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An Efficient Algorithm for Constructing Bayesian Optimal Choice Designs

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While Bayesian \mathcal{G} - and \mathcal{V} -optimal designs for the multinomial logit model have been shown to have better predictive performance than Bayesian \mathcal{D} - and \mathcal{A} -optimal designs, the algorithms for generating them have been too slow for commercial use. In this article, we present a much faster algorithm for generating Bayesian optimal designs for all four criteria while simultaneously improving the statistical efficiency of the designs. We also show how to augment a choice design allowing for correlated parameter estimates using a sports club membership study.

KEY WORDS: Alternating sample algorithm; Bayesian \mathcal{D} -, \mathcal{A} -, \mathcal{G} -, and \mathcal{V} -optimality; Conjoint choice design; Coordinate-exchange algorithm; Minimum potential design; Multinomial logit.

1. INTRODUCTION

Conjoint choice experiments are widely used in marketing to measure how the attributes of a product or service jointly affect consumer preferences. In a choice experiment, a product or service is characterized by a combination of attribute levels called a profile or an alternative. Respondents then choose one from a group of profiles called a choice set. They repeat this task for several other choice sets presented to them. All submitted choice sets make up the experimental design. The aim of a choice experiment is to estimate the importance of each attribute and its levels based on the respondents' preferences. The estimates are then exploited to mimic real marketplace choices by making predictions about consumers' future purchasing behavior.

Designing an efficient choice experiment involves selecting those choice sets that result in an accurately estimated model providing precise predictions. Kessels, Goos, and Vandebroek (2006) compared four different design criteria based on the multinomial logit model to reach this goal. They studied the predictive performance of the \mathcal{D} - and \mathcal{A} -optimality criteria versus the \mathcal{G} - and \mathcal{V} -optimality criteria. Special attention was paid to the \mathcal{G} - and \mathcal{V} -optimality criteria, which aim at making precise predictions. The authors were the first to work out these criteria for the multinomial logit model. On the other hand, the \mathcal{D} - and \mathcal{A} -optimality criteria focus on accurate parameter estimates. Until now, the \mathcal{D} -optimality criterion has been most often employed to construct efficient choice designs (see Huber and Zwerina 1996; Sándor and Wedel 2001).

Because the multinomial logit model is nonlinear in the parameters, the computation of the optimality criteria depends on the unknown parameter vector. To solve this problem,

Kessels et al. (2006) adopted a Bayesian design procedure as proposed by Sándor and Wedel (2001). Following these authors, they approximated the design criteria using a Monte Carlo sample from a multivariate normal prior parameter distribution. Monte Carlo sampling involves taking a large number of random draws from a probability distribution as a surrogate for that distribution. Like Sándor and Wedel (2001), Kessels et al. (2006) used 1,000 random draws. The four optimality criteria in the Bayesian context are labeled the \mathcal{D}_B -, \mathcal{A}_B -, \mathcal{G}_B -, and \mathcal{V}_B -optimality criteria. Kessels et al. (2006) implemented these criteria in a modified Fedorov algorithm (Cook and Nachtsheim 1980; Fedorov 1972) to construct \mathcal{D}_B -, \mathcal{A}_B -, \mathcal{G}_B -, and \mathcal{V}_B -optimal designs. We refer to their complete algorithm as the Monte Carlo modified Fedorov algorithm (MCMF).

Kessels et al. (2006) showed that the \mathcal{G}_B - and \mathcal{V}_B -optimality criteria outperform the \mathcal{D}_B - and \mathcal{A}_B -optimality criteria in terms of prediction accuracy. They warn, however, that the computation of \mathcal{G}_B - and \mathcal{V}_B -optimal designs is substantially more demanding than the search for \mathcal{D}_B - and \mathcal{A}_B -optimal designs. The long computing times resulting from MCMF make the \mathcal{G}_B - and \mathcal{V}_B -optimality criteria impractical to use. Also, the computational burden implies that the application of the \mathcal{D}_B -, \mathcal{A}_B -, \mathcal{G}_B -, and \mathcal{V}_B -optimality criteria to computerized conjoint choice studies is limited. Ideally, computerized conjoint studies use choice designs that are tailored to the individual respondents so that maximum information is obtained on the

individuals' preferences and thus on the heterogeneity between subjects.

The goal of this article is to present a novel design construction algorithm that is much faster than the MCMF algorithm employed by Kessels et al. (2006). The speed of the new algorithm allows the \mathcal{G}_B - and \mathcal{V}_B -optimality criteria to be used in practice, and it also makes it possible to apply individualized Bayesian optimal choice designs in web-based conjoint studies.

The new algorithm has four key features. First, it relies on a small designed sample of prior parameter vectors instead of the Monte Carlo sample of 1,000 draws. However, the algorithm still checks the designs produced by each random start using the Monte Carlo sample. Because it switches between calculating the objective function using these two different samples, the algorithm is called the alternating sample algorithm. Second, the algorithm is an adaptation of Meyer and Nachtsheim's (1995) coordinate-exchange algorithm, which is much faster than the modified Fedorov algorithm. Third, it involves a revised formula for the \mathcal{V}_B -optimality criterion so that its computation is even more efficient. Last, it uses an update formula to economically calculate the change in any of the optimality criteria for two designs that differ only in one profile. In this way, the optimality criterion values do not need to be recomputed from scratch.

The outline of the remainder of the article is as follows. Section 2 reviews the \mathcal{D}_B -, \mathcal{A}_B -, \mathcal{G}_B -, and \mathcal{V}_B -optimality criteria for the multinomial logit model. In Section 3, we present the alternating sample algorithm as an alternative to MCMF for faster computation of the optimal designs for all four criteria. We use the design example from Kessels et al. (2006) for comparison purposes. Section 4 discusses the four key features of the alternating sample algorithm. Section 5 shows how to deal with correlated prior parameter distributions in the context of augmenting an existing conjoint study on sports club membership. This application involves a more challenging scenario made possible by the new algorithm. Finally, Section 6 summarizes the results and suggests some opportunities for further research.

2. DESIGN CRITERIA FOR THE MULTINOMIAL LOGIT MODEL

To present our improved design construction approach, we start with an overview of the different design criteria for the multinomial logit model. The model requires a choice design matrix $\mathbf{X} = [\mathbf{x}'_{js}]_{j=1,\dots,J;s=1,\dots,S}$ where \mathbf{x}_{js} is a $k \times 1$ vector of the attribute levels of profile j in choice set s . A respondent's utility for that profile is modeled as $u_{js} = \mathbf{x}'_{js}\boldsymbol{\beta} + \varepsilon_{js}$ where $\boldsymbol{\beta}$ is a $k \times 1$ vector of parameters and ε_{js} is an iid extreme value error term. The multinomial logit probability a respondent chooses profile j in choice set s is $p_{js} = e^{\mathbf{x}'_{js}\boldsymbol{\beta}} / \sum_{t=1}^J e^{\mathbf{x}'_{ts}\boldsymbol{\beta}}$. The information matrix \mathbf{M} is the sum of the information matrices of the S choice sets \mathbf{M}_s as shown below:

$$\begin{aligned} \mathbf{M}(\mathbf{X}, \boldsymbol{\beta}) &= N \sum_{s=1}^S \mathbf{M}_s(\mathbf{X}_s, \boldsymbol{\beta}) \\ &= N \sum_{s=1}^S \mathbf{X}'_s (\mathbf{P}_s - \mathbf{p}_s \mathbf{p}'_s) \mathbf{X}_s, \end{aligned} \quad (1)$$

where $\mathbf{X}_s = [\mathbf{x}_{1s}, \dots, \mathbf{x}_{Js}]'$, $\mathbf{p}_s = [p_{1s}, \dots, p_{Js}]'$, $\mathbf{P}_s = \text{diag}[p_{1s}, \dots, p_{Js}]$ and N is the number of respondents. Kessels et al. (2006) implemented different design criteria or functions of the information matrix (1) for constructing optimal choice designs. This task is complicated by the fact that the information on the parameters depends on the unknown values of those parameters through the probabilities p_{js} . Therefore, the authors adopted a Bayesian design strategy that integrates the design criteria over a prior parameter distribution $\pi(\boldsymbol{\beta})$. The multivariate normal distribution $\mathcal{N}(\boldsymbol{\beta} | \boldsymbol{\beta}_0, \boldsymbol{\Sigma}_0)$ was chosen for this purpose.

The design criteria employed are the \mathcal{D} -, \mathcal{A} -, \mathcal{G} -, and \mathcal{V} -optimality criteria. The \mathcal{D} - and \mathcal{A} -optimality criteria both are concerned with a precise estimation of the parameters $\boldsymbol{\beta}$ in the multinomial logit model. The \mathcal{D} -optimality criterion aims at designs that minimize the determinant of the variance-covariance matrix of the parameter estimators, whereas the \mathcal{A} -optimality criterion aims at designs that minimize the trace of the variance-covariance matrix. The Bayesian \mathcal{D} -optimality criterion is

$$\mathcal{D}_B = \int_{\mathcal{R}^k} \{\det(\mathbf{M}^{-1}(\mathbf{X}, \boldsymbol{\beta}))\}^{1/k} \pi(\boldsymbol{\beta}) d\boldsymbol{\beta}, \quad (2)$$

with the \mathcal{D}_B -optimal design minimizing (2). The \mathcal{A}_B -optimal design minimizes

$$\mathcal{A}_B = \int_{\mathcal{R}^k} \text{tr}(\mathbf{M}^{-1}(\mathbf{X}, \boldsymbol{\beta})) \pi(\boldsymbol{\beta}) d\boldsymbol{\beta}. \quad (3)$$

The \mathcal{G} - and \mathcal{V} -optimality criteria were developed to make precise response predictions. These criteria are important in this context because predicting consumer responses is the goal of choice experiments. The \mathcal{G} - and \mathcal{V} -optimality criteria for the multinomial logit model were first elaborated by Kessels et al. (2006). They are defined with respect to a design region χ consisting of all Q possible choice sets of size J that can be composed from the candidate profiles: $\chi = \{\{\mathbf{x}_{1q}, \dots, \mathbf{x}_{Jq}\} | q = 1, \dots, Q\}$. A \mathcal{G} -optimal design minimizes the maximum prediction variance over the design region χ , whereas a \mathcal{V} -optimal design minimizes the average prediction variance over this region. Formally, the \mathcal{G}_B -optimality criterion is

$$\begin{aligned} \mathcal{G}_B &= \int_{\mathcal{R}^k} \max_{\mathbf{x}_{jq} \in \chi} \text{var}\{\hat{p}_{jq}(\mathbf{x}_{jq}, \boldsymbol{\beta})\} \pi(\boldsymbol{\beta}) d\boldsymbol{\beta} \\ &= \int_{\mathcal{R}^k} \max_{\mathbf{x}_{jq} \in \chi} \mathbf{c}'(\mathbf{x}_{jq}) \mathbf{M}^{-1}(\mathbf{X}, \boldsymbol{\beta}) \mathbf{c}(\mathbf{x}_{jq}) \pi(\boldsymbol{\beta}) d\boldsymbol{\beta}, \end{aligned} \quad (4)$$

where $\hat{p}_{jq}(\mathbf{x}_{jq}, \boldsymbol{\beta})$ denotes the predicted choice probability for \mathbf{x}_{jq} and

$$\mathbf{c}(\mathbf{x}_{jq}) = \frac{\partial p_{jq}(\mathbf{x}_{jq}, \boldsymbol{\beta})}{\partial \boldsymbol{\beta}} = p_{jq} \left(\mathbf{x}_{jq} - \sum_{t=1}^J p_{tq} \mathbf{x}_{tq} \right), \quad (5)$$

the partial derivative of the multinomial logit probability p_{jq} with respect to $\boldsymbol{\beta}$. The \mathcal{V}_B -optimality criterion is

$$\mathcal{V}_B = \int_{\mathcal{R}^k} \int_{\chi} \mathbf{c}'(\mathbf{x}_{jq}) \mathbf{M}^{-1}(\mathbf{X}, \boldsymbol{\beta}) \mathbf{c}(\mathbf{x}_{jq}) d\mathbf{x}_{jq} \pi(\boldsymbol{\beta}) d\boldsymbol{\beta}. \quad (6)$$

3. THE ALTERNATING SAMPLE ALGORITHM VERSUS MCMF FOR COMPUTING \mathcal{D}_B -, \mathcal{A}_B -, \mathcal{G}_B -, AND \mathcal{V}_B -OPTIMAL DESIGNS

We propose the alternating sample algorithm for generating \mathcal{D}_B -, \mathcal{A}_B -, \mathcal{G}_B -, and \mathcal{V}_B -optimal designs instead of the MCMF

algorithm employed by Kessels et al. (2006) (see Section 1). The alternating sample algorithm is much faster than MCMF so that for a given computing time the resulting designs outperform the designs produced by MCMF.

We illustrate the better results from the alternating sample algorithm versus MCMF using the design example of Kessels et al. (2006). These authors constructed \mathcal{D}_B -, \mathcal{A}_B -, \mathcal{G}_B -, and \mathcal{V}_B -optimal designs of two classes: $3^2 \times 2/2/12$ and $3^2 \times 2/3/8$. The design profiles in the two classes have a similar attribute structure with two attributes at three levels and one attribute at two levels. Hence, the sets of candidate profiles of the two classes comprise the same $3^2 \times 2 = 18$ profiles. The designs of the first class consist of 12 choice sets of size two, while the designs of the second class consist of eight choice sets of size three. So, the designs of both classes contain 24 profiles. Because we exploit this design example of 24 profiles to compare the alternating sample algorithm to MCMF, we refer to it as the comparison example and label it $3^2 \times 2/24$.

Using effects-type coding (see Kessels et al. 2006), the number of elements, k , in the parameter vector $\boldsymbol{\beta}$ is five. As prior parameter distribution, Kessels et al. (2006) proposed the multivariate normal distribution $\pi(\boldsymbol{\beta}) = \mathcal{N}(\boldsymbol{\beta}|\boldsymbol{\beta}_0, \boldsymbol{\Sigma}_0)$, with $\boldsymbol{\beta}_0 = [-1, 0, -1, 0, -1]'$ and $\boldsymbol{\Sigma}_0 = \mathbf{I}_5$. They approximated this distribution by drawing a Monte Carlo sample of $R = 1,000$ prior parameter vectors $\boldsymbol{\beta}^r$, $r = 1, \dots, R$, from it. The Bayesian optimal designs were then obtained from 200 random starts of the modified Fedorov algorithm. This algorithm iteratively improves the starting design by exchanging its profiles with profiles from the candidate set. To compute the \mathcal{G}_B - and \mathcal{V}_B -optimality criteria for the two-alternative designs, the design region χ consists of $Q = \binom{18}{2} = 153$ choice sets, whereas for the three-alternative designs, it includes $Q = \binom{18}{3} = 816$ choice sets.

Based on the same normal prior distribution we employed the alternating sample algorithm to reproduce the \mathcal{D}_B -, \mathcal{A}_B -, \mathcal{G}_B -, and \mathcal{V}_B -optimal designs for the comparison example. Besides the two- and three-alternative designs, we also generated four-alternative designs containing six choice sets. The design region χ in this case is quite extensive, involving $Q = \binom{18}{4} = 3,060$ choice sets. The optimal designs from the alternating sample algorithm appear in Tables A.1, A.2, and A.3 of the Appendix. Table 1 compares the criterion values of these designs with the criterion values obtained by Kessels et al. (2006) using the MCMF algorithm. The two-alternative \mathcal{D}_B -optimal designs from both algorithms are equivalent. However, in all the other cases with two and three alternatives, the designs generated with the alternating sample algorithm outperform the designs generated with MCMF.

The best criterion values from the alternating sample algorithm were the result of 1,000 random starts rather than the 200 random starts used to obtain the best criterion values from MCMF. Because the alternating sample algorithm is so much faster than MCMF, the extra random starts were still accomplished using far less computing time. The computing times for one random start of the alternating sample algorithm and MCMF appear in Tables 2(a) and 2(b), respectively. We performed all computations in MATLAB 7 using a Dell personal computer with a 1.60 GHz Intel Processor and 2 GB RAM.

Tables 2(a) and 2(b) show the huge reductions in computing time using the alternating sample algorithm. Particularly important are the reductions in computing time for the \mathcal{G}_B - and \mathcal{V}_B -optimality criteria, which make the construction of \mathcal{G}_B - and \mathcal{V}_B -optimal designs practically feasible. Even the four-alternative \mathcal{G}_B - and \mathcal{V}_B -optimal designs were generated quickly, whereas their computation was not doable with MCMF. Notice also the faster running time for the \mathcal{V}_B -optimality criterion compared with the \mathcal{G}_B -optimality criterion. This is due to a computational short cut in the calculation of the \mathcal{V}_B -optimality criterion, which we lay out in Section 4.3.

A comparison of the effectiveness of the alternating sample algorithm and MCMF appears in the plots of Figure 1. In these graphs, we plotted the estimated expected efficiencies of the two-alternative \mathcal{D}_B - and \mathcal{V}_B -optimal designs against the number of seconds of computing time. We expressed the number of seconds on a log-scale. These plots provide compelling evidence of the practical value of the alternating sample algorithm. The huge increase in speed created by the alternating sample algorithm overtly leads to more efficient designs in a given amount of computing time. This is especially the case for the prediction-based design criteria as illustrated by the plot for the \mathcal{V}_B -efficiencies. Note however, that the bend in the plot for the \mathcal{D}_B -efficiencies reveals that the alternating sample algorithm has a little difficulty making the final jump from 99% efficiency to 100% or global efficiency. Details on the calculation of the expected efficiency from a number of random starts can be found in the work of Kessels et al. (2006).

The plots for the two-alternative \mathcal{D}_B - and \mathcal{V}_B -optimal designs in Figure 1 are representative of the two-alternative \mathcal{A}_B - and \mathcal{G}_B -optimal designs, respectively. The plots for the three-alternative designs exhibit a similar pattern.

4. FEATURES OF THE ALTERNATING SAMPLE ALGORITHM

There are four features of the alternating sample algorithm that result in increased speed compared with MCMF. In order of importance, they are

Table 1. \mathcal{D}_B -, \mathcal{A}_B -, \mathcal{G}_B -, and \mathcal{V}_B -criterion values of the \mathcal{D}_B -, \mathcal{A}_B -, \mathcal{G}_B -, and \mathcal{V}_B -optimal designs for the comparison example $3^2 \times 2/24$ computed using the alternating sample algorithm and the Monte Carlo modified Fedorov algorithm

Optimal design	2 alternatives		3 alternatives		4 alternatives	
	Alternating sample	MCMF	Alternating sample	MCMF	Alternating sample	MCMF
\mathcal{D}_B	0.73024	0.73024	0.75362	0.76617	0.86782	–
\mathcal{A}_B	6.55212	6.60563	5.97903	6.02261	6.57135	–
\mathcal{G}_B	0.49887	0.51997	0.51051	0.51843	0.60494	–
\mathcal{V}_B	0.07184	0.07219	0.06267	0.06285	0.05728	–

Table 2. Computing times for one random start of the alternating sample algorithm and the Monte Carlo modified Fedorov algorithm to generate the Bayesian optimal designs for the comparison example $3^2 \times 2/24$.

(a) Alternating sample algorithm			
Design criterion	# Alternatives		
	2	3	4
\mathcal{D}_B	00:00:03	00:00:04	00:00:05
\mathcal{A}_B	00:00:03	00:00:04	00:00:05
\mathcal{G}_B	00:00:07	00:00:32	00:04:23
\mathcal{V}_B	00:00:03	00:00:05	00:00:08
(b) Monte Carlo modified Fedorov			
Design criterion	# Alternatives		
	2	3	4
\mathcal{D}_B	00:08:00	00:08:00	—
\mathcal{A}_B	00:08:00	00:08:00	—
\mathcal{G}_B	03:00:00	12:00:00	—
\mathcal{V}_B	03:00:00	12:00:00	—

NOTE: The times are expressed in hours:minutes:seconds.

1. a small designed sample of prior parameters,
2. a coordinate-exchange algorithm,
3. an efficient computation of the \mathcal{V}_B -optimality criterion, and
4. a fast update of the Cholesky decomposition of the information matrix.

The next sections discuss each of these in succession.

4.1 Small Designed Sample of Prior Parameters

In this section, we present a new method to approximate the integral related to a multivariate normal prior $\pi(\boldsymbol{\beta}) = \mathcal{N}(\boldsymbol{\beta}|\boldsymbol{\beta}_0, \boldsymbol{\Sigma}_0)$ in the definitions of the Bayesian optimality criteria. The solution of the integral with respect to a multi-

variate normal prior for the various criteria has not been accomplished analytically. In general, for models that are nonlinear in the parameters some numeric approximation to the integral is necessary (Chaloner and Verdinelli 1995).

Sándor and Wedel (2001) and Kessels et al. (2006) used a Monte Carlo estimate of the integral from 1,000 random draws of the prior. By the law of large numbers, such estimates are known to converge to the true value of the integral at a rate proportional to the square root of the number of draws. This necessitates a large number of draws to reduce the sample-to-sample variability to the point where different samples do not lead to different design choices. This approach is costly because the computing time for the Bayesian design is then roughly 1,000 times longer than the computing time for a locally optimal design (i.e., the design for one prior parameter vector).

To solve integrals related to a multivariate normal distribution for the construction of choice designs, Sándor and Wedel (2002) used samples based on orthogonal arrays (Tang 1993) and Sándor and Wedel (2005) constructed quasi-Monte Carlo samples (Hickernell, Hong, L'Ecuyer, and Lemieux 2000). In several cases, estimates using these methods are more efficient than Monte Carlo estimates so that it is possible to employ smaller samples to obtain the same accuracy (Sándor and András 2004; Sándor and Train 2004). There is also an extensive literature on quadrature, which is another approach to numerical integration. One such work is Sloan and Joe (1994), who discussed good lattice point methods. However, for integrals of functions in more than four dimensions, Monte Carlo estimates tend to outperform quadrature estimates (Geweke 1996; Monahan and Genz 1997).

4.1.1 A Designed Set of Sample Parameters. We propose to approximate the integrals in (2), (3), (4), and (6) with a designed sample of only a small number of parameter vectors. Assuming that the prior variance-covariance matrix $\boldsymbol{\Sigma}_0$ is proportional to the identity matrix, the multivariate normal distribution is spherically symmetric around the prior mean. As a result, every parameter has the same density on a k -dimensional

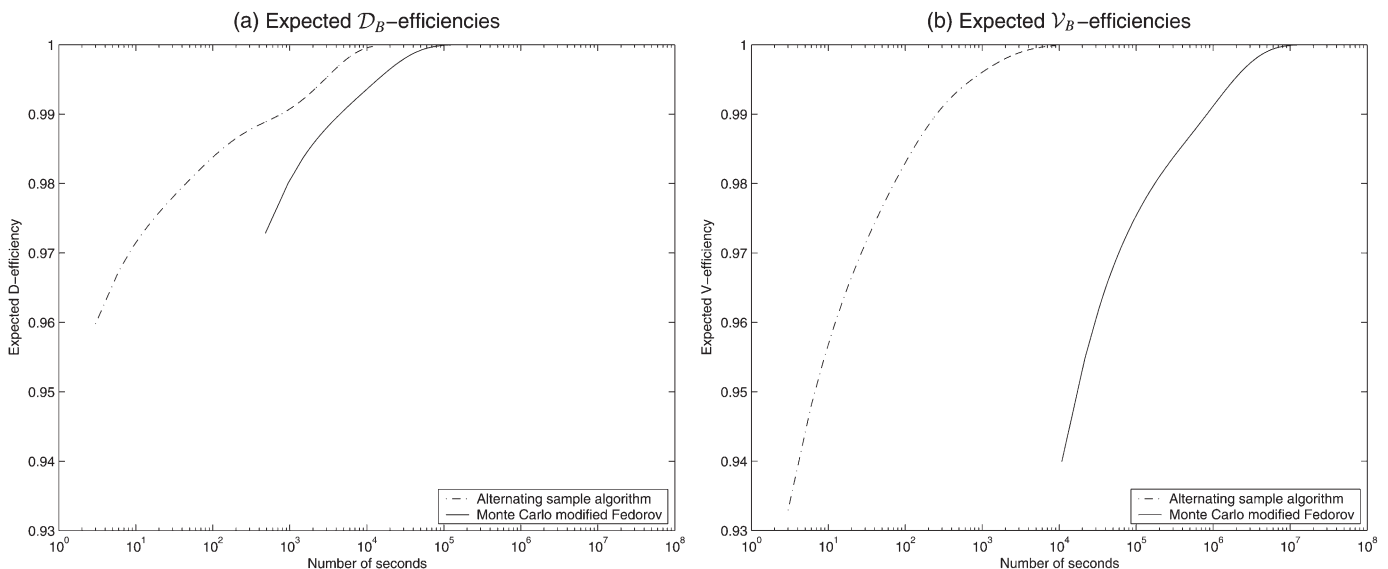


Figure 1. Estimated expected efficiencies against computation time of the alternating sample algorithm and the Monte Carlo modified Fedorov algorithm for producing the two-alternative \mathcal{D}_B - and \mathcal{V}_B -optimal designs.

hypersphere of a given radius. The parameter vectors we use are uniformly distributed on such a sphere. In this way, they sample the different directions away from the prior mean fairly.

The designed sample yields an approximation that is worse than the Monte Carlo sample of 1,000 draws. However, in the computation of Bayesian optimal designs, it is not necessary for the approximation of the integral to be accurate. All that is required is that the sign of the difference from a rough approximation corresponding to two slightly different designs matches the sign of the difference from a better approximation. In our examples, we chose 20 parameter vectors as a compromise between computation time and precision of the integral approximation. For the $3^2 \times 2/24$ example, the plot in Figure 2 illustrates that the systematic sample and the Monte Carlo sample largely agree on design improvements in a random start of the alternating sample algorithm.

The plot compares the \mathcal{V}_B -criterion value for the Monte Carlo sample with the \mathcal{V}_B -criterion value for the systematic 20-point sample. It depicts the course of one random start of the coordinate-exchange algorithm for the two-alternative designs. From a random starting design, the algorithm makes a sequence of changes, each of which improves the \mathcal{V}_B -criterion value for the systematic 20-point sample. By reevaluating each of these changes with the \mathcal{V}_B -criterion value for the Monte Carlo sample, we find out whether every change also leads to an improvement using the better approximation.

The starting design is represented by the point at the top right of the plot, which of all points has the highest or worst \mathcal{V}_B -criterion value according to the 20-point sample as well as the Monte Carlo sample. After making one change in the original design, the second point from the top right shows an improvement in the \mathcal{V}_B -criterion value for both samples. The points proceed from the top right to the bottom left of the plot. The point at the bottom left denotes the final and best design produced in the random start. Note that this point has the lowest

or best \mathcal{V}_B -criterion value as approximated by both samples. Furthermore, note that the drop in the \mathcal{V}_B -criterion value is not monotonic, indicating that the two approximations are not in complete agreement about the \mathcal{V}_B -criterion value of each change in the sequence.

Still, the agreement between the \mathcal{V}_B -criterion value for the Monte Carlo sample and the \mathcal{V}_B -criterion value for the systematic 20-point sample is clear from a correlation of 99%. Similar correlations are obtained using the coordinate-exchange algorithm with every other design criterion and with larger choice set sizes. However, this does not imply that designs that are optimal using the systematic 20-point sample are also optimal with respect to the Monte Carlo sample. The plot in Figure 3 demonstrates this.

Like the plot in Figure 2, the plot in Figure 3 displays the \mathcal{V}_B -criterion value for the Monte Carlo sample versus the \mathcal{V}_B -criterion value for the systematic 20-point sample. Now each point in the plot represents the best two-alternative design found in a single random start of the coordinate-exchange algorithm. Again, the algorithm used the \mathcal{V}_B -criterion value for the 20-point sample to generate the designs and the \mathcal{V}_B -criterion value for the Monte Carlo sample to reevaluate them. From the plot, we see that the worst design by both \mathcal{V}_B -criterion values is the same. On the other hand, the best design according to the \mathcal{V}_B -criterion value for the 20-point sample differs from the best design indicated by the \mathcal{V}_B -criterion value for the Monte Carlo sample.

In this case, the correlation between the \mathcal{V}_B -criterion values for the Monte Carlo sample and the \mathcal{V}_B -criterion values for the 20-point sample from the different random starts is only 66%. This result also applies to the other design criteria and larger choice set sizes. The fact that the correlation is not close to 100% means that it is important to reevaluate the design produced by the algorithm after each random start with one calculation of the objective function using the Monte Carlo sample. Therefore, our approach alternates between the small

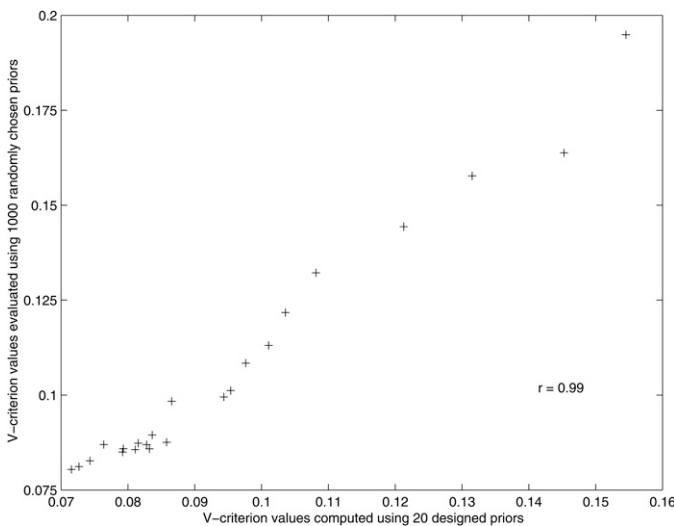


Figure 2. \mathcal{V}_B -criterion values according to the 1,000-point Monte Carlo sample versus the systematic 20-point sample and correlation between them. The points represent the course of one random start of the coordinate-exchange algorithm for the two-alternative designs using the 20-point sample.

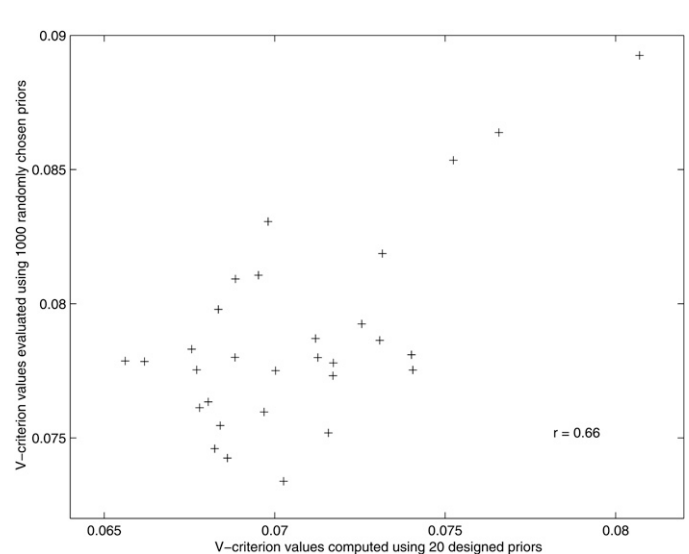


Figure 3. \mathcal{V}_B -criterion values according to the 1,000-point Monte Carlo sample versus the systematic 20-point sample and correlation between them. Each point represents a design produced from a different random start of the coordinate-exchange algorithm.

designed sample and the large Monte Carlo sample. Ultimately, the design with the best criterion value in terms of the Monte Carlo sample is selected.

Note that, if the correlation were near 100%, it would not be necessary to check the designs. Also, observe that because of the decrease in the number of prior parameters from 1,000 to 20 during a random start we save up to 98% of the computational work.

4.1.2 Constructing a Small Sample of Prior Parameters.

For any choice design problem, we can construct a small set of prior parameters using a minimum potential design (see SAS 2007, pp. 160–161). These designs were created using the commercial software JMP 7. For dimensions larger than three, the points of these designs will be uniformly distributed on a k -dimensional hypersphere at a radius of one away from the zero vector. So on the sphere, the minimum distance to a neighboring point from any of the design points will be roughly the same for all the points.

To understand how minimum potential designs are created, consider n points on a k -dimensional sphere around the zero vector. Each point, p , is labeled (z_{p1}, \dots, z_{pk}) . Let d_{ef} be the distance between the e th and f th points. That is

$$d_{ef} = \sqrt{\sum_{i=1}^k (z_{ei} - z_{fi})^2}. \quad (7)$$

The optimization problem is to find the $n \times k$ values of z_{pi} that minimize E_{pot} , the potential energy of the system:

$$E_{pot} = \sum_{e=1}^{n-1} \sum_{f=e+1}^n \left(d_{ef}^2 + \frac{1}{d_{ef}} \right). \quad (8)$$

In this expression, imagine the n points as electrons with springs attached to every point. Then, d_{ef}^2 is proportional to the energy stored in a spring when you pull it and $1/d_{ef}$ is the potential energy between two electrons. When the distance

between two points increases, d_{ef}^2 increases. When the distance between two points decreases, $1/d_{ef}$ increases.

For the comparison example, the minimum potential design with 20 points in a 5-dimensional space appears in Table 3. These points lie on a sphere of a radius of one around $[0, 0, 0, 0, 0]'$. The minimum distance for each point to the nearest point is 1.171. If this interpoint distance seems too large, then it can be reduced by increasing the number of points.

To properly approximate the prior distribution with a 20-point sample from the points of a minimum potential design, it is necessary to rescale these points for the prior variance-covariance matrix and the prior mean. If there is no correlation between the prior coefficients or $\Sigma_0 = \sigma_0^2 \mathbf{I}_k$, then the 20-point sample lies on a sphere with a radius that is proportional to the standard deviation σ_0 . Now, the effectiveness of the 20-point sample in the alternating sample algorithm depends on the radius specified, or the number of standard deviations away from the prior mean. That is to say, a well-chosen radius requires fewer random starts to reach the global optimum. To find the best radius for a spherical 20-point sample for any choice design problem, one could proceed as follows:

1. Do a number of random starts of the alternating sample algorithm for each of three radii.
2. Fit a quadratic function to the minimum criterion value found at each radius.
3. Choose the radius that minimizes the quadratic function.

For the comparison example, we performed 10 random starts for a radius of 1, 2, and 3. Recall that $\sigma_0 = 1$ for this example. The result for the \mathcal{V}_B -optimality criterion connected with two-alternative designs appears in Figure 4. Fitting a quadratic model to the minima results in a radius slightly larger than 2. We chose, however, a radius of 2 for simplicity. To illustrate the value of selecting a good radius, we compared the estimated expected efficiencies per number of random starts of the

Table 3. Minimum potential design of 20 points in 5 continuous factors for the comparison example.

Design point	z_1	z_2	z_3	z_4	z_5	Minimum distance	Nearest point	Radius
1	-0.17642	-0.57290	-0.19875	0.74536	-0.19600	1.17076	15	0.99281
2	-0.21775	0.81588	0.32619	-0.30104	-0.28759	1.17075	19	0.99281
3	-0.54891	-0.28739	-0.29445	0.17376	0.70655	1.17076	8	1.00000
4	-0.57116	0.06703	-0.27064	-0.77093	0.04122	1.17074	8	1.00000
5	-0.20011	-0.19572	-0.17339	-0.25973	-0.90384	1.17074	20	0.99281
6	0.00117	0.10528	0.59690	0.49371	-0.62360	1.17075	5	1.00000
7	-0.01228	0.13614	0.39319	-0.47950	0.76785	1.17076	13	0.99280
8	0.00528	-0.87552	-0.10638	-0.43810	0.15165	1.17074	4	0.99281
9	0.75353	-0.47946	-0.01214	0.10921	-0.43617	1.17076	16	1.00000
10	0.58274	0.19380	-0.32178	-0.71016	-0.08827	1.17075	20	0.99281
11	0.73699	0.47141	0.45742	0.07033	0.14296	1.17075	10	1.00000
12	-0.79511	-0.25333	0.54158	-0.02905	-0.04767	1.17077	13	0.99281
13	0.19427	-0.53359	0.65989	0.32602	0.36850	1.17075	17	1.00000
14	-0.00619	0.71761	-0.49688	-0.08192	0.48104	1.17075	2	1.00000
15	0.01039	-0.23327	-0.96643	-0.04302	-0.09815	1.17075	16	1.00000
16	0.60646	-0.18338	-0.34715	0.29484	0.61963	1.17075	15	0.99281
17	-0.19392	0.43870	0.30072	0.70409	0.42020	1.17075	13	0.99281
18	0.40102	0.49636	-0.41417	0.47335	-0.43591	1.17075	15	0.99281
19	-0.74200	0.35148	-0.35744	0.34145	-0.28555	1.17075	2	1.00000
20	0.17200	-0.17915	0.68369	-0.61868	-0.29685	1.17074	5	1.00000

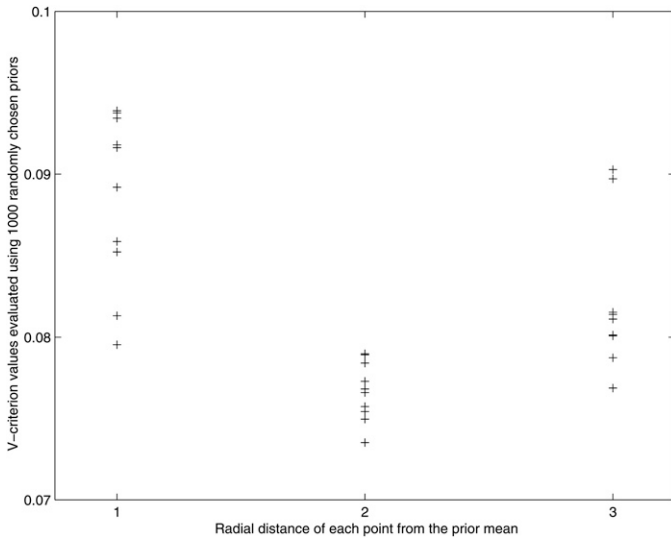


Figure 4. \mathcal{V}_B -criterion values of two-alternative designs from 10 random starts of the alternating sample algorithm using the 20-point samples for radii 1, 2, and 3.

two-alternative \mathcal{V}_B -optimal designs using the 20-point samples for radii 1 and 2, respectively. The plots based on 250 random starts appear in Figure 5. We clearly observe the higher expected efficiencies in case a radius of 2 is used as opposed to a radius of 1. We obtained similar results for any other optimality criterion in combination with any choice set size.

However, computing the “best” radius is not absolutely necessary. The heuristic of choosing a sphere radius that is twice the prior standard deviation worked well in all the examples we tried. The critical part of the alternating sample algorithm is that for each random start using the 20-point sample, one checks the resulting design with the larger Monte Carlo sample. So, no matter what radius one chooses, one will have a monotonically improving set of designs as the number

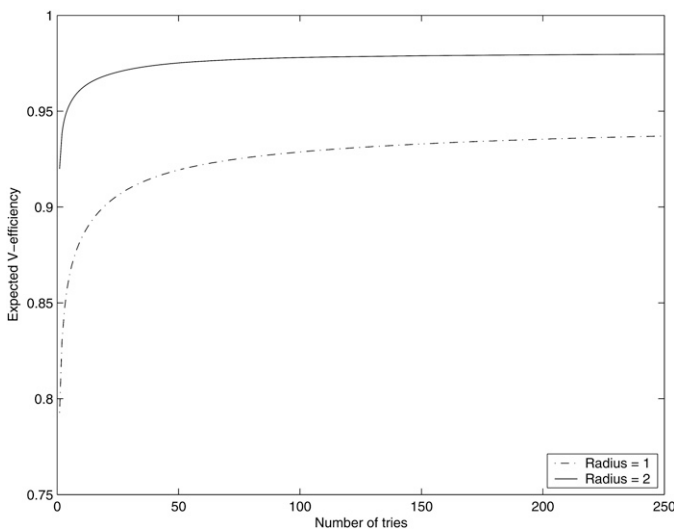


Figure 5. Estimated expected efficiencies per number of random starts of the two-alternative \mathcal{V}_B -optimal designs computed using the alternating sample algorithm with the 20-point samples for radii 1 and 2.

of random starts increases. Still, choosing a good radius increases the speed of the improvement over the random starts.

4.2 Coordinate-Exchange Algorithm

The alternating sample algorithm uses Meyer and Nachtsheim’s (1995) coordinate-exchange algorithm to generate Bayesian optimal designs. The coordinate-exchange algorithm has also been applied by Kuhfeld and Tobias (2005) to generate \mathcal{D} -efficient factorial designs for large choice experiments based on a linear model. As opposed to the modified Fedorov algorithm employed in Kessels et al. (2006), it allows the computation of choice designs with a large number of profiles, attributes, and/or attribute levels in a reasonable amount of time. The coordinate-exchange algorithm can be seen as a greedy profile exchange algorithm. Whereas the modified Fedorov algorithm possibly changes every “coordinate” or attribute level of a profile, the coordinate-exchange algorithm only changes one coordinate at a time. For each attribute level in the design, the coordinate-exchange algorithm tries all possible levels and chooses the level corresponding to the best value of the optimality criterion under consideration.

The algorithm begins by creating a random starting design. Improvements are made to the starting design by considering changes in the design on an attribute-by-attribute basis. For any attribute of a given profile in the current design, the objective function is evaluated over all the levels of that attribute. If the maximal value of the objective function is larger than the current maximum, then the current maximum is replaced and the profile’s current attribute level is replaced by the new level corresponding to the maximal value of the objective function. This attribute-by-attribute procedure continues until a complete cycle through the entire design is completed. Then, another complete cycle through the design is performed noting if any attribute level changes in the current pass. This continues until no changes are made in a whole pass or until a specified maximum number of passes have been executed.

In contrast with the modified Fedorov algorithm, the coordinate-exchange algorithm is a candidate-set-free algorithm. That is, it does not require the specification of a set of candidate profiles. This aspect becomes more important when the candidate set is very large because of a large number of attributes and/or attribute levels. The coordinate-exchange algorithm is also substantially faster than the modified Fedorov algorithm. It runs in polynomial time, whereas the modified Fedorov algorithm runs in exponential time. For the comparison example, this leads to roughly a factor of three speed increase of the coordinate-exchange algorithm over the modified Fedorov algorithm. For designs with more profiles, attributes, and/or attribute levels, this increase in speed becomes more pronounced.

4.3 Efficient Computation of the \mathcal{V}_B -Optimality Criterion

In the alternating sample algorithm, the \mathcal{V}_B -optimality criterion is implemented in an efficient way. For each prior vector of coefficients, it is possible to compute the average prediction variance without first computing the prediction variances for each profile $\mathbf{x}_{jq} \in \chi$ separately. A similar approach does not apply to the \mathcal{G}_B -optimality criterion because

finding the worst prediction variance requires the computation of all variances.

The prediction variance on the left of (9) is naturally a scalar since $\mathbf{c}(\mathbf{x}_{jq})$ is a $k \times 1$ vector and \mathbf{M}^{-1} a $k \times k$ matrix. The trace of a scalar is the scalar itself so that

$$\mathbf{c}'(\mathbf{x}_{jq})\mathbf{M}^{-1}\mathbf{c}(\mathbf{x}_{jq}) = \text{tr}(\mathbf{c}'(\mathbf{x}_{jq})\mathbf{M}^{-1}\mathbf{c}(\mathbf{x}_{jq})). \quad (9)$$

Now, $\text{tr}(\mathbf{ABC}) = \text{tr}(\mathbf{CAB})$ if \mathbf{A} , \mathbf{B} , \mathbf{C} are matrices such that \mathbf{ABC} is a square matrix and the matrix product \mathbf{CAB} exists. This equality is known as the cyclic property of the trace. Since the prediction variance is a scalar and $\mathbf{c}(\mathbf{x}_{jq})\mathbf{c}'(\mathbf{x}_{jq})$ is a $k \times k$ matrix that conforms with \mathbf{M}^{-1} ,

$$\text{tr}(\mathbf{c}'(\mathbf{x}_{jq})\mathbf{M}^{-1}\mathbf{c}(\mathbf{x}_{jq})) = \text{tr}(\mathbf{c}(\mathbf{x}_{jq})\mathbf{c}'(\mathbf{x}_{jq})\mathbf{M}^{-1}). \quad (10)$$

Let $\mathbf{W}_{jq} = \mathbf{c}(\mathbf{x}_{jq})\mathbf{c}'(\mathbf{x}_{jq})$. Because $\mathbf{c}(\mathbf{x}_{jq})$ does not depend on the design \mathbf{X} , \mathbf{W}_{jq} is not a function of \mathbf{X} either so that it only has to be computed once for each prior parameter vector. We now average the individual matrices \mathbf{W}_{jq} over all profiles $\mathbf{x}_{jq} \in \chi$ and denote the subsequent matrix by \mathbf{W} :

$$\mathbf{W} = \frac{1}{JQ} \sum_{j=1}^J \sum_{q=1}^Q \mathbf{W}_{jq}. \quad (11)$$

The average prediction variance across all profiles $\mathbf{x}_{jq} \in \chi$ for a given prior parameter vector is then

$$\int_{\chi} \mathbf{c}'(\mathbf{x}_{jq})\mathbf{M}^{-1}\mathbf{c}(\mathbf{x}_{jq})d\mathbf{x}_{jq} = \text{tr}(\mathbf{WM}^{-1}) \quad (12)$$

We refer to the work of Meyer and Nachtsheim (1995) for a similar expression of the \mathcal{V} -optimality criterion in the linear design setting.

So, to obtain the \mathcal{V}_B -optimality criterion, we have to compute \mathbf{W} for each prior parameter vector only once. The set of \mathbf{W} matrices can be reused from one random start to the next.

4.4 Updating the Cholesky Decomposition of the Information Matrix

Updating the Cholesky decomposition of the information matrix is an economical way to compute the \mathcal{D}_B -, \mathcal{A}_B -, \mathcal{G}_B -, and \mathcal{V}_B -criterion values of designs that differ only in one profile, and therefore one choice set, from another design. This is the case in the alternating sample algorithm, where at each step a new design is created by changing only one attribute level of a single profile (see Section 4.2).

If \mathbf{M} is a symmetric positive definite matrix, then its Cholesky decomposition is defined as

$$\mathbf{M} = \mathbf{L}'\mathbf{L}, \quad (13)$$

where \mathbf{L} is an upper triangular matrix named the Cholesky factor. Note that the information matrix \mathbf{M} is symmetric because it is the sum [from Equation (1)] of the information matrices of the S choice sets \mathbf{M}_s that are symmetric. Each of these \mathbf{M}_s is of the form $\mathbf{X}'_s\mathbf{C}_s\mathbf{X}_s$, where $\mathbf{C}_s = \mathbf{P}_s - \mathbf{p}_s\mathbf{p}'_s$ is symmetric.

We compute the \mathcal{D}_B -, \mathcal{A}_B -, \mathcal{G}_B -, and \mathcal{V}_B -criterion values of each of the designs as follows. For each prior parameter vector, we compute the information matrix \mathbf{M} through (1) and derive

its Cholesky factor \mathbf{L} . We update the Cholesky factor after every profile change with low rank updates based on the work of Bennett (1965) and implemented in the MATLAB function CHOLUPDATE. The update is low rank because only one choice set is changing at any step.

Using the Cholesky factors the four criterion values for each design can be obtained as shown below. In this way, we avoid recomputation of the information matrix through (1). For the comparison example $3^2 \times 2/24$, this procedure reduced the computing times by roughly a factor of three.

We now illustrate how the different design criteria rely on the Cholesky factor \mathbf{L} of the information matrix \mathbf{M} . For any parameter vector $\boldsymbol{\beta}^r$, the \mathcal{D} -optimality criterion becomes

$$\begin{aligned} \mathcal{D} &= (\det(\mathbf{M}^{-1}))^{1/k} = 1/(\det(\mathbf{M}))^{1/k} \\ &= 1/(\det(\mathbf{L}')\det(\mathbf{L}))^{1/k} = 1/\left(\prod_{i=1}^k l_{ii}\right)^{2/k}, \end{aligned} \quad (14)$$

where l_{ii} is the i th diagonal element of \mathbf{L} . Thus, to obtain the \mathcal{D}_B -criterion value of a design in which a profile has been changed, we do not need to recompute the information matrix for every prior parameter vector. Only an update of the Cholesky factor is required.

To show the dependency of the \mathcal{A}_B -, \mathcal{G}_B -, and \mathcal{V}_B -optimality criteria on the Cholesky factor \mathbf{L} , the Cholesky decomposition (13) has to be inverted. The inverse is given by

$$\mathbf{M}^{-1} = (\mathbf{L}'\mathbf{L})^{-1} = \mathbf{L}^{-1}(\mathbf{L}^{-1})'. \quad (15)$$

Because the Cholesky factor, \mathbf{L} , is triangular, inverting it is easier than inverting \mathbf{M} . Then, for any prior parameter vector, the \mathcal{A} -optimality criterion is

$$\mathcal{A} = \text{tr}(\mathbf{M}^{-1}) = \text{tr}(\mathbf{L}^{-1}(\mathbf{L}^{-1})') = \sum_{i=1}^k \sum_{j=i}^k m_{ij}^2, \quad (16)$$

where m_{ij} is the ij th element in \mathbf{L}^{-1} . So to obtain the \mathcal{A}_B -criterion value of a design in which a profile has been changed, we need to derive the new Cholesky factor for every prior parameter vector and take its inverse. This goes much faster than computing the new information matrix and inverting it.

In a similar manner, the \mathcal{G}_B - and \mathcal{V}_B -criterion values are obtained. The prediction variance of profile $\mathbf{x}_{jq} \in \chi$ is expressed as

$$\mathbf{c}'(\mathbf{x}_{jq})\mathbf{M}^{-1}\mathbf{c}(\mathbf{x}_{jq}) = \mathbf{c}'(\mathbf{x}_{jq})\mathbf{L}^{-1}(\mathbf{L}^{-1})'\mathbf{c}(\mathbf{x}_{jq}). \quad (17)$$

Here, $\mathbf{c}(\mathbf{x}_{jq})$ does not depend on the design \mathbf{X} and therefore only needs to be computed once for each prior parameter vector. The \mathcal{G}_B -criterion value is obtained by inserting (17) in (4). For the \mathcal{V}_B -optimality criterion, we performed some initial calculations that make its computation even more efficient as discussed previously.

5. DESIGNING A FOLLOW UP EXPERIMENT

The speed of the alternating sample algorithm makes the computation of Bayesian optimal designs feasible for more challenging problems of larger dimensions than the rather small comparison example $3^2 \times 2/24$. We illustrate this with the construction of a follow up design to the choice experiment on

Table 4. Parameter estimates and standard errors for the sports club membership choice experiment in Sándor and Wedel (2001)

Coefficient	Estimates	Standard error
Location 1	0.58	0.059
Location 2	−0.90	0.071
Period 1	−0.63	0.061
Period 2	0.05	0.057
Activities 1	−0.03	0.053
Activities 2	−0.35	0.060
Clubs 1	−0.15	0.057
Clubs 2	0.36	0.056
Price 1	0.54	0.062
Price 2	−0.02	0.055

sports club membership described in Sándor and Wedel (2001) and carried out at the University of Groningen in the Netherlands. The original experiment consisted of 30 choice sets of size two, half of which were obtained using the Bayesian \mathcal{D} -optimality criterion. The other 15 choice sets formed a non-Bayesian \mathcal{D} -optimal design. The Bayesian and the non-Bayesian \mathcal{D} -optimal design are displayed in Table A.4. The two designs were presented to each of the respondents in one session. The order of presentation of the choice sets from each design was alternated. The profiles in the experiment were configured from five three-level attributes. So in total, there are $3^5 = 243$ candidate profiles. This candidate set is much larger than the candidate set of 18 profiles employed in the comparison example.

We acquired data from 43 of the original 58 respondents from the authors of the original study, and analyzed it using the NLPCG subroutine in SAS. The parameter estimates and standard errors we obtained are given in Table 4. The variance-covariance matrix of the estimates is displayed in Table 5. We used the parameter estimates and their variance-covariance matrix as the mean and variance of the multivariate normal prior distribution $\pi(\boldsymbol{\beta})$ when designing the follow up study. We denote the vector of parameter estimates, which serves as the prior mean, by $\boldsymbol{\beta}_0$, and its covariance matrix by Σ_0 .

The procedure required to use $\boldsymbol{\beta}_0$ as the prior mean and Σ_0 as the prior variance in the alternating sample algorithm is as follows. First, randomly generate 1,000 parameter vectors from the standard normal distribution. If we denote any of these vectors by $\boldsymbol{\nu}$, then a random parameter vector $\boldsymbol{\beta}^r$ drawn from the multivariate normal distribution with mean $\boldsymbol{\beta}_0$ and variance Σ_0 can be constructed using

$$\boldsymbol{\beta}^r = \boldsymbol{\beta}_0 + \mathbf{D}'\boldsymbol{\nu}, \quad (18)$$

where \mathbf{D} is the Cholesky factor of the variance-covariance matrix Σ_0 , so that $\mathbf{D}'\mathbf{D} = \Sigma_0$.

Creating the designed sample of 20 parameter vectors using a minimum potential design and multiplying by 2 will put these vectors on the surface of a hypersphere of radius 2. Premultiplying the resulting vectors by the transpose of the Cholesky factor, \mathbf{D}' , moves them to the surface of a hyperellipsoid. This makes them have approximately the same correlation structure as the previously described Monte Carlo sample, because the minimum potential design is always nearly orthogonal. That is, the inner product of differing pairs of columns is close to zero. Finally, the designed sample needs to be recentered to the prior mean vector $\boldsymbol{\beta}_0$ by adding $\boldsymbol{\beta}_0$ to the outcome of the premultiplication by \mathbf{D}' .

We assumed that the original respondents were contacted for the follow up study and that they were asked to evaluate 10 additional choice sets. Together with the 30 choice sets of the original study, these choice sets make up the augmented design. We have constructed optimal follow up designs using the \mathcal{D}_B - and \mathcal{V}_B -optimality criteria and 1,000 random starts of the alternating sample algorithm. For this problem, χ consists of $Q = \binom{243}{2} = 29,403$ choice sets. The \mathcal{D}_B - and \mathcal{V}_B -optimal follow up designs are displayed in Table A.5 of the Appendix.

Table 6 shows the improvement in terms of estimation and prediction capability, as measured by the \mathcal{D}_B - and \mathcal{V}_B -criteria, due to the additional choice sets. The criteria depend on the prior mean vector, $\boldsymbol{\beta}_0$, and variance-covariance matrix, Σ_0 , in Table 4 and Table 5, respectively. As can be seen from the \mathcal{D}_B -criterion values, the \mathcal{D}_B - and \mathcal{V}_B -optimal augmented designs are nearly equivalent in terms of precision of estimation. The \mathcal{V}_B -optimal design is slightly more \mathcal{V}_B -efficient than the \mathcal{D}_B -optimal design.

In this application, the practical difference between the \mathcal{D}_B - and \mathcal{V}_B -optimal designs is minuscule. To check whether this result also holds in case of a smaller original design, we computed \mathcal{D}_B - and \mathcal{V}_B -optimal follow up designs of 10 choice sets both for the 15 choice sets of the Bayesian and the non-Bayesian \mathcal{D} -optimal design. These follow up designs appear in Table A.6 of the Appendix and the \mathcal{D}_B - and \mathcal{V}_B -criterion values of the augmented designs are given in Table 7. Although the differences in \mathcal{D}_B -efficiency and \mathcal{V}_B -efficiency are larger for these smaller design cases, we cannot conclude that there is any practical distinction between the \mathcal{D}_B - and \mathcal{V}_B -optimal designs.

Table 5. Variance-covariance matrix of the parameter estimates for the sports club membership choice experiment in Sándor and Wedel (2001)

	Location 1	Location 2	Period 1	Period 2	Activities 1	Activities 2	Clubs 1	Clubs 2	Price 1	Price 2
Location 1	0.00348	−0.00226	−0.00041	−0.00036	0.00031	0.00031	0.00031	0.00040	0.00031	−0.00009
Location 2	−0.00226	0.00510	0.00202	0.00058	−0.00013	0.00083	0.00010	−0.00067	−0.00130	−0.00009
Period 1	−0.00041	0.00202	0.00378	−0.00116	0.00005	0.00075	−0.00043	−0.00021	−0.00081	−0.00004
Period 2	−0.00036	0.00058	−0.00116	0.00329	−0.00020	0.00004	−0.00021	−0.00016	−0.00006	0.00001
Activities 1	0.00031	−0.00013	0.00005	−0.00020	0.00278	−0.00114	0.00002	0.00023	−0.00063	0.00029
Activities 2	0.00031	0.00083	0.00075	0.00004	−0.00114	0.00359	−0.00006	−0.00020	−0.00064	0.00011
Clubs 1	0.00031	0.00010	−0.00043	−0.00021	0.00002	−0.00006	0.00325	−0.00150	−0.00037	0.00003
Clubs 2	0.00040	−0.00067	−0.00021	−0.00016	0.00023	−0.00020	−0.00150	0.00315	0.00020	0.00037
Price 1	0.00031	−0.00130	−0.00081	−0.00006	−0.00063	−0.00064	−0.00037	0.00020	0.00381	−0.00163
Price 2	−0.00009	−0.00009	−0.00004	0.00001	0.00029	0.00011	0.00003	0.00037	−0.00163	0.00302

Table 6. \mathcal{D}_B - and \mathcal{V}_B -criterion values for the original and the augmented designs for the sports club membership study

Design	\mathcal{D}_B -criterion	\mathcal{V}_B -criterion
Original	0.12193	0.05103
\mathcal{D}_B -optimal augmented	0.08120	0.03263
\mathcal{V}_B -optimal augmented	0.08121	0.03240

We note, however, that the \mathcal{D}_B - and \mathcal{V}_B -criterion values of the designs match those of the larger original design shown in Table 6. The augmented designs use only 25 choice sets, whereas the larger original design has 30 choice sets. This shows the value of augmenting a small initial conjoint choice design, which allows one to update the knowledge about the unknown model parameters before spending all experimental resources.

6. CONCLUSION

In this article, we propose an alternating sample algorithm for producing \mathcal{D}_B -, \mathcal{A}_B -, \mathcal{G}_B -, and \mathcal{V}_B -optimal choice designs as an alternative to the MCMF algorithm employed by Kessels et al. (2006). Kessels et al. (2006) had shown that \mathcal{G}_B - and \mathcal{V}_B -optimal designs outperform \mathcal{D}_B - and \mathcal{A}_B -optimal designs for response prediction, which is central in choice experiments. However, using the MCMF algorithm for computing \mathcal{G}_B - and \mathcal{V}_B -optimal designs is even more cumbersome than searching for \mathcal{D}_B - and \mathcal{A}_B -optimal designs so that they suggested implementing the \mathcal{D}_B -optimality criterion in practice.

Unlike the MCMF algorithm, the new alternating sample algorithm makes the construction of \mathcal{G}_B - and \mathcal{V}_B -optimal designs practical and it allows the \mathcal{D}_B -, \mathcal{A}_B -, \mathcal{G}_B -, and \mathcal{V}_B -optimal designs to be embedded in web-based conjoint choice studies with individualized designs for the respondents. We prefer using \mathcal{V}_B -optimal designs because they minimize the average prediction variance and can be computed faster than \mathcal{G}_B -optimal designs. In general, the main improvement of the alternating sample algorithm over the MCMF algorithm is the approximation of the normal prior distribution by a designed sample of 20 parameter vectors instead of a Monte Carlo sample of 1,000 random draws. This saves up to 98% of the computational work within each random start of the algorithm. Nevertheless, we reevaluate the designs produced by each random start using the Monte Carlo sample and adapt the

design selection accordingly. This led us to call our method the alternating sample algorithm.

To further speed up the design generation, the alternating sample algorithm also uses a coordinate-exchange algorithm rather than a modified Fedorov algorithm. A coordinate-exchange approach saves time by avoiding the creation and use of a candidate set that grows exponentially with the number of attributes and attribute levels studied. Thus, the time savings of the coordinate-exchange algorithm increase with the number of profiles, attributes, and attribute levels. As a last way to accelerate the computations for any optimality criterion, the alternating sample algorithm incorporates an update formula to economically calculate the information matrix and the optimality criterion values of designs.

We also show how correlations between the parameter coefficients can be taken into account when computing the optimal choice designs. In case one suspects such correlations to be present, the multivariate normal prior distribution is elliptically symmetric around the prior mean. The small designed sample of parameters from a minimum potential design can then be linearly transformed to lie on the appropriate k -dimensional ellipsoid.

The computational speed of the alternating sample algorithm makes the use of individualized, adaptive Bayesian optimal conjoint choice designs in web-based surveys possible. Such an approach would involve generating an initial design for each respondent using one of the Bayesian optimality criteria, and augmenting that design choice set by choice set for each respondent individually exploiting the information contained within the choices made by that respondent in the course of the experiment. The procedure for augmenting an existing design outlined in Section 5 lends itself to be implemented in such a framework for creating individualized designs. To examine what is the best way to do this is, however, beyond the scope of this article. We expect that such an approach would allow an efficient estimation of mixed logit (Sándor and Wedel 2002) and latent class models (Andrews, Ainslie, and Currim 2002; Train 2003) that aim at modeling consumer heterogeneity. A related avenue for future research is to explore strategies for two-stage optimal choice experiments. One such strategy could be to use the \mathcal{D}_B -optimality criterion to design a pilot study, where the goal would be to get precise parameter estimates that can be used as prior information for the design of a follow up study. For the design of that follow up study, the use of the \mathcal{V}_B -optimality criterion might be more appropriate because the goal is typically to make predictions. Also, the efficiency of optimal designs with respect to the choice set size might be further investigated.

The alternating sample algorithm and all designs discussed in the article can be downloaded from the following URL: <http://www.ua.ac.be/Peter.Goos>.

ACKNOWLEDGMENTS

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Table 7. \mathcal{D}_B - and \mathcal{V}_B -criterion values for the smaller original designs and the augmented designs for the sports club membership study

Design	Original is Bayesian		Original is non-Bayesian	
	\mathcal{D}_B -criterion	\mathcal{V}_B -criterion	\mathcal{D}_B -criterion	\mathcal{V}_B -criterion
Original	0.27976	0.15158	0.31415	0.40521
\mathcal{D}_B -optimal augmented	0.12751	0.05178	0.12480	0.05082
\mathcal{V}_B -optimal augmented	0.12835	0.05158	0.12567	0.05049

APPENDIX: CHOICE DESIGN TABLES

Table A.1. Two-alternative Bayesian optimal designs for the $3^2 \times 2/24$ example

Choice set	Profile	\mathcal{D}_B			\mathcal{A}_B			\mathcal{G}_B			\mathcal{V}_B		
		Attribute			Attribute			Attribute			Attribute		
		1	2	3	1	2	3	1	2	3	1	2	3
1	I	1	2	2	2	1	2	1	2	2	1	3	2
	II	2	1	1	1	2	1	3	1	2	2	1	2
2	I	3	1	1	1	2	2	1	2	1	1	2	2
	II	2	3	2	2	1	1	2	3	1	2	3	2
3	I	2	3	2	2	2	2	2	1	1	2	2	2
	II	1	2	2	1	1	1	3	2	2	1	1	2
4	I	3	3	2	2	2	1	2	2	1	2	2	1
	II	2	2	1	3	1	1	1	3	1	1	3	2
5	I	2	2	2	2	1	1	1	2	1	1	1	1
	II	1	3	2	1	2	1	2	1	2	2	2	2
6	I	1	2	2	2	3	2	3	3	1	2	1	1
	II	3	1	2	3	2	1	2	1	1	3	1	2
7	I	3	1	2	1	2	2	2	3	2	1	2	2
	II	1	3	1	2	3	2	3	1	1	3	1	2
8	I	1	2	1	1	3	1	3	2	1	1	1	1
	II	2	1	2	3	1	2	1	1	1	3	3	2
9	I	2	2	2	1	1	1	3	1	2	1	2	1
	II	1	1	1	3	1	1	1	3	1	2	1	2
10	I	2	2	1	3	3	2	2	2	1	2	3	2
	II	1	1	1	2	1	1	3	3	2	3	1	1
11	I	3	2	1	2	2	2	2	2	2	3	2	2
	II	2	1	1	1	3	2	1	1	1	2	1	2
12	I	2	1	1	2	2	1	1	1	2	1	2	2
	II	3	2	2	1	1	1	2	1	1	3	1	1

Table A.2. Three-alternative Bayesian optimal designs for the $3^2 \times 2/24$ example

Choice set	Profile	\mathcal{D}_B			\mathcal{A}_B			\mathcal{G}_B			\mathcal{V}_B		
		Attribute			Attribute			Attribute			Attribute		
		1	2	3	1	2	3	1	2	3	1	2	3
1	I	2	1	1	1	2	1	2	1	1	3	1	1
	II	1	3	1	2	1	2	1	2	2	1	3	2
	III	1	2	2	1	3	2	1	3	1	2	2	1
2	I	2	3	2	1	1	1	2	2	1	3	1	1
	II	1	2	1	1	2	2	1	3	2	2	2	2
	III	3	1	2	2	2	1	3	2	2	3	2	2
3	I	1	2	1	2	2	2	2	3	1	3	1	2
	II	2	3	1	1	2	2	2	1	2	2	3	2
	III	1	3	2	1	1	1	3	3	1	2	2	1
4	I	3	2	2	1	2	1	1	1	1	1	3	1
	II	2	1	1	1	1	1	3	1	2	2	1	1
	III	1	3	2	2	1	1	2	3	2	1	2	2
5	I	2	1	2	2	2	1	3	2	1	1	1	1
	II	2	2	2	3	1	1	3	3	1	2	3	2
	III	1	1	1	1	3	1	1	3	1	3	2	2
6	I	3	3	2	1	2	1	1	2	1	3	3	2
	II	2	2	1	2	3	1	2	3	2	1	3	1
	III	1	1	1	3	3	2	2	3	1	2	1	2

(continued)

Table A.2. Continued

Choice set	Profile	\mathcal{D}_B			\mathcal{A}_B			\mathcal{G}_B			\mathcal{V}_B		
		Attribute			Attribute			Attribute			Attribute		
		1	2	3	1	2	3	1	2	3	1	2	3
7	I	3	1	2	2	3	2	1	1	1	1	3	2
	II	2	1	1	3	1	1	1	2	2	2	3	2
	III	3	2	1	3	3	1	2	1	2	1	2	2
8	I	1	2	1	2	1	1	2	1	1	3	2	1
	II	3	1	1	3	2	1	1	1	2	3	1	2
	III	2	2	2	1	2	1	2	2	1	1	1	1

Table A.3. Four-alternative Bayesian optimal designs for the $3^2 \times 2/24$ example

Choice set	Profile	\mathcal{D}_B			\mathcal{A}_B			\mathcal{G}_B			\mathcal{V}_B		
		Attribute			Attribute			Attribute			Attribute		
		1	2	3	1	2	3	1	2	3	1	2	3
1	I	2	2	2	2	3	2	2	3	1	3	1	1
	II	2	1	1	3	2	2	2	2	1	1	2	1
	III	3	1	2	2	2	2	1	3	1	2	1	1
	IV	3	2	1	1	1	1	1	2	2	3	2	2
2	I	2	1	2	1	3	1	3	2	1	3	2	2
	II	3	1	1	2	3	2	2	1	2	1	1	1
	III	3	2	2	1	3	2	1	1	1	2	3	2
	IV	1	2	1	2	1	1	3	1	1	2	2	2
3	I	2	2	1	3	1	1	1	3	2	2	3	1
	II	1	1	1	3	2	1	1	1	2	1	3	2
	III	1	3	2	1	2	2	1	2	1	2	1	2
	IV	3	1	2	2	1	1	2	2	2	1	2	1
4	I	1	2	1	2	2	1	2	1	1	3	3	1
	II	2	1	1	1	1	1	3	1	2	3	1	1
	III	1	3	1	3	1	2	1	2	2	1	3	1
	IV	2	3	2	1	3	2	2	3	2	2	2	2
5	I	3	2	2	3	2	2	2	3	1	2	2	1
	II	2	2	2	1	2	1	3	3	1	2	1	1
	III	2	3	2	3	1	1	3	1	1	1	3	2
	IV	1	1	1	1	1	1	3	3	2	3	1	2
6	I	1	2	2	1	3	1	3	1	2	2	3	2
	II	2	3	1	2	1	2	1	2	2	2	2	1
	III	1	3	1	2	3	1	2	1	2	1	2	2
	IV	2	1	1	1	2	1	1	1	1	1	3	1

Table A.4. Bayesian and non-Bayesian \mathcal{D} -optimal designs with 15 choice sets used by Sándor and Wedel (2001) for the sports club membership example

Non-Bayesian design							Bayesian design						
Choice		Attribute					Choice		Attribute				
set	Profile	1	2	3	4	5	set	Profile	1	2	3	4	5
1	I	3	2	1	2	3	2	I	1	3	1	2	3
	II	1	3	3	1	2		II	3	1	3	1	2
3	I	2	1	2	3	2	4	I	1	1	1	3	2
	II	1	3	1	1	3		II	3	2	2	1	3
5	I	1	1	1	3	1	6	I	3	3	1	3	1
	II	2	3	2	2	2		II	1	1	2	2	3
7	I	3	1	3	1	3	8	I	2	1	3	1	3
	II	2	2	2	2	1		II	1	3	2	2	1

(continued)

Table A.4. *Continued*

		Non-Bayesian design							Bayesian design				
Choice		Attribute					Choice		Attribute				
set	Profile	1	2	3	4	5	set	Profile	1	2	3	4	5
9	I	2	1	3	2	3	10	I	2	2	1	2	2
	II	1	2	2	3	1		II	1	3	3	3	1
11	I	3	2	1	3	1	12	I	1	2	3	1	1
	II	1	3	3	2	3		II	3	3	1	3	3
13	I	2	2	3	1	2	14	I	1	2	1	1	2
	II	1	3	1	2	1		II	2	3	3	2	1
15	I	1	1	3	2	2	16	I	2	3	1	1	2
	II	3	3	2	1	3		II	3	2	3	2	3
17	I	3	2	1	1	2	18	I	1	1	3	3	2
	II	2	3	2	3	1		II	2	2	1	1	1
19	I	1	3	2	2	2	20	I	2	3	3	2	2
	II	2	1	3	1	1		II	1	1	2	1	1
21	I	2	2	1	2	1	22	I	3	2	1	2	1
	II	3	1	2	3	3		II	2	3	2	1	3
23	I	3	1	1	1	1	24	I	3	1	2	2	1
	II	1	2	3	3	3		II	1	2	3	3	3
25	I	2	3	1	3	2	26	I	2	3	2	3	2
	II	3	1	2	2	3		II	3	1	1	2	3
27	I	1	2	3	1	1	28	I	2	1	1	1	1
	II	3	1	1	3	2		II	3	2	2	3	2
29	I	3	1	2	1	2	30	I	1	2	3	2	2
	II	2	3	1	3	3		II	3	1	2	3	3

Table A.5. \mathcal{D}_B - and \mathcal{V}_B -optimal follow up designs for the combined Bayesian and non-Bayesian \mathcal{D} -optimal design of Table A.4 used in the sports club membership example.

Choice set	Profile	\mathcal{D}_B -optimal					\mathcal{V}_B -optimal				
		Attribute					Attribute				
		1	2	3	4	5	1	2	3	4	5
31	I	3	3	3	3	3	1	1	2	2	2
	II	1	2	1	1	2	3	3	3	1	3
32	I	1	2	3	1	1	3	3	3	1	2
	II	3	3	1	2	2	1	2	1	2	3
33	I	1	1	1	3	3	3	3	1	3	3
	II	2	2	2	2	2	2	2	3	1	1
34	I	3	3	2	1	1	1	1	2	3	1
	II	1	2	1	2	3	3	2	1	1	2
35	I	1	2	2	3	1	3	2	2	3	1
	II	3	3	3	1	2	1	1	1	2	2
36	I	2	1	3	2	1	2	2	3	3	1
	II	3	2	2	3	2	1	3	2	1	3
37	I	2	2	3	3	1	1	3	2	1	1
	II	1	1	2	2	2	3	2	3	2	2
38	I	1	3	2	1	3	3	2	2	3	2
	II	3	1	3	3	1	2	3	3	1	3
39	I	1	3	1	1	3	3	3	2	2	2
	II	3	2	3	3	2	1	2	3	3	3
40	I	3	2	3	1	3	1	2	2	1	2
	II	1	1	2	3	1	3	1	3	3	1

Table A.6. \mathcal{D}_B - and \mathcal{V}_B -optimal follow up designs for the isolated Bayesian and non-Bayesian \mathcal{D} -optimal designs of Table A.4 used in the sports club membership example

Choice set	Profile	Original is Bayesian										Original is non-Bayesian									
		\mathcal{D}_B -optimal					\mathcal{V}_B -optimal					\mathcal{D}_B -optimal					\mathcal{V}_B -optimal				
		Attribute					Attribute					Attribute					Attribute				
		1	2	3	4	5	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5
31	I	3	3	2	1	3	2	1	3	3	1	1	3	2	1	2	1	3	1	1	3
	II	2	2	1	2	2	3	3	2	1	3	3	2	3	3	1	3	2	3	2	2
32	I	3	2	1	3	1	1	1	2	2	1	3	3	1	2	3	3	3	3	3	2
	II	1	3	2	1	2	3	3	1	1	2	1	2	2	1	1	1	2	2	1	1
33	I	3	3	3	3	3	3	1	2	1	2	2	1	2	1	1	2	1	1	2	2
	II	1	2	2	2	2	3	3	3	1	1	3	3	2	3	1	3	2	3	1	1
34	I	3	2	1	1	2	1	3	2	2	3	2	1	3	2	1	2	2	3	1	2
	II	2	1	3	2	1	3	2	1	3	1	3	3	2	3	2	3	1	2	2	1
35	I	2	2	3	2	3	1	3	3	1	3	3	1	3	2	2	3	3	1	2	3
	II	3	1	2	3	1	3	2	2	2	2	1	2	2	1	3	1	2	2	3	2
36	I	2	2	3	1	1	1	1	3	1	3	3	2	2	2	2	2	1	3	2	1
	II	1	1	1	2	3	2	3	2	2	1	1	3	1	1	3	3	3	2	3	2
37	I	3	2	2	3	2	2	2	1	2	3	1	2	1	2	3	1	2	1	3	3
	II	1	3	1	1	3	3	1	2	3	2	2	3	3	1	1	2	3	2	1	1
38	I	1	1	3	3	1	3	1	1	3	3	1	1	2	2	1	3	1	3	3	1
	II	3	3	2	2	2	2	2	3	1	2	3	2	3	3	2	1	2	2	1	3
39	I	3	1	3	1	2	2	2	3	3	3	3	2	3	1	3	3	2	3	3	3
	II	1	2	2	3	3	1	1	1	1	2	1	1	1	3	2	1	1	1	1	2
40	I	3	1	3	1	2	3	1	3	2	2	1	1	3	3	3	1	1	3	3	1
	II	2	3	2	3	1	1	2	2	3	1	2	3	1	1	2	3	2	1	2	2

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REFERENCES

- Andrews, R. L., Ainslie, A., and Currim, I. S. (2002), "An Empirical Comparison of Logit Choice Models with Discrete Versus Continuous Representations of Heterogeneity," *Journal of Marketing Research*, 39, 479–487.
- Bennett, J. M. (1965), "Triangular Factors of Modified Matrices," *Numerische Mathematik*, 7, 217–221.
- Chaloner, K., and Verdinelli, I. (1995), "Bayesian Experimental Design: A Review," *Statistical Science*, 10, 273–304.
- Cook, R. D., and Nachtsheim, C. J. (1980), "A Comparison of Algorithms for Constructing Exact \mathcal{D} -Optimal Designs," *Technometrics*, 22, 315–324.
- Fedorov, V. V. (1972), *Theory of Optimal Experiments*, New York: Academic Press.
- Geweke, J. (1996), "Monte Carlo Simulation and Numerical Integration", in *Handbook of Computational Economics* (Vol. 1, Chap. 15), eds. H. M. Amman, D. A. Kendrick, and J. Rust, Amsterdam: Elsevier Science, pp. 731–800.
- Hickernell, F. J., Hong, H. S., L'Ecuyer, P., and Lemieux, C. (2000), "Extensible Lattice Sequences for Quasi-Monte Carlo Quadrature," *SIAM Journal on Scientific Computing*, 22, 1117–1138.
- Huber, J., and Zwerina, K. (1996), "The Importance of Utility Balance in Efficient Choice Designs," *Journal of Marketing Research*, 33, 307–317.
- Kessels, R., Goos, P., and Vandebroek, M. (2006), "A Comparison of Criteria to Design Efficient Choice Experiments," *Journal of Marketing Research*, 43, 409–419.
- Kuhfeld, W. F., and Tobias, R. D. (2005), "Large Factorial Designs for Product Engineering and Marketing Research Applications," *Technometrics*, 47, 132–141.
- Meyer, R. K., and Nachtsheim, C. J. (1995), "The Coordinate-Exchange Algorithm for Constructing Exact Optimal Experimental Designs," *Technometrics*, 37, 60–69.
- Monahan, J., and Genz, A. (1997), "Spherical-Radial Integration Rules for Bayesian Computation," *Journal of the American Statistical Association*, 92, 664–674.
- Sándor, Z., and András, P. (2004), "Alternative Sampling Methods for Estimating Multivariate Normal Probabilities," *Journal of Econometrics*, 120, 207–234.
- Sándor, Z., and Train, K. (2004), "Quasi-Random Simulation of Discrete Choice Models," *Transportation Research B*, 38, 313–327.
- Sándor, Z., and Wedel, M. (2001), "Designing Conjoint Choice Experiments Using Managers' Prior Beliefs," *Journal of Marketing Research*, 38, 430–444.
- Sándor, Z., and Wedel, M. (2002), "Profile Construction in Experimental Choice Designs for Mixed Logit Models," *Marketing Science*, 21, 455–475.
- Sándor, Z., and Wedel, M. (2005), "Heterogeneous Conjoint Choice Designs," *Journal of Marketing Research*, 42, 210–218.
- SAS (2007), *JMP Design of Experiments Guide* (Release 7), SAS Institute Inc., Cary, NC, USA.
- Sloan, I. H., and Joe, S. (1994), *Lattice Methods for Multiple Integration*, Oxford, U.K.: Oxford University Press.
- Tang, B. (1993), "Orthogonal Array-Based Latin Hypercubes," *Journal of the American Statistical Association*, 88, 1392–1397.
- Train, K. E. (2003), *Discrete Choice Methods with Simulation*, Cambridge, U.K.: Cambridge University Press.