Bayesian-inspired mixed two- and four-level designs

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Abstract

Motivated by a Bayesian framework, we propose a new minimum aberration type criterion for designing experiments with two- and four-level factors. The Bayesian approach helps in overcoming the *ad hoc* nature of effect ordering in the existing minimum aberration type criteria. Moreover, the approach is also capable of distinguishing between qualitative and quantitative factors. Numerous examples are given to demonstrate the advantages of the proposed approach.

Some key words: Bayesian method; Minimum aberration; Qualitative factor; Quantitative factor.

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1 Introduction

A simple way to construct fractional factorial designs with two- and four-level factors is to modify a two-level full factorial design. However, very few studies have been carried out to understand the optimality properties of such designs. Minimum aberration criterion (Fries & Hunter, 1980) is the most popular criterion for selecting two-level fractional factorial designs. They are based on the effect hierarchy principle (Wu & Hamada, 2000, §3.5) that lower order effects are more important than higher order effects. It is not easy to apply this principle to the case of mixed two- and four-level factors because there is no natural ordering for the effects involving the three components of a four-level factor and the two-level factors. Wu & Zhang (1993) classified the effects into different types, depending on the number of four-level components they contain, and proposed an intuitive ordering. It will be described in the next section. There is, however, no strong justification for the effect ordering they proposed and its validity can be challenged. Moreover, their minimum aberration criterion becomes increasingly complicated as the number of four-level factors increases.

Another complication arises in dealing with four-level factors. Factors can be quantitative or qualitative. The existing factorial design theory focuses on qualitative factors (Mukerjee & Wu, 2006) and very little has been done on quantitative factors (e.g., Cheng & Ye, 2004). Neither the work of Cheng & Ye (2004) nor the work of Wu & Zhang (1993) addressed the case of four-level quantitative factors. Moreover, there is no existing theory available to accommodate both qualitative and quantitative factors in one design.

We propose a Bayesian approach to construct efficient mixed two-and four-level designs. Although it is motivated by a Bayesian framework, the final criterion that we propose is frequentist, in fact, very similar to minimum aberration type criterion.

2 Review of minimum aberration criterion

The simplest way to construct designs with mixed two- and four-level factors in 2^t runs is to start with a 2^t full factorial design and replace its three interaction columns of the form $(\alpha, \beta, \alpha\beta)$ by a four-level column according to the rule $(-,-,+) \rightarrow 0$, $(-,+,-) \rightarrow 1$, $(+,-,-) \rightarrow 2$, and $(+,+,+) \rightarrow 3$. By repeating this step for m mutually exclusive sets of the form $(\alpha, \beta, \alpha\beta)$ and additionally selecting p interaction columns, we can obtain a fraction of a $4^m 2^p$ factorial in 2^t runs. Hereafter such a design is simply referred to as a $(4^m 2^p, 2^t)$ design. This construction method is referred to as the method of replacement (Addelman, 1962; Wu, 1989; Mukerjee & Wu, 2006).

For instance, consider an original 2^4 full factorial design with four independent columns $1, 2, 3,$ and 4. Let $A = (1, 2, 12)$ be a four-level column which is obtained from the three two-level columns $1, 2,$ and 12 by the method of replacement. Denote $a_1 = 1$, $a_2 = 2$, and $a_3 = 12$ (with $a_3 = a_1 a_2$). Additionally selecting four two-level columns $3, 4, 23$ and 24, we can obtain a $(4^1 2^4, 2^4)$ design, denoted by d_1, which consists of the four-level column A and the four two-level columns. Let B, C, D, E represent the four two-level factors. It is easy to show that this design d_1 has the defining relation: $I = a_2 BD = a_2 CE = BCDE$. Thus, its defining contrast subgroup is

$G = \{I, a_2BD, a_2CE, BCDE\}$.

All words in the defining contrast subgroup G of a general $(4^12^p, 2^t)$ design d can be classified into two types. One type involves only the two-level factors and is called type 0, whereas the other type involves one component of the four-level factor A and some two-level factors and is called type 1. Let $A_{i0}(d)$ and $A_{i1}(d)$ be, respectively, the number of type 0 and type 1 words of length i in its defining contrast subgroup. The vector $W_1(d) = \{(A_{i0}(d), A_{i1}(d))\}_{i\geq 3}$ is the wordlength pattern of d. Thus, the wordlength pattern of the design d_1 just constructed is $W_1(d_1) = ((0,2),(1,0))$.

Wu & Zhang (1993) argued that a word of type 1 is less serious than a same-length word of type 0 because a less significant effect can be chosen to be part of the aliasing relations implied by the type 1 word than that implied by the type 0 word. Therefore the minimum aberration design is obtained by sequentially minimizing the wordlengths in the order: $A_{30}(d), A_{31}(d), A_{40}(d), A_{41}(d)\ldots$. For example, consider an alternative design $d_2 : A, 3, 4, 23, 134$. It has the wordlength pattern $W_1(d_2) = ((0,1),(0,2))$ and consequently has less aberration than d_1. In fact, it can be verified that d_2 has minimum aberration. The foregoing definition of minimum aberration can be extended to more than one four-level factor. For $(4^22^p, 2^t)$ designs, the words of the same length can be classified into three types. Type 0 is defined as before. Type 1 involves one component of any four-level factor and some two-level factors, while type 2 involves one component of the first four-level factor, one component of the second four-level factor and some two-level factors. The wordlength patterns have the nested structure of the form $W_2(d) = \{(A_{i0}(d), A_{i1}(d), A_{i2}(d))\}_{i\geq 3}$. The minimum aberration criterion now is to sequentially minimize the wordlengths in the order: $A_{30}(d), A_{31}(d), A_{32}(d), A_{40}(d), A_{41}(d), A_{42}(d), \ldots$.

As one can easily see, Wu & Zhang's definition of minimum aberration gets increasingly complicated as the number of four-level factors increases. Moreover, there are ambiguities in their classification and ordering of words. It is not clear if a type 1 word is really less serious than type 0. In addition, they assume that a_1, a_2, and a_3 have the same level of seriousness, i.e., one is not less or more serious than the other. This might be reasonable when the factor A is qualitative but not when it is quantitative. If A is a quantitative factor, then the three components can be approximately viewed as linear, quadratic, and cubic components of that factor (Wu & Hamada, 2000, §6.4). Naturally, linear effect should get more importance than quadratic effect and so forth, which is not considered in Wu & Zhang's approach. In this article, we propose a new Bayesian-inspired minimum aberration criterion for mixed two- and four-level designs that overcomes the forgoing limitations with the existing approach.

3 Bayesian optimal design criterion

3.1 Functionally induced priors

The key step in a Bayesian approach is to choose a meaningful prior distribution for the parameters. Directly postulating a prior distribution for all of the parameters in the linear model can be a daunting task. Joseph (2006) proposed a new approach, where a functional prior is postulated for the underlying transfer function and then the prior distribution for the parameters are induced from it. We briefly describe this approach below.

Suppose there are m four-level factors and p two-level factors. Let the output y is related to the factors $x = (x_1, x_2, \ldots, x_{m+p})'$ by the model $y = f(x) + e$, where $e \sim N(0, \sigma^2)$ is the random error in the output. Assume a stationary Gaussian process prior for the transfer function: $f(x) \sim GP(\mu_0, \sigma_0^2\psi)$, where μ_0 is the mean, σ_0^2 is the variance, and ψ is the correlation function. The correlation function is defined as $\psi(h) = \text{cor}\{f(x), f(x+h)\}$. This functional prior will be used for inducing the prior for the linear model parameters.

First, consider the case of a two-level design. Code the two levels of each factor by -1 and 1. The model matrix corresponding to the full factorial design of p two-level factors has 2^p columns. Denote the model parameters corresponding to the 2^p columns by β and approximate the transfer function by $f(x) = \mu_0 + u'\beta$, where $u = (u_0, u_1, \ldots, u_{2^p-1})'$ corresponds to the grand mean, main effects (me), two-factor interactions (2fi), and the pth-order interaction. Then, using an isotropic product correlation function

$$\psi(h) = \prod_{j=1}^{p} \psi_j(h_j) = \prod_{j=1}^{p} \rho^{h_j}, \quad h = (h_1, \ldots, h_p)',$$

Joseph (2006) showed that the prior distribution for β induced from the Gaussian process prior has a multivariate normal distribution with mean 0 and variance-covariance matrix $\tau^2 R$, where $\tau^2 = \sigma_0^2/(1+r)^p$, $r = (1-\rho)/(1+\rho)$, and $R = \text{diag}(1, r, \ldots, r^2, \ldots, r^p)$. Thus, the linear model parameters are independent with variances $\text{var}(\beta_0) = \tau^2$, $\text{var}(\beta_{\text{me}}) = \tau^2 r$, $\text{var}(\beta_{\text{2fi}}) = \tau^2 r^2$, etc. Because $r \in (0, 1)$, the variances decrease geometrically as the order of the effects increases, thus satisfying the effect hierarchy principle.

Similarly, it can be shown that the prior distribution for β in a design with four-level factors is $N(0, \tau^2 R)$, where τ^2 and R take different forms depending on the coding schemes and correlation functions. Because the choice of correlation function depends on the type of factor, viz. qualitative or quantitative, we present these results in later sections. When both two-level and four-level factors are present in the experiment, the prior distribution for β can be obtained by taking the Kronecker products of the R-matrices of two-level factors and four-level factors. As shown in Joseph & Delaney (2007), these functionally induced priors have simple forms and satisfy the effect hierarchy principle and thus are suitable for developing an optimal design criterion.

3.2 Optimal design criterion

Consider a mixed $(4^m 2^p, 2^t)$ design d which is constructed from an original 2^t full factorial design d_0. There are a total of 2^{2m+p} effects including the gross mean. Let G_0 be the defining contrast subgroup of d. It contains 2^k effects including I, where $k = 2m+p-t$. Then the remaining $2^{2m+p} - 2^k$ effects can be divided into $2^t - 1$ mutually exclusive aliasing sets, each being a coset of G_0. Denote them by $G_1, \ldots, G_{2^t-1}$ and the corresponding contrast coefficient variables by $u_1, \ldots, u_{2^t-1}$. Reorder $\beta = (\beta^{(0)\prime}, \ldots, \beta^{(2^t-1)\prime})'$, where $\beta^{(j)} = (\beta_1^{(j)}, \ldots, \beta_{2^k}^{(j)})'$ are the corresponding 2^k effect parameters in G_j. Here the components of β are ordered by grouping the effects belonging to the same aliasing set.

Let $Y = (y_1, \ldots, y_{2^t})'$ be the response values obtained from the 2^t runs. We want to fit the model

$$y = \mu_0 + \sum_{j=0}^{2^t-1} u^{(j)\prime} \beta^{(j)} + e, \tag{1}$$

where $u^{(j)}$ is a 2^k-dimensional column vector with each element being u_j and $e \sim N(0, \sigma^2)$. Assume that the e's are independent between different runs and σ^2 is known. Let U_d be the $2^t \times 2^{2m+p}$ model matrix corresponding to β in (1) generated from design d. Note that the columns of U_d are obtained from the u_j variables, where the 2^t values in each column depend on the design d.

Thus we have the following model in matrix form:

$$Y|\beta \sim N(\mu_0 1_{2^t} + U_d\beta, \sigma^2 I_{2^t}),$$

where 1_{2^t} denotes a 2^t-dimensional column of 1's and I_{2^t} denotes the identity matrix of order 2^t. Let the prior distribution of β be $N(0, \tau^2 R)$, where $\tau^2 = var(\beta_1^{(0)})$. Then, the posterior variance of β is given by

$$\text{var}(\beta|Y) = \tau^2 R - \tau^2 R U_d'(U_d R U_d' + \lambda I_{2^t})^{-1} U_d R,$$

where $\lambda = \sigma^2/\tau^2$.

Let H_t be the t-fold Kronecker product of a Hadamard matrix of order two. Note that H_t is simply the $2^t \times 2^t$ model matrix corresponding to $(u_0 = 1, u_1, \ldots, u_{2^t-1})$, i.e., the model matrix of a full factorial design containing all the main effects and interactions of the t two-level factors. Because the design d is constructed from a full factorial 2^t design, it is obvious that $U_d = H_t \otimes 1_{2^k}'$.

Suppose R has the completely diagonal form: $R = \text{diag}(R^{(0)}, \ldots, R^{(2^t-1)})$, where $R^{(j)} = \text{diag}(R_1^{(j)}, \ldots, R_{2^k}^{(j)})$ for $j = 0, 1, \ldots, 2^t - 1$, and $R_1^{(0)} = 1$. Since $H_t' H_t = H_t H_t' = 2^t I_{2^t}$, we have $U_d' H_t = (H_t' \otimes 1_{2^k}) H_t = 2^t I_{2^t} \otimes 1_{2^k}$. Therefore,

$$\begin{aligned}
\text{var}(\beta|Y) &= \tau^2 R - \tau^2 R U_d' H_t (H_t' U_d R U_d' H_t + \lambda H_t' H_t)^{-1} H_t' U_d R \\
&= \tau^2 R - \tau^2 R (I_{2^t} \otimes 1_{2^k}) [(I_{2^t} \otimes 1_{2^k}') R (I_{2^t} \otimes 1_{2^k}) + \lambda 2^{-t} I_{2^t}]^{-1} (I_{2^t} \otimes 1_{2^k}') R \\
&= \tau^2 R - \tau^2 \text{diag}(T_0, \ldots, T_{2^t-1}),
\end{aligned}$$

where $T_j = (V_j + \lambda 2^{-t})^{-1} \alpha_j \alpha_j'$, $\alpha_j = R^{(j)} 1_{2^k} = (R_1^{(j)}, \ldots, R_{2^k}^{(j)})'$, and $V_j = 1_{2^k}' R^{(j)} 1_{2^k} = \sum_{i=1}^{2^k} R_i^{(j)}$. Thus we obtain the following conclusion, where the upper bound follows from $(\lambda 2^{-t} + V_j - 2R_i^{(j)})^2 \geq 0$.

PROPOSITION 1. *If the prior variance-covariance matrix $\tau^2 R$ of β is diagonal, then the posterior variances of β's are given by*

$$var(\beta_i^{(j)}|Y) \;=\; \tau^2 R_i^{(j)} - \tau^2 (R_i^{(j)})^2 \left(\lambda 2^{-t} + V_j\right)^{-1} \leq \frac{\tau^2}{4}\left(\lambda 2^{-t} + V_j\right), \tag{2}$$

for $i = 1, \ldots, 2^k$ and $j = 0, 1, \ldots, 2^t - 1$.

A good design should make the posterior variances of the parameter estimates as small as possible. Therefore, we propose to find a design that minimizes the maximum posterior variance of $\beta_i^{(j)}$'s. Thus, our proposed optimal design criterion is to

$$\min_{d} \max_{i,j} \text{var}(\beta_i^{(j)}|Y).$$

In the next section we show that under certain conditions a minimum aberration type design minimizes the maximum of the posterior variances. This is a new minimum aberration criterion and differs from that of Wu & Zhang (1993). This criterion depends on the type of the four-level factor. Therefore it is developed for the qualitative, quantitative, and mixed qualitative-quantitative factors separately in the following sections.

4 Qualitative four-level factors

For a qualitative four-level factor, it is reasonable to assume equal correlation between any two levels. Thus, we choose $\psi_j(h_j) = \rho$ if $h_j \neq 0$ and 1 otherwise. Furthermore, we use the following coding for the four-level factor:

$$\begin{pmatrix} -1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & -1 \\ 1 & 1 & 1 \end{pmatrix}.$$

This coding makes it easier to relate and trace each component of four-level factors to a factorial effect in the original two-level design from which the mixed $(4^m 2^p, 2^t)$ design is generated (see Wu & Hamada, 2000, §6.3). The coding for the two-level factor is taken as $(-1, 1)$ and the correlation between the two levels is taken as ρ. Note that we assume the same correlation between the two levels of a two-level factor and between any two levels of a four-level factor. In reality, they could be different, but there is no way to know about it before conducting the experiment. Therefore, a priori we assume them to be the same.

Using the above correlation functions and coding schemes, it can be shown from Joseph & Delaney (2007) that the R matrix is diagonal with entries $R_i^{(j)} = r_1^{z_1} r_2^{z_2}$, where

$$r_1 = \frac{1-\rho}{1+\rho} \quad \text{and} \quad r_2 = \frac{1-\rho}{1+3\rho},$$

and z_1 and z_2 are the numbers of two-level factors and main effect components of four-level factors included in the effect $\beta_i^{(j)}$.

Note that the prior variance of the main effect of a two-level factor is proportional to r_1 and that of a four-level factor component is proportional to r_2, with a common proportionality constant τ^2. Since $r_1 > r_2$ for all $\rho \in (0,1)$, it is shown that the main effect of a two-level factor is more important than the components of a four-level factor. This justifies the intuitive explanation given by Wu & Zhang (1993) that a type 0 word should be considered more serious than type 1 word. However, Wu & Zhang could not quantify their level of seriousness or importance. Here, we have a quantification and therefore will be able to derive optimal design criteria in a less ambiguous way.

Our objective is to find a design that minimizes the maximum posterior variance of $\beta_i^{(j)}$'s. The posterior variance of $\beta_i^{(j)}$ depends on ρ, which is unknown to the investigator before conducting the experiment. Therefore, it will be good if we can find a design that is uniformly optimum for all $\rho \in (0,1)$. This is not always possible. In such cases, we choose the optimum design corresponding to the larger values of ρ, thereby preferring designs that work better for smooth functions.

Since the defining contrast subgroup G_0 contains the identity I, a word of length 0, while all other aliasing effect sets G_j do not, $V_0 \to 1$ and $V_j \to 0$ for all $j \neq 0$ as $\rho \to 1$. This means that for any design d, there exists a value $\rho'_d \in (0,1)$ such that $\max_{j\geq 0} V_j = V_0$ for all $\rho \in (\rho'_d, 1]$. Thus from (2) when $\rho > \rho'_d$, var$(\beta_i^{(j)}|Y) \leq \tau^2 R_i^{(j)} - \tau^2 (R_i^{(j)})^2 \left(\lambda 2^{-t} + V_0\right)^{-1}$ for all i and j, and the equality holds at least for $j = 0$. Also, $R_1^{(0)} = 1$ and $R_i^{(j)} \to 0$ for all other i and j as $\rho \to 1$. Thus, for any design d, there exists a value $\rho_d \in (0,1)$ such that $\max_{i,j}$ var$(\beta_i^{(j)}|Y) =$ var$(\beta_1^{(0)}|Y) = \tau^2 - \tau^2/(\lambda 2^{-t} + V_0)$ for $\rho > \rho_d$. Furthermore, there exist a finite number of designs of a given size. Thus, letting $\rho_0 = \max_d \rho_d$, we obtain the following conclusion.

PROPOSITION 2. *There exists a value* $\rho_0 \in (0,1)$ *such that for all* $\rho \in (\rho_0, 1]$, *a design that minimizes* V_0 *minimizes the maximum posterior variance of the parameters.*

Thus, our objective is to find a mixed $(4^m 2^p, 2^t)$ design that minimizes $V_0 = \sum_{i=1}^{2^k} R_i^{(0)}$. Noting that G_0 represents the defining contrast subgroup, we obtain

$$V_0 = \sum_{z_1=0}^{p} \sum_{z_2=0}^{m} r_1^{z_1} r_2^{z_2} N_{z_1,z_2},$$

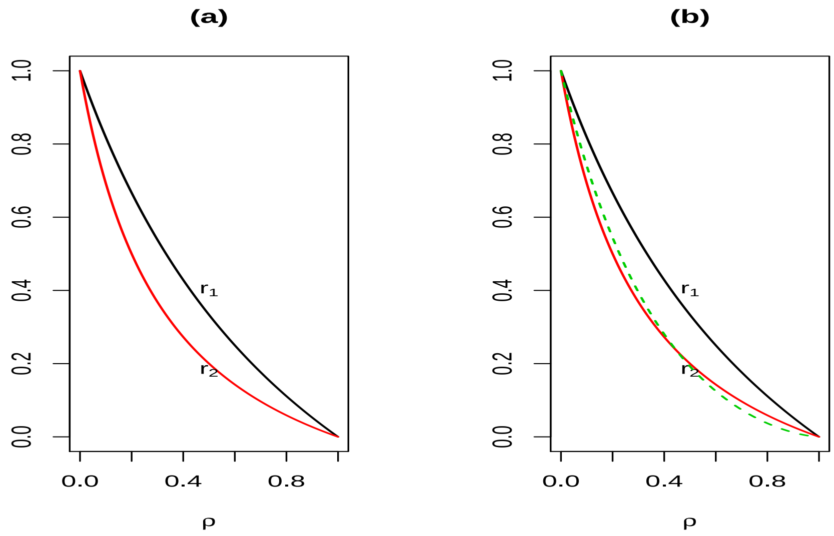

Figure 1: (a) The plot of r_1 and r_2 against ρ. (b) The plot of the approximation $r_2 \approx r_1^{1.5}$ (dashed).

where N_{z_1,z_2} is the number of words containing z_1 two-level factors and z_2 main effect components of four-level factors in its defining contrast subgroup. In Wu & Zhang's notation, $A_{i,j} = N_{i-j,j}$ with $N_{0,0} = 1$.

We can further simplify the foregoing objective function. It can be shown numerically that $r_2 \simeq r_1^{3/2}$ (see Figure 1). This suggests that a word containing three two-level factors has the same seriousness as a word containing two four-level components. For example, $a_1 b_1$ has the same seriousness as CDE. Under the above approximation, the objective function reduces to

$$V_0 \simeq \sum_{z_1=0}^{p} \sum_{z_2=0}^{m} r_1^{(2z_1+3z_2)/2} N_{z_1,z_2}.$$

Since $0 < r_1 < 1$, V_0 can be minimized by assigning unimportant (higher order) effects to the defining contrast subgroup. Thus, a design that minimizes V_0 tends to have fewer number of words N_{z_1,z_2} with smaller values $2z_1 + 3z_2$. This motivates us to define the following wordlength pattern for qualitative factor designs. They are the coefficients of $r_1^{z/2}$'s with z equal to $6, 7, 8, \ldots$. Note that only words of length three or more are considered. A mixed $(4^m 2^p, 2^t)$ design is called optimal if it sequentially minimizes the wordlength pattern. This is the proposed Bayesian-inspired minimum aberration design. In fact, the following can be proved, which is similar to the result in Joseph (2006) for two-level designs.

PROPOSITION 3. *There exists a value $\rho_0 \in (0, 1)$ such that a Bayesian-inspired minimum* *aberration design minimizes V_0 for all $\rho \in (\rho_0, 1]$.*

By putting Propositions 2 and 3 together, we find that the Bayesian-inspired minimum aberration design is a minimax design, which minimizes the maximum posterior variance of all the parameters.

For a mixed $(4^m 2^p, 2^t)$ design d with $m \leq 3$, the proposed wordlength pattern is given as the following sequence:

$$W_{13}(d) = (N_{30}, N_{21}, N_{12} + N_{40}, N_{03} + N_{31}, N_{22} + N_{50}, N_{13} + N_{41}, \ldots).$$

In particular, for a mixed $(4^1 2^p, 2^t)$ design d with one qualitative four-level factor, the wordlength pattern is reduced to

$$W_{11}(d) = (N_{30}, N_{21}, N_{40}, N_{31}, N_{50}, N_{41}, \ldots),$$

which is exactly the same as the wordlength pattern in Wu & Zhang (1993). This is a surprising and unexpected result. However, the similarity with Wu & Zhang's approach is only for the case of one four-level factor. The Bayesian-inspired minimum aberration criterion is different for two or more four-level factors and the difference sharpens as the number of four-level factors increases. For example, for a mixed $(4^2 2^p, 2^t)$ design d with two qualitative four-level factors, the wordlength pattern is reduced to

$$W_{12}(d) = (N_{30}, N_{21}, N_{12} + N_{40}, N_{31}, N_{22} + N_{50}, N_{41}, \ldots),$$

which is different from that of Wu & Zhang (1993). Note that, for two four-level factors, Wu & Zhang's approach requires the classification of words into three categories: type 0, type 1, and type 2, whereas our approach does not. The proposed approach is thus simpler than that of Wu & Zhang when there are more than one four-level factor.

Example 1. Consider the following two $(4^2 2^5, 2^5)$ designs for qualitative factors. The five independent columns are denoted by $1, 2, 3, 4, 5$ and all other columns are represented by their products. $A = (a_1, a_2, a_3) = (1, 2, 12)$ and $B = (b_1, b_2, b_3) = (3, 4, 34)$ represent the two four-level factors. Their generators are:

$$\begin{aligned} d_3: &\quad A, B, 5, 6 = 124, 7 = 234, 8 = 245, 9 = 1345; \\ d_4: &\quad A, B, 5, 6 = 14, 7 = 235, 8 = 1245, 9 = 1345. \end{aligned}$$

According to the Wu & Zhang's wordlength pattern,

$$\begin{aligned} W_2(d_3) &= ((0,0,2),(0,4,4),(0,2,2),(0,0,1)) \text{ and} \\ W_2(d_4) &= ((0,0,1),(1,4,6),(0,0,2),(0,0,0),(0,0,1)). \end{aligned}$$

Since $W_2(d_4) < W_2(d_3)$, d_4 is better than d_3. But based on the proposed wordlength pattern,

$$\begin{aligned} W_{12}(d_3) &= (0,0,2,4,4,2,2,0,1) \text{ and} \\ W_{12}(d_4) &= (0,0,2,4,6,0,2,0,0,0,1), \end{aligned}$$

and consequently d_3 is slightly better than d_4 owing to $W_{12}(d_3) < W_{12}(d_4)$.

In fact, designs d_3 and d_4 have the following defining relations with words of length 3 and 4:

$$\begin{aligned} d_3 : I &= a_3b_26 = a_2b_37 = a_1568 = b_1578 = a_3579 = b_3689 \\ &= a_2b_258 = a_1b_359 = a_1b_167 = a_3b_189; \\ d_4 : I &= a_1b_26 = 5789 = a_2568 = a_2679 = b_1678 = b_1569 \\ &= a_2b_157 = a_2b_189 = a_3b_258 = a_3b_279 = a_1b_359 = a_1b_378. \end{aligned}$$

Note that d_4 has one less word of the type a_2b_37 than d_4 and thus d_3 is considered better by Wu & Zhang. But d_4 has a word 5789 which has the same seriousness as that of a_2b_37, which is ignored by Wu & Zhang.

5 Quantitative four-level factors

For a quantitative four-level factor, the correlation should decrease as the distance between the levels increase. The following Gaussian correlation function is very popular: $\psi_j(h_j) = \rho^{h_j^2}$, $0 < \rho < 1$. In general, for a quantitative factor, the usual orthogonal-polynomial coding can be used. However, particularly in the case of four-level factors, the coding used in the previous section is more appropriate. Interestingly, the three components $(\alpha, \alpha\beta, \beta)$ can be approximately viewed as the linear, quadratic, and cubic components of the factor (Wu & Hamada, 2000, §6.4). Therefore, for a quantitative factor we denote the three components by (a_l, a_q, a_c) instead of (a_1, a_2, a_3).

For a two-level factor we use the same $(-1, 1)$ coding. We assume that the correlation between the two levels is ρ, which is the same as the correlation between two adjacent levels of a four-level factor. This assumption needs some clarification. It implies that a priori the impact of changing a level to its adjacent level has the same effect on the response for all factors, irrespective of whether it has two levels or four levels. Such an assumption is meaningful when a four-level factor can be assumed to explore a wider region than a two-level factor and that the four levels are equally spaced. On the other hand, if the four-level factor is considered for exploring the same region as a two-level factor, then it must be that this factor is more important than a two-level factor; otherwise there is no need to choose four levels for that factor. It is again reasonable to choose the same ρ between any two adjacent levels of a four-level factor and the two levels of a two-level factor.

Using the results in Joseph & Delaney (2007), it can be shown that the R matrix is approximately diagonal with elements $R_i^{(j)} = r_1^{z_1} r_l^{z_l} r_q^{z_q} r_c^{z_c}$, where

$$r_l = \frac{2+\rho-2\rho^4-\rho^9}{2+3\rho+2\rho^4+\rho^9},\ r_q = \frac{2-\rho-2\rho^4+\rho^9}{2+3\rho+2\rho^4+\rho^9},\ r_c = \frac{2-3\rho+2\rho^4-\rho^9}{2+3\rho+2\rho^4+\rho^9},$$

and z_1, z_l, z_q and z_c are, respectively, the numbers of two-level factors, linear, quadratic and cubic main effect components of four-level factors included in the effect $\beta_i^{(j)}$. It can be shown numerically that $r_l > r_q > r_c$ for all $\rho \in (0,1)$, which agrees with the intuition that a linear effect is more important than a quadratic effect and a quadratic effect is more important than a cubic effect. Moreover, $r_1 \approx r_q$. Thus, the main effect of a two-level factor has approximately the same importance as that of the quadratic effect of a four-level factor. This result is not intuitive and could not have been obtained in the traditional framework.

Furthermore, we can relate the importance of each effect through approximation. We obtain $r_l \approx r_1^{1/2}$, $r_q \approx r_1$, and $r_c \approx r_1^{3/2}$ (see Figure 2). This approximation also shows the very intuitive result that $r_q \approx r_l^2$ and $r_c \approx r_l^3$. We also checked these results by changing the Gaussian correlation function to the general exponential correlation function $\psi_j(h_j) = \rho^{h_j^\alpha}$. Although the results are affected by changing α, the foregoing approximations are quite reasonable when $\alpha \in [1,2]$.

Let N_{z_1,z_l,z_q,z_c} be the number of words containing z_1 two-level factors, z_l linear main effect components, z_q quadratic main effect components and z_c cubic main effect components of four-level factors in the defining contrast subgroup. In Wu & Zhang's notation, $A_{i,j} = \sum_{z_l+z_q+z_c=j} N_{i-j,z_l,z_q,z_c}$

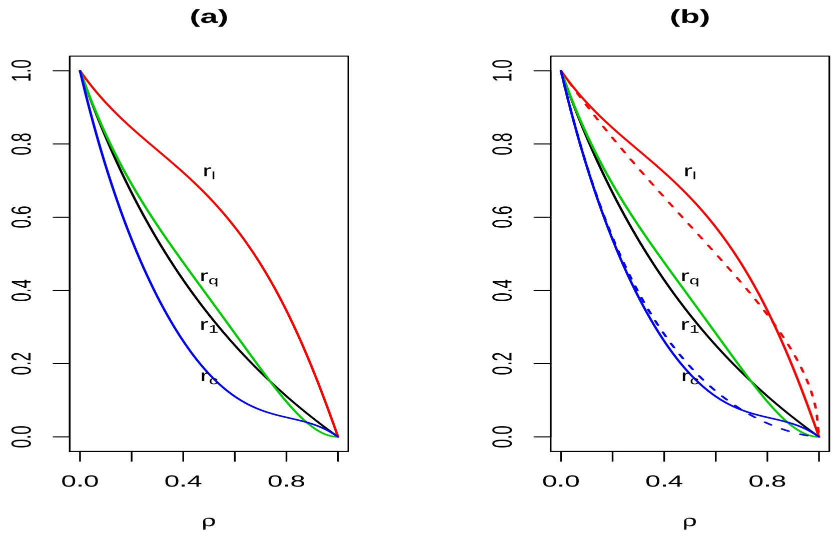

Figure 2: (a) The plot of r_1, r_l, r_q, and r_c against ρ. (b) The plot of the approximation $r_l \approx r_1^{.5}$ and $r_c \approx r_1^{1.5}$ (dashed).

with $N_{0,0,0,0} = 1$. Then

$$\begin{aligned} V_0 &= \sum_{z_1=0}^{p} \sum_{z_l+z_q+z_c=0}^{m} r_1^{z_1} r_l^{z_l} r_q^{z_q} r_c^{z_c} N_{z_1,z_l,z_q,z_c} \\ &\simeq \sum_{z_1=0}^{p} \sum_{z_l+z_q+z_c=0}^{m} r_1^{[z_l+2(z_1+z_q)+3z_c]/2} N_{z_1,z_l,z_q,z_c}. \end{aligned}$$

As in §4, for large enough ρ, the maximum posterior variance of the $\beta_i^{(j)}$'s is $\tau^2 - \tau^2/(\lambda 2^{-t} + V_0)$, which can be minimized by minimizing V_0. This can be achieved by assigning fewer number of words with smaller values of $z_l + 2(z_1 + z_q) + 3z_c$ to the defining contrast subgroup. Thus, we can define the following wordlength pattern for quantitative factor designs, which are the coefficients of $r_1^{z/2}$'s with the positive integer z starting from 3. A mixed $(4^m 2^p, 2^t)$ design is called Bayesian-inspired minimum aberration design if it sequentially minimizes the wordlength pattern. Again this design is quite different from Wu & Zhang's design, because their minimum aberration design makes sense only for qualitative factors.

For a mixed $(4^m 2^p, 2^t)$ design d with $m \leq 3$, the proposed wordlength pattern is given in detail as the following sequence:

$$\begin{aligned} W_{23}(d) &= (N_{0300}, N_{1200}+N_{0210}, N_{1300}+N_{2100}+N_{1110}+N_{0120}+N_{0201}, \\ &\quad N_{2200}+N_{1210}+N_{3000}+N_{2010}+N_{1020}+N_{0030}+N_{1101}+N_{0111}, \\ &\quad N_{2300}+N_{3100}+N_{2110}+N_{1120}+N_{1201}+N_{2001}+N_{1011}+N_{0021}+N_{0102}, \ldots). \end{aligned}$$

Example 2. Consider the following two $(4^2 2^5, 2^5)$ designs. Here, the five independent columns are also denoted by $1, 2, 3, 4, 5$ and all other columns are represented by their products. $A = (a_l, a_c, a_q) = (1, 2, 12)$ and $B = (b_l, b_c, b_q) = (3, 4, 34)$ represent the two sets of linear, cubic and quadratic main effect components of the two four-level quantitative factors. Their generators are:

$$\begin{aligned} d_4: &\quad A, B, 5, 6 = 14, 7 = 235, 8 = 1245, 9 = 1345; \\ d_5: &\quad A, B, 5, 6 = 24, 7 = 235, 8 = 145, 9 = 12345. \end{aligned}$$

If A and B are considered as two qualitative factors, then it can be verified that the two designs have the same wordlength pattern of Wu & Zhang (1993), i.e.,

$$W_2(d_4) = W_2(d_5) = ((0, 0, 1), (1, 4, 6), (0, 0, 2), (0, 0, 0), (0, 0, 1)).$$

On the other hand, according to the proposed wordlength pattern,

$$\begin{aligned} W_{23}(d_4) &= (0, 0, 0, 0, 1, 4, 3, 4, 2, 0, 0, 0, 1) \text{ and} \\ W_{23}(d_5) &= (0, 0, 0, 0, 0, 0, 14, 0, 0, 0, 0, 0, 0, 0, 1). \end{aligned}$$

So it is obvious that d_5 is much better than d_4 for quantitative factors owing to $W_{23}(d_5) < W_{23}(d_4)$.

It can be shown that both d_4 and d_5 have only one three-letter word: $a_l b_c 6$ and $a_c b_c 6$, respectively. Clearly the first one is a more serious aliasing, because the linear effect of A is much more important than its cubic effect. But this is not recognized in Wu & Zhang's approach, whereas our approach gives more importance to linear effects than cubic effects and declares the first aliasing as more serious and thus, selects d_5 as a better design. This confirms our intuition of what constitutes good designs for quantitative factors.

6 Mixed qualitative and quantitative four-level factors

Standard mathematical tools (Mukerjee & Wu, 2006) used for factorial designs, such as group theory and coding theory, treat all the factors as qualitative. Recently, Cheng & Ye (2004) used algebraic geometry methods to deal with quantitative factors. However, they did not consider the case of mixed qualitative and quantitative factors. Interestingly, this poses no challenge in our Bayesian framework.

Let there be m_1 qualitative four-level factors and m_2 quantitative four-level factors. Then, for factorial experiments based on a mixed $(4^{m_1+m_2}2^p, 2^t)$ design, the R matrix is approximately diagonal with elements $R_i^{(j)} = r_1^{z_1} r_2^{z_2} r_l^{z_l} r_q^{z_q} r_c^{z_c}$ with the same notation as before. For a mixed $(4^{m_1+m_2}2^p, 2^t)$ design d, let N_{z_1,z_2,z_l,z_q,z_c} be the number of words containing z_1 two-level factors, z_2 main effect components of m_1 qualitative four-level factors, and z_l linear main effect components, z_q quadratic main effect components and z_c cubic main effect components of m_2 quantitative four-level factors in its defining contrast subgroup. In Wu & Zhang's notation, $A_{i,j} = \sum_{z_2+z_l+z_q+z_c=j} N_{i-j,z_2,z_l,z_q,z_c}$ with $N_{0,0,0,0,0} = 1$. Then

$$\begin{aligned} V_0 &= \sum_{z_1=0}^{p} \sum_{z_2=0}^{m_1} \sum_{z_l+z_q+z_c=0}^{m_2} r_1^{z_1} r_2^{z_2} r_l^{z_l} r_q^{z_q} r_c^{z_c} N_{z_1,z_l,z_q,z_c} \\ &\simeq \sum_{z_1=0}^{p} \sum_{z_2=0}^{m_1} \sum_{z_l+z_q+z_c=0}^{m_2} r_1^{[z_l+2(z_1+z_q)+3(z_2+z_c)]/2} N_{z_1,z_2,z_l,z_q,z_c}. \end{aligned}$$

Thus, we define the wordlength pattern for mixed qualitative and quantitative designs as the coefficients of $r_1^{z/2}$'s with the positive integer z starting from 3. A mixed $(4^{m_1+m_2}2^p, 2^t)$ design is called a Bayesian-inspired minimum aberration design if it sequentially minimizes the corresponding wordlength pattern. As an example, for a mixed $(4^{1+1}2^p, 2^t)$ design d, the wordlength pattern is the following sequence corresponding to the coefficients of $r_1^{z/2}$'s with z starting from 5:

$$\begin{aligned} W_{31}(d) = & (N_{20100}, N_{30000} + N_{20010} + N_{11100}, N_{30100} + N_{21000} + N_{20001} + N_{11010}, \\ & N_{40000} + N_{30010} + N_{21100} + N_{11001}, N_{40100} + N_{31000} + N_{30001} + N_{21010}, \ldots). \end{aligned}$$

7 Tables of Bayesian-inspired minimum aberration designs

Without loss of generality, for qualitative factors we generally use $A = (a_1, a_2, a_3) = (1, 2, 12)$ and $B = (b_1, b_2, b_3) = (3, 4, 34)$ as the three contrast components of the first two four-level factors. But the third four-level factor is determined based on the rule of less aliasing among the three four-level factors. Then for $(4^m 2^p, 2^t)$ designs, we choose the third factor as $C = (c_1, c_2, c_3) = (1234, 14, 23)$

in 16 runs, $(5, 24, 245)$ in 32 runs and $(5, 6, 56)$ in 64 runs. For quantitative factors we choose the same sets of three columns as before, but the three columns represent the linear, cubic and quadratic effect components of the four-level factors. That is, $A = (a_l, a_c, a_q) = (1, 2, 12)$, $B = (b_l, b_c, b_q) = (3, 4, 34)$ and $C = (c_l, c_c, c_q) = (1234, 14, 23)$ in 16 runs, $(5, 24, 245)$ in 32 runs and $(5, 6, 56)$ in 64 runs. For mixed qualitative and quantitative $(4^{1+1}2^p, 2^t)$ designs, we use $A = (a_1, a_2, a_3) = (1, 2, 12)$ as the qualitative four-level factor and $B = (b_l, b_c, b_q) = (3, 4, 34)$ as the quantitative four-level factor.

Since the wordlength pattern W_{11} with one four-level factor coincides with the wordlength pattern W_1 of Wu & Zhang (1993), the optimal designs are consequently the same. By computer search, it is found that for two qualitative four-level factors, almost all the designs in Wu & Zhang (1993) are Bayesian-inspired minimum aberration designs, with the only exception given in Example 1. The Bayesian-inspired minimum aberration designs with three qualitative four-level factors are different from those of Wu & Zhang (1993) and are given in Table 1. The Bayesian-inspired minimum aberration designs for the case of quantitative four-level factors and mixed qualitative and quantitative four-level factors are given respectively in Tables 2 and 3. They are quite different from the minimum aberration designs of Wu & Zhang (1993). To save space, we list only the design generators of the two-level factors. The remaining two-level factors are assigned to the independent two-level columns not used by the four-level factors.

Table 1: Two-level generators of BIMA $4^3 2^{p-k}$ designs with qualitative four-level factors

k	16 runs	32 runs	64 runs
1	24	12345	246
2	24 134	1234 1235	245 1236
3	13 24 134	1235 145 345	245 236 1346
4	13 123 134 234	1234 1235 145 2345	235 1245 146 2346
5	13 123 24 134 234	124 234 235 145 12345	
6		124 134 234 235 145 12345	

Table 2: Two-level generators of BIMA $4^m 2^{p-k}$ designs with quantitative four-level factors

k	$m=1$	$m=2$	$m=3$
		16 runs	
1	234	24	24
2	23 134	23 124	24 134
3	23 24 134	23 14 234	123 24 134
4	23 24 134 1234	23 14 124 234	13 123 24 134
5	13 23 24 134 1234	23 14 24 124 234	13 123 24 134 234
6	13 23 14 24 134 1234	23 123 14 24 124 234	
7	13 23 14 24 134 234 1234	23 123 14 124 134 234 1234	
8	13 23 123 14 24 124 34 234	23 123 14 24 124 134 234 1234	
		32 runs	
1	2345	245	12345
2	245 1345	235 145	1234 1235
3	235 245 1345	235 145 12345	23 1234 1345
4	234 235 245 1345	24 235 145 12345	23 1234 1235 145
5	23 134 135 245 12345	14 234 235 1245 1345	23 124 25 1345 12345
6	23 24 134 135 1245 2345	124 234 135 1235 245 1345	23 14 124 1235 45 12345
		64 runs	
1	23456	2456	246
2	1345 2346	245 13456	24 236
3	234 1235 2456	245 1246 2356	24 236 146
4	234 235 1236 2456	245 1246 256 3456	245 236 146 12456

Table 3: Two-level generators of BIMA $4^{1+1}2^{p-k}$ designs for mixed qualitative and quantitative four-level factors

k	16 runs	32 runs	64 runs
1	24	245	2456
2	14 234	145 12345	12356 13456
3	14 124 234	235 145 12345	12346 12356 1456
4	23 14 124 234	24 235 145 12345	235 246 156 123456
5	23 123 134 234 1234	14 234 235 1245 1345	
6	13 23 123 134 234 1234	14 24 1234 25 135 1235	
7	13 23 123 14 134 234 1234		
8	13 23 123 14 124 134 234 1234		

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