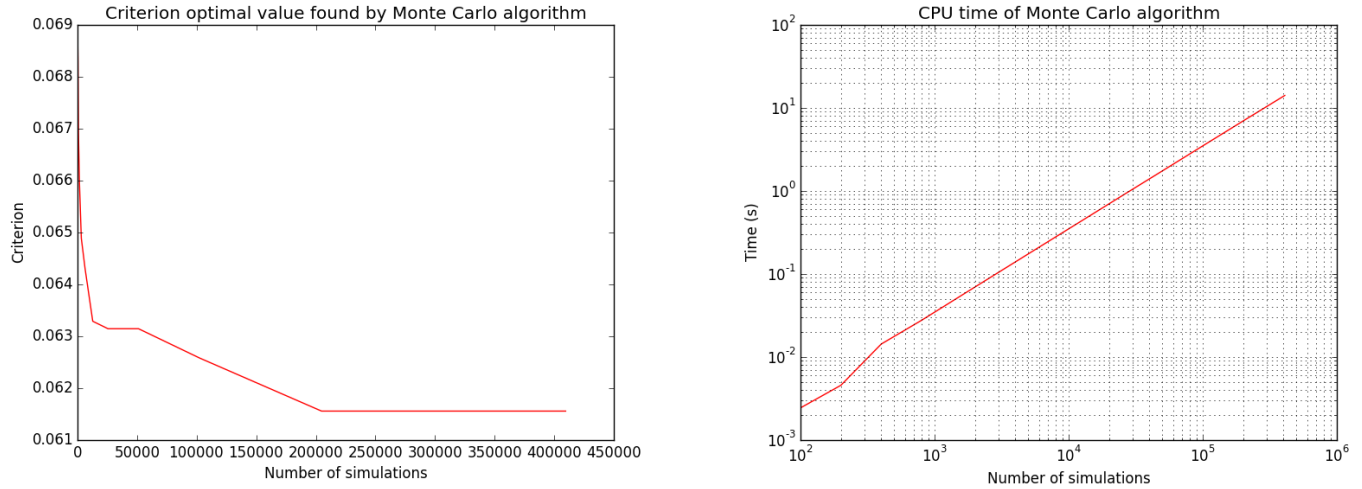


Figure 6: Scaling of Monte Carlo results when increasing number of simulations

Tests corresponding to use cases in table 1 are implemented and results obtained using Monte Carlo are given in table 2.

Dimension	Size	Criterion	Criterion value	CPU time (s)	Requirement
2	10	$C_2$	0.0643	0.72	$C_2 \leq 0.0664$
2	10	mindist	0.2666	0.47	$mindist \geq 0.272$
50	100	$C_2$	24.427	109.48	$C_2 \leq 22.176$
50	100	mindist	2.198	53.36	$mindist \geq 2.653$

Table 2: Monte Carlo results after  $N_{simu} = 10000$  simulations

We use  $N_{simu} = 10000$  simulations in order to get the optimal design (designs are not centered). As shown in

figure 6, 10000 iterations give a good solution for the small case; but in the larger case, it is expected that this number is way too small, so results are quite close to expectations.

In addition, we give design plots in dimension 2 only (in dimension 50, the interest is very limited).

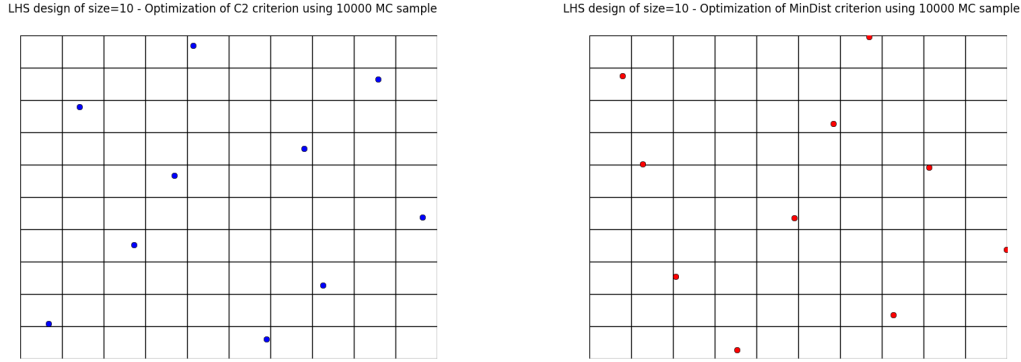


Figure 7: Monte Carlo results

### 5.5.2 Simulated annealing results

Using the `SimulatedAnnealingLHS` class and use cases described in table 1, tests are implemented and results are resumed in table 3. These are compared to those produced by `DiceDesign` R package in terms of criteria and CPU time.

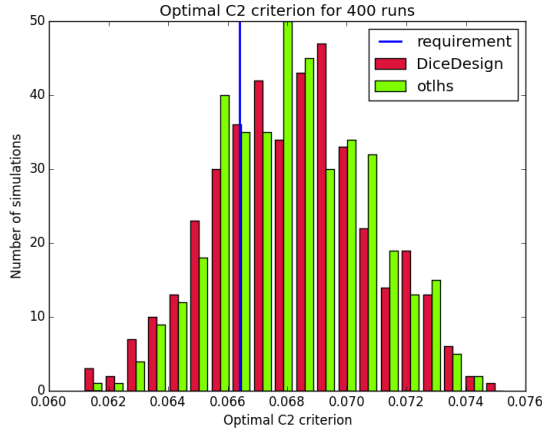
Test id	Requirement	otlhs		R	
		Criterion	CPU time (s)	Criterion	CPU time (s)
1	$C_2 \leq 0.0664$	0.0699	0.04	0.06153	89.8
2	$\text{mindist} \geq 0.272$	0.254	0.246	0.258	36.37
3	$C_2 \leq 22.176$	22.190	2.69	22.15	618.7
4	$\text{mindist} \geq 2.653$	2.643	55.8	2.64	220.6

Table 3: Numerical results obtained with the module

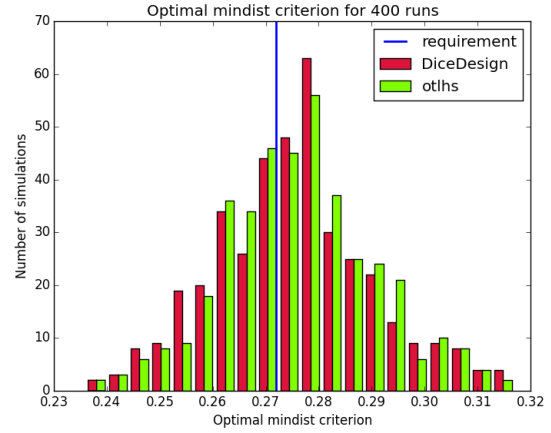
CPU time is much lower with *otlhs*. It must be noted that speedup of test 4 is not in par with speedups of other tests. We believe that this is not due to some performance problems, but is the combination of several factors:

1. R implementation of mindist is better than C2 because it does not contain loops, but only few high-level operations on matrices.
2. In *otlhs* implementations, mindist is slower than C2 because it calls `evaluate` instead of `perturbLHS`. It may be interesting to try with  $p = 5$  instead of  $p = 50$ , mindist would then be as fast as C2, and many restarts could be tried. Unfortunately, we did not have time to make these tests.

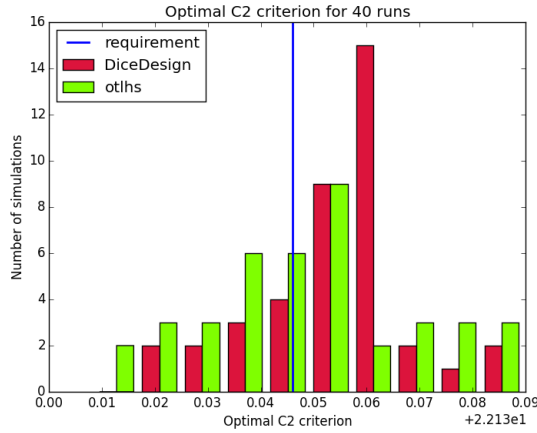
Results are close to expectations, but do not meet all requirements. In order to understand why *otlhs* results are sometimes out of bounds, we performed 400 runs of tests 1 and 2 with `DiceDesign` and *otlhs*, 40 runs of test 3 and 80 runs of test 4. Results are shown in figure 8. Diagrams look similar, thus in our opinion, *otlhs*



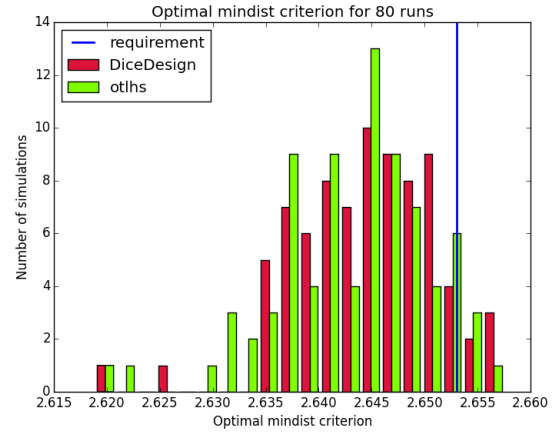
Comparison on 400 runs for test id 1



Comparison on 400 runs for test id 2



Comparison on 40 runs for test id 3



Comparison on 80 runs for test id 4

Figure 8: Results comparison with restarts

does meet requirements. Moreover, as *otlhs* is much faster than R, the same CPU budget will give better results with *otlhs*.

In addition, designs, optimized criterion convergence and elementary perturbation probability are given in figures 9, 10 and 11 (for dimension 50, only criterion history is displayed).

Results are very similar between the two implementations. It must be noted that there are many plots with probability 1. The reason is that DiceDesign accepts both row indices to be equal when checking for elementary perturbations.

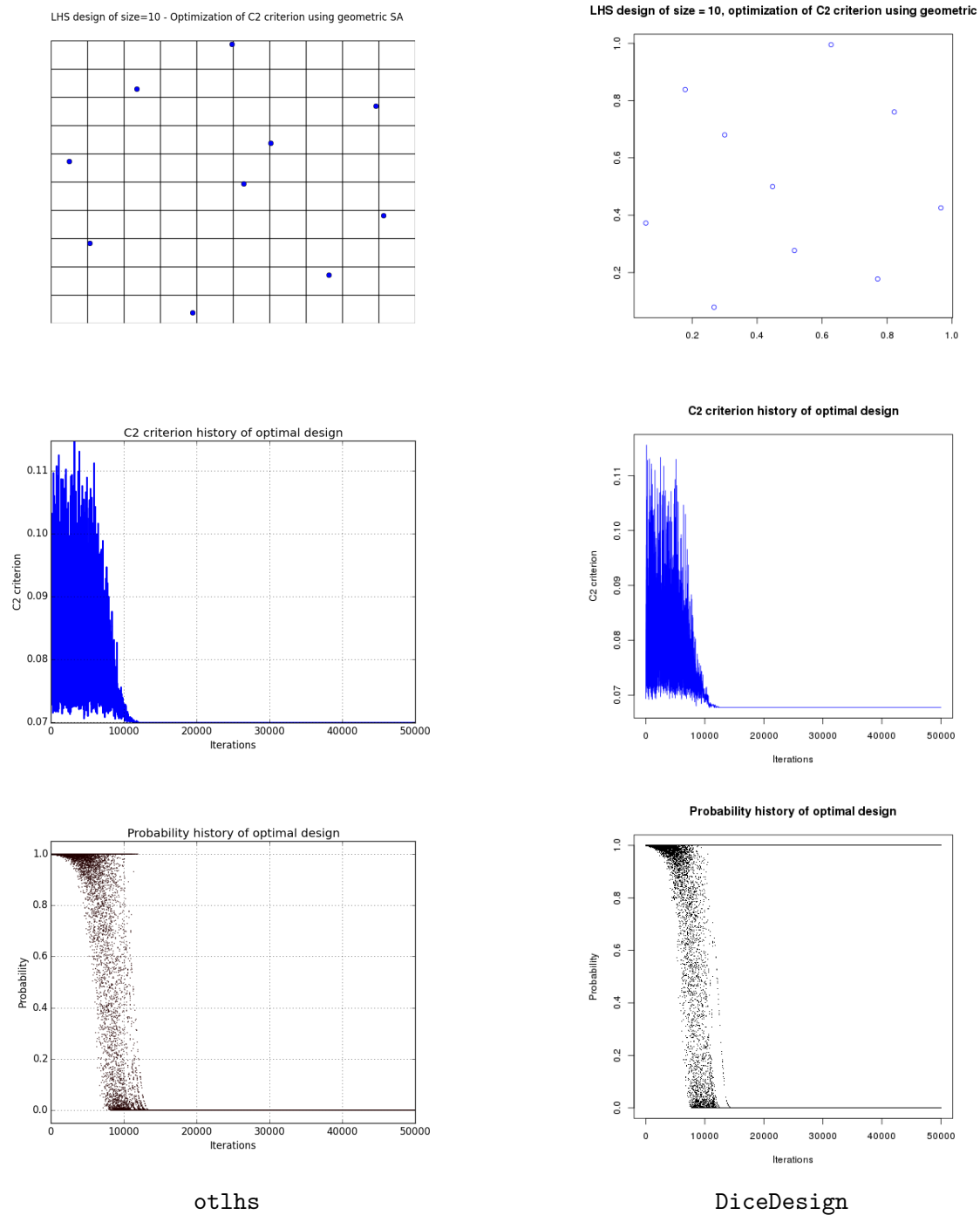


Figure 9: Simulated annealing results - Test id 1



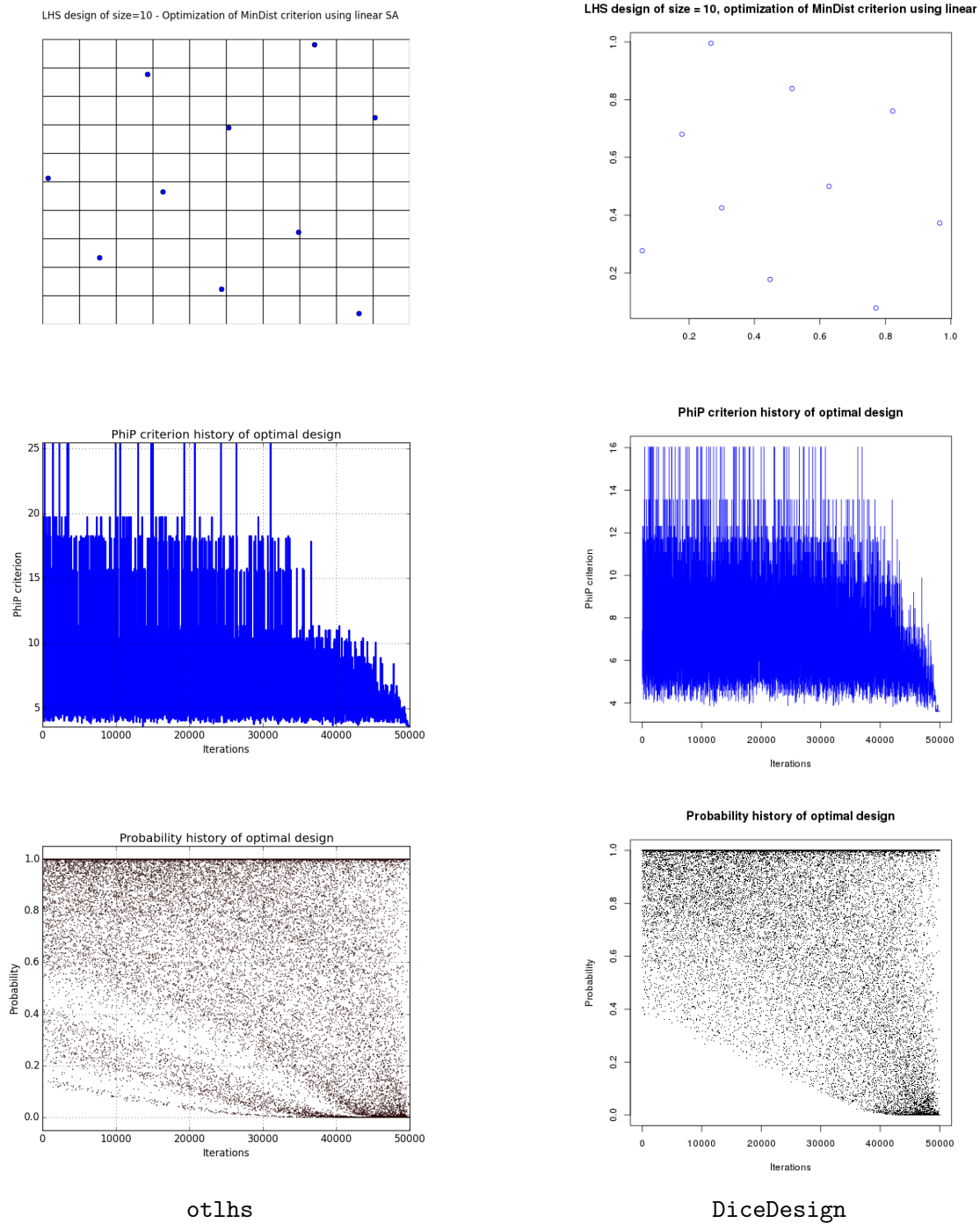


Figure 10: Simulated annealing results - Test id 2

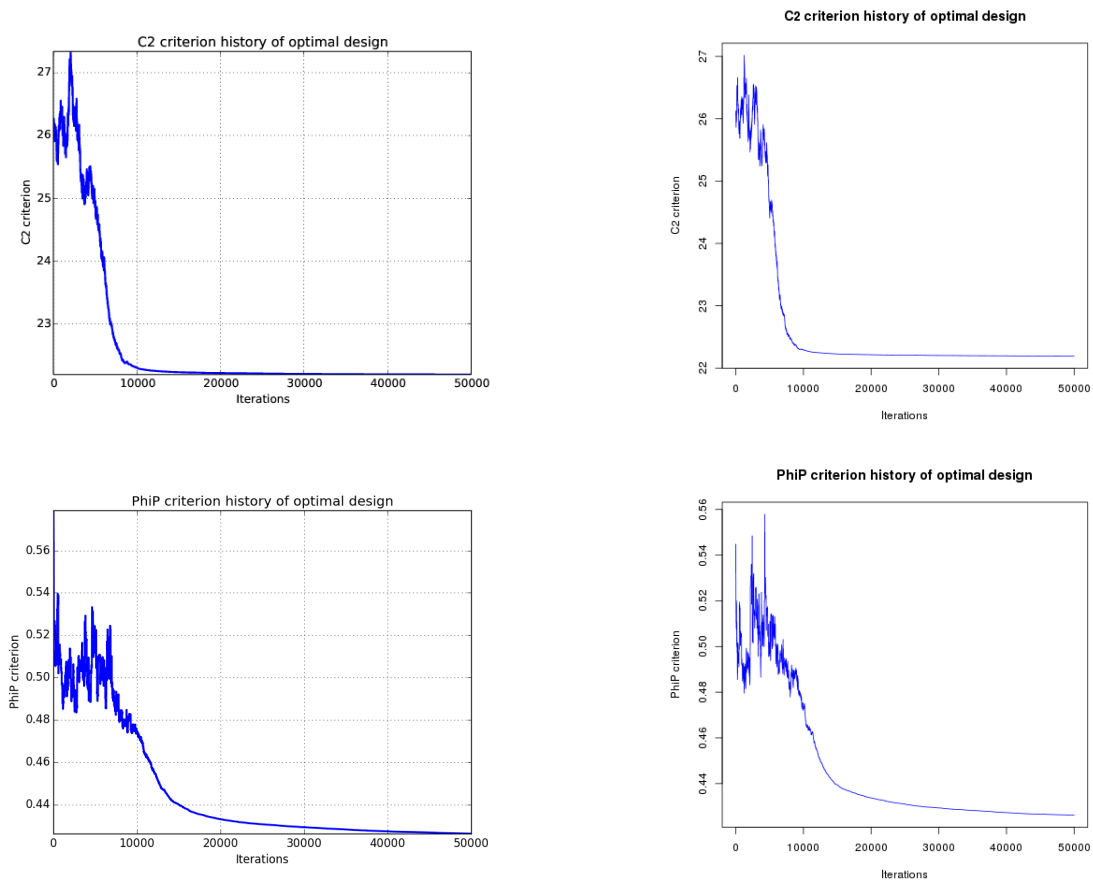


Figure 11: Simulated annealing criterion results - Test id 3 and 4