

Search for minimum aberration designs with uniformity

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Abstract

Uniform designs have been widely applied in engineering and sciences' innovation. When a lot of quantitative factors are investigated with as few runs as possible, a supersaturated uniform design with good overall and projection uniformity is needed. By combining combinatorial methods and stochastic algorithms, such uniform designs with flexible numbers of columns are constructed in this article under the wrap-around L_2 -discrepancy. Compared with the existing designs, the new designs and their two-dimensional projections not only have less aberration, but also have lower discrepancy. Furthermore, some novel theoretical results on the minimum-aberration, uniform and uniform projection designs are obtained.

Keywords Discrepancy · Projection · Stochastic algorithm · Uniform design

1 Introduction

In many industrial, scientific, medical and engineering innovations, experiments with a large number of quantitative factors but limited resources occur frequently. One of the most critical problems in such experiments is to effectively screen out the variables that have the most substantial effect on the responses so that better statistical models can be consequently obtained. To achieve this goal, constructing good experimental designs with high factor-to-run ratios in advance is of particular importance. How to efficiently construct designs for such experiments is a challenging problem.

Uniform designs (UDs) are common choices in various fields of experiments due to their robust performances (Fang et al. 2006a). The main idea of uniform designs is to scatter the design points uniformly among the experimental domain

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by minimizing a measure called discrepancy. Among many discrepancies, the centered L_2 -discrepancy, the wrap-around L_2 -discrepancy (Hickernell 1998a, b) and the mixture discrepancy (Zhou et al. 2013) are the most popular ones and constructions of the corresponding uniform designs have been paid much attention by researchers recently. Traditional construction methods of uniform designs can be broadly classified into two categories—combinatorial methods and algorithmic optimizations. The former require no or little computation but are restricted to only a few special parameters, whereas the latter can be applied in general cases but usually suffer from heavy computational burden when the target design is large. On the UD homepage (http://web.stat.nankai.edu.cn/cms-ud/UD/UniformDesign.html), one can find many designs produced by the threshold-accepting algorithm described in Fang et al. (2006b), but these designs do not have large numbers of runs or columns.

The (generalized) minimum aberration (MA for short, see Xu and Wu 2001) criterion is commonly used for fractional factorials. Recently, Tang et al. (2012), Tang and Xu (2013) and Zhou and Xu (2014) have showed that for a fractional factorial design, when all possible level permutations are considered, the average discrepancy is linearly connected with the generalized wordlength pattern (Xu and Wu 2001). Therefore, MA designs tend to have lower discrepancies on average. Based on this theory, these authors proposed the level permutation method and efficiently obtained many unsaturated and saturated uniform designs from orthogonal arrays with less aberration.

The vast majority of the literature on the construction of uniform designs, including the work mentioned above, mainly considers unsaturated and saturated cases. Supersaturated designs have received much attention in the past two decades because of their run size economy and mathematical novelty (Ai et al. 2007). Obviously, uniformity can be used to assess and optimize supersaturated designs. Uniform supersaturated designs provide a solution for the aforementioned scenario of interest in this article, i.e., when there are many quantitative factors, when experimentation is relatively expensive, and when the effect sparsity principle holds. However, to the best of our knowledge, few studies have addressed the construction of uniform supersaturated designs. Fang et al. (2002) constructed multi-level uniform supersaturated designs under a discrete discrepancy, but his designs are only suitable for experiments involving nominal factors. For experiments with quantitative inputs where other discrepancies like the centered L_2 -discrepancy and the wrap-around L_2 -discrepancy are more appropriate, Fang et al. (2017) proposed an adjusted threshold-accepting algorithm to construct supersaturated uniform designs. Their method takes the column juxtaposition of an orthogonal array D_a and a balanced design D_b as the starting design, then iteratively updates D_b while keeping D_a unchanged, with the goal of minimizing the discrepancy of the whole design. Finally, level permutations are performed for both D_a and D_b to reduce the discrepancy further. This approach is flexible, but quickly becomes ineffective when the number of columns in D_h increases.

This article presents a new efficient approach to constructing uniform supersaturated designs which can accommodate a larger number of columns. Roughly speaking, our method can be decomposed into two steps. The first step constructs supersaturated MA designs with many columns by combining both combinatorial



methods and an algorithmic optimization. The second step permutes the levels of designs constructed in the first step to further reduce their discrepancies. Section 2 reviews the uniformity, projection uniformity and MA criteria. Sections 3 and 4 are devoted to the two steps of the proposed new design method, respectively. More specifically, Sect. 3 proposes a local search heuristic algorithm for searching MA designs with a more flexible number of columns, and also constructs several classes of supersaturated MA designs in explicit form with generalized Hadamard matrices and saturated mixed orthogonal arrays. Section 4 obtains supersaturated uniform designs through level permutations. Additionally, in this section, a numerical comparison with the adjusted threshold-accepting algorithm by Fang et al. (2017) is also given. Section 5 concludes with some remarks, and Appendix contains all technical proofs. Throughout, we focus on the wrap-around L_2 -discrepancy as the measure of uniformity, but it is worth mentioning that the method can be similarly extended to other discrepancies.

2 Uniformity, projection uniformity and minimum aberration

This section gives a brief review of the criteria used in our uniform supersaturated design construction. We call an $N \times n$ matrix D an orthogonal array with N runs, n factors and strength t ($n \ge t \ge 1$), denoted by $OA(N, s^n, t)$, if each column of D has s levels from a set of s elements, say $\{0, \ldots, s-1\}$, such that all possible level combinations occur equally often as rows in every $N \times t$ submatrix. Typically, an $OA(N, s^n, 1)$ is called a balanced design and referred to as an (N, s^n) -design for brevity. An (N, s^n) -design is saturated if N - 1 = n(s - 1) and supersaturated if N - 1 < n(s - 1).

Uniformity under the wrap-around L_2 -discrepancy is a popular measure of space-fillingness in both computer and physical experimental designs. By Hickernell (1998a), the wrap-around L_2 -discrepancy of an (N, s^n) -design $D = (d_{i,j})$ can be expressed as

$$\mathrm{WD}(D) = -\left(\frac{4}{3}\right)^n + \frac{1}{N^2} \sum_{i_1=1}^N \sum_{i_2=1}^N \prod_{j=1}^n \left[\frac{3}{2} - \frac{1}{s} |d_{i_1,j} - d_{i_2,j}| + \frac{1}{s^2} (d_{i_1,j} - d_{i_2,j})^2\right].$$

Throughout, a design D is said to be *uniform* if it has the minimum wrap-around L_2 -discrepancy.

An *n*-dimensional uniform design focuses on good one-dimensional projections as well as *n*-dimensional uniformity. Sun et al. (2019) proposed the uniform projection criterion to optimize the two-dimensional projection uniformity. Similar to Sun et al. (2019), the *uniform projection criterion* under the wrap-around L_2 -discrepancy is defined as

$$PWD(D) = \frac{2}{n(n-1)} \sum_{|v|=2} WD(D_v),$$
 (1)



where v is a subset of $\{1, 2, ..., n\}$, |v| denotes the cardinality of v and D_v is the projection design of D onto dimensions indexed by the elements of v. The PWD defined in (1) is the average WD value of all two-dimensional projections of D. A design D achieving the minimum PWD(D) value is a *uniform projection design*.

Minimum aberration is the standard criterion for evaluating fractional factorial designs aiming at minimizing the aliasing of higher-order interactions on the main effects. Let D be an (N, s^n) -design. Consider the ANOVA model

$$Y = X_0 \alpha_0 + X_1 \alpha_1 + \dots + X_n \alpha_n + \epsilon,$$

where *Y* is the vector of *N* responses, α_0 is the intercept, X_0 is an $N \times 1$ vector of 1's, α_1 is the vector of all main effects, α_j ($j \ge 2$) is the vector of all *j*-factor interactions, X_j is the matrix of orthonormal contrast coefficients for α_j , and ϵ is the random error. Denote $n_j = (s-1)^j \binom{n}{j}$ and $X_j = (x_{ik}^{(j)})_{N \times n_j}$, then the generalized wordlength pattern of the design *D* can be defined by

$$A_j(D) = N^{-2} \sum_{k=1}^{n_j} \left| \sum_{i=1}^N x_{ik}^{(j)} \right|$$
 for $j = 0, \dots, n$.

It is obvious that $A_0(D)=1$ by definition. For two designs $D^{(1)}$ and $D^{(2)}$, $D^{(1)}$ is said to have less aberration than $D^{(2)}$ if there exists an integer $r\in\{1,2,\ldots,n\}$, such that $A_r(D^{(1)}) < A_r(D^{(2)})$ and $A_i(D^{(1)}) = A_i(D^{(2)})$ for $i=1,\ldots,r-1$. $D^{(1)}$ is said to have (generalized) *minimum aberration* (MA) if there is no other design with less aberration than $D^{(1)}$.

3 Search for MA designs

Our method constructs and optimizes a supersaturated design under the MA criterion in the first step and focuses on the uniformity and projection uniformity in the second step. This section is devoted to the first step of the construction.

3.1 A local search heuristic algorithm

For an (N, s^n) -design D, denote $\delta^D_{i_1, i_2}$ as the coincidence number of the i_1 th and i_2 th rows of D, i.e., the number of positions where rows i_1 and i_2 take the same value. We obtain a theoretical result which transforms the problem of searching MA designs into an optimization problem.

Theorem 1 An (N, s^n) -design D has MA if and only if there exists a constant c > 0 such that for any $z \in (1, 1 + c)$, D is a solution to the optimization problem of minimizing



$$\phi_z(D) = \sum_{1 \le i_1 < i_2 \le N} z^{\delta^D_{i_1, i_2}}.$$
 (2)

Theorem 1 can be proved using Lemma A.2 in Tang et al. (2012), and the details are postponed to Appendix. This result is of great practical value as it simplifies the original multi-objective optimization MA searching problem to a single objective $\phi_{\tau}(D)$ -function minimization problem.

Based on Theorem 1, the lower bound of $\phi_z(D)$ is obtained as follows.

Theorem 2 For an (N, s^n) -design D and any z > 1,

$$\phi_{z}(D) \ge h(z, nN(N-s)/(2s), N(N-1)/2),$$

where $h(z, M, m) = z^{\lfloor M/m \rfloor} (m \lfloor M/m \rfloor + m - M) + z^{\lfloor M/m \rfloor + 1} (M - m \lfloor M/m \rfloor), \lfloor x \rfloor$ is the largest integer not exceeding x. The equality holds if and only if the difference among all δ_{i_1, i_2}^D , $i_1 < i_2$, does not exceed one.

When solving the optimization problem (2) with an appropriately selected z, MA or nearly MA designs with any number of columns can be obtained. Now we propose a local search heuristic algorithm, referred to as Algorithm 1, for solving this optimization problem. Let τ be the number of iterations, and T_1, \ldots, T_{τ} be the sequence of the thresholds. Choose $\tau = IJ$, where I and J are the numbers of outer and inner iterations, respectively. Then, the sequence of the thresholds is determined as follows: $T_1 = \cdots = T_J$, $T_{J+1} = \cdots = T_{2J} = \gamma T_1$, $T_{2J+1} = \cdots = T_{3J} = \gamma^2 T_1$, and so on, where $\gamma = (T_{\tau}/T_1)^{\overline{J-1}}$. Here, the values $T_1 = 0.01$ and $T_{\tau} = 10^{-6}$ are chosen as default for the initial and terminal thresholds, respectively. In each iteration, assume that the design \widetilde{D} is obtained by exchanging $d_{i,j}$ and $d_{i,j}$ ($d_{i,j} \neq d_{i,j}$) of the current design D. Let $v_1 = \{r : d_{rj} = d_{i,j} \text{ and } r \neq i_1\}$ and $v_2 = \{r : d_{rj} = d_{i,j} \text{ and } r \neq i_2\}$ for convenience. Then a one-point update formula for

$$\nabla = \phi_{\tau}(\widetilde{D}) - \phi_{\tau}(D)$$

can be simplified to

$$\nabla = (z - 1) \left[\sum_{r \in v_1} \left(z^{\delta_{i2,r}^D} - z^{\delta_{i_1,r}^D - 1} \right) + \sum_{r \in v_2} \left(z^{\delta_{i_1,r}^D} - z^{\delta_{i_2,r}^D - 1} \right) \right]. \tag{3}$$

It is easy to calculate that the complexity of each iteration is only O(N/s). As a comparison, the adjusted threshold-accepting algorithm proposed by Fang et al. (2017) iteratively optimizes D_b to minimize the discrepancy of the whole design $D = (D_a, D_b)$, and the corresponding complexity of ∇ in each iteration is O(N). During the iterations, once the lower bound in Theorem 2 is achieved, the process will be terminated.



Algorithm 1 The stochastic algorithm for searching an MA or nealy MA (N, s^n) -design

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1: Initialize \tau, z and the sequence of thresholds T_1, \ldots, T_\tau \in (0, 1).

2: Let D^{(0)} be an MA (N, s^{n_0})-design and D^{(1)} be a random (N, s^{n-n_0})-design. Take D = (D^{(0)}, D^{(1)}) as the column juxtaposition of D^{(0)} and D^{(1)}.

3: Let D^{\min} := D. Compute \phi_z(D).

4: for i = 1 to \tau do

5: Generate a new design \widetilde{D} \in \mathcal{N}(D|D^{(0)}) and compute \nabla = \phi_z(\widetilde{D}) - \phi_z(D).

6: if \nabla < \phi_z(D) \cdot T_i, then let D = \widetilde{D}.

7: if \phi_z(D) < \phi_z(D^{\min}), then let D^{\min} := D.

8: end for
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Traditional local search heuristic algorithm (see Fang et al. 2006b) needs to optimize all columns, which leads to too large search space. The results are often stuck in bad local optimums, especially when the number of columns is large. In order to improve efficiency, we use a new neighborhood in Algorithm 1. Let D be an (N, s^n) -design. Let $D = (D^{(0)}, D^{(1)})$ be a column partition of D such that $D^{(0)}$ consists of the first n_0 columns and $D^{(1)}$ consists of the remaining $n - n_0$ columns. The new neighborhood set, called neighborhood of D given $D^{(0)}$ and denoted by $\mathcal{N}(D|D^{(0)})$, is defined to be the set of all designs obtained from D through exchanging two distinct elements within the same column of $D^{(1)}$. Here, $D^{(0)}$ is taken as an MA design with as many columns as possible, and only $D^{(1)}$ is updated in the iterative process. Utilizing such a new neighborhood can help reduce the size of searching space significantly.

From Theorem 1, when z-1 is positive and small enough, the solution to the optimization problem (2) is just an MA design. At the same time, when z is too close to 1, the difference between distinct $\phi_z(D)$ values will be tiny. As the computational error accumulates during the iterative process, the algorithm may fail. By testing many different values, we eventually recommend taking z in the interval (1.1, 1.2).

3.2 Some theoretical results

Algorithm 1 starts with an (N, s^n) -design D which is comprised of an MA (N, s^{n_0}) -design matrix $D^{(0)}$ and a random (N, s^{n-n_0}) -design. A key point in this algorithm is that we should choose an appropriate MA design $D^{(0)}$. It follows that the number of columns of $D^{(0)}$ determines the number of remaining columns that need to be optimized and therefore determines the size of searching space. The larger the number n_0 is, the smaller the searching space of $D^{(1)}$ becomes. For large searching space, the algorithm needs more iterations and longer running time and is more likely to get stuck in bad local optimums. To avoid this situation, $D^{(0)}$ should be taken as an MA design with as many columns as possible. In this subsection, we provide some theoretical results and combinatorial constructions of MA designs with as many columns as possible.

The first construction is based on generalized Hadamard matrices, which is a special class of difference schemes. An $N \times n$ difference scheme, denoted by



D(N, n, s), is an array with entries from an abelian group \mathcal{A} of s elements, such that every element of \mathcal{A} appears equally often in the vector difference between any two columns of the array. In particular, a D(N, N, s) is also called a generalized Hadamard matrix. Because the entries are from some abelian group \mathcal{A} . When \mathcal{A} is not $\{0, 1, ..., s-1\}$, one should convert these symbols to $\{0, 1, ..., s-1\}$ after the construction of MA designs. No conversion is necessary if $\mathcal{A} = \{0, 1, ..., s-1\}$.

Let D' be a generalized Hadamard matrix D(N, N, s). Note that subtracting any column from each column of D' also yields a D(N, N, s). Without loss of generality, assume D' has the form

$$D' = \left[\mathbf{0}_N, D_0\right],\,$$

where $\mathbf{0}_N$ is the vector of N zeros. It follows from the proof of Theorem 6.5 of Hedayat et al. (1999) that the transpose of D' is again a D(N, N, s). As a consequence, $\delta_{i_1,i_2}^{D_0} = N/s - 1$ for any $i_1 < i_2$. By Theorems 1 and 2, D_0 is an MA (N, s^{N-1}) -design. Let D_1, \ldots, D_k be k (N, s^{N-1}) -designs generated by randomly permuting rows of D_0 and $D = (D_1, \ldots, D_k)$ be their column juxtaposition. Simple calculation shows that $\delta_{i_1,i_2}^D = k(N/s - 1)$ for any $i_1 < i_2$, which implies D is an MA design. Moreover, adding one balanced column to or removing one column from D also results in an MA design. We summarize the above results in the following theorem.

Theorem 3 If a generalized Hadamard matrix D(N, N, s) exists, then for any integer $k \ge 1$, there exists an MA (N, s^n) -design, where n = k(N - 1) or $n = k(N - 1) \pm 1$.

Theorem 3 is actually constructive. Consider the case of s being a power of a prime p, say $s = p^u$, $u \ge 1$. From Theorem 6.6 of Hedayat et al. (1999), there exists a $D(p^m s, p^m s, s)$ for any integer $m \ge 0$. By using Corollary 6.39 and Theorem 6.63 of Hedayat et al. (1999), there also exist a $D(2s^m, 2s^m, s)$ and a $D(4s^m, 4s^m, s)$ for any integer $m \ge 1$. If q is a prime power and a difference scheme D(q+1,q+1,s) exists, then by Theorem 6.64 of Hedayat et al. (1999), there exists a $D(q^m(q+1),q^m(q+1),s)$ for any integer $m \ge 0$. Combining these facts with Theorem 3, a large number of MA designs can be immediately obtained.

It is known that there exists a difference scheme D(s, s, s) for any prime power s. Let D_1 be a saturated $OA(N, s^q, 2)$ and D_2 be a difference scheme D(s, k, s), $2 \le k \le s$, without identical rows, both with entries from the Galois field GF(s). From Corollary 1 of Sun et al. (2011), the Kronecker sum $D_1 \oplus D_2^T$ is a (kN, s^{qs}) -design with coincidence numbers being q and q-1, and thus is an MA design by Theorem 2. We summarize all the above results in the following corollary.

Corollary 1 Suppose p is a prime and $s = p^u$ is a prime power with $u \ge 1$.

(i) For any $m \ge 0$ and $k \ge 1$, there exists an MA $(p^m s, s^n)$ -design, where $n = k(p^m s - 1)$ or $n = k(p^m s - 1) \pm 1$.



(ii) For any $m \ge 1$ and $k \ge 1$, there exists an MA $(2s^m, s^n)$ -design, where $n = k(2s^m - 1)$ or $n = k(2s^m - 1) \pm 1$.

- (iii) For any $m \ge 1$ and $k \ge 1$, there exists an MA $(4s^m, s^n)$ -design, where $n = k(4s^m 1)$ or $n = k(4s^m 1) \pm 1$.
- (iv) If q is a prime power and a generalized Hadamard matrix D(q+1,q+1,s) exists, then for any $m \ge 0$ and $k \ge 1$, there exists an MA $((q+1)q^m, s^n)$ -design, where $n = k((q+1)q^m 1)$ or $n = k((q+1)q^m 1) \pm 1$.
- (v) For any $m \ge 2$ and $2 \le k \le s$, there exists an MA (ks^m, s^n) -design, where $n = s(s^m 1)/(s 1)$.

The following result is an immediate corollary of Corollary 1 (iv).

Corollary 2 If s and s-1 are both prime powers, then for any $m \ge 0$ and $k \ge 1$, there exists an MA $((s-1)^m s, s^n)$ -design, where $n = k((s-1)^m s - 1)$ or $n = k((s-1)^m s - 1) \pm 1$.

The second construction uses saturated mixed orthogonal arrays. A mixed orthogonal array with N runs, n_1 factors at s_1 level, n_2 factors at s_2 level and strength t, denoted by $OA(N, s_1^{n_1} s_2^{n_2}, t)$, is an $N \times (n_1 + n_2)$ matrix in which every $N \times t$ submatrix contains all possible level combinations as rows with the same frequency. An $OA(N, s_1^{n_1} s_2^{n_2}, t)$ is called saturated if and only if $N - 1 = n_1(s_1 - 1) + n_2(s_2 - 1)$.

Suppose $s \ge 3$ is a prime power. From Theorem 6.33 of Hedayat et al. (1999), there exists a generalized Hadamard matrix D(2s, 2s, s), say D'. By using D', a saturated mixed $OA(2s^2, s^{2s}(2s)^1, 2)$, say D_1 , can be constructed from Theorem 9.15 of Hedayat et al. (1999). After replacing the 2s-level factor of D_1 with another two or three specific s-level factor, an MA $(2s^2, s^{2s+2})$ - or $(2s^2, s^{2s+3})$ -design can be obtained. From Theorem 8 of Xu and Wu (2005), there also exists an MA $(2s^2, s^{s^2+s})$ -design, denoted by D_2 . If s is even, by appending an s-level factor to D_2 , we can get another MA $(2s^2, s^{s^2+s+1})$ -design. Combining these facts with Corollary 1 (ii), a large number of MA $(2s^2, s^n)$ -designs can be constructed.

Theorem 4 For any prime power $s \ge 3$ and $k \ge 0$, there exists an MA $(2s^2, s^n)$ -design, where $n = k(2s^2 - 1) + 2s + 2$, $k(2s^2 - 1) + 2s + 3$ or $k(2s^2 - 1) + s^2 + s$. In particular, if s is even, there also exists an MA $(2s^2, s^n)$ -design, where $n = k(2s^2 - 1) + s^2 + s + 1$.

By Theorems 3, 4 and Corollaries 1, 2, many supersaturated MA designs can be constructed in explicit form. For example, for any $k \ge 1$, MA $(18, 3^n)$ -designs with n = 17k - 9, 17k - 8, 17k - 5, 17k - 1, 17k, 17k + 1 and MA $(32, 4^n)$ -designs with n = 31k - 21, 31k - 20, 31k - 11, 31k - 10, 31k - 1, 31k, 31k + 1 are obtained.

Theorem 2 shows that an (N, s^n) -design D is an MA design if the difference among all coincidence numbers between distinct rows does not exceed one. This condition is equivalent to that of an (N, s^n) -design to be an $E(f_{NOD})$ -optimal design in the literature of supersaturated designs, see, e.g., Liu and Cai (2009). There is abundant literature constructing $E(f_{NOD})$ -optimal designs, see, e.g., Lu et al. (2002),



Lu et al. (2003), Fang et al. (2004), Georgiou and Koukouvinos (2006), Sun et al. (2011) and Liu and Liu (2012). Based on these existing $E(f_{NOD})$ -optimal designs, we can further construct MA designs under some special parameters. For illustration, we consider the case of s=6, which is a non-prime power. Lu et al. (2002) and Lu et al. (2003) provided $E(f_{NOD})$ -optimal (6m, 6^{6m-1})-designs with equal coincidence numbers for $2 \le m \le 7$. Then, using arguments similar to those before Theorem 3, we obtain the following result.

Corollary 3 For any $2 \le m \le 7$ and $k \ge 1$, there exists an MA $(6m, 6^n)$ -design, where n = k(6m - 1) or $n = k(6m - 1) \pm 1$.

4 MA designs with uniformity

In this section, we discuss how to further generate the uniform and uniform projection supersaturated designs based on the MA designs constructed in Sect. 3.

There is a close relationship between MA and uniformity. When considering all possible level permutations for each factor of an (N, s^n) -design D, we obtain $(s!)^n$ designs. Denote the set of these designs as $\mathcal{P}(D)$. Following Zhou and Xu (2014), the average WD value of all designs in $\mathcal{P}(D)$ can be expressed as

$$\overline{\text{WD}}(D) = -\left(\frac{4}{3}\right)^n + \left(\frac{8s^2 + 1}{6s^2}\right)^n \sum_{j=0}^n \left(\frac{s+1}{8s^2 + 1}\right)^j A_j(D).$$

Similarly, for an (N, s^n) -design D, we establish the relationship between the average PWD value of all designs in $\mathcal{P}(D)$, denoted by $\overline{\text{PWD}}(D)$, and the generalized word-length pattern of D as follows:

$$\overline{\text{PWD}}(D) = \frac{16s^2 + 1}{36s^4} + \frac{2}{n(n-1)} \left(\frac{s+1}{6s^2}\right)^2 A_2(D). \tag{4}$$

For an (N, s^n) -design D with s = 2 or 3, level permutation does not alter its PWD value. Thus, it follows that an (N, s^n) -design D with s = 2 or 3 is a uniform projection design if and only if D has the minimum A_2 value. Notice that the WD value of an (N, s^n) -design D with s = 2 or 3 can be reformulated as

$$WD(D) = -\left(\frac{4}{3}\right)^n + \frac{1}{N}\left(\frac{8s-1}{6s}\right)^n + \frac{2}{N^2}\left(\frac{8s-1}{6s}\right)^n \phi_z(D),\tag{5}$$

where z = 9s/(8s - 1). Combining Theorems 1, 2 and equations (4) and (5), we immediately obtain the following result which shows the optimality of a class of designs under multiple criteria.

Theorem 5 For an (N, s^n) -design D with s = 2 or 3, if the difference among all $\delta^D_{i_1, i_2}$, $i_1 < i_2$, does not exceed one, then D is an MA, uniform and uniform projection design.



Theorem 5 is very useful in determining a two- or three-level MA, uniform and uniform projection design. For example, the designs with two- or three-levels, produced by Theorems 3, 4 and Corollaries 1, 2, have the property that the number of coincidences between any two rows differs by at most one. From Theorem 5, they are all MA, uniform and uniform projection designs. For many other parameters, optimal designs under the MA, WD and PWD criteria simultaneously can also be constructed in explicit form. We list these results in Corollary 4. To save space, we postpone the construction details to the proof in Appendix.

Corollary 4 Suppose s = 2 or 3 and the wrap-around L_2 -discrepancy is used.

- (i) For any $m \ge 3$ and k, there exists an MA, uniform and uniform projection (s^m, s^n) -design, where $n = k(s^m 1)/(s 1)$ or $n = k(s^m 1)/(s 1) \pm 1$.
- (ii) For any $m \ge 3$ and k < s, there exists an MA, uniform and uniform projection (ks^{m-1}, s^n) -design, where $n = (s^m 1)/(s 1) 1$.
- (iii) For any n, there exists an MA, uniform and uniform projection (s^2 , s^n)-design.
- (iv) For any $n \le s$ and k < s, there exists an MA, uniform and uniform projection (ks, s^n) -design.
- (v) For any $m \ge 2$ and $2 \le k \le s$, there exists an MA, uniform and uniform projection (ks^m, s^n) -design, where $n = s(s^m 1)/(s 1)$.

Corollary 4 can be viewed as an extension of Theorem 2 of Xu and Wu (2005). Our focus here is the optimality on not only the MA but also the WD and the PWD criteria. Theorem 5 and Corollary 4 are very powerful in obtaining many MA, uniform and uniform projection designs with a large number of columns. Here is an example.

Example 1 Let D be a saturated $OA(27, 3^{13}, 2)$. The design D and another two designs obtained by adding one balanced column to D and removing one column from D are three MA, uniform and uniform projection designs. Taking the last column of D as the branching column, we obtain 3 fractions according to the levels of the branching column. After removing the branching column, the row juxtaposition of the first 2 fractions forms an MA, uniform and uniform projection (18, 3¹²)-design. From Corollary 1 and Theorem 4, MA, uniform and uniform projection $(18, 3^n)$ -designs for n = 8, 9, 16, 17, 18 are obtained. We can also construct MA, uniform and uniform projection (12, 3^n)-designs for n = 10, 11, 12 by using Corollary 1 (iii) or Corollary 2. Table 1 lists the WD, PWD and A_2 values of the above optimal designs and the comparable designs on the UD homepage. It can be seen that designs obtained by our method have smaller WD, PWD and A2 values than the corresponding designs on the UD homepage for almost all cases except for the cases of $(12, 3^{10})$, $(12, 3^{12})$, $(18, 3^8)$ and $(18, 3^9)$. For the cases of $(12, 3^{10})$, $(12, 3^{12})$, $(18, 3^8)$ and $(18, 3^9)$, designs obtained by our method and those on UD homepage have the same WD, PWD and A_2 values.



Table 1 Comparisons between the optimal $(N, 3^n)$ -designs under the MA, WD and PWD criteria simultaneously and the designs on UD homepage

		Our d	lesigns	UD homepage					
N	n	WD	10 ² PWD	A_2	Source	WD	10 ² PWD	A_2	
12	10	3.56	5.0823	9	Co 1 (iii)	3.56	5.0823	9	
12	11	5.52	5.0823	11	Co 1 (iii)	5.53	5.0848	11.2	
12	12	8.67	5.0973	15	Co 1 (iii)	8.67	5.0973	15	
18	8	1.25	4.9824	0.5	Th 4	1.25	4.9824	0.5	
18	9	1.97	4.9954	1.5	Th 4	1.97	4.9954	1.5	
18	12	7.25	5.0224	6	Co 4 (ii)	7.27	5.0248	6.3	
18	16	38.4	5.0412	15	Co 1 (ii)	38.6	5.0434	15.5	
18	17	57.6	5.0412	17	Co 1 (ii)	58.0	5.0456	18.1	
18	18	87.2	5.0479	21	Co 1 (ii)	87.4	5.0493	21.4	
27	12	6.30	4.9726	0	Co 4 (i)	6.45	4.9855	1.6	
27	13	9.38	4.9726	0	Co 4 (i)	9.68	4.9885	2.3	
27	14	14.3	4.9846	2	Co 4 (i)	14.5	4.9925	3.3	

A boldfaced value indicates a smaller WD value than that listed on UD homepage

Now, we turn to the case of designs with more than three levels. Different from the two- and three-level cases, when s > 3, theoretical results like Theorem 5 and Corollary 4 will not hold. To achieve uniformity or projection uniformity, we construct supersaturated designs by permuting levels of MA designs obtained in Sect. 3. Here, Algorithm 2, proposed by Tang and Xu (2013), is used for level permutations.

Algorithm 2 The level permutation algorithm for improving uniformity

- 1: Initialize τ , δ and u_0 .
- 2: Input staring design D^c and let $D^{\min} := D^c$.
- 3: for i = 1 to τ do
- 4: Choose a random integer j. Generate a new design D^{new} by randomly exchanging all elements of two distinct levels within the jth column of D^c .
- 5: Compute $\nabla = \text{WD}(D^{new}) \text{WD}(D^c)$ and generate $u \ (u \in U[0,1])$.
- 6: if $\nabla < 0$ or $(\nabla < \delta \text{ and } u < u_0)$, then let $D^c := D^{new}$.
- 7: **if** $WD(D^c) < WD(D^{\min})$, **then** let $D^{\min} := D^c$.
- 8: end for

As a baseline method, the adjusted threshold accepting (TA) algorithm, proposed by Fang et al. (2017), can be divided into three steps as follows:

Step 1: Let D_a be an $OA(N, s^{n_0}, 2)$ and D_b be a random (N, s^{n-n_0}) -design. Take $D = (D_a, D_b)$ as their column juxtaposition.

Step 2: Minimize WD(D) by iteratively updating D_b while keeping D_a unchanged.



[&]quot;Th" and "Co" represent "theorem" and "corollary," respectively

Step 3: Use Algorithm 2 to further reduce the value of WD(D).

To compare our method with the adjusted TA algorithm, the constructions of $(32,4^n)$, n = 20-53, $(64,4^n)$, n = 62-64, $(50,5^n)$, n = 48-50, $(125,5^n)$, n = 123-125, and $(98,7^n)$, n = 96-98, uniform designs are investigated. Five designs $OA(32,4^9,2)$, $OA(64,4^{21},2)$, $OA(50,5^{11},2)$, $OA(125,5^{31},2)$ and $OA(98,7^{15},2)$ are taken as the D_a for the adjusted TA algorithm. Among them, the $OA(125, 5^{31}, 2)$ is constructed by Theorem 3.16 of Hedayat et al. (1999), and the others can be found from Sloane's website (http://neilsloane.com/oadir/). For our method, the supersaturated MA designs are constructed by Corollary 1, Theorem 4 or Algorithm 1. When using Algorithm 1, set z = 1.15 and take the MA designs obtained by Corollary 1 and Theorem 4 to be the initial designs $D^{(0)}$. We also set I = 100 and $J = 10^4$ as the numbers of outer and inner iterations, respectively, for Algorithm 1 and the adjusted TA algorithm. For a fair comparison, in each case, both methods are repeated 100 times. The calculation is done by using the Matlab program on a personal computer with a 2.8 GHz CPU processor and 8 Gb memory. Tables 2 and 3 list the WD, PWD and A_2 values of the best results and the total time T in seconds for both methods. It can be seen that our approach acquires less running time in all cases and obtains smaller A_2 values than the adjusted TA algorithm in almost all cases. Moreover, our designs and their two-dimensional projections tend to have lower discrepancies, in particular as the number of columns increases.

When orthogonal arrays do not exist, the adjusted TA algorithm cannot be carried out, but the construction method in this article is still applicable as long as MA designs exist. For example, for constructing a uniform $(3^m4, 4^n)$ - or $(4^m5, 5^n)$ -design, one can use Corollary 2 and Algorithm 1 to construct an MA design and then permute its levels. However, in such cases, the adjusted TA algorithm fails as no orthogonal arrays exist. Hence, the construction method of this article is applicable to a wider range of parameters.

5 Concluding remarks

In this paper, we study the issue of constructing designs for computer or physical experiments involving many quantitative factors subject to a limited number of runs. We provide a solution by proposing a construction approach of supersaturated uniform designs. The main idea of our approach is to construct a supersaturated minimum-aberration design first and then permute its levels to further improve the uniformity and projection uniformity. A local search heuristic algorithm is proposed for constructing large-size minimum-aberration designs with a flexible number of columns. Furthermore, by using the generalized Hadamard matrices and saturated mixed orthogonal arrays, several classes of supersaturated minimum-aberration designs are given in explicit form. By permuting levels of those designs, many supersaturated uniform designs are obtained. Compared with the existing adjusted threshold-accepting algorithm, our method is more efficient and the resulting uniform supersaturated design and its two-dimensional projections outperform under both the MA and wrap-around L_2 -discrepancy criteria.



Table 2 Comparisons with the adjusted TA algorithm in Fang et al. (2017) when constructing $(32, 4^n)$ -designs

	Our metho	od		Adjusted TA					
n	10^{-3} WD	10^2 PWD A_2		Source	T(s)	10^{-3} WD	10 ² PWD	A_2	T(s)
20	0.10681	2.8297	30	Th 4	122	0.10700	2.8303	33.3	459
21	0.15964	2.8296	34	Th 4	123	0.16073	2.8319	38.2	458
22	0.23962	2.8309	39	Al 1	365	0.24150	2.8337	43.1	463
23	0.35993	2.8326	45	Al 1	363	0.36213	2.8349	48.2	461
24	0.54385	2.8364	51	Al 1	368	0.54291	2.8360	53.0	461
25	0.81645	2.8381	57	Al 1	366	0.81406	2.8371	58.6	464
26	1.22347	2.8392	63	Al 1	367	1.22022	2.8383	65.1	465
27	1.83267	2.8401	69	Al 1	367	1.82882	2.8393	71.3	469
28	2.74403	2.8407	75	Al 1	368	2.74011	2.8402	77.4	471
29	4.10668	2.8412	81	Al 1	370	4.10501	2.8411	84.5	472
30	6.14426	2.8414	87	Co 1(ii)	126	6.14848	2.8419	91.8	474
31	9.17314	2.8407	93	Co 1(ii)	127	9.21136	2.8427	99.3	481
32	13.7700	2.8424	102	Co 1(ii)	129	13.7970	2.8434	106.5	476
33	20.6397	2.8433	111	Al 1	385	20.6712	2.8442	115.4	474
34	30.9206	2.8439	120	Al 1	382	30.9669	2.8448	123.7	478
35	46.3310	2.8446	129	Al 1	379	46.3839	2.8454	132.0	476
36	69.4221	2.8453	138	Al 1	380	69.4874	2.8460	140.9	476
37	104.041	2.8461	147	Al 1	380	104.104	2.8465	150.1	480
38	155.884	2.8466	156	Al 1	380	155.980	2.8471	159.7	481
39	233.587	2.8471	165	Al 1	383	233.707	2.8475	169.3	485
40	349.960	2.8475	174	Al 1	384	350.182	2.8480	179.9	487
41	524.414	2.8479	184	Th 4	136	524.785	2.8485	190.7	488
42	785.872	2.8483	195	Th 4	138	786.393	2.8489	199.7	489
43	1178.08	2.8489	205.9	Al 1	404	1178.66	2.8494	212.6	490
44	1766.00	2.8494	217	Al 1	399	1766.41	2.8498	223.7	491
45	2646.95	2.8498	229	Al 1	399	2647.42	2.8501	234.5	494
46	3967.79	2.8502	241	Al 1	399	3968.16	2.8504	246.1	493
47	5947.91	2.8506	253.3	Al 1	397	5948.60	2.8508	259.5	495
48	8916.75	2.8510	265.5	Al 1	402	8917.54	2.8512	272.0	492
49	13367.6	2.8514	278	Al 1	399	13368.2	2.8515	284.7	497
50	20040.4	2.8516	290.6	Al 1	402	20042.0	2.8518	297.8	497
51	30047.5	2.8520	303	Th 4	134	30049.0	2.8521	309.3	510
52	45046.2	2.8521	316	Th 4	139	45052.6	2.8524	323.9	513
53	67544.3	2.8525	330	Al 1	419	67548.8	2.8526	336.9	511

A boldfaced value indicates a smaller WD value than that obtained by the adjusted TA Column "source" indicates the construction methods of supersaturated MA designs "Th," "Al" and "Co" represent "theorem," "algorithm" and "corollary," respectively



Table 3	Comparisons	with the	adjusted	TA	algorithm	in	Fang	et :	al.	(2017)	when	constructing	some
large-sized designs													

			Our method				Adjusted TA				
S	N	n	WD	10 ² PWD	A_2	Source	T(s)	WD	10 ² PWD	A_2	T(s)
4	64	62	1.30580e+09	2.8137	183	Co 1(i)	208	1.30658e+09	2.8148	195.4	705
4	64	63	1.95674e+09	2.8138	189	Co 1(i)	195	1.95789e+09	2.8150	203.1	614
4	64	64	2.93288e+09	2.8143	198	Co 1(i)	206	2.93416e+09	2.8152	211.4	623
5	50	48	5.67723e+06	1.8196	282	Co 1(ii)	250	5.68182e+06	1.8203	301.7	629
5	50	49	8.51251e+06	1.8196	294	Co 1(ii)	248	8.52125e+06	1.8206	314.7	635
5	50	50	1.27715e+07	1.8202	310	Co 1(ii)	254	1.27797e+07	1.8209	330.6	645
5	125	123	3.65025e+19	1.7968	732	Co 1(i)	584	3.65026e+19	1.7975	791.7	1150
5	125	124	5.47536e+19	1.7968	744	Co 1(i)	581	5.47537e+19	1.7975	804.2	1140
5	125	125	8.21303e+19	1.7969	760	Co 1(i)	583	8.21304e+19	1.7975	821.2	1142
7	98	96	8.19422e+14	0.9290	1425	Co 1(ii)	460	8.19434e+14	0.9295	1527.5	954
7	98	97	1.22914e+15	0.9290	1455	Co 1(ii)	457	1.22916e+15	0.9296	1562.1	952
7	98	98	1.84372e+15	0.9291	1491	Co 1(ii)	456	1.84374e+15	0.9296	1598.8	954

A boldfaced value indicates a smaller WD value than that obtained by the adjusted TA Column "source" indicates the construction methods of supersaturated MA designs. "Co" represents "corollary"

Our method is suitable especially for constructing uniform designs with a large number of columns. Suppose there exists an MA (N, s^{n_0}) -design satisfying that all coincidence numbers are equal. Then, for any n, let $g = \lfloor n/n_0 \rfloor$ and $r = n - gn_0$, we can search an MA or nearly MA (N, s^r) -design by Algorithm 1 and then append it to the column juxtaposition of g MA (N, s^{n_0}) -designs. At last, full factor level permutations are performed to improve the uniformity. Notice that there exist many designs with equal coincidence numbers. These designs include saturated OAs, the (N, s^{N-1}) -designs obtained by Corollaries 1, 2 and many $E(f_{NOD})$ -optimal supersaturated designs in the literature. All these designs make our method powerful and effective.

The wrap-around L_2 -discrepancy is chosen as the measure of uniformity, but the main results of this paper can be easily extended to other discrepancies. The range of z in the optimization problem is summarized through practice. Logically, z should change with the scale of the optimization problem, which can be further studied in the future.

Appendix

To prove Theorem 1, we need the following lemma from Tang et al. (2012).

Lemma 1 For an (N, s^n) -design D, denote δ_{i_1, i_2}^D as the number of places where the i_1 th and i_2 th rows of D take the same value. Then, for any real number z > 1, we have



$$\sum_{i_1,i_2=1}^N z^{\delta^D_{i_1,i_2}} = N^2 \left(\frac{z+s-1}{s}\right)^n \sum_{i=0}^n \left(\frac{z-1}{z+s-1}\right)^i A_i(D).$$

Proof of Theorem 1 Since there are altogether finite (N, s^n) -designs, we just need to prove that for any two (N, s^n) -designs D_1 and D_2 , D_1 has less aberration than D_2 if and only if there exists a constant c > 0, such that $\phi_z(D_1) < \phi_z(D_2)$ for any $z \in (1, 1 + c)$. Note that there exists a constant M > 0 such that $A_i(D) < M$ for any i and any (N, s^n) -design D. Moreover, from Lemma 1, we have

$$\phi_z(D_1) - \phi_z(D_2) = \frac{N^2}{2} \left(\frac{z+s-1}{s}\right)^n \sum_{i=0}^n \left(\frac{z-1}{z+s-1}\right)^i \left[A_i(D_1) - A_i(D_2)\right].$$

By noting that $\lim_{z\to 1^+}(z-1)/(z+s-1)=0$, the desired result immediately follows.

Proof of Theorem 2 Suppose that z > 1 and that x_1, \ldots, x_m are nonnegative integers satisfying $\sum_{i=1}^m x_i = M$. According to the properties of convex functions, we obtain that

$$\sum_{i=1}^{m} z^{x_i} \ge h(z, M, m)$$

with equality if and only if all x_i 's equal $\lfloor M/m \rfloor$ or $\lfloor M/m \rfloor + 1$. From Corollary 2 of Xu (2003), we have

$$\sum_{1 \leq i_1 < i_2 \leq N} \delta^D_{i_1,i_2} = \frac{nN(N-s)}{2s}.$$

Combining the above formulas, the desired result follows.

Proof of Theorem 4 For a prime power $s \ge 3$, let α be a primitive element of the Galois field GF(s). Write the elements of GF(s) as $\alpha_0 = 0$, $\alpha_1 = \alpha$, $\alpha_2 = \alpha^2, \ldots$, $\alpha_{s-1} = \alpha^{s-1} = 1$. By Theorem 6.33 of Hedayat et al. (1999), there exists a D(2s, 2s, s), say D, with entries from GF(s). Let $\mathbf{b} = (\alpha_0, \ldots, \alpha_{s-1})^T$ and \mathbf{d} be a vector of length $2s^2$ with the form

$$\mathbf{d} = (0, \dots, 2s - 1, 0, \dots, 2s - 1, \dots, 0, \dots, 2s - 1)^{T}.$$

Let $D^{(0)} = \mathbf{b} \oplus D$ and $D^* = [D^{(0)}, \mathbf{d}]$, where \oplus denotes the Kronecker sum. By Theorem 9.15 of Hedayat et al. (1999), D^* is a saturated mixed $OA(2s^2, s^{2s}(2s)^1, 2)$.

It follows from Lemma 1 of Butler (2005) that the coincidence numbers of any two runs in $D^{(0)}$ take only two values, 0 or 2. More precisely, $\delta_{i_1,i_2}^{D^{(0)}}=2$ if $\delta_{i_1,i_2}^{\mathbf{d}}=0$, and $\delta_{i_1,i_2}^{D^{(0)}}=0$ if $\delta_{i_1,i_2}^{\mathbf{d}}=1$. Let $\tilde{\mathbf{d}}_0,\tilde{\mathbf{d}}_1,\tilde{\mathbf{d}}_2$ be three s-level columns of length $2s^2$ with entries from GF(s). The entries of $\tilde{\mathbf{d}}_i$, i=0,1,2, are obtained by $f_i(\mathbf{d})$, where the $f_i(\cdot)$'s are three maps from $\{0,1,\ldots,2s-1\}$ to GF(s) given by



$$f_i(j) = \begin{cases} \alpha_j & \text{if } 0 \le j \le s - 1, \\ \alpha_i + \alpha_{j-s} & \text{if } s \le j \le 2s - 1. \end{cases}$$

Let $D_1 = [D^{(0)}, \tilde{\mathbf{d}}_0, \tilde{\mathbf{d}}_1]$ and $D_2 = [D^{(0)}, \tilde{\mathbf{d}}_0, \tilde{\mathbf{d}}_1, \tilde{\mathbf{d}}_2]$. It can be verified that for any $i_1 < i_2, \delta_{i_1, i_2}^{D_1}$ and $\delta_{i_1, i_2}^{D_2}$ takes only two values 2 or 3. From Theorems 1 and 2, D_1 and D_2 are MA $(2s^2, s^{2s+2})$ - and $(2s^2, s^{2s+3})$ -designs, respectively.

Let $D^{(1)}$ be a saturated $OA(s^3, s^{s^2+s+1}, 2)$. Taking the last column of $D^{(1)}$ as the branching column, we obtain s fractions according to the levels of the branching column. After removing the branching column, let D_3 be the row juxtaposition of the first two fractions. From Theorem 8 of Xu and Wu (2005), D_3 is an MA $(2s^2, s^{s^2+s})$ design satisfying that $\delta^{D_3}_{i_1,i_2} = s$ if the i_1 th and i_2 th runs are from the same fraction, and $\delta^{D_3}_{i_1,i_2} = s + 1$ otherwise. Moreover, if s is even, append a balanced column to D_3 , such that the first s/2 levels belong to the first fraction, and the rest s/2 levels belong to the second fraction. It can be checked that the resulting design, denoted by D_4 , is an MA design with coincidence numbers being s or s+1.

At last, by Corollary 1, there exists an MA $(2s^2, s^{2s^2-1})$ -design with coincidence numbers being 2s-1. From Theorems 1 and 2, appending D_1 , D_2 , D_3 or D_4 to the column juxtaposition of several MA $(2s^2, s^{2s^2-1})$ -designs also forms an MA design. Hence, the conclusion of Theorem 4 follows.

Proof of Corollary 4 Mukerjee and Wu (1995) observed that for a saturated $OA(N, s^q, 2)$ H with q = (N-1)/(s-1), $\delta_{i_1, i_2}^H = (N-s)/[s(s-1)]$ for any $i_1 < i_2$. Let D_1, \ldots, D_k be k saturated $OA(N, s^q, 2)$'s and $D = (D_1, \ldots, D_k)$ be their column juxtaposition. It can be seen that $\delta_{i_1, i_2}^D = k(N-s)/[s(s-1)]$ for any $i_1 < i_2$. Then, from Theorem 5, D is an MA, uniform and uniform projection design. Moreover, adding one balanced column to or removing one column from D also results in an MA, uniform and uniform projection design. Thus, part (i) follows.

Next, we prove part (ii). Similar to Lin (1993), taking any column of a saturated $OA(N, s^q, 2)$ as the branching column, we obtain s fractions according to the levels of the branching column. After removing the branching column, the fractions have the properties that the row juxtaposition of any k fractions forms a (kNs^{-1}, s^{q-1}) -design of which the number of coincidences between any two rows differs by at most one. From Theorem 5, such a design is an MA, uniform and uniform projection design.

Now we turn to part (iii). It is known that the number of coincidences between any two rows of an $OA(s^2, s^n, 2)$, $1 \le n \le s + 1$, is either 0 or 1. So the column juxtaposition of any number of saturated $OA(s^2, s^q, 2)$'s and one $OA(s^2, s^n, 2)$ is an MA, uniform and uniform projection design.

Part (iv) follows by part (iii) and the same argument of part (ii).

Part (v) follows from Corollary 1 (v) and Theorem 5.

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