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Construction of space-filling designs using WSP algorithm for high dimensional spaces

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ABSTRACT

In the computer experiments setting, if the relationship between the response and the inputs is unknown, then the purpose is to use designs that spread the points at which the response is observed evenly throughout the region. These designs are called space-filling designs (SFD) and the most known are Latin Hypercubes (random, orthogonal, optimized) and low discrepancy sequences. But, simulation codes becoming more and more complex, high dimensional optimal designs are needed to study a high number of parameters (more than 20 parameters) and the construction proves difficult. The aim of this study is to explore a construction method of new space-filling designs for high dimensional spaces. After a short presentation of the criteria considered to quantify the intrinsic quality of the designs, the generation of these designs using WSP algorithm is presented. As the first step consists in generating candidate points, the influence of the initial set of points is investigated in dimension 20 and the final designs are compared with others space-filling designs. Then, designs are proposed in dimension 20, 30, 40 and 50 and the study of the intrinsic quality of these new space-filling designs highlights the robustness of this generation method in high dimensional spaces.
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1. Introduction

In the last decade, the uniform designs of experiments based on space filling have been more frequently used since experimental designs methods started being applied in numerical experiments. In domains such as the oil industry, astronomy, optics, the nuclear industry, etc., the experiments are expensive and time consuming. Therefore, phenomena are often studied using numerical simulations, but the time of calculation can be very long because the models are increasingly complex, involving a large number of coefficients. This statement of fact reveals that it would be advantageous to plan and organize the simulations as done in the domain of experiments and working in high dimension is now essential. Nevertheless high dimensional experimental designs are not widely used and their study looks promising. Uniform space-filling designs (SFD) [1,2], which spread the computer runs evenly throughout the space studied, seem to be well adapted to numerical simulations. Generally, however, the classical methods to build these experimental designs – such as low discrepancy sequences [3–7], good lattice points [8–11], Latin Hypercubes [12–16], orthogonal Latin Hypercube [17–19]– have been described for low dimensional spaces, often fewer than ten dimensions. This is usually because the algorithms require too long calculations in high dimensions [20].

In this work, we propose a construction method allowing the generation of high dimensional designs. First we present the criteria commonly used to evaluate the intrinsic quality of space-filling designs, then we present the so called WSP designs based on Wootton, Sergent, Phan-Tan-Luu's algorithm. Finally, we compare different space-filling designs in dimensions 20, 30, 40, 50.

2. Construction of space-filling designs

2.1. Measures of uniformity

When the dimension is higher than 2, the uniformity of the space filling cannot be visually evaluated. It is thus necessary to use measures in order to know if the distribution is uniform and if the space of the variables is well filled. Among the various criteria proposed in the literature, the most used are:

– The Euclidean distance, *MinDist*[21,22]:

$$MinDist = \min_{x_i \in X} \min_{\substack{x_k \in X \\ k \neq i}} dist\left(x^i, x^k\right)$$

with, $X = \{x^1, x^2, ..., x^n\} \subset [0,1]^d$, a set of n points in d dimensions.

A higher value of *Mindist* should correspond to a more regular scattering of design points and ensures that a point is never too close to another point.

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- The cover measure, *Cov*[23]:

$$Cov = \frac{1}{\overline{\gamma}}\left(\frac{1}{n}\sum_{i=1}^{n}\left(\gamma_i - \overline{\gamma}\right)^2\right)^{1/2}$$

with, $\gamma_i = \min_{k \neq i} dist(x^i, x^k)$ and $\overline{\gamma} = \frac{1}{n}\sum_{i-1}^{n} \gamma_i$.

A low value of *Cov* corresponds to a distribution close to a regular grid and ensures that the points fill up the space.

We can plot these values, *Mindist* and *Cov*, to distinguish between distributions of points (random, cluster, ordered, etc.). The *empirical* repartition is reported on Fig. 1[24].

In the (*MinDist, Cov*) plane, the best space-filling designs correspond to a quasi-periodical distribution which presents the best compromise between a regular grid (space filling) and a random distribution (uniformity). These designs are characterized by a low value of *Cov* and a high value of *Mindist*, which means that the desirable area is at the bottom, on the right.

This plot presents a repartition of the different point distributions similar to the cartography of the Minimum Spanning Tree approach [24]. This approach is based on a graph constructed from the set of points of an experimental design, considering two parameters: the mean and the standard deviation of the edges length of the Minimum Spaning Tree associated to the studied design.

This leads to conclude that these two criteria – *MinDist and Cov* – are sufficient to assess the quality of a space-filling design.

2.2. WSP designs

The construction of WSP designs is based on a selection of well-distributed points in accordance with the algorithm proposed by Sergent and al [25–27]. In this algorithm, the points are selected from a set of candidate points so as to be at a preset minimal distance (d_{min}) from every point in the defined multidimendional parameters space, already included in the design.

2.2.1. Algorithm

Step 1 generate a set of N candidate points
Step 2 calculate the distances (D_{ij}) matrix of the N points
Step 3 choose an initial point O and a distance d_{min}
Step 4 eliminate the points I such as: $D_{OI} < d_{min}$
Step 5 the point O is replaced by the nearest point among the remaining points
Step 6 repeat the steps 4 and 5 until there are no more points to choose.

In this way, the space of the variables will be "full" and covered the most uniformly possible. Fig. 2 illustrates this algorithm in a 2D space.

It's important to point out that, since the algorithm doesn't add any point, the initial candidate points is important and must be spread evenly throughout the studied space.

2.2.2. Impact of the candidate points

As the first step of the WSP algorithm is to generate a set of candidate points, the question arises on the impact of the choice of these candidate points as for their number and their distribution. To answer this question, different types of candidate point distributions were tested and for some distributions, the number of points in the departure set was investigated too. This comparison was performed in high dimensional space: D = 20, with a number of points arbitrarily fixed to 400 (20 points by dimension).

– Study of the influence of the candidate points distribution**:**

We selected eight initial distributions with 3000 candidate points: stochastic designs such as random distributions, random Latin Hypercubes, Strauss designs [28] and deterministic designs such as low discrepancy sequences (Halton [4], Hammersley [5], Faure [3], Sobol [7]) and maximin Latin Hypercubes [13,29–31,17,32,15,33–35]. For each set of points, the criteria presented in Section 2.1 were calculated (Table 1). In the case of non deterministic designs, such as random designs, random LHS and Strauss designs, the distribution of the points can be slightly different each time we generate a design. Consequently, for these designs we generated 20 designs and we considered the mean and the standard deviation (reported in brackets).

This table shows a large variation of the uniformity criteria. For example, *MinDist* varies from 0.194 (Faure low discrepancy sequence) to 0.690 (Sobol low discrepancy sequence) and *Cov* varies from 0.085 (Sobol low discrepancy sequence) to 0.830 (Faure low discrepancy sequence). With regard to these measures, Faure low discrepancy sequence appears as the worst intrinsic quality design.

From these different sets of points, the WSP selection algorithm was performed and a final subset, with around 400 points, was selected. Table 2 reports the comparison of the intrinsic qualities of the final designs.

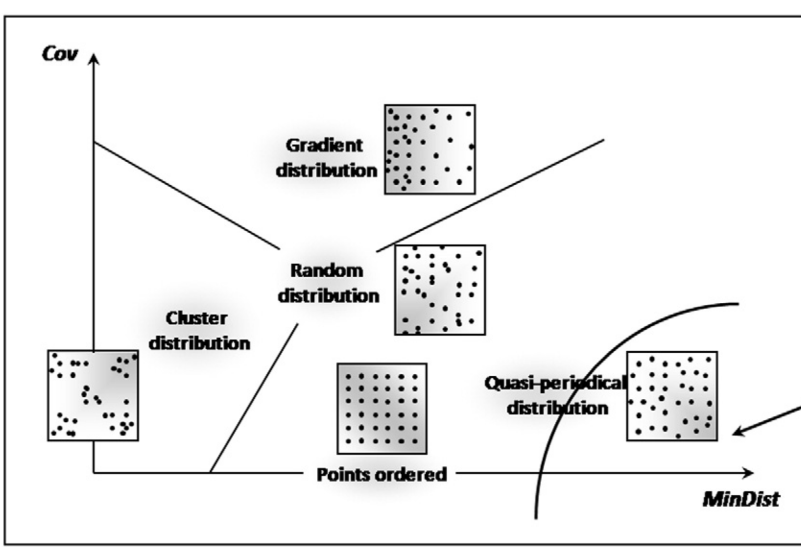

Fig. 1. Empirical repartition of different space-filling designs using *MinDist* and *Cov* criteria. The desirable designs have a high value of *MinDist*, corresponding to sufficiently distant points, and a low value of *Cov*, corresponding to a regular distribution.

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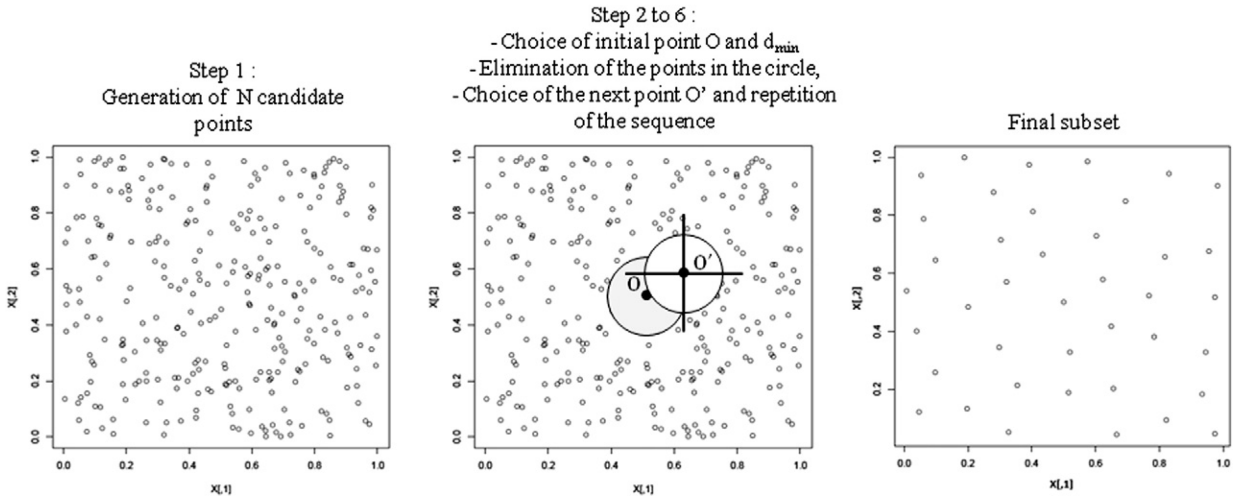

Fig. 2. Illustration of WSP algorithm in 2D space.

As regards the non deterministic distributions, the 20 final designs are very similar in terms of uniformity measure since the standard deviations become very low.

To illustrate the impact of the WSP selection algorithm on the values of *MinDist* and *Cov*, these values are plotted for the initial and final designs (Fig. 3).

Fig. 3 clearly shows that the eight initial designs (N = 3000 points) present very different intrinsic qualities and, after the selection algorithm, the eight final designs with around 400 points are equivalent in terms of the *MinDist* and *Cov* criteria (*MinDist* ≈ 1.3 and *Cov* ≈ 0.024). We can conclude that the type of the initial distribution has no impact on the intrinsic quality of the design after the selection algorithm.

– Study of the influence of the number of candidate points:

As mentioned above, the WSP algorithm is a selection procedure and doesn't add any point. Consequently, the initial distribution must uniformly fill the studied space because if some areas are not well covered, they will be poorly represented in the final design and the presence of voids could be prejudicial for a subsequent response surface. In this section, we study the impact of the number of points of the initial set and, for a same type of initial distribution the number of candidate points has been studied from 500 to 3000 points. As the nature of the initial set of points is non influential, only 4 types of design (Hammersley low discrepancy sequence, Faure low discrepancy sequence, random LHS and random distribution) are considered. Like in the first study, the d_{min} of the selection algorithm was optimized to obtain final designs with around 400 points. The uniformity criteria were calculated for each final design, varying the number of points of the initial design. Results are reported in Table 3 and on Fig. 4. For comparison, the criteria were calculated for each type of distribution with 400 points without the WSP selection algorithm: the values are reported in the lines highlighted in gray in Table 3. It can be noticed that the final designs after WSP selection algorithm (N ≈ 400 points) present better values of the criteria than the different considered designs with a same number of points. For example, *MinDist* varies from 0.194 for a Faure low discrepancy sequence with 400 points to 1.290 for a design with 400 points after the selection algorithm on a Faure low discrepancy sequence (N = 3000) and *Cov* varies from 0.470 (Faure low discrepancy sequence, N = 400) to 0.020 (WSP, N = 400).

The scatter plot of each design versus the number of candidate points shows large variation in the *Cov* and *MinDist* criteria. This leads to conclude that the number of candidate points may have a great impact on the quality of the final subset. More precisely, Fig. 4 shows that the intrinsic quality of the designs improves significantly (the *mindist* increases and the cover measure decreases) when the number of candidate points increases up to a threshold value beyond which the addition of points becomes useless (no more variation of the criteria). In this 20 dimensional study, we thus observe that from 2000 candidate points, the addition of supplementary points in the initial set has no influence on the qualities of the final design with around 400 points. This presence of a horizontal asymptote can be observed whatever the type of initial distribution.

Moreover, it is interesting to note the variation of the uniformity measures between a uniform design (Hammersley sequence, N = 400, *MinDist* = 0.512 and *Cov* = 0.280) and a design after selection on an

Table 1
Mindist and *Cov* criteria of the initial 20 dimensional distributions with 3000 points. For the non deterministic designs, the mean value and the standard deviation in brackets are reported.

Design	*MinDist* ↗	*Cov* ↘
Random distribution	0.585	0.095
	(0.0648)	(0.0024)
Random LHS	0.589	0.096
	(0.0550)	(0.0016)
Maximin LHS	0.627	0.095
Halton sequence	0.512	0.232
Hammersley sequence	0.512	0.237
Faure sequence	0.194	0.830
Sobol sequence	0.690	0.085
Strauss design	0.597	0.096
	(0.0485)	(0.0016)

Table 2
MinDist and *Cov* criteria of 20 dimensional designs after WSP selection algorithm with the respective number of points. For the non deterministic designs, the mean value and the standard deviation in brackets are reported.

Design	Number of points	*MinDist* ↗	*Cov* ↘
Random distribution	401.6	1.319	0.023
	(3.80)	(0.0031)	(0.0016)
Random LHS	400.6	1.319	0.023
	(2.87)	(0.0025)	(0.001)
Maximin LHS	402	1.320	0.027
Halton sequence	395	1.290	0.027
Hammersley sequence	399	1.292	0.024
Faure sequence	400	1.290	0.020
Sobol sequence	397	1.320	0.022
Strauss design	400.3	1.318	0.023
	(1.68)	(0.0041)	(0.0016)

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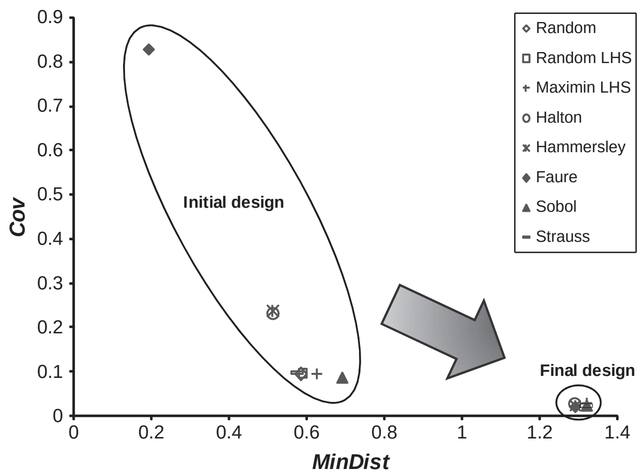

Fig. 3. Comparison of *MinDist* and *Cov* values for eight types of designs. The initial designs (N = 3000 points) present a large variation of the criteria whereas the resulting designs, after WSP selection algorithm (N = 400 points) are equivalent.

initial distribution at 500 points (from Hammersley sequence, N = 399, *MinDist* = 0.670 and *Cov* = 0.172). The addition of only 100 points to generate a set of candidate points for the selection algorithm significantly enhances the quality of the final design and thus leads to a sort of "repairing".

Finally, by analyzing the intrinsic quality of the final designs, we can conclude from both studies that the type of the initial distribution has no importance, even if it is a random distribution, but only if the number of points of the initial distribution is sufficient. The number of candidate points depends on the number of required points in the final design, but we could advise to consider a number of candidate points equal to at least 5 to 10 times the final set.

Table 3
Mindist and *Cov* values of the 20 dimensional designs after WSP selection varying the number of candidate points. For each type of design, the first line, highlighted in gray, corresponds to the distribution with 400 points without the WSP selection algorithm.

Design	Number of points in the candidate set	Number of points in the final subset	*MinDist* ↗	*Cov* ↘
RANDOM		400	0.695	0.100
	500	401	1.075	0.057
	1000	398	1.220	0.031
	1500	401	1.255	0.028
	2000	398	1.290	0.027
	2500	401	1.302	0.024
	3000	395	1.322	0.024
RLHS		400	0.819	0.096
	500	402	1.061	0.062
	1000	402	1.205	0.041
	1500	402	1.254	0.030
	2000	403	1.275	0.028
	2500	398	1.307	0.023
	3000	401	1.322	0.023
HAMMERSLEY		400	0.512	0.280
	500	399	0.670	0.172
	1000	401	1.160	0.037
	1500	399	1.220	0.028
	2000	400	1.250	0.027
	2500	399	1.284	0.025
	3000	399	1.292	0.024
FAURE		400	0.194	0.47
	500	420	0.975	0.080
	1000	407	1.030	0.072
	1500	399	1.185	0.027
	2000	403	1.243	0.023
	2500	401	1.265	0.021
	3000	400	1.290	0.020

2.3. Comparison of space-filling designs in 20 dimensional space

The previous studies have allowed us to trend towards an optimized WSP selection algorithm and it seems to us interesting to compare, in terms of intrinsic quality criteria, space-filling designs constructed using this algorithm with space-filling designs customarily used in numerical simulation.

The designs selected for the comparison, with 400 points in a 20 dimensional space, are the most common designs used for numerical experiments. Koehler and Owen (1996) and Franco [28] proposed an overview of space filling-designs and we have retained:

- Random designs: designs obtained by simple application of a random function,
- Maximin designs (Covd): optimal designs based on the maximin distance,
- Dmax designs (dmax): designs which maximize the determinant of the covariance matrix (Shewry & Wynn (1987), Currin et al. (1988).
- Latin Hypercube designs, with and without optimization (ilhs, mlhs, rlhs),
- Strauss designs: designs created using a Strauss procedure, which considers the repulsion between two points to maximize the space filling (Franco, 2008). Different types of Strauss designs were considered, with and without optimization.
- Low discrepancy sequences (Faure, Hammersley, Halton, Sobol).

For designs with a stochastic procedure or requiring an optimization (random, LHS, maximin, Dmax and Strauss designs), 5 designs were generated and all the criteria values are reported on Fig. 5.

For comparison, different designs based on WSP selection algorithm were constructed from Strauss designs and low discrepancy sequences (Hammersley, Halton, Faure, Sobol) with 3000 candidate points. The measures of uniformity –*DistMin* and *Cov* – were calculated for each design and the values are reported on Fig. 5.

This plot underlines the relative position of the different designs and allows the intrinsic quality of the designs to be compared. We can conclude that, in high dimension, the low discrepancy sequences appear as the worst intrinsic quality designs, designs as Covd, Latin Hypercubes, Dmax seem to be equivalent and group together and, located at the bottom on the right of the plot, Strauss and WSP designs appear as the best designs in terms of space-filling designs. Moreover, it must point out that some algorithms require too long calculations or are not conceivable: for instance, building a design with WSP algorithm requires around 2 s compared to a cover design or a Strauss design (without optimization) that require 220 s or 630 s respectively (calculation on a HP Z600 workstation).

2.4. Construction in high dimension

The previous studies were performed in 20D and allowed us to answer the questions that had arisen on the impact of the initial set of points. From these conclusions, we constructed WSP designs in 30, 40 and 50D and calculated the respective criteria. Actually, as the algorithm is based on the calculation of the distances between the points of an initial set, it is easily applied to the study of high dimensional spaces as 30D, 40D or 50D and even more. We present designs for these dimensions with 10 points or 20 points per dimension in the final designs. The candidate points were generated using Sobol low discrepancy sequences with 5000 to 7000 candidate points (the final designs are available on simple request to the authors). The classical criteria –*MinDist* and *Cov*– were calculated and are reported in Table 4 and on Fig. 6. For comparison, we calculated the criteria for another space-filling design with the same number of points, a Sobol sequence which seems to be the best low discrepancy sequence.

As mentioned above, in high dimensional spaces, it's difficult to build some classical space-filling designs such as Latin Hypercubes.

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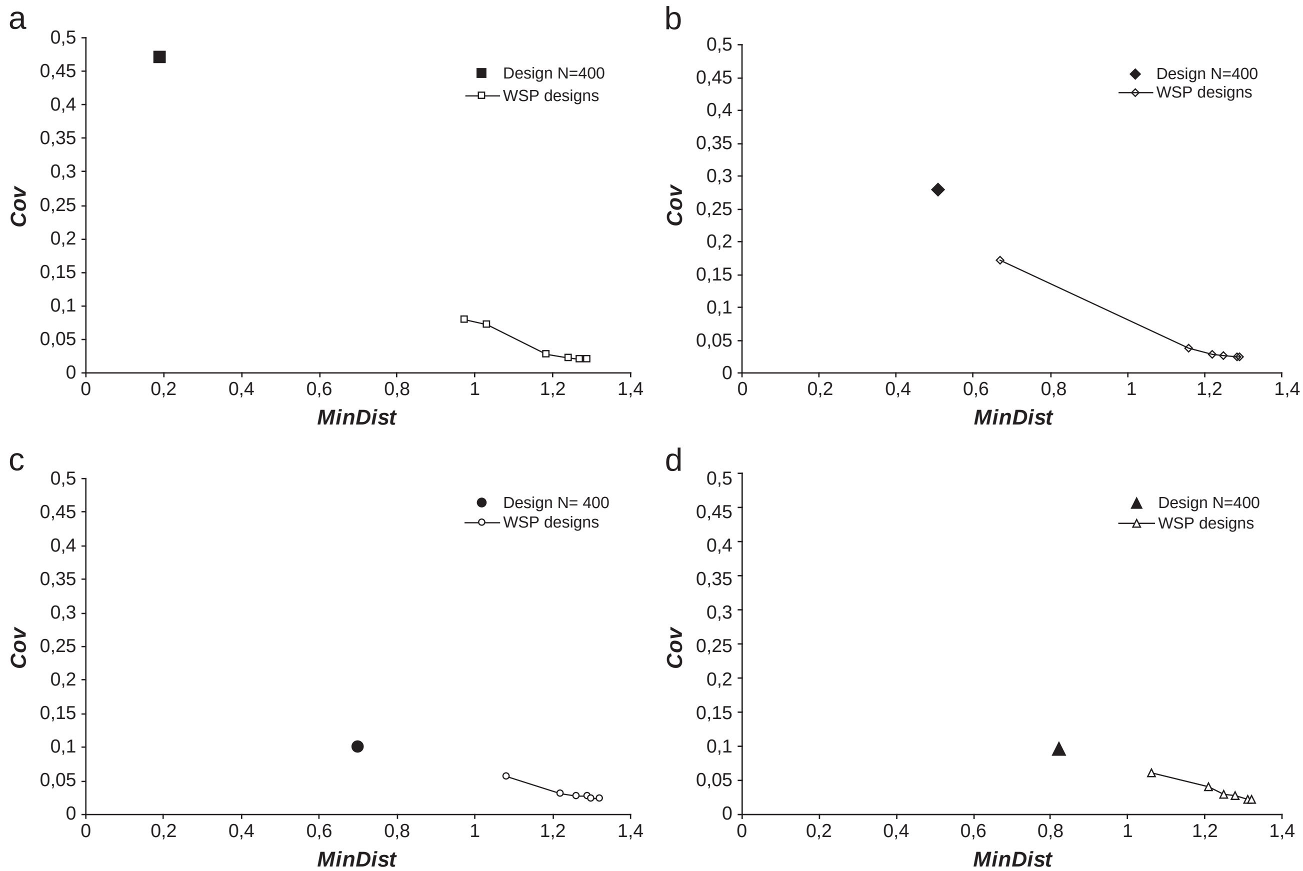

Fig. 4. *MinDist* and *Cov* for designs (N = 400 points) after WSP selection algorithm from four initial distributions: random distribution (a), RLHS design (b), Hammersley sequence (c) and Faure sequence (d), with a variation of the number of points in the initial set from 500 to 3000.

Only some designs can be generated, such as some low discrepancy sequences, but Table 4 and Fig. 6 point out that the designs built by the WSP selection algorithm present better intrinsic quality better than the classical low discrepancy sequences.

3. Conclusion

The space-filling designs are now recognized as suitable for computer experiments, but the main obstacle is the high dimensionality of the problem and the algorithms of classical designs require too long calculations in high dimensions or are not conceivable for some of them. The new space filling designs based on WSP algorithm presented in this paper, propose a set of points uniformly spread in the space selected from a set of candidate points so as to be at a preset minimal distance from every point in the defined multidimendional parameters space already included in the design. The analysis of intrinsic quality criteria of these designs varying the number of points and the type of the candidate set leads to conclude that the type of the initial distribution has no importance if the number of points is sufficient. This conclusion reveals the robustness of the algorithm, even in high dimensional spaces. The comparison of these designs to the classical space-filling designs shows a better quality regarding the

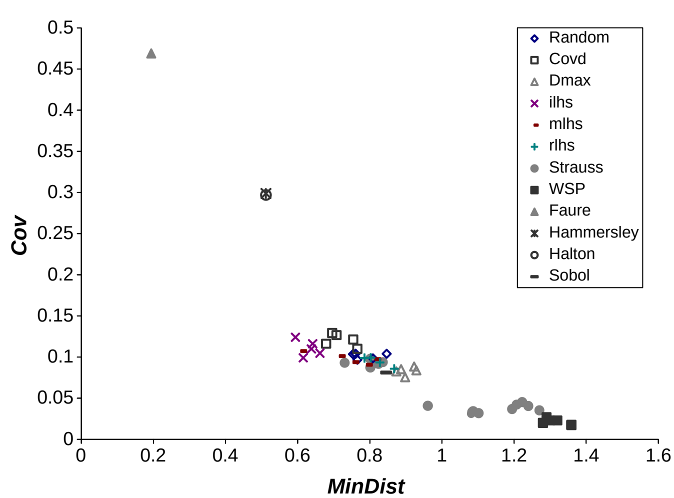

Fig. 5. *MinDist* and *Cov* criteria for different types of space-filling designs (N = 400 points) in a 20 dimensional space.

Table 4
Mindist and *Cov* values for two designs: a low discrepancy Sobol sequence and a design using WSP selection algorithm. The results are presented for two cases, 10 and 20 points per dimension.

Dimension	Number of points of the design	Design	*MinDist* ↗	*Cov* ↘
30D	309	WSP	1.76	0.021
	300	Sobol	1.20	0.077
	605	WSP	1.71	0.022
	600	Sobol	1.20	0.069
40D	398	WSP	1.99	0.022
	400	Sobol	1.42	0.069
	800	WSP	1.94	0.024
	800	Sobol	1.29	0.065
50D	501	WSP	2.22	0.019
	500	Sobol	1.66	0.059
	1000	WSP	2.17	0.022
	1000	Sobol	1.57	0.059

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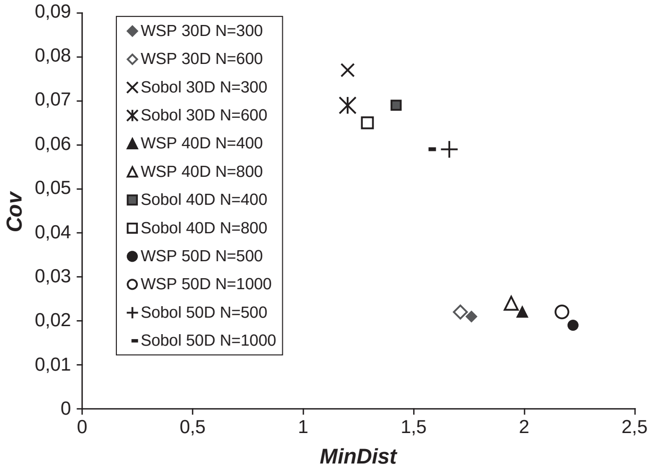

Fig. 6. *MinDist* and *Cov* criteria for Sobol and WSP designs in 30D (N = 300 or 600 points), 40D (N = 400 or 800 points), 50D (N = 500 or 1000 points) spaces.

uniform repartition and the good fill-up of the space. The advantage of this algorithm is the ability to build uniform designs in high dimensional spaces with short calculation time.

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