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Bayesian D-optimal supersaturated designs

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Abstract

We introduce a new class of supersaturated designs using Bayesian D-optimality. The designs generated using this approach can have arbitrary sample sizes, can have any number of blocks of any size, and can incorporate categorical factors with more than two levels. In side by side diagnostic comparisons based on the $E(s^2)$ criterion for two-level experiments having even sample size, our designs either match or out-perform the best designs published to date. The generality of the method is illustrated with quality improvement experiment with 15 runs and 20 factors in 3 blocks.

Keywords: Blocking; Exchange algorithm; Model robust designs; Ridge regression; Screening designs

1. Introduction

In process characterization studies engineers often need to distinguish between a few factors that have substantial effects (*active* factors) and many other factors that do not have an effect (*inert* factors). The goal of screening experiments is to separate active from inert factors. When each run is expensive and there are many factors, it is desirable to find a way to reduce the total number of experimental runs. Supersaturated designs fit the bill here, since they have fewer runs than factors.

Consider a common screening model of the form

$$\mathbf{y} = \beta_0\mathbf{1} + \beta_1\mathbf{x}_1 + \cdots + \beta_k\mathbf{x}_k + \boldsymbol{\varepsilon} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}, \tag{1}$$

where $\mathbf{y}$ is an $n \times 1$ vector of observations, $\mathbf{x}_i$ is an $n \times 1$ vector of settings for the ith factor, the design matrix $\mathbf{X}$ is $n \times [p = (k + 1)]$, $\boldsymbol{\beta}$ is the $p \times 1$ vector of coefficients to be estimated, and $\boldsymbol{\varepsilon}$ is the noise vector. In a two-level factorial design, each factor setting can be coded as ± 1 (or simply $\pm$). The design is then determined by the $n \times k$ matrix, $\mathbf{S}$, of elements ± 1. Each row of $\mathbf{S}$ constitutes a *run*. When $n = p$, the design is called a *saturated* design and the design matrix $\mathbf{X}$ is $n \times n$. We use ξ to denote an experimental design, and indicate the dependence of $\mathbf{X}$ on ξ by $\mathbf{X}_\xi$.

To obtain an unbiased estimate of the main effect of each factor, the number of experiments must equal or exceed p. Thus, a common classical screening approach is to use the smallest fractional factorial or Plackett–Burman (1946)

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design capable of fitting the screening model. However, the ability to independently estimate the main effects of all the factors is unnecessary if the goal is simply to identify the few active factors. If the effect sparsity assumption holds, the use of slightly biased parameter estimates will still allow one to accomplish the screening goal while significantly reducing the amount of experimental work.

Of course the idea of using supersaturated designs for screening is not new. Satterthwaite (1959) was the first to consider the use of such designs. Booth and Cox (1962) proposed minimizing the maximum pairwise correlation as optimization criterion. They also introduced the $E(s^2) = \sum_{i>j} \mathbf{x}_i'\mathbf{x}_j/(k(k-1)/2)$ criterion as a diagnostic measure. More recently, Lin (1991, 1993) proposed a class of special supersaturated designs that can be easily constructed using half-fractions of the Hadamard matrices. These designs can examine $k = N - 2$ factors with $n = N/2$ runs, where N is the order of the Hadamard matrix used. Nguyen (1996) showed the relationship between the singular values of the $\mathbf{X}$ matrix and the $E(s^2)$ criterion. Using a columnwise interchange algorithm, he also extended Lin's (1993) list of designs that match a lower bound for $E(s^2)$ where the $k = 2(n-1)$. Recent advances in supersaturated design can be found in Lin (1999, 2000) and references therein.

In this paper, we propose a new class of supersaturated designs using Bayesian D-optimality, building on our recent work of Lin (1993, 1995), DuMouchel and Jones (1994), and Meyer and Nachtsheim (1995). This new class of designs has several advantages:

1. It can incorporate categorical or blocking factors at more than two levels.
2. It works for arbitrary sample sizes, including odd sample sizes, and is not restricted to powers of two or multiples of four.
3. It can require the estimability of subsets of terms.
4. The computer algorithm for building these designs is fast. Since the algorithm works in polynomial time, practitioners can obtain their designs immediately.

This paper is organized as follows. Section 2 describes Bayesian D-optimality for supersaturated design and discusses the computational requirements of the algorithm. Section 3 compares Bayesian supersaturated with existing designs for many cases using several diagnostic measures including one new measure inspired by Nguyen (1996). We show that Bayesian D-optimal supersaturated designs perform equivalently or out-perform $E(s^2)$-optimal designs on all measures except that they do not necessarily minimize the maximum pairwise correlations between factors. The application example introduced in Section 4 demonstrates all the advantages listed above. Finally, a discussion and conclusion are given in Section 5.

2. Bayesian D-optimal supersaturated designs

In factor screening applications, the model is unknown by definition. This complicates the use of classical optimal design criteria because of the underlying assumption that the form of the true model is known. In recent years, however, there has been growing interest in the development of optimality criteria that reflect model uncertainty. Cheng et al. (1999) introduced the estimation capacity (EC) criterion in the context of minimum aberration designs, which considers the percentage of alternative or potential models that are estimable. Li and Nachtsheim (2000) constructed model robust factorial designs, building on the work of Cheng et al. (1999), Läuter (1974, 1976), and Cook and Nachtsheim (1982). The criteria considered in these papers involved the average efficiency of a design, where the average is taken over a set of m potential models. Let w_i denote the weight (or prior probability) assigned to the ith model. The model robust design criterion is given by

$$\phi(\xi) = \sum_{i=1}^{m} w_i e_i(\xi), \tag{2}$$

where $e_i(\xi)$ is a measure of the efficiency or optimality of the design ξ for model i.

Bayesian methods are ideally suited to deal with model uncertainty. Bayesian design generally requires three components: a prior distribution $p(\boldsymbol{\beta})$ for the unknown parameter vector $\boldsymbol{\beta}$; the distribution of the responses, given the unknown parameters, $p(\mathbf{y}|\boldsymbol{\beta})$; and a utility (or risk) function of the form $\mathrm{U}(d, \boldsymbol{\beta}, \xi, \mathbf{y})$, where d is the terminal

decision. Then, for any design ξ in the design space Ξ, the expected utility of the best decision d in action space D is $\mathrm{U}(\xi) = \int_{\mathbf{y}} \max_{d\in D} \int_{\boldsymbol{\beta}} \mathrm{U}(d, \boldsymbol{\beta}, \xi, \mathbf{y}) p(\boldsymbol{\beta}|\xi)\, \mathrm{d}\boldsymbol{\beta}\, \mathrm{d}\mathbf{y}$. The Bayesian optimal design ξ_{B} maximizes the expected utility:

$$\xi_{\mathrm{B}} = \arg\, \max_{\xi\in\Xi} \mathrm{U}(\xi). \tag{3}$$

In the supersaturated case, we adopt fairly standard assumptions for a normal linear model. Taking $\sigma^2 = 1$ without loss of generality, the prior distribution is $\boldsymbol{\beta} \sim N(\boldsymbol{\beta}_0, \mathbf{R}^{-1})$, the conditional distribution of y given $\boldsymbol{\beta}$ is $\mathbf{y}|\boldsymbol{\beta} \sim \mathrm{N}(\mathbf{X}\boldsymbol{\beta}, \mathbf{I})$, and the posterior distribution for $\boldsymbol{\beta}$ given $\mathbf{y}$ is $\boldsymbol{\beta}|\mathbf{y} \sim \mathrm{N}(\boldsymbol{\beta}^*, \mathbf{D}_\xi))$, where $\boldsymbol{\beta}^* = (\mathbf{X}'_\xi\mathbf{X}_\xi + \mathbf{R})^{-1}(\mathbf{X}'_\xi\mathbf{y} + \mathbf{R}\boldsymbol{\beta}_0)$ and $\mathbf{D}_\xi = (\mathbf{X}'_\xi\mathbf{X}_\xi + \mathbf{R})^{-1}$.

When utility is based on Shannon information (Lindley, 1956), the Bayesian optimal design ξ_{B} satisfies (Chaloner and Verdinelli, 1995):

$$\xi_{\mathrm{B}} = \arg\, \max_{\xi\in\Xi} |\mathbf{X}'_\xi\mathbf{X}_\xi + \mathbf{R}|. \tag{4}$$

Note that maximizing $|\mathbf{X}'_\xi\mathbf{X}_\xi + \mathbf{R}|$ is equivalent to maximizing $|\mathbf{M}_\xi + n^{-1}\mathbf{R}|$, where $\mathbf{M}_\xi = \mathbf{X}'_\xi\mathbf{X}_\xi/n$ is the normalized information matrix. This form of the objective function shows that when either n is large ($n \to \infty$) or when little prior information about $\boldsymbol{\beta}$ is available ($\mathbf{R} \to \mathbf{0}$), the Bayesian approach reduces to classical D-optimality.

Model uncertainty in the Bayesian context has been incorporated in a number of ways. Spezzaferri (1988) developed a Bayesian approach for designing experiments when there are dual objectives of parameter estimation and discrimination between two alternative models. Ponce De Leon and Atkinson (1991) also considered the two-model discrimination problem based on a different utility function.

DuMouchel and Jones (1994) incorporated model uncertainty into criterion (4) through their choice of prior $p(\boldsymbol{\beta})$. They divided the set of model terms into two sets. Primary terms are assumed to be present in the true model. Potential terms are those that may or may not be present. For example, in a larger screening experiment, the primary terms might correspond to the intercept and p_1 first-order effects. The potential terms might correspond to the two-factor interactions. Primary terms are assumed to be active, and since no direction is assumed for their effects, DuMouchel and Jones employ a diffuse prior with arbitrary prior mean and prior variance tending to infinity. For the $p_2 = p - p_1$ potential terms, a prior mean of zero and variance τ^2 is assumed, reflecting the belief that parameters are unlikely to be large. For this prior distribution, the information matrix of the parameters is $\mathbf{R} = \mathbf{K}/\tau^2$, where:

$$\mathbf{K} = \begin{pmatrix} \mathbf{0}_{p_1\times p_1} & \mathbf{0}_{p_1\times p_2} \\ \mathbf{0}_{p_2\times p_1} & \mathbf{I}_{p_2\times p_2} \end{pmatrix}. \tag{5}$$

Criterion (4) is then

$$\xi_{\mathrm{B}} = \arg\, \max_{\xi\in\Xi} |\mathbf{X}'_\xi\mathbf{X}_\xi + \mathbf{K}/\tau^2|. \tag{6}$$

Note that when $n < p$, $|\mathbf{X}'_\xi\mathbf{X}_\xi| = 0$. However, $|\mathbf{X}'_\xi\mathbf{X}_\xi + \mathbf{K}/\tau^2|$ will be positive for appropriate choice of design.

The DuMouchel–Jones criterion (6) is directly applicable to the supersaturated design problem. We consider two cases. In the first case, all terms except the intercept are potential terms. In this situation, the experimenter is unsure as to the presence of any of the factors to be included in the experiment. In the second case, we assume that the first $p_1 - 1$ factors are known to be active and the remaining p_2 factors are to be screened—and are therefore potential effects. In the latter case, designs produced guarantee the separate estimability of all of the primary terms. Note that n must be greater than p_1.

We use the coordinate exchange algorithm (Meyer and Nachtsheim, 1995) to optimize criterion (6), although in theory any exact design algorithm could be substituted. The coordinate exchange algorithm is useful here because it does not require the construction of candidate sets. Most exchange algorithms such as DETMAX improve a design criterion iteratively through exchanges of runs in the design with a "best" new point selected from a candidate set. For problems considered here, the processing of relevant candidate sets can become computationally prohibitive. For example, the candidate set for a supersaturated design problem involving 20 factors would normally be based on the 2^{20} (more than 10^6) vertices of the hypercube $[-1, 1]^{20}$. (Because the model is first-order, we use a grid size of 2 in our implementation of the coordinate exchange algorithm.) Avoiding the use of candidate sets reduces execution time by several orders of magnitude. We note that if balanced designs are required, the columnwise–pairwise (CP) algorithm of Li and Wu (1997) could be similarly implemented, also without requiring the construction of candidate sets .

Because exchange algorithms do not guarantee convergence to the globally optimal design, we strongly advocate the use of multiple random starting designs. Normally a few dozen are sufficient, although we employ 100 random starts for the detailed comparisons discussed in the next section. Also, for the DuMouchel–Jones criterion, we have found that the optimal designs are relatively insensitive to the choice of prior variance τ^2. All examples herein employ $\tau^2 = 5$.

3. Comparisons

In this section we examine the performance characteristics of Bayesian D-optimal supersaturated designs. We do so by comparing our designs with the best designs (in terms of the $E(s^2)$ criterion) published to date, as reported in Table 2 of Nguyen (1996). The design diagnostics are:

1. $E(s^2)$.
2. Average correlation $\bar{r} = \sqrt{\sum_{i=1}^{k-1}\sum_{j=i+1}^{k}(r_{ij})^2/(k(k-1)/2)}$.
3. Maximum absolute correlation $\max|r|$.
4. Our new diagnostic, c, described below.
5. Bayesian D-optimal objective function $D_{\text{Bayes}} = |\mathbf{X}'\mathbf{X} + \mathbf{K}/\tau^2|$.

Among them, the first three criteria are the-smaller-the-better type; while the last two criteria are the-larger-the-better type.

Nguyen showed that minimizing the $E(s^2)$ criterion is like trying to make all the singular values of $\mathbf{S}$ equal while keeping their sum of squares constant. His designs achieve this goal whenever $k = 2(n-1)$. This suggests the criterion:

$$c = \frac{(n-1)\prod_{i=1}^{n-1} s_i^{2/(n-1)}}{nk}, \tag{7}$$

where s_i is the ith largest singular value of $\mathbf{S}$. This criterion ranges from zero to one and achieves its upper bound for Nguyen's designs where $k = 2(n-1)$. Note that in (7) we have assumed that the maximum rank of $\mathbf{S}$ is $n-1$. This is the case for the classes of supersaturated designs discussed here. For example, use of the $E(s^2)$ criterion restricts the search to balanced designs, so that all columns of $\mathbf{S}$ sum to one. For the Bayesian D-optimal designs we created, the maximum rank of $\mathbf{S}$ is $n-1$ because the intercept is a primary term, and it must be separately estimable from the main effects.

Of the 21 designs in Table 2 of Nguyen (1996), 14 have $k = 2(n-1)$ and are optimal by the $E(s^2)$ criterion. These designs are also at least locally Bayesian D-optimal designs. To demonstrate this we started by perturbing a Nguyen design. The perturbation involved adding a uniform random number on the interval [0, 0.1] to each -1 setting and subtracting a uniform random number on the same interval from each $+1$ setting. Applying the coordinate exchange algorithm of the previous section to the perturbed Nguyen design returned the original Nguyen design in every case.

Table 1 compares Bayesian D-optimal designs to Nguyen's $E(s^2)$-optimal designs for the seven cases tabulated by Nguyen where $k \neq 2(n-1)$. The criterion values for the Bayesian D-optimal designs meet or exceed those for the

Table 1
Comparison of Bayesian D-optimal versus Nguyen's $E(s^2)$-optimal designs

k	n	$E(s^2)$[a]	$\bar{r}$[a]	$\max\|r\|$[a]	c[b]	D_{Bayes}[b]
16	12	4.8 (5.2)	0.181 (0.190)	0.48 (0.33)	0.99 (0.97)	6.37 (6.32)
18	12	5.96 (5.96)	0.203 (0.203)	0.33 (0.33)	0.98 (0.98)	4.85 (4.85)
24	12	7.83 (7.83)	0.233 (0.233)	0.67 (0.33)	0.99 (0.98)	2.008 (2.004)
24	18	6.68 (7.13)	0.145 (0.148)	0.45 (0.33)	0.98 (0.96)	9.93 (9.87)
30	18	9.14 (9.37)	0.168 (0.170)	0.45 (0.33)	0.983 (0.978)	5.74 (5.73)
30	24	7.72 (7.92)	0.116 (0.117)	0.33 (0.33)	0.97 (0.96)	15.32 (15.30)
36	18	10.78 (10.91)	0.183 (0.183)	0.56 (0.56)	0.988 (0.986)	3.185 (3.182)

Criterion values for Nguyen's designs are given in parentheses.

[a]The smaller, the better.

[b]The larger, the better.

$E(s^2)$-optimal designs for all criteria except the maximum absolute correlation. In three of the seven cases, the values are the same, in three cases the difference is moderate (0.48 versus 0.33 or 0.45 versus 0.33) and in one case the Nguyen design does substantially better (0.67 versus 0.33). Note that many Bayesian D-optimal designs have lower values of $E(s^2)$ than the $E(s^2)$-optimal designs. This is due to the fact that the $E(s^2)$-optimal designs are constrained to be balanced. Relaxing this constraint allows the Bayesian D-optimal design to improve on the "$E(s^2)$-optimal" values. The final column in Table 1 shows that the $E(s^2)$-optimal designs also do quite well by the Bayesian criterion.

These examples indicate that in cases where n and k are even, and where supersaturated designs have been generated based on $E(s^2)$ or other combinatorial properties, the Bayesian designs perform comparably. The example in the next section demonstrates the flexibility and generality of the Bayesian approach.

4. Example

A six sigma team needed to investigate a process that tends to shift in level from day to day. This process makes very expensive parts at the rate of 5 parts per day. The plant manager has agreed to allow 3 days for experimentation. A brainstorming session reveals 20 factors that may affect the response of interest. It is likely that only a few of these 20 factors are active, but the team does not know which.

A standard approach would be to attempt to convince the plant manager to allow 4 days for experimentation and run 4 blocks with 4 runs per block for a total sample size of 16. This approach would also require the removal of at least 8 of the 20 factors from consideration. This solution has several disadvantages.

1. It increases the cost of the experiment.
2. By increasing the number of blocks (days) required, it makes the experiment more difficult to implement.
3. The process used to reduce the number of experimental factors may eliminate key active factors from further consideration.

Taken together, these issues may dampen management's enthusiasm for actually conducting the experiment.

The Bayesian D-optimal design shown in Table 2 provides a solution to the problem exactly as posed. To construct this design, we first designate the blocking factor as a primary effect and the 20 continuous factor main effects as potential effects. A starting design is generated by choosing 15 points at random from the $[-1, 1]^{20}$ hypercube and then distributing the points into three blocks of size 5. The design in Table 2 is the best design found by the coordinate exchange algorithm using 40 random starts. To give some indication of the computing time required, the average execution time per random start was about one second on a 1.7 Ghz personal computer.

Table 2
Bayesian D-optimal supersaturated design for 15 runs and 20 factors in 3 blocks

Block	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	−	−	−	−	+	−	+	+	−	+	−	+	+	+	−	+	+	+	+	−
1	−	+	−	−	−	+	+	−	+	−	+	−	+	+	+	+	−	−	−	−
1	+	+	+	+	−	−	−	+	+	+	+	−	−	−	+	+	+	+	+	−
1	+	−	−	−	+	−	−	−	−	+	+	−	−	−	−	−	−	−	−	+
1	−	−	+	+	−	+	+	+	+	−	−	+	−	−	−	−	+	−	−	+
2	+	+	−	−	+	+	+	+	+	+	−	−	−	−	+	+	+	+	−	+
2	−	+	+	−	−	−	−	+	+	+	+	+	+	+	−	−	−	+	−	+
2	−	+	+	+	+	−	+	−	−	−	+	−	−	+	−	+	+	−	+	+
2	+	−	+	+	+	+	+	−	+	+	+	+	+	−	+	−	−	−	+	−
2	+	−	−	+	−	−	−	+	−	−	−	+	−	+	+	+	−	−	−	−
3	+	+	−	−	−	−	+	+	−	−	+	+	+	−	+	−	+	−	+	+
3	−	−	+	+	+	+	−	+	−	−	+	−	+	−	+	+	−	+	−	+
3	−	+	−	+	+	−	+	+	+	+	+	+	−	−	−	+	−	−	−	−
3	+	+	−	+	+	+	−	−	+	−	−	+	−	+	−	−	−	+	+	+
3	+	−	+	−	−	−	−	−	+	+	−	−	+	+	−	+	+	−	−	−

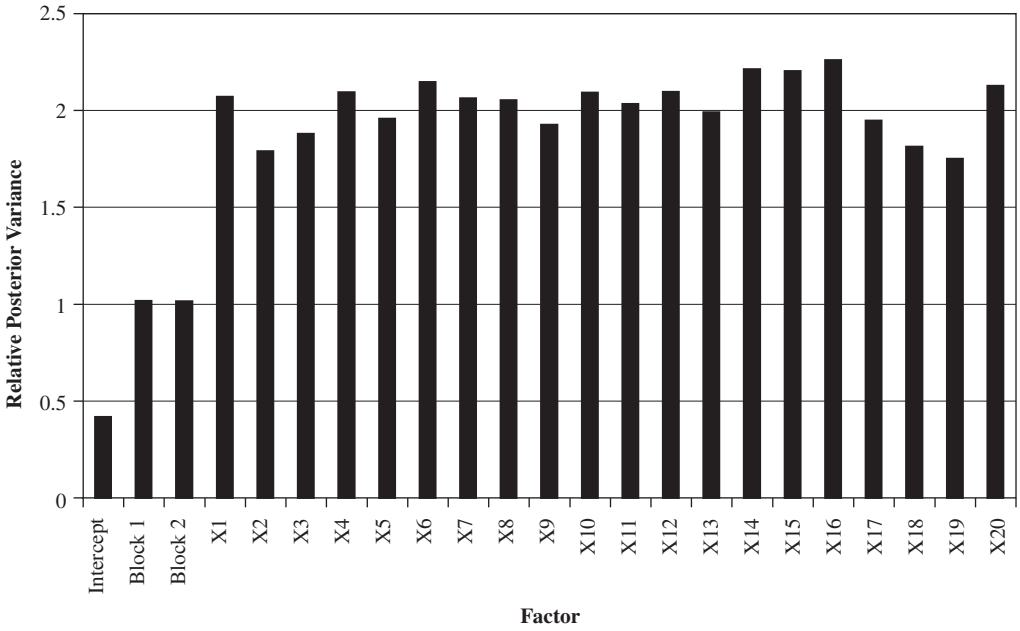

Fig. 1. Posterior variances for all estimated effects.

We first note that for each block and for every continuous factor, there are either 2 or 3 +s. In this sense the design is "nearly" balanced within blocks; thus factor effects are nearly orthogonal to block effects. Among factor effects, the average correlation measure $\bar{r}$ for this design is 0.185, and the maximum absolute correlation is 0.49. The relative posterior variances of the coefficients are displayed in Fig. 1. The figure shows that the variances of the estimates cluster into three groups. For the intercept term (i.e., the mean) the relative posterior variance is less than 0.5; for the two block effects, the relative posterior variances are about 1.0; and for the 20 factor effects the posterior variances are about 2.0. Clearly, the variances of the three primary effects (mean and block effects) are considerably smaller than those of the 20 potential effects. This reflects the fact that, for these factors, the corresponding diagonal elements of $\mathbf{K}$ are zero. Among the potential factors, there is little variation in the posterior variances—all are in the vicinity of 2.0. Thus, the design leads to parameter estimates having roughly uniform precision, and to a reduction in the (relative) variances of the parameters from prior values of $\tau^2 = 5$ to posterior values of approximately 2.0.

While the analysis of the data obtained from such an experiment is not the subject of this paper, we comment that a fully Bayesian treatment would lead to the use of a generalized ridge estimator. As discussed above, the relative posterior variances of the estimated parameters are displayed in Fig. 1. Other approaches as discussed in Lin (2000) and Chen and Lin (1998) could be applied as well.

5. Discussion and conclusion

We have applied Bayesian D-optimality to the problem of supersaturated design. The resulting designs compare favorably to balanced $E(s^2)$-optimal designs for many criteria including $E(s^2)$.

We recommend these designs, not only for their excellent statistical properties but for their applicablilty to a much broader set of problems than has been possible to date. To our knowledge there have been no published supersaturated designs with arbitrary numbers of runs. More importantly, we are not aware of any prior work enabling the construction of optimally blocked supersaturated designs for arbitrary numbers of blocks and block sizes. One member of the current author team has considered the development of supersaturated designs for factors with more than two levels (Fang et al., 2000), but until now there has been no general approach for constructing supersaturated designs for factors having arbitrary numbers of levels. Bayesian D-optimal design provides a framework for doing all of these things.

Better yet, the coordinate exchange algorithm generates these designs quickly so that there is no need to resort to books of tabulated designs.

Our method is currently implemented in the JMP software published by SAS Institute Inc. All designs discussed in the paper are can be downloaded from the following URL: http://www.smeal.psu.edu/faculty/dkl5/BayesSSD.

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