Bayesian Model Robust Designs

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Abstract

In industrial experiments, cost considerations will sometimes make it impractical to design experiments so that effects of all the factors can be estimated simultaneously. Therefore experimental designs are frequently constructed to estimate main effects and a few pre-specified interactions. A criticism frequently associated with the use of many optimality criteria is the specific reliance on an assumed statistical model. One way to deal with such a criticism may be to assume that instead the true model is an approximation of an unknown element of

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a known set of models. In this paper, we consider a class of designs that are robust for change in model specification.

This paper is motivated by the belief that appropriate Bayesian approaches may also perform well in constructing model robust designs and by the limitation of such approaches in the literature. I will use the traditional Bayesian design method for parameter estimation and incorporates a discrete prior probability on the set of models of interest. Some examples and comparisons with existing approaches will be provided.

Key Words: Optimal design, Optimal Bayesian design, General Equivalence Theorem, Design region, Design criteria, Exchange algorithm, Sequential and non-sequential algorithm, A-, D- and E-optimality, Exact design, Approximate design, Model Robust Design.

1 Introduction

An experiment is a process comprised of trials where a single trial consists of measuring the values of the r responses, or output variables $y_1, \ldots, y_r$. These response variables are believed to depend upon the values of the m factors or explanatory variables $x_1, \ldots, x_m$. However, the relationship between the factors and the response variable is obscured by the presence of unobserved random errors $\epsilon_1, \ldots, \epsilon_r$.

The basic idea in experimental design is that statistical inference about the quantities of interest can be improved by appropriately selecting the values of the control variables. In general these values should be chosen to achieve small variability for the estimator of interest.

A major challenge in the general domain of statistics is the construction of experimental designs that are optimal with respect to some criteria consistent with the goal of the study. The derivation of these criteria involves for the most part the specification of a model considered as the true model. However, in most practical applications, the model is not known. Often, the true model can then be assumed to approximate an unknown element of a known set of models. Then a design can be derived with the requirement that it will be robust for change in model specification. This is the issue of model robust designs.

In this paper, we will review the notion of the optimal experimental design and the model robust optimal designs. Then, we will introduce a new approach that uses some Bayesian ideas to construct some model robust designs. I will present some concrete examples and comparisons with existing approaches.

2 Model Robust Optimal Design

One situation involving model robust design was well described by Li and Nachtsheim (2000) concerning an industrial experiment that was conducted at an automotive company. The goal of the project was to reduce the leakage of a clutch slave cylinder. The factors body inner diameter, body outer diameter, seal inner diameter and seal outer diameter were thought to be potentially significant. Due to cost considerations, the management allowed for only 8 runs. The engineers believed that a small number (here 2) of two factors interactions were likely to be significant, but these interactions are not known. Thus the set of possible models contains all main effects plus 2 two-factors interactions. The goal of the experiment from a model robust design prospective is then to seek an eight run design that performs well for all of the models of the defined set of possible models.

A typical methodology for this problem would be the use of an orthogonal fractional factorial design, say, a 2^{4-1} resolution IV design with a defining relation I=1234. Such a design allows the estimation of the four main effects as well as the confounded pairs 12=34, 13=24, 14=23. However, this design may be of great interest if it is known in advance that the only interactions likely to be present are, for example, those involving factor 1. Since the experimenters were seeking a design capable of estimating models containing all main effects and any pair of two-factor interactions, the 2^{4-1} fractional factorial design may be misleading. Because, there are $\binom{4}{2} = 6$ two-factor interactions, the number of possible models that include all main effects and 2 two-factor interactions is $\binom{6}{2} = 15$. These models are listed in in Table 1.

If we used the 2^{4-1}_{VI} fractional factorial design, only some of the candidate models are estimable. It turns out that models (5), (8) and (10) are not estimable. Nachtsheim and Li (200) considered the notion of estimation capacity (EC) of a design defined as being the ratio of the number of estimable models to the number of possible models (following Sun 1993 and Cheng, Steinberg, and Sun 1999). They found that EC=12/15=80%. A natural question arises: Is there a better design for which the estimation capacity is larger than 80%?

Nachtsheim and Li (2000) developed the notion of model-robust factorial designs ($MRFD$'s) using a frequentist approach as an alternative to the

Table 1: Possible models for the 2^{4-1} resolution IV fractional factorial design models

Model	Main effects	Interaction
1	1 2 3 4	12 13
2	1 2 3 4	12 14
3	1 2 3 4	12 23
4	1 2 3 4	12 24
5	1 2 3 4	12 34
6	1 2 3 4	13 14
7	1 2 3 4	13 23
8	1 2 3 4	13 24
9	1 2 3 4	13 34
10	1 2 3 4	14 23
11	1 2 3 4	14 24
12	1 2 3 4	14 34
13	1 2 3 4	23 24
14	1 2 3 4	23 34
15	1 2 3 4	24 34

standard maximum-resolution fractional factorial designs. They considered an upper bound g on the number of likely two factor interactions. Then they selected a $MRFD$ that guarantees that models including all main effects and any combination of up to g interactions will be estimable. This methodology has the advantage of eliminating the explicit need for the choice of a confounding scheme as specified by the defining relation in the fractional factorial design case. The $MRFD$ are robust with regard to change in model specification and they are not necessary orthogonal.

The methodology is the following: Let m be the number of main effects. The focus here is on the construction of designs that allow the estimation of all main effects and g or fewer two-factors interactions. These models are contained in a known set denoted by F_g. The number of such models in F_g is $d = \binom{t}{g}$, where $t = m(m-1)/2$ is the number of two-factors interactions. If we define $e_i(\xi(\text{n}))$ as the efficiency of design $\xi(n)$ when the true model $f_T = f_i$, an optimal design $\xi^*(n)$ is robust for F_g if

$$\xi^*(n) = arg \max \sum w_i e_i(\xi(n)) \tag{2.1}$$

where $w_i \geq 0$ is the weight assigned to model f_i, and $\sum w_i = 1$. Basically, a design $\xi^*(n)$ is model robust if it maximizes the average efficiency over the model space. The maximization is taken over the space of n-point exact designs. The efficiency e_i will depend on the basic criterion under consideration by the experimenter. Nachtsheim and Li considered two optimality criteria, EC_g and IC_g.

For $EC_g - Optimality$:

$w_1 = w_2 = ... = w_d = 1/d$ and

$$e_i = \begin{cases} 1 & \text{if } f_i \text{ is estimable,} \\ 0 & \text{otherwise.} \end{cases} \tag{2.2}$$

For $IC_g - Optimality$:

The efficiency $e_i(\xi)$ of the design $\xi(n)$ for model f_i is given by

$$e_i = (\frac{D_i(\xi(n))}{D_i(\xi_i^*(n))})^{\frac{1}{p_i}} \tag{2.3}$$

where $\xi_i^*(n)$ is the D-optimal design for model f_i, $D_i(\xi(n)) = |X_i'X_i|$ is the determinant of the information matrix for design $\xi(n)$ and model f_i, p_i is the dimension of the parameter space for model f_i. It is assumed that a nonsingular optimal design $\xi_i^*(n)$ exist for each $f_i \in F_g$.

Lauter (1974) proposed a number of generalized criteria, among which was the maximization of the average, taken on the model space, of the log of the determinant. Motivated by a similar problem concerning the estimation of uranium content in calibration standards, Cook and Nachtsheim (1982) developed the notion of model robust linear optimal design in a situation in which, a priori, the exact degree of the polynomial regression model is not known. DuMouchel and Jones (1994) proposed a Bayesian approach in which they defined the notion of primary and potential models.

3 Proposed Approach to Bayesian Model Robust Design

3.1 Bayesian Optimal Design

Chaloner and Verdinelli (1995) noted that experimental design is one situation where it is meaningful within Bayesian theory to average over the sample space. Since the sample has not yet been observed, the averaging over what is unknown applies. Following Raiffa and Schlaifer (1961), Lindley (1956 and 1972) presented a decision-theoretic approach to the experimental design situation as follows. For a design ξ chosen from some set χ, a data $\mathbf{y}$ from a sample space Y will be observed. Given $\mathbf{y}$, a decision d will be chosen from some set D. The selection of ξ and the choice of a terminal decision d constitute the important parts of the process. The unknown parameters θ are elements of the parameter space Θ. A general utility function is then defined in the form of U(d,θ,ξ,$\mathbf{y}$). Considering a prior distribution of $p(\theta)$ on the parameter space, the probability distribution function of the data $p(y|\theta)$ and the utility function (or risk function); for any design ξ, the expected utility of the best decision is given by:

$$U(\xi) = \int_Y \max_{d \epsilon D} \int_\Theta U(d, \theta, \xi, \mathbf{y}).p(\theta \mid \mathbf{y}, \xi).p(\mathbf{y} \mid \xi) d\theta d\mathbf{y} \tag{3.1}$$

The Bayesian experimental design is then the design ξ^* maximizing $U(\xi)$:

$$U(\xi^*) = \max_{\xi \epsilon \chi} \int_Y \max_{d \epsilon D} \int_\Theta U(d, \theta, \xi, \mathbf{y}).p(\theta \mid \mathbf{y}, \xi).p(\mathbf{y} \mid \xi) d\theta d\mathbf{y} \tag{3.2}$$

Then the choice of the design can be regarded as a decision problem and is equivalent to the selection of the design that maximizes the expected utility with the goals ranging from estimation to prediction and so on. Lindley's (1956) work led several authors (Stone 1959a, b; DeGroot, 1962, 1986; Bernado, 1979) to consider the expected gain in Shannon information given by an experiment as a utility function (Shannon, 1948). In doing so, they proposed choosing a design that maximizes the expected gain in Shannon information or, equivalently, maximizes the expected Kullback-Leibler divergence between the posterior and the prior distributions $\int \int \log(\frac{p(\theta|\mathbf{y},\xi)}{p(\theta)}) p(\mathbf{y}, \theta \mid \xi) d\theta d\mathbf{y}$. Since the prior distribution does not depend on the optimal design

ξ maximizes:

$$U(\xi) = \int\int \log p(\theta \mid \mathbf{y}, \xi) p(\mathbf{y}, \theta \mid \xi) d\theta d\mathbf{y} \tag{3.3}$$

Consider the problem of choosing a design ξ for a normal linear regression model. The data $\mathbf{y}$ are a vector of n observations, where $\mathbf{y}|\ \theta,\sigma^2 \sim \boldsymbol{N}$ $(\mathbf{X}\theta,\sigma^2\mathrm{I})$, θ is a vector of k unknown parameters, σ^2 is known and I is the $n \times n$ identity matrix. Let's suppose that the prior information is such that $\theta|\ \sigma^2$ is normally distributed with mean θ_0 and variance-covariance matrix $\sigma^2 R^{-1}$, where the $k \times k$ matrix R is known. Recall the matrix $\frac{X'X}{n}$ is the information matrix also denoted by M(ξ). The posterior distribution for θ is also normal with mean vector $\theta^* = (X'X + R)^{-1}(X'\mathbf{y} + R\theta_0)$ and covariance matrix σ^2D(ξ)= $\sigma^2(X'X + R)^{-1}$; $D(\xi)$is a function of the design ξ and the prior precision $\sigma^{-2}R$. A standard calculation leads to:

$$U(\xi) = (-\frac{k}{2}) \log 2\pi + \frac{1}{2} \log \det(\sigma^{-2}(nM(\xi) + R)) + \frac{-k}{2} \tag{3.4}$$

Maximizing this utility therefore reduces to maximizing the function:

$$\phi_B(\xi) = \det\{nM(\xi) + R\} = \det\{X'X + R\} \tag{3.5}$$

This criterion is known as Bayes D-optimality.

3.2 Model Robust Bayesian Designs

We propose an approach based on the model robust design situation and the general Bayesian optimal design idea that has the advantage of extending the Bayesian D-optimality to more than one candidate model. For parameter estimation purposes, a utility function based on the Shannon information or the expected Kullback divergence between the prior and the posterior is considered. We specify a prior probability that each model is true and conditionally on this probability, prior distributions for the parameters are also specified. We also assume that the model prior probability is independent of the joint distribution of the the data (response variable) and the parameter given the design.

We define this class of designs as the Bayesian Model Robust Designs ($BMRD$'s) . We denote by X_i, the design matrix for the model f_i for every $i \ \epsilon\{1, ..., d\}$. The prior distribution of each model f_i is $p(i) = w_i$ for each $i \ \epsilon\{1, ..., d\}$. The prior distribution of the parameter θ given i is given by $\theta \ |i \sim N(\theta_{0i}, \ \sigma^2 R_i^{-1})$, where the $k \times k$ matrix R_i is known. The posterior distribution of θ given $\mathbf{y}$ and i is $\theta|\mathbf{y}, i, \ \xi \sim N(\theta_i^*, \ \sigma^2 D_i)$ where θ_i^* $= (X'_{i,\xi} X_{i,\xi} + R_i)^{-1}(X'_i \mathbf{y} + R_i \theta_{0i})$ and $\sigma^2 D_i = \sigma^2(X'_{i,\xi} X_{i,\xi} + R_i)$. We have the requirement that $\sum_{i=1}^{d} w_i = 1$. Let μ be a counting measure associated with the variable i. The expected utility function for the class of linear models considered will be:

$$
\begin{aligned}
U(\xi) &= \int\int\int \log p(\theta \mid \mathbf{y}, i, \xi)\} p(\mathbf{y}, \theta, i \mid \xi) d\theta d\mathbf{y} \mu(di) \\
&= \int\int\int \log p(\theta \mid \mathbf{y}, i, \xi)\} p(\mathbf{y}, \theta \mid i, \xi) p(i) d\theta d\mathbf{y} \mu(di) \\
&= \sum_{i=1}^{d} \int\int \log p(\theta \mid \mathbf{y}, i, \xi) p(\mathbf{y}, \theta \mid i, \xi) p(i) d\theta d\mathbf{y} \\
&= \sum_{i=1}^{d} w_i \int\int \{\log p(\theta \mid \mathbf{y}, i, \xi)\} p(\mathbf{y}, \theta \mid i, \xi) d\theta d\mathbf{y} \\
&= \sum_{i=1}^{d} w_i \{-\frac{k}{2}\log(2\pi) - \frac{k}{2} + \frac{1}{2}\log\det(\sigma^{-2}(X'_{i,\xi}X_{i,\xi} + R_i)\} \\
&= \sum_{i=1}^{d} w_i \log\{det(\sigma^{-2}(X'_{i,\xi}X_{i,\xi} + R_i))\} + \sum_{i=1}^{d} w_i \{\frac{k}{2} + \frac{k}{2}\log(2\pi)\}
\end{aligned}
$$

Therefore the criteria for finding the Bayesian Model Robust Optimal design is reduced then to maximizing the function:

$$
\phi_{BR}(\xi) = \sum_{i=1}^{d} w_i \log\{\det(\sigma^{-2}(X'_{i,\xi}X_{i,\xi} + R_i))\} \qquad (3.6)
$$

3.2.1 Model Priors

The model prior is the probability assigned to each of the models of interest. Based on prior knowledge of such experiments, this prior can be assigned uniformly on each of the models. We denoted this as the uniform model robust Bayesian design.

We can also based our choice of priors on the use of hierarchical model priors as advocated by Chipman, Hamada and Wu (1997). The prior for all the candidate models is derived from the prior on the main effects and the different interactions. A vector δ of zeros and ones having the same length as the parameter θ capture the importance of all the models.

As a simple example, consider a model including three main effects A, B, C and three two-factor interactions AB, AC and BC. The importance of the term AB will depend on whether whether the main effects A and B are included or not in the model. If they are included in the model, the interaction is more likely, otherwise, the interaction seems less plausible and more difficult to explain. The prior on δ is then expressed as $\delta = (\delta_A, ..., \delta_{BC})$ as follows.

$$Pr(\delta) = Pr(\delta_A)Pr(\delta_B)Pr(\delta_C)Pr(\delta_{AB} \mid \delta_A, \delta_B)Pr(\delta_{AC} \mid \delta_A, \delta_C)Pr(\delta_{BC} \mid \delta_B, \delta_C) \tag{3.7}$$

The *conditional independence* and the *inheritance principle* are required in this approach. The conditional independence states that conditional on first order terms, the second order terms (δ_{AB},δ_{AC},δ_{BC}) are independent. The main effects are also assumed to be independent. The inheritance principle assumes that the importance of a term depends only on those from which it was formed, implying

$$Pr(\delta_{AB} \mid \delta_A, \delta_B, \delta_C) = Pr(\delta_{AB} \mid \delta_A, \delta_B) \tag{3.8}$$

With this setup, it is necessary to specify $P(\delta_{AB} = 1 \mid \delta_A, \delta_B)$ for the four possibilities

$$\begin{cases} p_{00} & \text{if } (\delta_A, \delta_B) = (0,0), \\ p_{01} & \text{if } (\delta_A, \delta_B) = (0,1), \\ p_{10} & \text{if } (\delta_A, \delta_B) = (1,0), \\ p_{11} & \text{if } (\delta_A, \delta_B) = (1,1). \end{cases} \tag{3.9}$$

Typically, the value p_{11} will be the largest among the p_{ij}'s since A and B are active in this case.

As an example, consider a simple two-level experiment involving two factors, A and B. We assume that for any main effects A and B, we have the following prior probabilities $P(\delta_A = 1) = P(\delta_B = 1) = 0.4$. Then, for the two-factors interactions, we specify the following probabilities in (7.4) as p_{01} = p_{10} = 0.1, p_{11} = 0.25, p_{00} = 0.01.

Now, we consider two main effects A and B. We are interested in the set of all possible models including A or B and/or their interaction. The following table gives a list of the possible models along with their prior based on the

Table 2: Prior table for all possible models with at most two main effects and one two factors interaction.

Models	A	B	AB	Prior Computation	Prior
1	0	0	0	$(0.6)^2(0.99)$	0.3564
2	1	0	0	$(0.4)(0.6)(0.9)$	0.2260
3	0	1	0	$(0.4)(0.6)(0.9)$	0.2260
4	0	0	1	$(0.6)^2(0.1)$	0.0036
5	1	1	0	$(0.4)^2(0.75)$	0.1200
6	0	1	1	$(0.4)(0.6)(0.1)$	0.0240
7	1	0	1	$(0.4)(0.6)(0.1)$	0.0240
8	1	1	1	$(0.4)^2(0.25)$	0.0400

priors on A, B and the hierarchical priors stated above. In the table, each model is represented by $\delta = (\delta_A, \delta_B, \delta_{AB})$ where $\delta_A, \delta_B, \delta_{AB}$ take the values 0 or 1.

3.2.2 Examples with two-level factors

Uniform model robust Bayesian design

In what follows, we consider only two-level experiments. We will use +1 and -1 to denote the levels of each of the factors (main effects). The known model set in consideration is comprised of models containing m main effects and a specified number g of two factor interactions for a specific number n of runs. In the examples that follow, the prior distribution of the parameters $p(\theta \mid i)$ follows a normal distribution with mean θ_{0i} and variance covariance-matrix $\sigma^2 R_i^{-1}$, where the $k \times k$ matrix R_i^{-1} is the matrix $c * I_{k\times k}$, $I_{k\times k}$ is the $k \times k$ identity matrix, k is the dimension of the parameter vector θ_{0i} and c is a constant. We considered an arbitrary prior $p(i)$ given by $p(i) = \frac{1}{d}$ for each model where d is the number of candidate models considered. The signs + and - denote respectively the high and low levels of each of the main effects. The X's represent the main effects of the factors in consideration in the examples. The examples are constructed using the coordinate exchange algorithm with 100 starting designs selected at random. The best design among the 100 resulting designs is chosen to be the optimal design. The design tables are stated in the Table 3 and presented in the Appendix.

The performances of the FFD, the $MRFD$ and $BMRD$ are assessed using the information capacity, estimation capacity and the Bayesian model robust-based criteria as shown in the tables 4, 5, 6 and 7.

The proposed Bayesian model robust criteria values for the Bayesian

Table 3: Summary table of the constructed designs

Design tables in Appendix	n	m	g	c
9	6	3	2	1, 3, 10, 100
10	6	4	1	100
11	8	4	3	1
12	8	5	2	3

Table 4: Comparison table between the FFD, $MRFD$ and the $BMRD$ for $n = 8$, $c = 10$, $g = 1$ and $m = 4$

m	Designs	IC_1	EC_1	BR_1
4	FFD	1.000	1.00	8.32
4	$MRFD$	1.000	1.00	11.78
4	BMRD	0.7071	1.00	13.905

Table 5: Comparison table between the FFD, $MRFD$ and the $BMRD$ for $n = 8$, $c = 10$, $g = 2$ and $m = 4$

m	Designs	IC_2	EC_2	BR_2
4	FFD	0.800	0.800	6.452
4	$MRFD$	0.758	1.00	10.653
4	BMRD	0.6729	0.800	12.305

Table 6: Comparison table between the FFD, $MRFD$ and the $BMRD$ for $n = 8$, $c = 10$, $g = 1$ and $m = 5$

m	Designs	IC_1	EC_1	BR_1
5	FFD	0.400	0.400	5.053
5	$MRFD$	0.822	1.00	10.975
5	BMRD	0.6427	1.00	12.412

Table 7: Comparison table between the FFD, $MRFD$ and the $BMRD$ for $n = 8$, $c = 10$, $g = 2$ and $m = 5$

m	Designs	IC_2	EC_2	BR_2
5	FFD	0.089	0.089	4.51
5	$MRFD$	0.508	0.733	9.73
5	BMRD	0.5540	0.9556	11.02

model robust designs exceeded all those for the Model Robust Factorial Designs and the Fractional Factorial Designs. The information capacity and the estimation capacity criterion values of the Bayesian model robust designs exceed most of the values of the Fractional Factorial Designs and just few of the values of the Model Robust Factorial Designs. Indeed, for the estimation capacity criteria, the Bayesian model robust designs produced performed better than the related fractional factorial designs. This is the indication that the Bayesian model robust designs produced by the proposed approach do well compared to designs produced by other criteria and perform sometimes better with respect to the Model robust factorial design criterion proposed by Li and Nachtsheim (2000). They produced reasonably good estimation and information capacity efficiencies. The values of efficiency get better for large values of m, g. However, the resulting designs are definitely sensitive to the choice of the model and parameter priors.

Hierarchical model robust Bayesian design

Considering all the different models in the table 2 above with their respective priors, the related Bayesian model robust design for $n = 8$ runs and $c = 10$ appears in the table 12 of the Appendix. This design is balanced and is the replicated two level two by two factorial design. It is the same as the design produced by the model robust factorial design using the information capacity criteria in this case.

Appendix

Table8: Uniform Design matrix for $n = 6, m = 3, g = 2, c \in \{1, 3, 10, 100\}$

1	-	+	+
2	-	-	+
3	+	-	-
4	-	+	-
5	+	-	+
6	+	-	-

Table9:Uniform Design matrix for $n = 6, m = 4, g = 1, c = 100$

1	+	-	+	+
2	-	-	-	-
3	+	-	-	-
4	+	+	-	+
5	+	+	+	-
6	-	+	+	+

Table10: Uniform Design matrix for $n = 8, m = 4, g = 3, c = 1$

1	-	+	+	+
2	+	-	+	+
3	+	+	+	-
4	-	-	-	+
5	+	+	-	+
6	+	-	-	-
7	-	-	+	-
8	-	+	-	-

Table11: Uniform Design matrix for $n = 8, m = 5, g = 2, c = 3$

1	-	-	+	-	-
2	+	-	+	+	-
3	+	-	-	-	+
4	+	+	+	-	-
5	-	+	-	-	+
6	-	+	+	+	+
7	-	+	-	+	-
8	-	-	-	+	+

Table12: Hierachical Design matrix for $n = 8, c = 10$

Design points	X_1	X_2
1	+	-
2	+	+
3	+	-
4	-	-
5	-	+
6	-	-
7	+	+
8	-	+

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