Statistica Sinica **21** (2011), 1379-1396

ROBUST UNIFORM DESIGN WITH ERRORS IN THE DESIGN VARIABLES

Peter Winker and Dennis K. J. Lin

University of Giessen and Pennsylvania State University

Abstract: Uniform design has become a standard tool in experimental design over the last two decades. Its properties are analyzed for a situation when the actual values of the control variables are subject to some error in factor level values. A closed form for the expected discrepancy is established, under some mild assumptions. A thorough Monte Carlo study is conducted under various potential scenarios. Some general properties have been revealed. Both theoretical and simulation results are consistent. The robustness of uniform design under error in control variables is also investigated. It is shown that uniform designs are highly robust with regard to uniformly distributed errors in design variables.

Key words and phrases: Error in design variables, robust design, threshold accepting, uniform design.

1. Introduction

Uniform Design (*UD*) has received a great deal of interest in both theoretical and practical aspects since the 1980s (Fang and Lin (2003); Fang, Li and Sudjianto (2006)). Typically, uniform experimental design (*UD*) is used before further analysis or modeling, i.e., when no information on the actual relationship is known. Then, the aim is to cover the experimental domain as uniformly as possible with a limited number of design points. The *UD* has advantages: it can explore relationships between the response and the factors with a reasonable number of runs; it is insensitive to different model specifications. The *UD* is essentially one kind of fractional factorial design with the uniformity property (see, e.g., Fang et al. (2000)). For practical use, a large number of uniform designs have been constructed and tabulated. Some of them are listed on the website `http://www.math.hkbu.edu.hk/UniformDesign`.

In practical applications of experimental design, however, it is not always possible to set the design variables exactly to the values suggested by a given design. In general, the setting of factor levels in an experiment can be subject to errors, called errors in factor levels or errors in design variables. There is a range of possibilities. For example, in some applications it is feasible to set the factor levels to target values only in the same way as in the experiment. There, no consideration regarding robustness of the design with regard to such errors is relevant. On the other hand, in some processes the setting of factor levels might be subject to different errors from those in the experiment. Then, a more complex analysis might be required.

Among these possibilities, in our paper we concentrate on the case where factor levels might be subject to random errors in the experiment, but can be set accurately in the process. Examples include physical experiments, e.g., in agriculture, when it comes to define water level or temperature, and the outcome of computer simulations which might depend on the actual choice of pseudo-random numbers. If the experimenter is faced with this situation, the best she can do is find a design which is as uniform as possible in mean over all possible realizations of the random errors in design variables.

The following research issues are discussed.

- When the setting of factor levels is subject to some noise, what is the impact of running a uniform design?
- How robust is uniform design to this type of error in design variables?
- What is the most robust uniform design, i.e., a U-type design which is least sensitive to errors in design variables or a U-type design which is least sensitive to errors in design variables, while still keeping a reasonably low discrepancy? Thereby, a l-level U-type design $V(n, l^d)$ is given by a $n \times d$ matrix, where n is the number of runs, d the dimension of the design space, and each column has the same number of entries of $(2k-1)/2l$ for $k = 1, \ldots, l$. Throughout, we consider the case $n = l$.

Box (1963) and Draper and Beggs (1971) are perhaps the first to address the errors in factor levels in linear models and design of experiments. Donev (2004) discusses the effects of errors in setting the factor levels on the optimality of the designs actually used as compared to the originally planned designs. It is shown that, when considering D-optimality as criterion, the expected quality of the designs might be affected. Thereby, it is assumed that a polynomial model is fitted to the data. Then, robustness is defined in terms of minimizing the sum of the variances of the estimated responses (Donev (2004, p. 574)). Obviously, this definition depends on the model considered. This idea of robustness does not apply to situations in which some independent variables are not subject to control, as discussed, e.g., by López-Fidalgo and Garcet-Rodríguez (2004).

The rest of this paper is organized as follows. In Section 2 we provide some theoretical results on the robustness of Uniform Designs. Empirical evidence on robustness properties is provided in Section 3. Section 4 presents a method for the construction of U-type designs with a small expected discrepancy under errors in design variables. We provide both empirical results and a comparison with standard uniform designs. Section 5 summarizes the main findings and points at possible areas of future research.

2. Robustness of Uniform Designs

When assessing the quality of a design before and after adding noise to design variables, a formal criterion is required. Many discrepancy measures have been proposed for this purpose. The centered L_2-discrepancy (CD_2), proposed by Hickernell (1998), is commonly accepted as most appropriate (Fang, Li and Sudjianto (2006)), and is used here. Other discrepancy criteria can be investigated in a similar manner, if desired.

Let V denote a design matrix consisting of n points in the d-dimensional unit cube C^d. Then, a formal definition of CD_2 has

$$(CD_2(V))^2 = \sum_{u \neq \emptyset} \int_{C^u} \left[\frac{N(V \cap J_w(v_u))}{n} - Vol(J_w(v_u)) \right]^2 dv_u, \tag{2.1}$$

where u is any non-empty subset of the coordinate indices $\{1, \cdots, d\}$, $|u|$ denotes the cardinality of u, C^u is the $|u|$-dimensional unit cube involving the coordinates in u, $N(V \cap A)$ counts the number of points of V falling in A, v_u is the projection of $v \in V$ on C^u, and $J_w(v_u)$ is the hyper-rectangle in C^u containing the points between v_u and the nearest vertex of C^u.

Specifically, for each point in C^u, the difference of two ratios is calculated: (1) the number of design points lying in the rectangle formed by this point and the nearest vertex of C^u over the total number of design points n, and (2) the volume of this rectangle and the volume of C^u which is one. For a uniform design, these differences should be small. The measure is given by integrating over all points in the experimental region while considering all lower dimensional projections C^u.

The evaluation of objective function (2.1) appears to be quite complex. However, based on results provided by Hickernell (1998), the following formula can be obtained (Fang, Li and Sudjianto (2006)):

$$\begin{aligned}(CD_2(V))^2 = \left(\frac{13}{12}\right)^d - \frac{2}{n} \sum_{k=1}^{n} \prod_{i=1}^{d} \left[1 + \frac{1}{2}\left|v_{ki} - \frac{1}{2}\right| - \frac{1}{2}\left|v_{ki} - \frac{1}{2}\right|^2 \right] \\ + \frac{1}{n^2} \sum_{k=1}^{n} \sum_{j=1}^{n} \prod_{i=1}^{d} \left[1 + \frac{1}{2}\left|v_{ki} - \frac{1}{2}\right| + \frac{1}{2}\left|v_{ji} - \frac{1}{2}\right| - \frac{1}{2}\left|v_{ki} - v_{ji}\right| \right].\end{aligned} \tag{2.2}$$

Assume that a UD is selected, i.e., a design minimizing the objective function (2.2). Furthermore, suppose that there are errors in design variables, i.e., that the values suggested by the *UD* can be implemented for the practical application only with some random errors. One might think of examples like fixing the temperature for a chemical reaction or the amount of fertilizer provided to some plants. Our interest is to what extent such errors in design variables might impair the properties of the *UD*, in particular with regard to its discrepancy as measured by (2.2).

Now, suppose the experimental levels of the *UD* are contaminated with errors, namely, $\tilde{v}_{ki} = v_{ki} + \tau_{ki}$, where the τ_{ki} are independently distributed random variables such that $\tilde{v}_{ki}$ still belongs to the d-dimensional unit cube. For example, the τ_{ki} might be uniformly distributed on $(-\delta, \delta)$ where $\delta < 1/2n$ is a positive constant. We relax this assumption for the empirical study in Section 3. The centered discrepancy for the actual design $\tilde{V} = (\tilde{v}_{ki})_{ki}$ becomes, from (2.2),

$$
\begin{aligned}
(CD_2(\tilde{V}))^2 = \left(\frac{13}{12}\right)^d - \frac{2}{n}\sum_{k=1}^{n}\prod_{i=1}^{d}\left[1 + \frac{1}{2}\left|v_{ki} + \tau_{ki} - \frac{1}{2}\right| - \frac{1}{2}\left|v_{ki} + \tau_{ki} - \frac{1}{2}\right|^2\right] \\
+\frac{1}{n^2}\sum_{k,j=1}^{n}\prod_{i=1}^{d}\left[1 + \frac{1}{2}\left|v_{ki} + \tau_{ki} - \frac{1}{2}\right| + \frac{1}{2}\left|v_{ji} + \tau_{ji} - \frac{1}{2}\right|\right. \\
\left. -\frac{1}{2}\Big|(v_{ki} - v_{ji}) + (\tau_{ki} - \tau_{ji})\Big|\right].
\end{aligned}
$$

Since the errors are assumed to be i.i.d., the expectation of $(CD_2(\tilde{V}))^2$ can be written as

$$
\begin{aligned}
\mathrm{E}\left[(CD_2(\tilde{V}))^2\right] = \left(\frac{13}{12}\right)^d - \frac{2}{n}\sum_{k=1}^{n}\prod_{i=1}^{d}\left[1+\frac{1}{2}\mathrm{E}\left|v_{ki}+\tau_{ki}-\frac{1}{2}\right|-\frac{1}{2}\mathrm{E}\left|v_{ki}+\tau_{ki}-\frac{1}{2}\right|^2\right] \\
+\frac{1}{n^2}\sum_{k,j=1}^{n}\prod_{i=1}^{d}\left[1+\frac{1}{2}\mathrm{E}\left|v_{ki}+\tau_{ki}-\frac{1}{2}\right|+\frac{1}{2}\mathrm{E}\left|v_{ji}+\tau_{ji}-\frac{1}{2}\right|\right. \\
\left. -\frac{1}{2}\mathrm{E}\Big|(v_{ki}-v_{ji})+(\tau_{ki}-\tau_{ji})\Big|\right].
\end{aligned}
$$

Under the assumption of uniformly distributed τ_{ki}, we are able to prove (see Appendix A) the following.

Theorem 1. *For $\delta < 1/2n$ and all $v_{ki} \neq 1/2$, we have*

$$
\begin{aligned}
E\left[CD_2(\tilde{V}))^2\right] = \left(\frac{13}{12}\right)^d - \frac{2}{n}\sum_{k=1}^{n}\prod_{i=1}^{d}\left[1 + \frac{1}{2}\left|v_{ki} - \frac{1}{2}\right| - \frac{1}{2}\left|v_{ki} - \frac{1}{2}\right|^2 - \frac{1}{6}\delta^2\right] \\
+\frac{1}{n^2}\sum_{k,j=1}^{n}\prod_{i=1}^{d}\left[1 + \frac{1}{2}\left|v_{ki} - \frac{1}{2}\right| + \frac{1}{2}\left|v_{ji} - \frac{1}{2}\right| - \frac{1}{2}\left|v_{ki} - v_{ji}\right|\right].
\end{aligned}
$$

Recall that for a U-type design with n runs and $l = n$ levels, each experimental variable is coded as $[1/(2n), 3/(2n), \ldots (2n-1)/(2n)]$. Thus, imposing the constraint $\delta < 1/2n$ ensures that all design points will stay within the unit cube, even though they may not be exactly located at the designated position.

In other words, under errors in experimental variables, $\tilde{v}_{ki} = v_{ki} + \tau_{ki}$ with $\tau_{ki} \sim \text{Unif}(-\delta, \delta)$, the resulting discrepancy is expected to be greater than the original discrepancy. When such an error in experimental variables is small, i.e., $\delta < 1/2n$, the difference between the resulting discrepancy and the original discrepancy is a function of d, n and δ^2.

For larger δ or for alternative distributions (for example, normal or beta distributions), however, we are unable to obtain a closed form expression of $\text{E}[(CD_2(\tilde{V}))^2]$. We will address these cases via a Monte Carlo study which is presented in the next section. In particular, it will be verified (numerically) that $E[(CD_2(\tilde{V}))^2]$ is indeed an increasing function of δ, d, as well as n.

3. Empirical Study

To analyze the actual distribution of the CD_2 discrepancy when design points are subject to errors in design variables, we conducted a Monte Carlo simulation. The procedure is summarized in Algorithm 1. (1:) fix a run size n, the number of factors d and the number of levels l. Here, we concentrated on the case that the number of levels is equal to the run size ($l = n$). (2:) search for a U-type design V exhibiting the lowest CD_2 discrepancy using the Threshold Accepting algorithm introduced in Fang et al. (2000). Given that no lower bounds are available for the CD_2 discrepancy in the case that $l > 4$ (for $l = 2$, lower bounds are provided by Fang, Lu and Winker (2003), for $l = 3, 4$ by Fang et al. (2006)), no formal proof of optimality can be given for the resulting designs. Nevertheless, at least, they are close to uniformity, i.e., exhibiting very low discrepancy. When constructing V, we still assumed the deterministic setting, i.e., without noise in input variables.

For the Monte Carlo simulation (3: to 11:), in each replication i, a uniform random error from $[-\delta, \delta]$ was added to each element of the design matrix V. Obviously, the uniform distribution can be replaced by another distribution in step (6:). We report some results for the normal and beta distributions in Section 5. For larger values of δ, the modified design points might leave the unit cube. Therefore, in (7:), such points are put on the boundary introducing some additional bias. Then (10:), for the modified design matrix $\tilde{V}$ the discrepancy CD_2 is calculated and stored. Finally (12:), after running all Monte Carlo replications (1,000,000 for the present application), statistics on the distribution of these CD_2 values were calculated and are reported here.

Algorithm 1 Simulation of CD_2 under Errors-in-Variables.

1: Initialize run size n, number of factors d and number of levels $l = n$.
2: Find uniform design $V = (v)_{ij}$ by solving: $\min_{V \in \text{U-type designs}} CD_2(V)$.
3: **for** $i = 1$ to $I_{\max}$ **do**
4:   **for** $j = 1$ to n **do**
5:     **for** $k = 1$ to d **do**
6:       Draw random error $\tau \sim U(-\delta, \delta)$.
7:       $(\tilde{V})_{jk} = \max(\min((v)_{jk} + \tau, 1), 0)$.
8:     **end for**
9:   **end for**
10:   Calculate $CD_2(\tilde{\mathbf{V}})$
11: **end for**
12: Report statistics on distribution of CD_2.

The range δ for the uniform noise added to the design points varied from 0 to 0.25 in all cases. Given the definition of design points for a U-type design with n runs, for $\delta < 1/2n$, the boundary control in (7:) was not active. For n and d, we analyzed the following combinations: (A) $d = 2$, $n = 10, \ldots, 30$; (B) $d = 3$, $n = 10, \ldots, 30$; (C) $n = 10$, $d = 2, \ldots, 9$; and (D) $n = 20$, $d = 2, \ldots, 19$.

Figure 1 shows kernel density estimates (f) of the distribution of CD_2 for different values of δ and the problem instance $d = 2$ and $n = 10$ from set (A). The vertical line indicates the discrepancy of the optimized design. As expected, adding noise to the design points increases the discrepancy. Thereby, both the mean and the variance of the CD_2 values increase for growing values of δ, as predicted by Theorem 1 for small values of δ.

Summarizing the results from Figure 1 and similar plots for the other problem instances (not listed here) the following trends can be identified.

- both the mean and the variance of CD_2 increase as δ increases for all considered combinations of d and n;
- both the mean and the variance of CD_2 decrease as n increases for $d = 2$ and $d = 3$ and all considered values of δ;
- both the mean and the variance of CD_2 increase as d increases for $n = 10$ and $n = 20$ and all considered values of δ.

When starting with an optimized U-type design (or a uniform design), an increase of the mean and the standard deviation of CD_2 when adding noise to the design points has to be expected. Thus, a proper definition of robustness is required for further analysis. One way of defining robustness is by comparison with random designs. Thus, we define a U-type design V to be robust under addition of uniform random noise $\tau \sim \text{Unif}(-\delta, \delta)$ at level p (p-δ-robust) if

$$q_{1-p}(D(V + \tau)) \leq q_p(D(R)) \,, \tag{3.1}$$

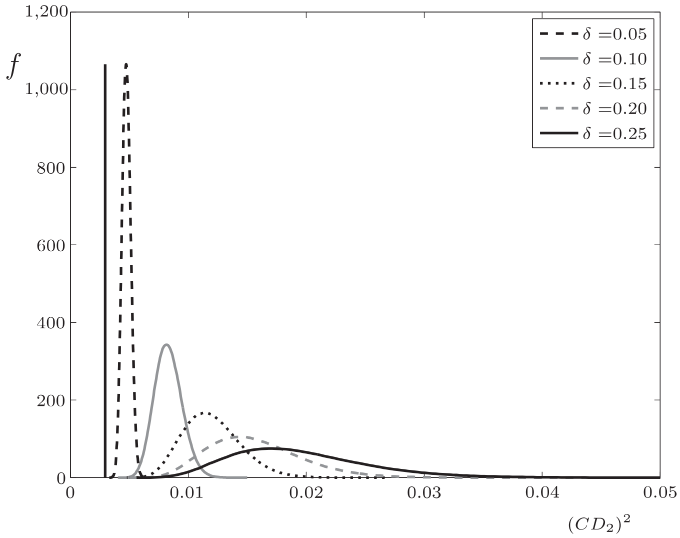

Figure 1. Distribution of CD_2 values for increasing δ ($d = 2, n = 10$).

where q_{1-p} and q_p denote the $1-p$ and p-quantiles respectively, D is the discrepancy measure considered (CD_2), and R is a random design with n points drawn uniformly from $[0,1]^d$. This condition implies that, even after adding some errors to the design variables, an upper quantile of the resulting distribution of the CD_2 values of the uniform design plus noise ($V + \tau$) is still lower than the corresponding lower quantile of the distribution for the randomly generated designs.

Next, we can define the maximum noise level still satisfying p-δ-robustness, i.e.,

$$\delta_p^*(V) = \max_{\delta}\{V \text{ is } p\text{-}\delta\text{-robust}\}\,. \tag{3.2}$$

Figure 2 summarizes the findings for our test cases in groups (A) – (D) for $p = 0.05$ (solid lines) and $p = 0.01$ (dashed lines). These values were determined by successively increasing δ until V was not p-δ-robust anymore. Then, the algorithm went back to the previous value of δ and the step size was decreased. The procedure was iterated until $\delta_p^*(V)$ had been approximated up to at least 4 digits precision. The large values found for $\delta_{0.05}^*$ and $\delta_{0.01}^*$ have to be interpreted relative to the design space which is $[0,1]^d$. Therefore, when starting with an optimized U-type design (or a uniform design if available), even after adding a substantial amount of noise, the resulting design most of the time was still significantly better than a random design. The findings for the normal and beta distributions considered were similar (see Appendix B), except for heavily skewed distributions (e.g., beta(1,3) and beta(2,5)) and $p = 0.01$ resulting in substantial lower, but still positive values of δ^*.

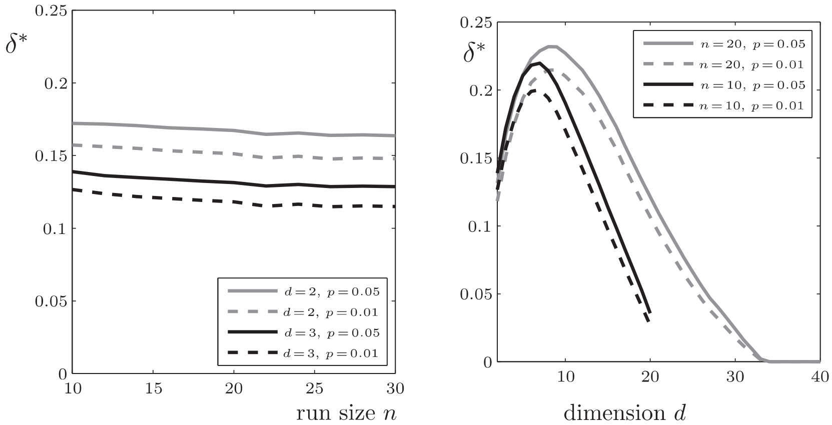

Figure 2. $\delta^*_{0.05}(V)$ and $\delta^*_{0.01}(V)$ for optimized U-type designs in (A) – (D).

Table 1. Regression model for $\delta^*_p(V)$.

Explanatory	$\delta^*_{0.05}$			$\delta^*_{0.01}$		
Variable	Coeff.	t-Stat.	p-Value	Coeff.	t-Stat.	p-Value
Const.	0.1328	5.397	0.0000	0.1247	5.504	0.0000
d	0.0221	8.169	0.0000	0.0199	7.982	0.0000
n	-0.0030	-1.255	0.2172	-0.0033	-1.482	0.1467
d^2	-0.0015	-18.776	0.0000	-0.0014	-19.752	0.0000
n^2	$3.6 \cdot 10^{-5}$	0.667	0.5089	$3.8 \cdot 10^{-5}$	0.762	0.4509
dn	0.0003	2.226	0.0320	0.0004	2.854	0.0069
R^2		0.93			0.93	

For given d, the values of δ^*_p tended to marginally decrease with growing n (left plot), while the dependence on d was not monotonic (right plot). In order to model the dependence of δ^*_p on d and n, a second order polynomial with cross terms was fitted. The results are summarized in Table 1. The partial impact of n was not significantly different from zero both for $p = 0.05$ and $p = 0.01$, confirming what might have been expected from the visual inspection. By contrast, the partial impact of d was highly significant both in levels (d), squared terms (d^2) and interaction term (dn). For fixed n, growing dimension d first allows more noise prior to coming close to a low quantile of random designs. However, this effect decreased due to a negative effect of the squared term. It should be noted that for $d > n$, the values of δ^*_p eventually converge to zero, e.g., for $d > 34$ when $n = 20$ (results available on request). The quadratic approximation was fitted only for the case $d < n$ and cannot be used to extrapolate for $d > n$.

4. Construction of Robust U-type Designs

In the previous section, the properties of uniform designs have been analyzed when some noise is added to the variables. Alternatively, one might be interested in constructing designs achieving a high degree of robustness under errors in design variables. In this section, such an approach is presented.

As above, we assume that the values of the design points are subject to some random error τ. We still consider U-type designs, for which the number of levels l is assumed to be equal to the number of runs n. Of course, this constraint might be relaxed in future work, but appears to be reasonably representative given the broad use being made of U-type designs in practical applications. Then, for given dimension d and number of runs n, we try to find the U-type design with $l = n$ levels minimizing the expected discrepancy, i.e., instead of solving $\min_{V \in U\text{-type}} D(V)$ the objective becomes

$$\min_{V \in U\text{-type}} E(D(V + \tau)) \,, \tag{4.1}$$

where D is some measure of discrepancy – CD_2 for the present application – and τ is the random error added to V, assumed independent uniform over $[-\delta, \delta]$ in each coordinate of each design point, with those components of V leaving the unit cube being fixed at the boundary. The method can be used for other distributions as well.

Instead of concentrating solely on the expected discrepancy, we might also take into account its variance, e.g., by minimizing mean squared error,

$$\min_{V \in U\text{-type}} \left\{ [E(D(V + \tau))]^2 + Var(D(V + \tau)) \right\} . \tag{4.2}$$

Given that – except for small $\delta < 1/2n$ and a uniform distribution – no closed form solutions for $E(D(V + \tau))$ and – in general – for $Var(D(V + \tau))$ are available, we evaluated these moments by means of Monte Carlo integration, i.e., we generated a large number of random drawings of τ and replaced $E(D(V + \tau))$ and $Var(D(V + \tau))$ by the resulting sample moments. In fact, we used antithetic variates in these simulations to improve the approximation quality for the rather modest number of replications which is feasible within the heuristic optimization framework. Let $\tilde{f}(V)$ denote these Monte Carlo estimates. Given that the optimization is run with regard to V, a highly complex optimization problem results, tackled again using a Threshold Accepting implementation. Some implementation details are presented in the following subsection, while first results are summarized in Subsection 4.2.

Algorithm 2 Pseudo-code for the Threshold Accepting implementation.

1: Generate (randomly) initial U-type design V^{c}, initialize $I_{\max}$ and $T_i, i = 1, \ldots, I_{\max}$
2: **for** $i = 1$ to $I_{\max}$ **do**
3: Select $V^{\mathrm{n}} \in \mathcal{N}(V^{\mathrm{c}})$ (neighbor to current solution)
4: Obtain approximation $\tilde{f}(V^{\mathrm{n}})$ of objective function (4.1) or (4.2) by Monte Carlo simulation
5: **if** $\tilde{f}(V^{\mathrm{n}}) < \tilde{f}(V^{\mathrm{c}}) + T_i$ **then** $V^{\mathrm{c}} = V^{\mathrm{n}}$
6: **end for**

4.1. Implementation details

Algorithm 2 describes the Threshold Accepting implementation for the generation of robust U-type designs.

The algorithm proceeds similar to the one used for obtaining low discrepancy U-type designs (Fang et al. (2000)). It starts with a random initial U-type design V^{c} (1:) that is slightly modified in each iteration (3:). However, the objective function cannot be evaluated analytically for most cases, but has to be approximated by means of Monte Carlo simulation (4:) as pointed out above. For $\delta < 1/2n$ and uniformly distributed error terms, the approximation in (4:) can be replaced by the exact value from Theorem 1. This results in a tremendous speed up of the algorithm that was used to run the algorithm for such problem instances ($\delta = 0.01$, $\delta = 0.02$ for $n \leq 20$) with a large number of iterations. However, given the high robustness of uniform designs, the properties of the robust U-type designs obtained were almost identical to those of the uniform designs.

Then, the modified design V^{n} became the current solution if the value of $\tilde{f}$ was lower than for the old candidate solution. It was also accepted if $\tilde{f}$ increased by no more than the current value of the threshold T_i (5:). This threshold acceptance step was required to avoid getting stuck in local optima. At the same time, it accounts for the Monte Carlo variance that is inevitable in approximating $\tilde{f}$ (for another application of threshold accepting in the context of simulated objective functions, see Winker, Gilli and Jeleskovic (2007)). The implementation might be improved by fine tuning the threshold sequence as a function of the Monte Carlo variance, that in turn might be decreased over the number of iterations by increasing the number of random drawings. This refinement was not used in the current implementation. Instead we used up to 1,000 drawings for the Monte Carlo simulation in each step and values of $I_{\max}$ of up to 500,000.

4.2. Results and comparison

Given the high computational load of Algorithm 2 due to the double loop structure, we did not try to construct robust U-type designs for all cases in groups (A) – (D) and many different values of δ. Instead, we concentrated on a few

Table 2. Properties of robust U-type designs with regard to Bias (objective function (4.1)).

		Designs optimized for $\delta = 0.05$				Designs optimized for $\delta = 0.25$			
d	n	$\hat{\mu}_{0.05}$	$\hat{\mu}_{0.25}$	$\hat{\sigma}^2_{0.05}$	$\hat{\sigma}^2_{0.25}$	$\hat{\mu}_{0.05}$	$\hat{\mu}_{0.25}$	$\hat{\sigma}^2_{0.05}$	$\hat{\sigma}^2_{0.25}$
2	10	1.0042	1.0010	1.0044	1.0023	1.9716	1.0195	3.1950	1.0671
2	20	1.0595	1.0017	1.0852	1.0067	2.4730	1.0021	3.4741	1.0430
2	30	1.1081	0.9992	1.1785	0.9962	3.4238	0.9641	3.8106	1.0188
3	10	1.0324	0.9991	1.0500	1.0037	1.7303	1.0108	2.7589	1.0355
3	20	1.1497	1.0106	1.2650	1.0142	1.8834	1.0012	2.4649	0.9787
3	30	1.1866	0.9961	1.3043	1.0009	2.0839	0.9970	2.7201	1.0158
5	10	1.0934	1.0044	1.1725	1.0065	1.5364	0.9990	2.2837	0.9626
7	10	1.0313	0.9674	0.8130	0.8836	1.4388	0.9519	1.5970	0.7792
9	10	0.9166	0.8897	0.4959	0.7117	1.2459	0.8667	0.9981	0.5709
7	20	1.1707	0.9982	1.3369	0.9570	1.7765	1.0103	2.7630	0.9126
11	20	1.0188	0.9102	0.6334	0.7117	1.3078	0.8807	1.2127	0.5477
15	20	0.8059	0.7592	0.2537	0.5023	1.0007	0.7002	0.5491	0.2887
19	20	0.5948	0.5788	0.1145	0.3525	0.7497	0.5016	0.2897	0.1363

typical examples, i.e., $n \in \{10, 20, 30\}$ in group (A) and (B), $d \in \{2, 3, 5, 7, 9\}$ in group (C), and $d \in \{2, 3, 7, 11, 15, 19\}$ in group (D). Furthermore, we considered one value of δ well below δ^* for all problem instances (0.05) and one above (0.25). Given the high degree of robustness of optimized U-type designs reported in Section 3, we expect only minor improvements for small values of δ (0.05), while larger uncertainty about the actual design points (0.25) might allow for larger gains from robustification.

Tables 2 and 3 report the findings for the designs optimized for bias and MSE, i.e., objective functions (4.1) and (4.2), respectively. We compared the performance of the robust U-type designs with the uniform designs presented above. The columns headed by $\hat{\mu}_{0.05}$ and $\hat{\mu}_{0.25}$ report the ratio of the CD_2 values of the robust U-type designs to the CD_2 value of the uniform designs, where for the robust U-type designs uniform noise with δ equal to 0.05 and 0.25 was added, respectively. To obtain these values, 1,000,000 random draws were used. Thus, entries smaller than one indicate a higher robustness of the result obtained by the method described in this section. The same interpretation applies to the ratios of the variances reported in the columns headed by $\hat{\sigma}^2_{0.05}$ and $\hat{\sigma}^2_{0.25}$.

The results provide support for the high degree of robustness found for the uniform designs in the previous section. In fact, for small designs, the method was not able to suggest designs with a higher level of robustness to low (0.05) or high (0.25) level of noise in design variables. The algorithm often suggests designs resulting even in a higher mean and variance. This, of course, is due to the highly complex double loop optimization problem, that does not always allow to come up with the global optimum. Theoretically, the results should be

Table 3. Properties of robust U-type designs with regard to MSE (objective function (4.2)).

		Designs optimized for $\delta = 0.05$				Designs optimized for $\delta = 0.25$			
d	n	$\hat{\mu}_{0.05}$	$\hat{\mu}_{0.25}$	$\hat{\sigma}^2_{0.05}$	$\hat{\sigma}^2_{0.25}$	$\hat{\mu}_{0.05}$	$\hat{\mu}_{0.25}$	$\hat{\sigma}^2_{0.05}$	$\hat{\sigma}^2_{0.25}$
2	10	1.0125	1.0010	1.0101	1.0029	2.0511	1.0273	3.4729	1.0997
2	20	1.1004	0.9970	1.1267	0.9989	2.6833	0.9876	3.7447	1.0364
2	30	1.1008	0.9992	1.0448	1.0017	3.4206	0.9797	3.8000	1.0284
3	10	1.0335	0.9975	1.0738	1.0025	1.7045	1.0130	2.8784	1.0432
3	20	1.1503	0.9961	1.2821	0.9899	2.4733	0.9942	3.7322	1.0279
3	30	1.2050	1.0045	1.3588	1.0007	2.3151	1.0123	2.6615	0.9938
5	10	1.0747	1.0145	1.0945	1.0201	1.7796	1.0214	2.8634	1.0257
7	10	1.0459	0.9765	0.8630	0.9099	1.3677	0.9611	1.5811	0.7942
9	10	0.9219	0.8766	0.4590	0.6726	1.1533	0.8635	0.8563	0.5736
7	20	1.2045	0.9947	1.4828	0.9472	1.6715	1.0175	2.4162	0.9228
11	20	1.0243	0.8976	0.6282	0.6665	1.3161	0.8811	1.1956	0.5319
15	20	0.8075	0.7559	0.2698	0.4968	1.0316	0.7039	0.5671	0.2892
19	20	0.5966	0.5809	0.1182	0.3567	0.7194	0.5046	0.2760	0.1486

at least as good as for the uniform design as the latter is within the search space. In fact, increasing the number of iterations $I_{\max}$ for a few selected cases with ratios larger than one resulted in ratios much closer to one.

From the designs optimized with regard to a low level of noise, only for $d = 9, n = 10$ and $d = 15, n = 20$ and $d = 19, n = 20$, the expected value of CD_2 was slightly lower than for the uniform design, while the variance was reduced substantially in these cases. When the designs were optimized with regard to a higher level of noise, the design for $d = 11, n = 20$ also was slightly more robust than the uniform design, while the variance was reduced for the high level of noise case even for some of the smaller problem instances.

The findings were qualitatively similar for the second objective function considered, i.e., when minimizing the mean squared error of the discrepancy values.

To summarize our findings, we might conclude that the uniform design is not robust only in the sense described in the previous section, i.e., in comparison with random designs. It is also not possible to find U-type designs of higher degree of robustness by explicit optimization for smaller problem instances. Only for larger problem instances, in particular when the dimension gets close to the number of points, more robust designs might be constructed in the way described in this section.

5. Discussion

Uniform design has received a great deal of attention in the recent literature. Much of its theoretical development, practical value, as well as performance in applications has been reported (see, for example, Fang and Lin (2003)). These studies are based on the ideal situation where the experimental variables can be set exactly at the designated values. In some practical applications, however, the setting of factor level values might be subject to some errors. In this paper, we investigate the robustness of uniform design under such an error in experimental variable situation.

The expected L_2-discrepancy (CD_2) was derived, its closed form is available when the error is relatively small. A thorough Monte Carlo study was conducted under various scenarios. Furthermore, the search for the most robust U-type design was attempted. An algorithm for construction of robust U-type designs was proposed. The search results under the assumption of uniform error distribution, however, indicate that the uniform design is rather robust for small n and d. Only for larger d, in particular, when d approaches n, relevant improvements can be achieved by explicitly searching for robust U-type designs.

Future research will concentrate on the generalization of the closed form expressions for the expected value under uniform errors for the case of larger errors $(\delta \geq 1/2n)$ and other distributional assumptions, e.g., normally distributed error terms. Then, the construction of robust U-type designs will become much more efficient as the inner Monte Carlo simulation loop in the optimization routine can be avoided. Otherwise, e.g., for other objective functions like the mean squared error, it might also be worth considering further improvements of the optimization heuristics taking into account the approximation error of the Monte Carlo integration in the inner loop.

Acknowledgement

We thank Jianfeng Yang for help on Lemma 1. We are also indebted to the Editor and an associate editor of this journal, as well as two reviewers, for their helpful comments on a previous version of the paper. Financial support from the DFG through grant No. 62201080 (Mercator Lin) and the EU Commission through MRTN-CT-2006-034270 COMISEF is gratefully acknowledged.

Appendix A: Proof of Theorem 1

For the proof of Theorem 1 we use the following Lemma.

Lemma 1. *For $\tau, \upsilon \sim U(-\delta,\delta)$ independent, we find*

(i) $$E\,|\tau + c| = \begin{cases} -c & , \mathit{if}\ \ c \leq -\delta, \\ \frac{\delta^2+c^2}{2\delta} & , \mathit{if}\ \ -\delta < c < \delta, \\ c & , \mathit{if}\ \ c \geq \delta\,. \end{cases}$$

(ii) $$E\,|\tau + c|^2 = \frac{1}{3}\delta^2 + c^2\,.$$

(iii) $E\,|\tau - \upsilon + c| =$

$$E\,|\tau + \upsilon + c| = \begin{cases} -c & , \mathit{if} \;\; c \le -2\delta, \\ \frac{1}{12\delta^2}(8\delta^3 + 6\delta c^2 + c^3) & , \mathit{if} \;\; -2\delta < c \le 0, \\ \frac{1}{12\delta^2}(8\delta^3 + 6\delta c^2 - c^3) & , \mathit{if} \;\; 0 \le c < 2\delta, \\ c & , \mathit{if} \;\; c \ge 2\delta\,. \end{cases}$$

Proof of Lemma 1.

(i) $\mathrm{E}|\tau + c| = (1/2\delta)\int_{-\delta}^{\delta}|x + c|dx$

(1) $c \le -\delta \Rightarrow x + c \le 0$
$\mathrm{E}|\tau + c| = -(1/2\delta)\int_{-\delta}^{\delta}(x + c)dx = -c.$

(2) $-\delta \le c \le \delta$
$\mathrm{E}|\tau + c| = (1/2\delta)\int_{-\delta}^{-c} -(x + c)dx + (1/2\delta)\int_{-c}^{\delta}(x + c)dx = (\delta^2 + c^2)/2\delta.$

(3) $c \ge \delta$ $\mathrm{E}|\tau + c| = c.$

(ii) $\mathrm{E}|\tau + c|^2 = (1/2\delta)\int_{-\delta}^{\delta}(x + c)^2dx = (1/3)\delta^2 + c^2.$

(iii) $\mathrm{E}|\tau - \upsilon + c| = \mathrm{E}|\tau + \upsilon + c| = (1/4\delta^2)\int_{-\delta}^{\delta}\int_{-\delta}^{\delta}|x + y + c|dxdy$

(1) $c \le -2\delta \Rightarrow x + y + c \le 0$

$$\begin{aligned}\int_{-\delta}^{\delta}\int_{-\delta}^{\delta}|x + y + c|dxdy &= -\int_{-\delta}^{\delta}dx\int_{-\delta}^{\delta}(x + y + c)dy \\ &= -\int_{-\delta}^{\delta}2\delta(x + c)dx = -4\delta^2 c.\end{aligned}$$

(2) $c \ge 2\delta \Rightarrow x + y + c \ge 0$
Similar to case (1), we have

$$\int_{-\delta}^{\delta}\int_{-\delta}^{\delta}|x + y + c|dxdy = 4\delta^2 c.$$

(3) $-2\delta \le c \le 0$

$$\begin{aligned}&\int_{-\delta}^{\delta}\int_{-\delta}^{\delta}|x + y + c|dxdy = \int_{-\delta}^{\delta}\int_{-\delta}^{\delta}|x - y + c|dxdy \\ &\quad = \int_{-\delta}^{-\delta-c}dx\int_{-\delta}^{\delta}-(x - y + c)dy + \\ &\quad\quad \int_{-\delta-c}^{\delta}dx\left[\int_{-\delta}^{x+c}(x - y + c)dy + \int_{x+c}^{\delta}-(x - y + c)dy\right] \\ &\quad = \int_{-\delta}^{-\delta-c}-2\delta(x + c)dx + \int_{-\delta-c}^{\delta}\left[\frac{1}{2}(x + \delta + c)^2 + \frac{1}{2}(x - \delta + c)^2\right]dx\end{aligned}$$

$$= (\delta c^2 - 2\delta^2 c) + \frac{1}{3}(8\delta^3 + c^3 + 6\delta^2 c + 3\delta c^2)$$
$$= \frac{1}{3}(8\delta^3 + 6\delta c^2 + c^3).$$

(4) $0 \le c \le 2\delta$

$$\int_{-\delta}^{\delta}\int_{-\delta}^{\delta} |x+y+c| dxdy = \int_{-\delta}^{\delta}\int_{-\delta}^{\delta} |x-y+c| dxdy$$
$$= \int_{-\delta}^{\delta-c} dx \left[\int_{-\delta}^{x+c} (x-y+c)dy + \int_{x+c}^{\delta} -(x-y+c)dy\right] +$$
$$\int_{\delta-c}^{\delta} dx \int_{-\delta}^{\delta} (x-y+c)dy$$
$$= \int_{-\delta}^{\delta-c} \left[\frac{1}{2}(x+\delta+c)^2 + \frac{1}{2}(x-\delta+c)^2\right] dx + \int_{\delta-c}^{\delta} 2\delta(x+c)dx$$
$$= \frac{1}{3}(8\delta^3 - c^3 + 3\delta c^2 - 6\delta^2 c) + (2\delta^2 c + \delta c^2)$$
$$= \frac{1}{3}(8\delta^3 + 6\delta c^2 - c^3).$$

Proof of Theorem 1. We proof the following slightly more general version of Theorem 1 including the case that some $v_{ki} = 1/2$:

Proposition 1. *For $\delta < 1/2n$, we have*

$$E\left[CD_2(\tilde{V}))^2\right] = \left(\frac{13}{12}\right)^d$$
$$- \frac{2}{n}\sum_{k=1}^{n}\prod_{i=1}^{d}\left[1+\frac{1}{2}\left(I_{(v_{ki}-1/2)}\left|v_{ki}-\frac{1}{2}\right|+\left(1-I_{(v_{ki}-1/2)}\right)\frac{\delta}{2}\right) - \frac{1}{2}\left|v_{ki}-\frac{1}{2}\right|^2 - \frac{1}{6}\delta^2\right]$$
$$+ \frac{1}{n^2}\sum_{k,j=1}^{n}\prod_{i=1}^{d}\left[1 + \frac{1}{2}\left(I_{(v_{ki}-1/2)}\left|v_{ki} - \frac{1}{2}\right| + \left(1 - I_{(v_{ki}-1/2)}\right)\frac{\delta}{2}\right)\right.$$
$$\left. + \frac{1}{2}\left(I_{(v_{ji}-1/2)}\left|v_{ji} - \frac{1}{2}\right| + \left(1 - I_{(v_{ji}-1/2)}\right)\frac{\delta}{2}\right) - \frac{1}{2}\left|v_{ki} - v_{ji}\right|\right],$$

where

$$I_{(v_{ki}-1/2)} = \begin{cases} 1, & \text{if } v_{ki} - \frac{1}{2} \neq 0, \\ 0, & \text{if } v_{ki} - \frac{1}{2} = 0\,. \end{cases}$$

Proof of Proposition 1. Note that $\delta < 1/2n$ and $v_{ki} \neq 1/2$ implies that $|v_{ki} - 1/2| > \delta$. Then the results for the first sum of products follows directly from Lemma 1 (i) and (ii). For the second sum of products, again the results for the first two expected values follow directly from Lemma 1 (i). For $v_{ki} = 1/2n$ the expected values become $\delta/2$ again from Lemma 1 (i). Consider the last term, $E|(v_{ki} - v_{ji}) + (\tau_{ki} - \tau_{ji})|$. If $k = j$, the term becomes zero. If $k \neq j$, τ_{ki} and τ_{ji} are independent by assumption. Then, (iii) of Lemma 1 applies. Furthermore, as we consider U-type designs with $l = n$ levels, $k \neq j$ implies $v_{ki} \neq v_{ji}$. Then, for $\delta < 1/2n$, the difference $(v_{ki} - v_{ji})$ is larger than 2δ in absolute terms. Hence, the expectation becomes $|v_{ki} - v_{ji}|$.

Appendix B: Results for Alternative Distributions

The analysis presented in Section 3 was repeated for the normal and beta distributions. Some typical shapes of beta distributions are considered with the parameter combinations (a, b) provided in Table B.1.

The distributions were all scaled such that the noise added to the designs had mean zero and a variance equal to the one of the uniform distribution for a given value of δ. Consequently, the results can be compared directly. Figure B.1 shows the resulting values of δ^* for the problem instances (A) – (D) analyzed in Section 3 for the normal distribution and the beta distribution with parameters $(1, 1)$, $(1, 3)$ and $(1, 1.5)$. Thereby, the solid lines correspond to $p = 0.05$ and the dashed lines to $p = 0.01$. Furthermore, for the plots with different run size n (first row), the grey lines correspond to $d = 2$, while the dark lines represent $d = 3$. For the plots with varying dimension d (second row), the grey lines show results for $n = 20$, while the dark lines provide information for the problem instances with $n = 10$.

For $p = 0.05$ we found only minor differences in the values of δ^* and their dependence on the run size n and the dimension d, as compared to the results for the uniform distribution (beta(1,1)). However, when considering a more binding case of p-δ-robustness for $p = 0.01$ (dashed lines), we found that the maximum level of δ satisfying this constraint (δ_p^*) was much smaller for heavily skewed distributions (e.g., beta(1,3)), while similar for symmetric distribution. The functional form of the dependency on n and d, respectively, remained the same also for $p = 0.01$.

References

Box, G. E. P. (1963). The effect of error in the factor levels and experimental design. *Technometrics* **5**, 247-262.

Donev, A. N. (2004). Design of experiments in the presence of errors in factor levels. *J. Statist. Plann. Inference* **126**, 569-585.

Draper, N. R. and Beggs, W. J. (1971). Errors in the factor levels and experimental design. *Ann. Math. Statist.* **41**, 46-56.

Table B.1. Parameters (a, b) of beta distribution.

a	b	
1	1	Unif(0,1) (symmetric)
0.5	1	squared of Unif(0,1) – strictly decreasing
0.5	0.5	Jeffrey's prior for proportion – U-shaped
1	3	strictly convex
1	1.5	strictly concave
2	2	unimodal

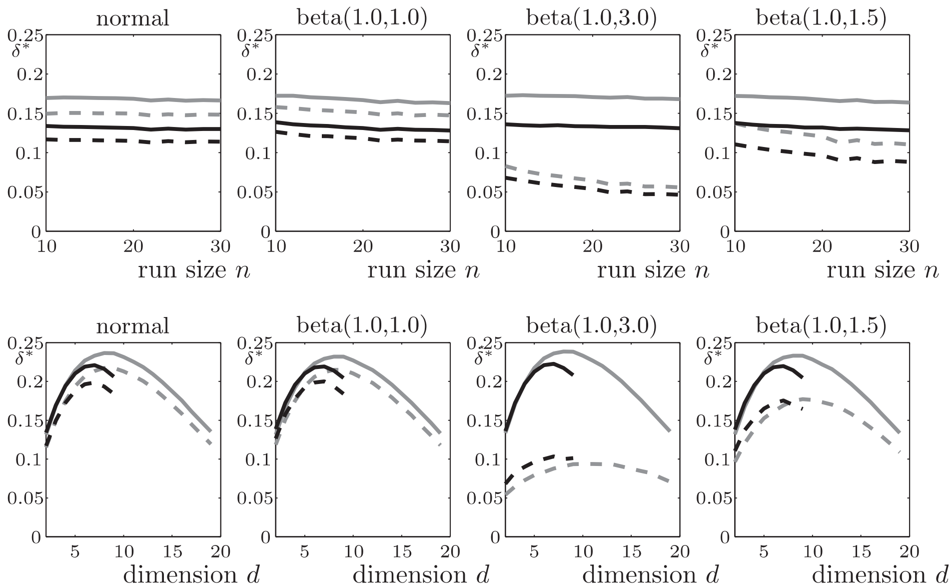

Figure B.1. $\delta^*_{0.05}(V)$ and $\delta^*_{0.01}(V)$ for optimized U-type designs in (A) – (D).

Fang, K.-T., Maringer, D. Tang, Y. and Winker, P. (2006). Lower bounds and stochastic optimization algorithms for uniform designs with three or four levels. *Math. Computation* **75**, 859-878.

Fang, K.-T., Li, R. and Sudjianto, A. (2006). *Design and Modeling for Computer Experiments.* Chapman & Hall, Boca Raton, FL.

Fang, K.-T., Lin, D. K. J., Winker, P. and Zhang, Y. (2000). Uniform design: Theory and application. *Technometrics* **42**, 237-248.

Fang, K.-T. and Lin, D. K. J. (2003). Uniform experimental design and its applications in industry. In *Handbook of Statistics in Industry* (Edit by C.R. Rao and R. Khattree), 131-170. North Holland, New York.

Fang, K.-T., Lu, X. and Winker, P. (2003). Lower bounds for centered and wrap–around L_2–discrepancies and construction of uniform designs by threshold accepting. *J. Complexity* **19**, 692-711.

Hickernell, F. J. (1998). A generalized discrepancy and quadrature error bound. *Math. Computation* **67**, 299-322.

López-Fidalgo, J. and Garcet-Rodríguez, S. A. (2004). Optimal experimental designs when some independent variables are not subject to control. *J. Amer. Statist. Assoc.* **99**, 1190-1199.

Winker, P., Gilli, M. and Jeleskovic, V. (2007). An objective function for simulation based inference on exchange rate data. *J. Economic Interaction and Coordination* **2**, 125-145.

Department of Economics, University of Giessen, Licher Str. 64, 35394 Giessen, Germany.

E-mail: Peter.Winker@wirtschaft.uni-giessen.de

Department of Statistics, Pennsylvania State University, University Park, PA 16801, USA.

E-mail: DennisLin@psu.edu

(Received March 2009; accepted March 2010)