ON THE USE OF MINIMUM-BIAS COMPUTER EXPERIMENTAL DESIGNS

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ABSTRACT
Computer experimental designs are used to generate data in metamodeling of multiresponse engineering systems. Metamodels, which are also called surrogate models, offer more efficient prediction of system responses but add errors when used as surrogates for the simulators. Error sizes depend on computer experimental designs. Only bias errors are incurred in deterministic computer experiments; however, the majority of experiments reported in the literature are not optimized for minimum bias. Box and Draper–the pioneers of the response surface methodology–originated the work on minimum bias designs in the late 1950's. Space-filling designs such as the Latin hypercubes are mainly in current use; sometimes even in response surface models. This work is a practical study via a number of analytical and electronic circuit examples on the use of minimum bias designs for response surface metamodels. Some minimum bias designs in hypercuboidal spaces are also introduced.

Keywords: Experimental design, minimum bias design, Latin hypercube design, response surface models

1. INTRODUCTION

Computer experimental designs are sampling techniques used to determine combinations of design variables to generate metamodels (also known as surrogate models) of complex engineering systems responses. Different sampling techniques are used to generate metamodels using simulation output for system responses for points in the experimental design. For deterministic simulations, errors introduced by the metamodels are systematic, or bias, errors caused by the deficiency of the metamodel in truly representing the response. Contrary to data in practical experiments, no variance-related error components are present in computer experiments.

Experimental designs can be categorized into classical designs and the more recent space-filling designs (Chen et. al 2006). Classical designs such as factorial designs (Myers and Montgomery 1995) and central composite designs (Box and Wilson 1951) are primarily used in response surface modeling methods. Space-filling designs such as the Latin hypercube designs (Mckay, Beckman, and Conover 1979) aim at uniformly scattering the points over the design variables space.

Different system response complexities require different metamodel types in order to adequately accommodate the underlying behavior and reduce bias errors. Hence, different metamodel types exist depending on the underlying response. Response surface models and kriging metamodel types receive much coverage in the current literature on the design and analysis of computer experiments. Other types, considered to be equally competitive in current usage according to (Simpson et al. 2008) include multivariate adaptive splines, radial basis functions, neural networks, and support vector regressors. The study in (Chen et al. 2006) concludes that no one metamodel type stands out. A similar conclusion is made in (Wang 2003), stating that no one metamodel type is definitely superior to others. According to (Goel et. al 2007), the consensus among researchers is that no single metamodel type can be considered the most effective for all responses. Nonetheless, (Wang 2003) also concludes that kriging and second-order polynomial response surfaces are the most intensively investigated metamodels. Based on a Google Scholar search, the work in (Simpson et al. 2008) concludes that response surface models are the favorite methods in structural optimization disciplines. While (Viana and Haftka 2008) conclude in a Google Scholar search that the distinction between metamodels diminished after an initial popularity for response surface and artificial neural networks techniques; they nonetheless acknowledge that response surface models are the favorite techniques in structural optimization.

The review in (Chen et. al, 2006) on the design and modeling of computer experiments investigated experimental design methods and their relation to the various types of metamodels used in computer experiments. The review presented conclusions from attempts by many researches to determine the most appropriate experimental design for the selected metamodel type. Based on their own computational study tests on the available options, (Chen et. al, 2006) conclude that response surface model designs such as the central composite designs and the Box-Behnken designs are "good only" for response surface models, while all other experimental designs (space-filling designs such as the Latin hypercube samples) are appropriate for all metamodels other than the response surface models. It is noteworthy to mention here that minimum bias designs were not included in the review by (Chen et. al 2006).

A Google Scholar search similar to those in (Simpson et al. 2008) and (Viana and Hafka 2008) was conducted in this work in April, 2011. The results are shown in Table 1 for response surface models and in Table 2 for kriging metamodels.

Table 1: Search Results Related to Response Surface Models Using Google Scholar

Search Phrase	Number of Publications	
	2000-2011	2005-2011
approximation OR metamodel OR surrogate AND "response surface"	12800	9090
"experimental design" AND "response surface"	15400	12400
"minimum bias design" AND "response surface"	24	14
"Latin hypercube" AND "response surface"	2210	1720

Table 2: Search Results Related to Kriging Metamodels Using Google Scholar

Search Phrase	Number of Publications	
	2000-2011	2005-2011
approximation OR metamodel OR surrogate AND "kriging"	9360	6790
"experimental design" AND "kriging"	1830	1340
"Latin hypercube" AND "kriging"	1370	1130

The results in Tables 1-2 lead to the following general possible interpretations with regard to experimental designs and metamodeling methods:

- Response surface models of the 1950's still compete with the more recent metamodels such as the kriging type. As seen in Table 1, the number of publications with "response surface" in combination with any of the words approximation, metamodel, or surrogate since 2000 is about 12,800. The majority of these publications (9,090) appeared in the last half of the last decade from 2005 to 2011. The corresponding statistics for "kriging" metamodels are 9,360 for the period 2000-2011, with 6,790 of these publications appearing in the period 2005-2011.
- From the other tables entries, of the 15,400 papers since 2000 having the phrase "response surface" AND "experimental design", only 24 papers mention "minimum bias designs" while 2,210 papers talk about "Latin hypercube" designs. What are the reasons for the unpopularity of minimum bias computer designs? During the times minimum bias designs were presented in articles in the late 1950's and early 1960's (Box and Draper 1959; Draper and Lawrence 1965), experiments were conducted in the laboratories, and hence the reasons for avoiding large experimental designs are obvious. However, the recent space-filling designs used in computer experiments of today can have larger sizes than most of minimum bias designs, so reasons attributed to size for ignoring these designs are ruled out.

There are two main objectives for the work presented in this paper:

- To show that minimum bias computer experimental designs *can potentially* give more accurate response surface models than the widely used space-filling designs of comparable size. This is demonstrated via analytical functions and electronic circuits.
- To introduce some minimum bias computer experimental designs for hypercuboidal spaces of dimensions 2 to 6.

The remainder of this paper is organized as follows: section 2 demonstrates through analytical examples the motives for using minimum bias designs. Section 3 deals with error types due to variance and bias, presenting basis which are subsequently applied to cuboidal design spaces to construct minimum bias designs. Some of these designs are then used in the electronic circuit examples of section 4. Conclusions are given in section 5.

2. MOTIVATION

Sample points in a minimum bias experimental design are located in the design region such that the design's moments satisfy certain conditions as outlined in the next section. In this section, analytic examples are used to demonstrate the superiority vis-à-vis prediction accuracy of metamodels based on minimum bias designs (MBD) in comparison to models derived using other experimental designs such as the Latin hypercube (LHC) designs.

Figure 1 shows four experimental designs used to derive a first-order response surface for the response given in Equation (1):

$$y = 5 + 2x_1 - x_2 + 0.5x_1^2 + 3x_1x_2 + x_2^2 \; ; \; x \in [-1,+1] \quad (1)$$

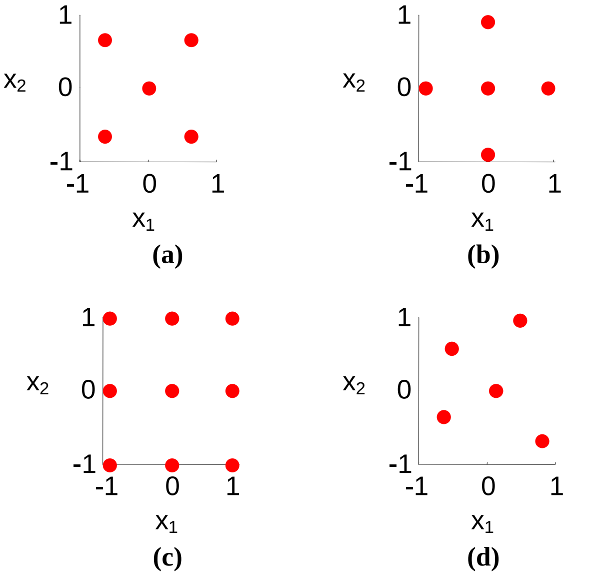

Figure 1: Experimental Designs (a) MBD 1 (b) MBD 2 (c) FAC (d) LHC

Two MBDs are shown in parts (a) and (b); part (c) depicts the standard response surface model design known as factorial design (FAC), and a LHC design is shown in part (d).

Metamodels built using these designs are validated using a 21x21 sample. See Table 3.

Table 3: Validation Results Corresponding to the Four Experimental Designs in Figure 1

Experimental Design	Figure 1 Part	RMSE
MBD 1	a	1.160
MBD 2	b	1.160
FAC	c	1.243
LHC	d	1.381

As shown in the table, the lowest root mean square error (RMSE) is obtained using any of the two MBDs. To demonstrate the relation between RMSEs for MBDs and LHCs, 100 metamodels are fitted using 100 different LHC samples. RMSEs for these metamodels are compared to the RMSE obtained if a MBD is used; see Figure 2. In the figure, the RMSEs shown are normalized to the RMSE for the MBD (the dotted line at 1.0).

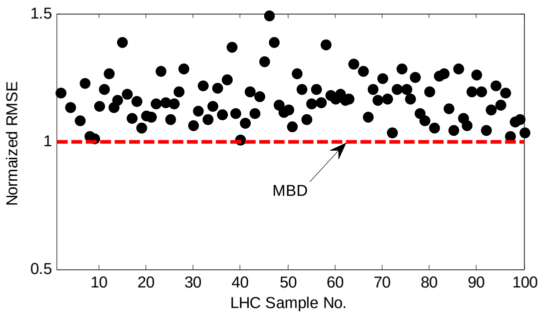

Figure 2: Normalized RMSEs for 100 LHC Designs.

The results depicted in the figure clearly demonstrate the superiority of MBDs. Unfortunately, this is not always the case. To illustrate, the above metamodeling activities are repeated for the response in Equation (2) (see Figure (3) for function plot):

$$y = \sum_{i=1}^{9} a_i (x-900)^{i-1} \quad ; \quad x \in [905,995] \qquad (2)$$

where $a_1 = -659.23$, $a_2 = 190.22$, $a_3 = -17.802$, $a_4 = 0.82691$, $a_5 = -0.01885$, $a_6 = 0.0003463$, $a_7 = -3.2446 \times 10^{-6}$, $a_8 = 1.6606 \times 10^{-8}$, and $a_9 = -3.5757 \times 10^{-11}$.

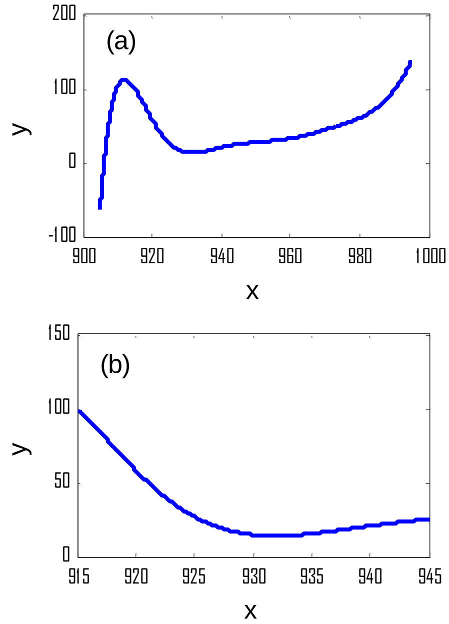

Figure 3: Function Plot for $y(x)$ in Equation (2) for: (a) $x \in [905,995]$ (b) $x \in [915,945]$

In Figure (4) RMSEs for 100 different metamodels built using 100 different LHC samples are compared to the RMSE for the metamodel derived using a MBD (each LHC sample has the same size as the MBD).

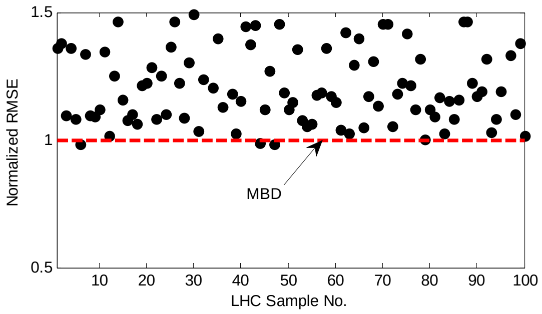

Figure 4: Normalized RMSEs for 100 LHC Designs for the Function in Figure 3(a).

The figure shows that RMSE for the MBD case is not always lower (a few points are below the dotted line at 1.0 corresponding to the normalized RMSE for the MBD). However, for most of the 100 LHC samples, their RMSEs are worse by comparison to the MBD sample. The reason for the discrepancy between results of the similar metamodeling activities summarized by Figures 2 and 4 are attributed to the underlying response being modeled. As it will be shown, MBDs result in least errors provided the underlying assumptions for deriving MBDs are satisfied. Usually, the derivation assumes that the complexity of the response is such that it is higher than the response surface metamodel that fits it by one order; e.g., the response follows a third-order polynomial if the metamodel fitted is a second-order polynomial. Obviously, as the design variables space narrows down, such assumption about orders becomes more valid (see Figure 3). This is demonstrated in Figure 5, which is similar to Figure 4 except now the design space for the response is narrowed down to $x \in [915,945]$ from $x \in [905,995]$ in Equation (2).

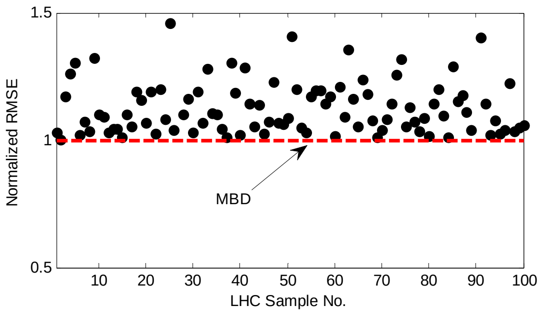

Figure 5: Validation Results for the Function in Figure 3(b).

3. MINIMUM BIAS DESIGNS

There are two sources for errors in metamodels: (i) noise in the experimental design data used to fit the metamodel; and (ii) inadequacy of the metamodel. Accordingly, errors are categorized as: (i) variance, and (ii) bias errors, respectively. In practical experiments, variance errors are the assumed error source while bias errors are the only source of errors in computer experiments.

Standard response surface designs such as the central composite designs are derived ignoring bias errors; i.e., derivations in this case assume that the fitted metamodel adequately represents the response. In minimum bias designs, however, it is customary to assume that the true response is a one-order higher polynomial than the metamodel. Thus, if the metamodel is a second-order polynomial then the MBD is derived assuming a third-order polynomial response.

There is no intention in this paper to provide rigorous mathematical treatment for MBD derivations. Such derivations originated in the pioneering work by Box and Drapper in 1950's (Box and Draper 1959), with more recent treatment in (Goel et. al 2008) and (Abdelbasit and Butler 2006). The results are presented in terms of satisfying the necessary and sufficient conditions for MBD derivation in terms of the so-called design moments.

(Draper and Lawrence 1965) applied the above mathematical conditions in (Box and Draper 1959) to derive MBDs for cuboidal regions. They used parameterized experimental design sets to build first and second-order MBDs. However, many of the tabulated results involve sets with parameters outside the assumed coded design space boundaries. This may be inappropriate in many practical engineering system design problems; for example, negative transistor widths cannot be implemented in practice.

Our work (also for cuboidal design spaces) involves the parameterized experimental design sets mentioned shortly later on in this section. However, solutions for the parameters resulting in practical MBD sets (i.e., with none of the parameters outside the design space) are taken when the mathematical conditions related to design moments are applied. The sets are used to construct second and third-order MBDs.

Consider a k-dimensional space with design (input) variables $x_1, x_2, ..., x_k$. It is assumed that the space is coded such that $-1 \le x_1, x_2, ..., x_k \le +1$. Second and third-order MBDs in our work are constructed using combinations of the following sets: $C(0^k)$, $F(\alpha^k)$, and $S(\alpha^a, \beta^{k-a})$. Explanation for this notation is provided in Table 4.

Table 4: Notation Used

Notation	Meaning	#points	Notes
$C(0^k)$	a design point at the center	1	$x_1 = ... = x_k = 0$
$F(\alpha^k)$	factorial design	2^k	See Table 5 for $k = 3$
$S(\alpha^a, \beta^{k-a})$	All k permutations of factorial designs with a variables at α and $k-a$ variables at β	$k2^k$	See Table 6 for $k = 3$

Table 5: $F(\alpha^k)$ Factorial Design for $k = 3$

$x_1 = \pm\alpha$	$x_2 = \pm\alpha$	$x_3 = \pm\alpha$
$-\alpha$	$-\alpha$	$-\alpha$
$-\alpha$	$-\alpha$	$+\alpha$
$-\alpha$	$+\alpha$	$-\alpha$
$-\alpha$	$+\alpha$	$+\alpha$
$+\alpha$	$-\alpha$	$-\alpha$
$+\alpha$	$-\alpha$	$+\alpha$
$+\alpha$	$+\alpha$	$-\alpha$
$+\alpha$	$+\alpha$	$+\alpha$

Table 6: $S(\alpha^a, \beta^{k-a})$ Design for $k = 3$ with $a = 1$

$x_1 = \pm\alpha$, $x_2 = \pm\beta$, $x_3 = \pm\beta$			$x_1 = \pm\beta$, $x_2 = \pm\alpha$, $x_3 = \pm\beta$			$x_1 = \pm\beta$, $x_2 = \pm\beta$, $x_3 = \pm\alpha$		
x_1	x_2	x_3	x_1	x_2	x_3	x_1	x_2	x_3
$-\alpha$	$-\beta$	$-\beta$	$-\beta$	$-\alpha$	$-\beta$	$-\beta$	$-\beta$	$-\alpha$
$-\alpha$	$-\beta$	$+\beta$	$-\beta$	$-\alpha$	$+\beta$	$-\beta$	$-\beta$	$+\alpha$
$-\alpha$	$+\beta$	$-\beta$	$-\beta$	$+\alpha$	$-\beta$	$-\beta$	$+\beta$	$-\alpha$
$-\alpha$	$+\beta$	$+\beta$	$-\beta$	$+\alpha$	$+\beta$	$-\beta$	$+\beta$	$+\alpha$
$+\alpha$	$-\beta$	$-\beta$	$+\beta$	$-\alpha$	$-\beta$	$+\beta$	$-\beta$	$-\alpha$
$+\alpha$	$-\beta$	$+\beta$	$+\beta$	$-\alpha$	$+\beta$	$+\beta$	$-\beta$	$+\alpha$
$+\alpha$	$+\beta$	$-\beta$	$+\beta$	$+\alpha$	$-\beta$	$+\beta$	$+\beta$	$-\alpha$
$+\alpha$	$+\beta$	$+\beta$	$+\beta$	$+\alpha$	$+\beta$	$+\beta$	$+\beta$	$+\alpha$

MBDs for $k = 2-6$ (generated by applying the sufficient and necessary conditions in the references mentioned at the beginning of this section to the above design sets) are given in Table 7 for second-order MBDs and in Table 8 for third-order designs. Add one center point $C(0^k)$ for each row in the tables to complete the MBD.

Table 7: Second-Order MBDs

k	$F(\alpha^k)$	$S(\alpha^a, \beta^{k-a})$		
	α	α	β	a
2	-	0.418	0.759	1
3	-	0.816	0.434	1
4	-	0.868	0.448	1
5	-	0.913	0.460	1
6	0.620	0.973	0.450	1

Table 8: Third-Order MBDs

k	$F(\alpha^k)$	$S_1(\alpha^a, \beta^{k-a})$			$S_2(\alpha^a, \beta^{k-a})$		
	α	α	β	a	α	β	a
2	0.685	0.255	0.741	1	-	-	-
3	-	0.775	0.252	1	0.378	0.763	1
4	-	0.844	0.305	1	0.202	0.743	1
5	0.724	0.801	0.311	1	-	-	-
6	-	0.951	0.287	1	0.194	0.742	1

Note that the size of second-order MBDs in Table 7 is $1 + k2^k$ points for $k \le 5$.

4. APPLICATION TO ELECTRONIC CIRCUIT MODELING

In this section two electronic circuits are modeled using MBDs and the results are compared to LHC designs. The two circuits are the amplifier and filter in Figure 6.

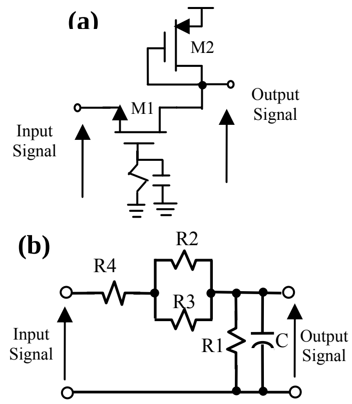

Figure 6: Two Electronic Circuits: (a) Amplifier (b) Filter.

The gain (the ratio of output signal to the input signal) $A_{amplifier}$ of the amplifier, and the maximum gain A_{filter} and bandwidth BW_{filter} of the filter are modeled using the appropriate MBDs in Table 7, with $k = 2$ for the amplifier and $k = 5$ for the filter. Figure 7(a) shows RMSE comparisons for $A_{amplifier}$ for the region $W_1 \in [2,200]$ and $W_2 \in [2,200]$, where W_1 and W_2 are the width of the two amplifier transistors M1 and M2 in Figure 6(a). When the space is narrowed down to $W_2 \in [2,20]$ for W_2, RMSEs become worse (by comparison to RMSE for the MBD) for more of the 100 LHC samples as demonstrated in part (b) of Figure 7. This is expected as demonstrated earlier for the function in Figure (3).

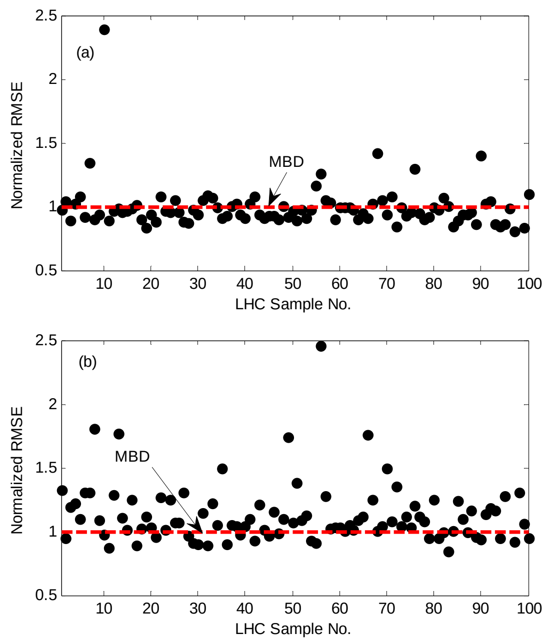

Figure 7: Results for the Amplifier Circuit: (a) for the Region $W_1 \in [2,200]$ and $W_2 \in [2,200]$ (b) for the Narrower Region $W_1 \in [2,200]$ and $W_2 \in [2,20]$.

Results for RMSEs for the filter circuit are shown in Figure 8. Note that while the results give advantage for the MBD for A_{filter} as shown in part (a); however, part (b) of the figure shows that RMSEs for the LHC samples are lower for BW_{filter}. This is the worst case obtained in our work. Nonetheless, even for this case the RMSE for all 100 LHC samples is nearly 90% on average of the RMSE obtained using MBD as can be inferred from Figure 8(b).

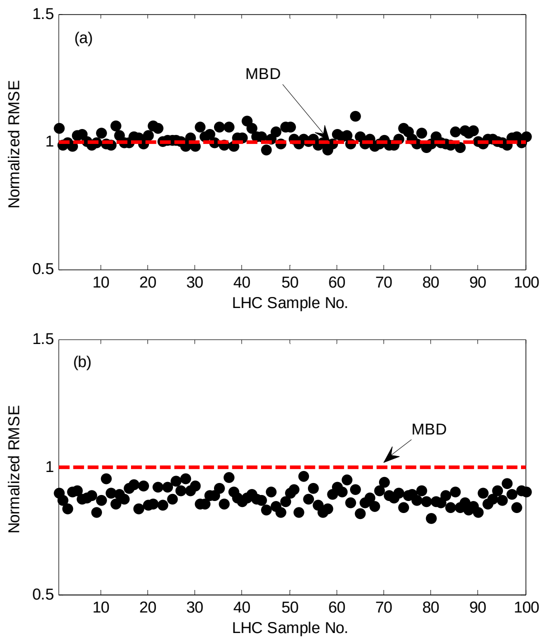

Figure 8: Results for the Filter Circuit: (a) A_{filter} (b) BW_{filter}.

5. CONCLUSIONS

Metamodels are appropriate surrogates for simulators in the design of complex engineering systems provided that the errors incurred are acceptable. Bias errors due to metamodel inadequacy result in inaccurate metamodels when computer experimental data are used to construct these metamodels. This paper demonstrated that minimum bias computer experimental designs are potentially superior in response surfaces by comparison to space-filling designs such as the popular Latin hypercube samples. Also, the paper introduced minimum bias designs for normalized hypercuboidal spaces. The list of these designs is by no means exhaustive, and more work is needed to expand the list for higher-dimension spaces and higher-order minimum bias designs.

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