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Two-level factorial designs for searching dispersion factors and estimating location main effects

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Abstract

In factorial experiments, changing the level of a factor might, in certain applications, change the variance of the response variable. Such factors are called *dispersion factors* in this article. There have been several publications on the analysis methodology for identifying dispersion factors in unreplicated factorial experiments. However, the design optimality issues for the search and identification of dispersion factors seem to be relatively unexplored. In this study, we focus on the two-level factorial experiment in which there is at most one dispersion factor whose identity is not known a priori. The task is to estimate all location main effects and simultaneously identify the dispersion factor, if any. We propose a likelihood-based criterion for selecting the design from a class of competing designs using which one can estimate all location main effects and also correctly identify, with as high a probability as possible, the identity of the dispersion factor (if one exists). It is shown that, if attention is restricted to the class of regular 2^{n-p} fractional factorial designs, then a large run size design of high resolution may be required to achieve our goal. As an alternative, we consider the class of simple arrays due to its appealing symmetry property and flexibility in run size. Additionally, the trade-off of efficiency between identification of the dispersion factor and estimation of the location main effects is under investigation. The situation involving multiple dispersion factors is also discussed.

MSC: 62K15

Keywords: Mixed linear model; Robust design; Design resolution; Orthogonal design; Simple array

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1. Introduction

Although *homogeneity of variance* is a standard assumption in most analysis of variance models, it is not uncommon to encounter situations where the variance of the response variable changes from one experimental setting to another. Often a small number of factors are responsible for such changes. These factors are called *dispersion factors*. Changing the level of a dispersion factor will change the variance of the response variable when all other factor levels are kept fixed.

Recently, the problem of identification of dispersion factors in a factorial experiment setting has attracted much attention. In order to keep the cost of experimentation affordable, it is of interest to develop approaches for identifying dispersion factors using unreplicated two-level factorial designs. Box and Meyer (1986) develop an informal approach in identifying unusually large dispersion effects by studying the logarithm of the ratio of the residual variances. Montgomery (1990) uses the normal plot on these statistics to achieve the same goal. Wang (1989), Bergman and Hynên (1997), Liao (2000) and McGrath and Lin (2001a) provide significance tests for dispersion effects from unreplicated two-level fractional factorial experiments. Furthermore, Pan (1999) and McGrath and Lin (2001b) discuss the impact of confounding between location effects and dispersion effects when using unreplicated two-level factorial designs. After discussing the structural bias and the estimation bias for various methods, Brenneman and Nair (2001) suggest some iterative strategies for model selection and estimation of the dispersion effects. All of these studies focus on analysis methodology and do not address the issue of design selection. However, Liao and Iyer (2000) consider design optimality issues for estimation of dispersion effects using the class of regular 2^{n-p} fractional factorial designs, denoted by FFDs (2^{n-p}). This paper explores properties of two-level fractional factorial designs for screening dispersion factors, and simultaneously estimating location main effects. Specific attention is given to the situation that there exists at most one dispersion factor, since this may provide guidance for constructing good designs for more general situations.

Section 2 describes the notation used in this article and defines simple arrays. Section 3 formulates a mixed linear model to describe the dispersion effects in a two-level factorial experiment where a single factor, whose identity is unknown, is responsible for the dispersion effects. The goal of the study is to not only estimate the location main effects, but also correctly identify the dispersion factor if one exists. To this end, we develop a performance measure that quantifies the ability of a design to discriminate the correct model from a set of n candidate models, each of which treat one of the n factors as the dispersion factor. Section 4 evaluates the performance of FFDs(2^{n-p}). Also a simulation study is conducted to investigate the relationship between the performance measure developed and the probability of correct search for the dispersion factor. Section 5 considers the use of simple arrays in searching for a dispersion factor. Section 6 contains a comparison between FFDs(2^{n-p}) and simple arrays. Restricted maximum likelihood estimation (REML) for estimating the dispersion effect is also discussed. Finally, we close the paper with some issues for the further study, including data analysis related to the proposed performance measure and the situation involving multiple dispersion factors.

2. Preliminaries

We first describe the notation used in this article. We use $F_1, F_2, \ldots, F_n$ to denote the n two-level factors. $F_1, F_2, \ldots, F_n$ also represent the main effects of the corresponding factors. The expression $F_1^{e_1}F_2^{e_2}\cdots F_n^{e_n}$ represents a general factorial effect with e_i's being 0 or 1. If e_i is 1, then F_i appears in the factorial effect, otherwise it does not. If all e_i's are 0, then the factorial effect denotes the grand mean μ.

2.1. *Regular 2^{n-p} fractional factorial designs*

When the number of factors n is large, it is uneconomical to conduct an experiment that uses all 2^n possible treatment combinations. A regular fractional factorial design with $N = 2^{n-p}$ treatment combinations is commonly used based on a suitably chosen list of p independent design generators. Such fractional factorial designs are typically described using the identity alias relations. For instance, the design described by the alias relations

$$F_1F_2F_3 = F_4F_5F_6 = F_1F_2F_3F_4F_5F_6 = I$$

represents a regular fractional factorial design with n factors and run size equal to $N = 2^{n-2}$. The resolution of a design depends upon the alias relations. In general, a two-level regular fractional factorial design is said to be of *resolution d* if the smallest word-length of any factorial effect that is aliased with the general mean μ is equal to d. For instance, the above design is a design of resolution III.

2.2. *Simple arrays*

A deficiency of FFDs(2^{n-p}) is that their run size N must be a power of 2. Consequently, the run size for the smallest acceptable design can still be very large and economically unfeasible. To address such issues, it is desirable to study classes of designs that allow for more flexible run sizes and at the same time possess appealing symmetry properties and allow for estimation of effects of interest. So Plackett and Burman (1946) designs are commonly used for screening of important factors responsible for location effects. In this study, we consider the simple array that is defined below.

A *simple array* with 2 symbols, N runs and strength n, is an $N \times n$ matrix with elements $+1$ or -1 such that, two n-tuples which have the same number of +1's occur equal number of times as a row of the matrix. Let *weight* of an n-tuple be the number of +1's in the n-tuple. And *equivalence class* of weight k is defined by the set consisting of the $\binom{n}{k}$ n-tuples with weight k, for $k = n, n-1, \ldots, 1, 0$. Then a simple array, denoted by $\mathrm{SA}(N, n)$, can be simply expressed as its index set $\boldsymbol{\omega} = (\omega_n, \omega_{n-1}, \ldots, \omega_1, \omega_0)$, where ω_k represents the frequencies of occurrence of equivalence class of weight k in the $N \times n$ matrix. Clearly, the run size of such a design is given by

$$N = \omega_n\binom{n}{n} + \omega_{n-1}\binom{n}{n-1} + \cdots + \omega_1\binom{n}{1} + \omega_0\binom{n}{0}.$$

For instance, the array given below is a simple array SA$(11, 3)$ with index set $\boldsymbol{\omega} = (\omega_3, \omega_2, \omega_1, \omega_0) = (2, 1, 1, 3)$.

$$\begin{bmatrix} +1 & +1 & +1 \\ +1 & +1 & +1 \\ +1 & +1 & -1 \\ +1 & -1 & +1 \\ -1 & +1 & +1 \\ +1 & -1 & -1 \\ -1 & +1 & -1 \\ -1 & -1 & +1 \\ -1 & -1 & -1 \\ -1 & -1 & -1 \\ -1 & -1 & -1 \end{bmatrix}.$$

3. A performance measure for designs

In this study, it is assumed that two-factor and higher-order interactions for mean response are all zero. Regarding the dispersion response, we first consider that there is exactly one of the n factors responsible for the dispersion effects in the experiment. Changing the level of the dispersion factor in a treatment combination results in a change in variance of the response. That is, when this factor is set at its high level the variance of the response is σ^2_{H}, and when it is set at its low level the variance is σ^2_{L}. Both σ^2_{H} and σ^2_{L} are positive numbers. Which specific one of the n factors is responsible for this dispersion effect is not known. We shall use a mixed linear model to describe this situation.

Let $\gamma_0 = (\sigma^2_{\mathrm{H}} + \sigma^2_{\mathrm{L}})/2$ and $\gamma_1 = (\sigma^2_{\mathrm{H}} - \sigma^2_{\mathrm{L}})/2$. Then there are n possible candidate models. Suppose F_k has the dispersion effect so that the kth model can be described as follows:

$$\begin{aligned} &E(\boldsymbol{y}) = \boldsymbol{X\beta}, \\ &V(biy) = \gamma_0 \boldsymbol{I}_N + \gamma_1 \boldsymbol{D}_k, \end{aligned} \tag{3.1}$$

where $\boldsymbol{y}$ is the observation vector corresponding to the design used in the experiment; $\boldsymbol{\beta}$ is the $(n+1) \times 1$ parameter vector consisting of the grand mean μ and the main effects for mean response; $\boldsymbol{X}$ is the model matrix with elements $+1$ or -1 determined by the design; and $\boldsymbol{I}_N$ is the identity matrix of order N. The matrix $\boldsymbol{D}_k$ is a diagonal matrix whose diagonal elements correspond to the levels of F_k in the treatment combinations. The jth diagonal element of $\boldsymbol{D}_k$ is $+1$ or -1 according as whether F_k occurs at its high level or low level, respectively, in observation j.

Now let l_k, for $k = 1, 2, \ldots, n$, be the log-likelihood of the n possible candidate models described in (3.1) on the assumption that the observation vector $\boldsymbol{y}$ has a multivariate normal distribution. Then the log-likelihood ratio for a test of the null hypothesis

$$\mathrm{H}_0\colon \text{model } i \text{ is true}$$

versus the alternative hypothesis

$$\mathrm{H}_\mathrm{a}\colon \text{model } j \text{ is true}$$

is $\hat{l}_i - \hat{l}_j$, where $\hat{l}_i$ and $\hat{l}_j$ are the values of l_i and l_j evaluated at maximum likelihood estimates (MLEs) of the parameters in models *i* and *j*, respectively. The value of this ratio tends to be large when model *i* is the true model. Therefore, the conditional expectation of $\hat{l}_i - \hat{l}_j$ under the assumption that model *i* is the true model, denoted by $E(\hat{l}_i - \hat{l}_j|M_i)$, can be used as a measure of information for discriminating in favor of model *i* against model *j* when model *i* is true. Note that designs which maximize this magnitude are called *T-optimum* by Atkinson and Donev (1992, p. 229), to emphasize the connection with testing models. As shown in their book, the T-optimum design provides the most powerful test for lack of fit test of model *j* when model *i* is true.

This study attempts to find designs that make the magnitude of $E(\hat{l}_i - \hat{l}_j|M_i)$ as large as possible for each $j \neq i$. These designs should possess satisfactory performance in identifying model *i* as the true model from the *n* possible candidate models, when model *i* is indeed the true model. By examining this discrimination measure for each $i = 1, 2, \ldots, n$, we expect to find good designs for searching and identifying the unknown true model.

The mixed linear model of (3.1) can be rewritten as

$$E(\boldsymbol{y}) = \boldsymbol{X\beta},$$

$$V(\boldsymbol{y}) = \gamma_0 \boldsymbol{H}_k, \tag{3.2}$$

where $\boldsymbol{H}_k = \boldsymbol{I}_N + \rho \boldsymbol{D}_k$, $\rho = \gamma_1/\gamma_0$, and $-1 < \rho < 1$. Due to the nonexistence of closed form solutions for the MLEs of $\boldsymbol{\beta}$, γ_0 and ρ for the mixed linear model described in model (3.2), we proceed as follows. Suppose that the value of ρ is known. Under the *k*th mixed linear model, we have the MLEs of $\boldsymbol{\beta}$ and γ_0 given by

$$\tilde{\boldsymbol{\beta}}_k = (\boldsymbol{X}'\boldsymbol{H}_k^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{H}_k^{-1}\boldsymbol{y}, \tag{3.3}$$

$$\tilde{\gamma}_{0k} = \frac{1}{N}(\boldsymbol{y} - \boldsymbol{X}\tilde{\boldsymbol{\beta}}_k)'\boldsymbol{H}_k^{-1}(\boldsymbol{y} - \boldsymbol{X}\tilde{\boldsymbol{\beta}}_k), \tag{3.4}$$

for $k = 1, 2, \ldots, n$. We shall use the notation $\tilde{l}_k$ to denote the log-likelihood evaluated at $\tilde{\boldsymbol{\beta}}_k$ and $\tilde{\gamma}_{0k}$. Then we have

$$\tilde{l}_k = -\frac{N}{2}\ln(2\pi) - \frac{1}{2}\ln(|\boldsymbol{H}_k|) - \frac{N}{2}\ln(\tilde{\gamma}_{0k}) - \frac{N}{2}. \tag{3.5}$$

The Taylor expansion of Eq. (3.5) in $(\tilde{\gamma}_{0k} - \gamma_0)$ yields the following linearization:

$$\begin{aligned}\tilde{l}_k &\simeq -\frac{N}{2}\ln(2\pi) - \frac{1}{2}\ln(|\boldsymbol{H}_k|) - \frac{N}{2}\ln(\gamma_0) - \frac{N}{2\gamma_0}(\tilde{\gamma}_{0k} - \gamma_0) - \frac{N}{2}\\ &\simeq -\frac{N}{2}\ln(2\pi) - \frac{1}{2}\ln(|\boldsymbol{H}_k|) - \frac{N}{2}\ln(\gamma_0) - \frac{1}{2\gamma_0}(\boldsymbol{y} - \boldsymbol{X}\tilde{\boldsymbol{\beta}}_k)'\boldsymbol{H}_k^{-1}(\boldsymbol{y} - \boldsymbol{X}\tilde{\boldsymbol{\beta}}_k).\end{aligned} \tag{3.6}$$

So $\tilde{l}_k$ can be approximated as a quadratic form in $\boldsymbol{y}$. For a given design, the value of $E(\tilde{l}_i - \tilde{l}_j|M_i)$ can be evaluated approximately using expression (3.6).

4. Performance of regular 2^{n-p} fractional factorial designs

First, using the discrimination measure developed in the previous section, we discuss the performance of FFDs(2^{n-p}), since they are most commonly used for studying the dispersion effects in the literature. We have the following result whose proof is given in the appendix.

Proposition 4.1. *Consider the family of mixed linear models given in* (3.2) *corresponding to a* FFD(2^{n-p}) $\mathscr{D}$. *Then, an approximation for the conditional expectation* $E(\tilde{l}_i - \tilde{l}_j|M_i)$ *of* $\tilde{l}_i - \tilde{l}_j$ *when model i is the true model, is given by*

$$E(\tilde{l}_i - \tilde{l}_j|M_i) \simeq \frac{\rho^2}{2\gamma_0(1-\rho^2)}(N - 2n + 2a_j), \tag{4.1}$$

where a_j *is the number of identity alias relations of the form* $F_j F_u F_v = I$ *that hold for* $\mathscr{D}$, *with* i, j, u *and* v *all distinct and* $u < v$.

Expression (4.1) demonstrates that the discrimination power for searching the dispersion factor can be strongly related to the inherent alias structure of the FFD(2^{n-p}). For fixed N and n, the expected value $E(\tilde{l}_i - \tilde{l}_j|M_i)$ increases as the number a_j of three-factor interactions in the defining relations involving the *j*th factor but not the *i*th factor increases. We thus have the following interesting observations:

(1) The ability to successfully identify the true dispersion factor, say factor i, can be improved by making the remaining $n-1$ factors uniformly involved in more alias relations of word-length 3; and simultaneously making the responsible factor F_i free to the full extent possible from the alias relations of word-length 3.
(2) When in fact the effect of the dispersion factor is negligible, i.e. the value of ρ is close to 0, the design with a higher probability to identify the dispersion factor is more likely to falsely identify a factor as the dispersion factor.
(3) If the run size N is comparatively large relative to the number of factors n, then the alias structure has less impact on the discrimination power. Also the probability of false identification of the dispersion factor can be reduced.

A natural question that arises is, whether these observations still hold when ρ is unknown but is estimated from data. The following simulation study is conducted to examine this question. We consider the two cases: (i) $N = 16$ and $n = 5$ and (ii) $N = 32$ and $n = 6$. For these two cases, we identify a set of nonisomorphic designs according to the values of a_i and $\sum_{j \neq i}^{n} a_j$ and use the numerical method described in Hocking (1985) to compute the MLEs of the parameters in (3.2) under each of the n possible models. Then the log-likelihood is evaluated at the MLEs of the parameters. According to the *likelihood rule*, model i is chosen as the true model if $\hat{l}_i$, the log-likelihood evaluated at the MLEs computed under model i, is greater than or equal to $\hat{l}_j$ for all $j \neq i$.

For convenience, let τ be the ratio of the variance corresponding to the high level of the dispersion factor to the variance corresponding to its low level, i.e. $\tau = \sigma^2_{\mathrm{H}}/\sigma^2_{\mathrm{L}}$. So $\rho = (\tau - 1)/(\tau + 1)$. For each given design, 10,000 simulated data sets are used to calculate the log-likelihood values for each model and the proportion of times the correct model is chosen as the true model by the likelihood rule stated above is computed. This is done for values of τ from 1 to 30 in steps of 1. Note that the case $\tau = 1$ corresponds to the situation where there is no factor responsible for any dispersion effect. In other words, $\tau = 1$ corresponds to having the homogeneity of variance condition hold. So, in this case, each factor should have equal probability of being chosen as the dispersion factor for an ideal design. The results are as follows.

Example 4.1 (*The case* $N = 16$ *and* $n = 5$). Without loss of generality, we take factor F_5 to be the dispersion factor. The following is a complete list of the nonisomorphic designs of resolution III or higher according to the values of a_5 and $\sum_{j \neq 5}^{n} a_j$.

$$\mathscr{D}_1\colon F_1F_2F_3 = I,$$

$$\mathscr{D}_2\colon F_1F_2F_3F_4 = I,$$

$$\mathscr{D}_3\colon F_1F_2F_3F_4F_5 = I,$$

$$\mathscr{D}_4\colon F_1F_2F_5 = I.$$

These designs have the following parameters:

Design	Resolution	a_5	$\sum_{j \neq 5}^{n} a_j$
$\mathscr{D}_1$	III	0	3
$\mathscr{D}_2$	IV	0	0
$\mathscr{D}_3$	V	0	0
$\mathscr{D}_4$	III	1	2

The result is graphed in Fig. 1, which strongly supports observations (1) and (2) made above. Note that when $\tau = 1$, i.e. there is no dispersion factor, the probability of correct search should be equal to 0.20 if the test is unbiased. Designs $\mathscr{D}_2$ of resolution IV and $\mathscr{D}_3$ of resolution V seem to be less biased since they do not have any three-factor interactions appearing in the defining relations.

Example 4.2 (*The case* $N = 32$ *and* $n = 6$). For this case, factor F_6 is taken to be the true dispersion factor. The following contains some nonisomorphic designs of resolution from III to V:

$$\mathscr{D}_5\colon F_1F_2F_3 = I,$$

$$\mathscr{D}_6\colon F_1F_2F_3F_4 = I,$$

$$\mathscr{D}_7\colon F_1F_2F_3F_4F_5 = I,$$

$$\mathscr{D}_8\colon F_1F_2F_6 = I.$$

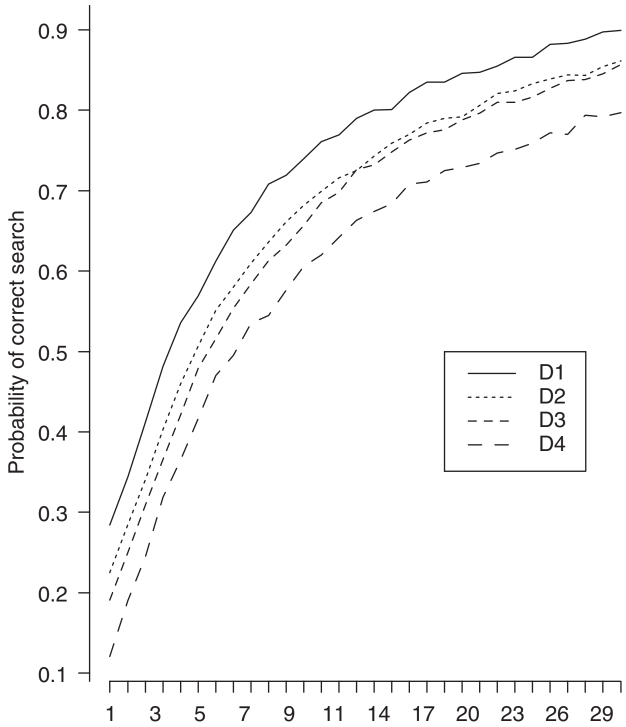

Fig. 1. The performance of designs $\mathscr{D}_1$, $\mathscr{D}_2$, $\mathscr{D}_3$ and $\mathscr{D}_4$. The horizontal axis represents $\tau = \sigma^2_{\mathrm{H}}/\sigma^2_{\mathrm{L}}$.

These designs have the following parameters:

Design	Resolution	a_6	$\sum_{j \neq 6}^{n} a_j$
$\mathscr{D}_5$	III	0	3
$\mathscr{D}_6$	IV	0	0
$\mathscr{D}_7$	V	0	0
$\mathscr{D}_8$	III	1	2

Fig. 2 shows that all the designs have very similar success rates for correct identification of the dispersion factor F_6. This is because run size $N = 32$ requires only a single defining relation since $n = 6$. Therefore, the performance of these large run size designs is almost free from their inherent alias structures. This supports observation (3) made above.

Based on the above discussions, one major issue arises when using a FFD(2^{n-p}). On the one hand, the "main effects only" model under consideration usually suggests the use of a resolution III design to keep the run size small. On the other hand, good designs for

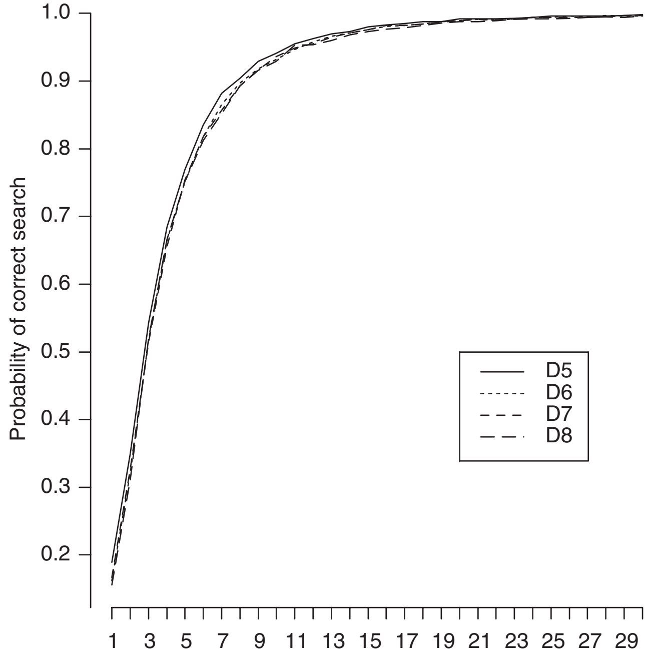

Fig. 2. The performance of designs $\mathscr{D}_5$, $\mathscr{D}_6$, $\mathscr{D}_7$ and $\mathscr{D}_8$. The horizontal axis represents $\tau = \sigma_{\mathrm{H}}^2/\sigma_{\mathrm{L}}^2$.

screening the dispersion factor should avoid the three-factor interactions involving possible dispersion factors in its alias relations. Since the identity of the dispersion factor is usually unknown before an experiment is conducted, the larger run size designs with resolution IV or higher may be required for realizing good performance under this setting.

5. Performance of simple arrays

Since any one of the factors may be the dispersion factor, it is desirable to use designs that are invariant under relabeling of the factors. The class of simple arrays possesses such a symmetry property, so it is one of the classes of designs suitable for screening the dispersion factor. We have the following result on the performance of simple arrays using the discrimination criterion of Section 3. The proof of this result involves straightforward algebra and is similar to the proof of Proposition 4.1, so we omit the proof.

Proposition 5.1. *Consider the family of mixed linear models given in* (3.2) *corresponding to a simple array* $\mathrm{SA}(N, n)$ *with index set* $\boldsymbol{\omega}=(\omega_n, \omega_{n-1}, \ldots, \omega_1, \omega_0)$. *Then an approximation for the conditional expectation* $E(\tilde{l}_i - \tilde{l}_j|M_i)$ *of* $\tilde{l}_i - \tilde{l}_j$, *when model i is the true model, is given by*

$$E(\tilde{l}_i - \tilde{l}_j|M_i) \simeq \frac{1}{2\gamma_0}\left[\frac{1}{1-\rho^2}(\mathrm{Tr1} - \mathrm{Tr2}) - (N-n-1)\right], \tag{5.1}$$

where

$$\mathrm{Tr1} = N + (1-\rho)m_1 - \rho^2 m_2,$$

$$\mathrm{Tr2} = (1+\rho^2)\mathrm{Tr}(\boldsymbol{C}) - \rho(1-\rho^2)\mathrm{Tr}(\boldsymbol{C}_1) - 2\rho^2\mathrm{Tr}(\boldsymbol{C}_2),$$

$$\boldsymbol{C} = (\boldsymbol{M} - \rho\boldsymbol{M}_1)^{-1}\boldsymbol{M};\ \boldsymbol{C}_1 = (\boldsymbol{M} - \rho\boldsymbol{M}_1)^{-1}\boldsymbol{M}_1;\ \boldsymbol{C}_2 = (\boldsymbol{M} - \rho\boldsymbol{M}_1)^{-1}\boldsymbol{M}_2,$$

where

$$\boldsymbol{M} = \begin{bmatrix} m_0 & m_1\mathbf{1}_n' \\ m_1\mathbf{1}_n & \boldsymbol{M}^* \end{bmatrix} \quad \textit{with } \boldsymbol{M}^* = m_0\boldsymbol{I}_n + (m_2 - m_0)\boldsymbol{J}_n,$$

$$\boldsymbol{M}_1 = \begin{bmatrix} m_1 & m_0 & m_2\mathbf{1}_{n-1}' \\ m_0 & m_1 & m_1\mathbf{1}_{n-1}' \\ m_2\mathbf{1}_{n-1} & m_1\mathbf{1}_{n-1} & \boldsymbol{M}_1^* \end{bmatrix} \quad \textit{with } \boldsymbol{M}_1^* = m_1\boldsymbol{I}_{n-1} + (m_3 - m_1)\boldsymbol{J}_{n-1},$$

$$\boldsymbol{M}_2 = \begin{bmatrix} m_2 & m_1 & m_1 & m_3\mathbf{1}_{n-2}' \\ m_1 & m_2 & m_0 & m_2\mathbf{1}_{n-2}' \\ m_1 & m_0 & m_2 & m_2\mathbf{1}_{n-2}' \\ m_3\mathbf{1}_{n-2} & m_2\mathbf{1}_{n-2} & m_2\mathbf{1}_{n-2} & \boldsymbol{M}_2^* \end{bmatrix}$$
$$\textit{with } \boldsymbol{M}_2^* = m_2\boldsymbol{I}_{n-2} + (m_4 - m_2)\boldsymbol{J}_{n-2},$$

where $\mathbf{1}_s$ *is the* $s \times 1$ *vector and* $\boldsymbol{J}_s$ *is the* $s \times s$ *matrix with every element being* 1. *Moreover,* m_0, m_1, m_2, m_3 and m_4 *are functions of the index set given by* $m_0 = N$; $m_1 = \lambda_4 + 2\lambda_3 - 2\lambda_1 - \lambda_0$; $m_2 = \lambda_4 - 2\lambda_2 + \lambda_0$; $m_3 = \lambda_4 - 2\lambda_3 + 2\lambda_1 - \lambda_0$; *and* $m_4 = \lambda_4 - 4\lambda_3 + 6\lambda_2 - 4\lambda_1 + \lambda_0$, *where* $\lambda_i = \sum_{j=0}^{n}\omega_j\binom{n-4}{j-i}$, *for* $i = 0, 1, 2, 3, 4$.

Obviously, the values of $E(\tilde{l}_i - \tilde{l}_j|M_i)$ of expression (5.1) are all the same for any $1 \leqslant i \neq j \leqslant n$. Nonetheless, it is not immediately obvious that the value of $E(\tilde{l}_i - \tilde{l}_j|M_i)$ is independent of parameter ρ. That is, we are unable to analytically verify that a simple array has the highest value of $E(\tilde{l}_i - \tilde{l}_j|M_i)$ for a fixed value of ρ is also the best design for other values of ρ. Fortunately, empirical evidence based on an examination of a large number of cases, indicates that, for fixed n and N, the design that has the largest value of $E(\tilde{l}_i - \tilde{l}_j|M_i)$ at one ρ value always has the largest values for a wide range of ρ values. For details, the reader is referred to Liao (1994). Therefore, for practical convenience, it is reasonable to determine good designs for searching the dispersion factor based on some specified ρ value. In this study, we specify $\tau = \sigma_{\mathrm{H}}^2/\sigma_{\mathrm{L}}^2 = 12$, i.e. $\rho = 11/13$ to obtain the desired simple array for given n and N. A list of simple arrays obtained for $n = 4$ with $9 \leqslant N \leqslant 16$ and $5 \leqslant n \leqslant 8$ with $(2n+1) \leqslant N \leqslant 32$ is given in Liao (1994).The simulation approach is the same as that described in the previous section. In Table 1 we report the obtained designs for $n = 5$ with $11 \leqslant N \leqslant 20$.

There are at least two advantages of using the simple arrays chosen. First, the designs chosen exist for any given N. Second, the symmetry property of the designs chosen leads to *unbiased* identification when in fact there are no dispersion effects. For example, Table 1 shows that the simulated probabilities of correct search for all the designs are very close to the expected probability 0.20 for the situation that $\tau = 1$.

Table 1
Some chosen simple arrays and their simulated probabilities of correct search for $n = 5$

Simple array	N	$\tau = \sigma^2_{\mathrm{H}}/\sigma^2_{\mathrm{L}}$							
		1	2	4	8	12	16	20	30
(0, 2, 0, 0, 0, 1)	11	0.203	0.261	0.344	0.436	0.490	0.527	0.526	0.620
(1, 2, 0, 0, 0, 1)	12	0.203	0.259	0.342	0.434	0.489	0.527	0.556	0.610
(2, 2, 0, 0, 0, 1)	13	0.199	0.259	0.337	0.434	0.494	0.532	0.563	0.622
(3, 2, 0, 0, 0, 1)	14	0.208	0.271	0.352	0.453	0.513	0.554	0.584	0.636
(0, 0, 1, 0, 1, 0)	15	0.194	0.224	0.327	0.479	0.583	0.653	0.704	0.778
(0, 3, 0, 0, 0, 1)	16	0.210	0.323	0.478	0.632	0.717	0.767	0.802	0.856
(0, 3, 0, 0, 0, 2)	17	0.195	0.271	0.440	0.629	0.722	0.767	0.815	0.870
(0, 3, 0, 0, 0, 3)	18	0.209	0.252	0.429	0.621	0.721	0.778	0.817	0.871
(1, 3, 0, 0, 0, 3)	19	0.193	0.257	0.435	0.633	0.729	0.782	0.821	0.875
(0, 0, 1, 1, 0, 0)	20	0.200	0.292	0.472	0.683	0.792	0.847	0.881	0.929

Note that the simple arrays are expressed by their index sets $\boldsymbol{\omega} = (\omega_n, \omega_{n-1}, \ldots, \omega_1, \omega_0)$.

6. A comparison between SA(N, n) and FFD(2^{n-p})

It is of interest to compare the chosen simple arrays with the FFDs(2^{n-p}) for fixed $N = 2^{n-p}$. Table 2 is a comparison between the simple array chosen for $n = 5$ and $N = 16$ and the FFD(2^{5-1}) of resolution V.

It can be seen that the performance of the simple array is slightly better than that of the regular design of resolution V. This can be due to the fact that the SA($N = 16, n = 5$) with index set $\boldsymbol{\omega} = (0, 3, 0, 0, 0, 1)$ includes three replicates for each treatment combination of the equivalence class of weight 4. When the main focus of the experiment is to identify the dispersion factors, the replication of treatment combinations may become intimately connected with the successful and correct search. This point is also pointed out in Pan (1999). On the other hand, the design with more power in identification of the dispersion factor may lead to a less efficiency in estimation of the location main effects. We thus use the following efficiency index, according to D-optimality criterion, to compare the designs.

$$D_{\mathrm{e}} = \frac{|\boldsymbol{X}'(V(\boldsymbol{y}))^{-1}\boldsymbol{X}|^{1/v}}{N\gamma_0}. \tag{6.1}$$

D_{e} is the relative efficiency, for the MLE of $\boldsymbol{\beta}$ with v elements, of the underlying design to the orthogonal design with run size N under the assumption of homogeneous variance. Note that $v = n + 1$ for model (3.2). The D_{e} for the simple array and the FFD(2^{5-1}) of resolution V is reported in Table 3. Obviously, the FFD(2^{5-1}) is much more efficient in estimating the location main effects.

As shown in Wolfinger and Tobias (1998), Nelder and Lee (1991, 1998) and Brenneman and Nair (2001), REML has less bias than MLE in dispersion estimation. This is because that REML accounts for the loss of degrees of freedom due to estimating the location effects first prior to estimating the dispersion effects. Another advantage of REML over MLE is that MLE may not converge in case where REML does. Specifically, this may occur in highly designs where the number of location and dispersion parameters is very close or even equal

Table 2
Simulated probabilities of correct search for the SA($N=16, n=5$) with index set $\boldsymbol{\omega}=(0,3,0,0,0,1)$ and the FFD(2^{5-1}) determined by defining relation $F_1F_2F_3F_4F_5=I$

Design	$\tau=\sigma_{\mathrm{H}}^2/\sigma_{\mathrm{L}}^2$							
	1	2	4	8	12	16	20	30
SA($N=16, n=5$)	0.210	0.323	0.478	0.632	0.717	0.767	0.802	0.856
FFD(2^{5-1})	0.192	0.250	0.366	0.554	0.657	0.732	0.776	0.857

Table 3
D_{e} of (6.1) for the SA($N=16, n=5$) with index set $\boldsymbol{\omega}=(0,3,0,0,0,1)$ and the FFD(2^{5-1}) determined by defining relation $F_1F_2F_3F_4F_5=I$

Design	$\tau=\sigma_{\mathrm{H}}^2/\sigma_{\mathrm{L}}^2$							
	1	2	4	8	12	16	20	30
SA($N=16, n=5$)	0.787	0.496	0.312	0.197	0.150	0.124	0.107	0.082
FFD(2^{5-1})	1.000	0.735	0.580	0.482	0.439	0.413	0.395	0.365
Ratio of D_{e}	0.787	0.674	0.538	0.408	0.342	0.300	0.270	0.223

The ratio of D_{e} of the SA($N=16, n=5$) to that of the FFD(2^{5-1}) is also reported.

to N. REML is thus considered for estimation of the dispersion effect in (3.4). The REML corresponding to (3.4) is given by

$$\tilde{\gamma}_{0k}(\mathrm{REML})=\frac{1}{N-(n+1)}(\boldsymbol{y}-\boldsymbol{X}\tilde{\boldsymbol{\beta}}_k)'\boldsymbol{H}_k^{-1}(\boldsymbol{y}-\boldsymbol{X}\tilde{\boldsymbol{\beta}}_k). \tag{6.2}$$

The REML takes $n+1$ location parameters (the constant term plus n main effects) into account. As a result, it does not change the choice of designs if one replaces MLE of (4.1) by REML of (6.2) in calculation of the performance measure $E(\tilde{l}_i-\tilde{l}_j|M_i)$. However, REML should be used in the simulation comparison of this study. An iterative algorithm is developed to compute the REML estimates for the dispersion parameters in model (3.2). This algorithm is derived from the restricted log-likelihood, the Cox and Reid (1987) adjusted profile likelihood, presented in Nelder and Lee (1998). Hence, we redo the simulation study of Table 2 using the algorithm. The results are displayed in Table 4.

Interestingly, the results in Table 4 are different from those in Table 2. From Table 4, the FFD(2^{5-1}) slightly outperforms the SA($N=16, n=5$). After checking the averages of estimates of the dispersion parameters based on the 10,000 simulated data sets, we find that the REMLs are less biased than MLEs as expected. For example, when σ_{L}^2 and σ_{H}^2 are specified as 1.0 and 4.0, the averages of REMLs are 1.1160 and 3.9267, respectively, using the FFD(2^{5-1}). The corresponding averages of MLEs are 0.6705 and 3.3444. Consequently, resolution V design is preferred for both location and dispersion identification based on Tables 3 and 4. Nonetheless, the simple arrays are still quite useful for run sizes that are not a power of 2.

Table 4
Simulated probabilities of correct search for the SA($N=16, n=5$) with index set $\boldsymbol{\omega}=(0,3,0,0,0,1)$ and the FFD(2^{5-1}) determined by defining relation $F_1F_2F_3F_4F_5=I$ using the REML method

Design	$\tau=\sigma_{\mathrm{H}}^2/\sigma_{\mathrm{L}}^2$							
	1	2	4	8	12	16	20	30
SA($N=16, n=5$)	0.194	0.256	0.374	0.529	0.616	0.680	0.714	0.784
FFD(2^{5-1})	0.201	0.244	0.395	0.557	0.654	0.726	0.778	0.847

7. Concluding remarks

It is to be emphasized that several important issues regarding the design choice for screening the important factors, responsible for location and dispersion effects, have been raised in the present paper. The following discusses some of them that will be investigated in a future research.

Box and Meyer (1986) suggest the use of the likelihood principle for deciding which of the design factors is a dispersion factor after using an informal test. Our criterion, which is based on the log-likelihood ratio for testing the hypothesis, may be also possibly used to identify the dispersion effects once the experimental data are available. We may proceed as follows.

Step 1: Identify active location effects using half-normal plots. This is still based on the assumption of homogeneity of variance. Let $\boldsymbol{\beta}_0$ denote the identified active location effects.

Step 2: Conduct forward selection for active dispersion factors using maximum likelihood ratio tests. First consider the following test:

$$\mathrm{H}_0\colon E(\boldsymbol{y})=\boldsymbol{X}\boldsymbol{\beta}_0,\quad V(\boldsymbol{y})=\gamma_0\boldsymbol{I}_N,$$

$$\mathrm{H}_1\colon E(\boldsymbol{y})=\boldsymbol{X}\boldsymbol{\beta}_0,\quad V(\boldsymbol{y})=\gamma_0\boldsymbol{H}_k$$

for $k=1,2,\ldots,n$. Note that H_1 is the same as model (3.2) except for the difference in the included active location effects. Let $\hat{l}_0$ and $\hat{l}_k$ denote the log-likelihood estimates of H_0 and H_1, respectively. It is well known that $-2(\hat{l}_0-\hat{l}_k)$ approximates to χ^2 distribution with 1 degree of freedom for large N. This approximation is often quite accurate for small N. See McCullagh and Nelder (1989, p. 471). Hence, we may identify the dispersion factor as the one corresponding to the smallest p-value among the χ^2 tests. Certainly the p-value must be less than a nominal significance level. In the next test, H_0 is the model identified in the first test, and H_1 is the H_0 model adapted by adding one of the remaining $(n-1)$ factors to the dispersion part. The procedure can be performed sequentially until no additional dispersion effects are found to be significant. The performance of the above method shall be assessed and compared with others.

There is a concern that the assumptions on model (3.2) under study may restrict the practical applications of the results. For the location part, it may be sufficient to consider only main effects at the initial stage of the experiment. But for the dispersion part, it may be required to investigate the situation involving multiple dispersion factors. We now simply consider the situation that there are two factors involving dispersion effects. So the following mixed model modified from (3.2) can fit this case.

$$E(\boldsymbol{y}) = \boldsymbol{X\beta},$$

$$V(\boldsymbol{y}) = \gamma_0 \boldsymbol{H}_{(k_1,k_2)},$$

where $\boldsymbol{H}_{(k_1,k_2)} = \boldsymbol{I}_N + \rho_1 \boldsymbol{D}_{k_1} + \rho_2 \boldsymbol{D}_{k_2}$ and $-1 < \rho_1, \rho_2 < 1$ for all $1 \leqslant k_1 \neq k_2 \leqslant n$. There are $\binom{n}{2}$ possible candidate models. According to the performance measure presented in Section 3, one needs to calculate the expectation of log-likelihood $\tilde{l}_{(k_1,k_2)}$ as (3.6). Even for this simple extension, the calculation becomes very complicated. Specifically, we cannot obtain a closed form of $(\boldsymbol{X}'\boldsymbol{H}^{-1}_{(k_1,k_2)}\boldsymbol{X})^{-1}$, see (A.6) in the appendix, when using FFDs(2^{n-p}). This causes a difficulty in analytically evaluating the performance of FFDs(2^{n-p}) for screening of multiple dispersion factors based on the measure. However, the principle that the FFDs(2^{n-p}) with higher resolution has better performance in both screening dispersion factors and estimating location effects could still hold, assuming that there is no prior information available on which factors may be responsible for the dispersion effects. For the class of simple arrays, it is still possible to evaluate the designs based on the proposed measure for fixed values of dispersion parameters ρ_1 and ρ_2. But there is no guarantee that the chosen simple array based on a set of fixed values of ρ_1 and ρ_2 is also the best for others.

Even though the main results obtained in this study are on the single dispersion factor model, they have shed some light on how the defining relations used in constructing a FFD(2^{n-p}) are related to the efficiency of the search for multiple dispersion factors. This is also helpful in identifying other possible alternative classes of designs for studying dispersion effects. However, other possible performance measures for choosing designs to detect dispersion factors need to be investigated. A criterion that is robust to the assumed model like *minimum aberration criterion* presented by Fries and Hunter (1980) for location effects would be preferable.

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Appendix A. Proof of Proposition 4.1

First, we state the following lemmas that will be needed in the proof of Proposition 4.1.

Lemma A.1. *Let matrix* $\boldsymbol{Z}_k = \boldsymbol{X}'\boldsymbol{D}_k\boldsymbol{X}$, *where* $\boldsymbol{X}$ *and* $\boldsymbol{D}_k$ *are the same as described in Eq.* (3.1). *Also express* $\boldsymbol{X} = [\boldsymbol{x}_0|\boldsymbol{x}_1|\boldsymbol{x}_2|\cdots|\boldsymbol{x}_n]$, *where* $\boldsymbol{x}_0$ *is a column vector with all elements* +1*'s*, $\boldsymbol{x}_i$ *are column vectors of* +1*'s and* -1*'s depending on the levels of factor i. Clearly*, $\boldsymbol{Z}_k$ *is a square matrix of size* $(n+1) \times (n+1)$ *with its* (g, h) *element equal to the triplet* $\boldsymbol{x}_k \circ \boldsymbol{x}_g \circ \boldsymbol{x}_h = \sum_{l=1}^{N} x_{lk}x_{lg}x_{lh}$ *(general dot product), for* $g, h = 0, 1, 2, \ldots, n$. *Note that* *the rows and columns of* $\mathbf{Z}_k$ *are labeled from* 0 *to* n. *The matrix* $\mathbf{Z}_k$, $k = 1, \ldots, n$, *has the following properties*:

1. $\mathbf{Z}_k$ *is symmetric with* 0'*s on the diagonal and its off-diagonal elements are* 0 *or* N. *The elements in* $(0, k)$ *and* $(k, 0)$ *positions are equal to* N *since* $\boldsymbol{x}_k \circ \boldsymbol{x}_0 \circ \boldsymbol{x}_k = N$, *and the elements in* (g, h) *and* (h, g) *positions are equal to* N *if the alias relation* $F_k F_g F_h = I$ *holds for the design*, *and are* 0 *otherwise*.
2. *If* $F_k F_g F_h = I$ *and* $F_k F_u F_v = I$ *then* $F_g F_h F_u F_v = I$. *Since we use designs of resolution* III *or higher*, *it follows that* g, h, u, v *must be distinct. This implies that each column or each row in* $\mathbf{Z}_k$ *has at most one nonzero element.*
3. $\mathbf{Z}_k^2$ *is a diagonal matrix. The elements in* $(0, 0)$, (k, k), (g, g), *and* (h, h) *positions are equal to* N^2 *if the alias relation* $F_k F_g F_h = I$ *holds for the design.*
4. $\mathbf{Z}_k^3 = N^2 \mathbf{Z}_k$.

Based on the above properties, it is easy to verify the following lemma.

Lemma A.2. *Let* $\mathbf{Z}_i = \boldsymbol{X}'\boldsymbol{D}_i\boldsymbol{X}$, $\mathbf{Z}_j = \boldsymbol{X}'\boldsymbol{D}_j\boldsymbol{X}$ *and* $\mathbf{Z}_{ij} = \boldsymbol{X}'\boldsymbol{D}_i\boldsymbol{D}_j\boldsymbol{X}$. *Suppose that* k *and* k' *are distinct elements of the set* $\{i, j, ij\}$. *Then*

1. $\mathrm{Tr}(\mathbf{Z}_k) = 0$,
2. $\mathrm{Tr}(\mathbf{Z}_k^2) = 2N^2(a_k + 1)$,
3. $\mathrm{Tr}(\mathbf{Z}_k \mathbf{Z}_{k'}) = 0$,

where $\mathrm{Tr}(\boldsymbol{B})$ *denotes the trace of matrix* $\boldsymbol{B}$. *If* $k = i$ *or* $k = j$, *then* a_k *is the number of alias relations of the design of the form* $F_k F_u F_v = I$ *with* $u < v$. *If* $k = ij$, *then* a_k *is the number of alias relations of the design of the form* $F_i F_j F_u F_v = I$ *with* $u < v$.

Now we prove Proposition 4.1. The conditional expectation of $\tilde{l}_k$ described in (3.6) can be simplified as

$$E(\tilde{l}_k | M_i) \simeq -\frac{N}{2} \ln(2\pi) - \frac{1}{2} \ln(|\boldsymbol{H}_k|) - \frac{N}{2} \ln(\gamma_0) - \frac{1}{2\gamma_0} \mathrm{Tr}(\boldsymbol{A}_k \boldsymbol{H}_i),$$

where

$$\boldsymbol{A}_k = \boldsymbol{H}_k^{-1} - \boldsymbol{H}_k^{-1}\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{H}_k^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{H}_k^{-1}.$$

Then we have

$$E(\tilde{l}_i - \tilde{l}_j | M_i) \simeq -\frac{1}{2} (\ln |\boldsymbol{H}_i| - \ln |\boldsymbol{H}_j|) - \frac{1}{2\gamma_0} [\mathrm{Tr}(\boldsymbol{A}_i \boldsymbol{H}_i) - \mathrm{Tr}(\boldsymbol{A}_j \boldsymbol{H}_i)]. \tag{A.1}$$

The designs of resolution III or higher are used to estimate the parameters in the models, so

$$|\boldsymbol{H}_k| = |\boldsymbol{I}_N + \rho \boldsymbol{D}_k| = (1 - \rho)^{N/2}(1 + \rho)^{N/2} \tag{A.2}$$

for $k = 1, 2, \ldots, n$, and

$$\begin{aligned}\mathrm{Tr}(\boldsymbol{A}_i\boldsymbol{H}_i) &= \mathrm{Tr}(\boldsymbol{H}_i^{-1} - \boldsymbol{H}_i^{-1}\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{H}_i^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{H}_i^{-1})\boldsymbol{H}_i \\ &= \mathrm{Tr}(\boldsymbol{I}_N) - \mathrm{Tr}(\boldsymbol{I}_{n+1}) \\ &= N - (n+1), \end{aligned} \tag{A.3}$$

$$\mathrm{Tr}(\boldsymbol{A}_j\boldsymbol{H}_i) = \mathrm{Tr}(\boldsymbol{H}_j^{-1}\boldsymbol{H}_i) - \mathrm{Tr}(\boldsymbol{X}'\boldsymbol{H}_i^{-1}\boldsymbol{X})^{-1}(\boldsymbol{X}'\boldsymbol{H}_j^{-1}\boldsymbol{H}_i\boldsymbol{H}_j^{-1}\boldsymbol{X}), \tag{A.4}$$

where

$$\begin{aligned}\mathrm{Tr}(\boldsymbol{H}_j^{-1}\boldsymbol{H}_i) &= \frac{1}{1-\rho^2}\,\mathrm{Tr}(\boldsymbol{I}_N - \rho\boldsymbol{D}_j)(\boldsymbol{I}_N + \rho\boldsymbol{D}_i) \\ &= \frac{1}{1-\rho^2}\,\mathrm{Tr}(\boldsymbol{I}_N - \rho\boldsymbol{D}_j + \rho\boldsymbol{D}_i - \rho^2\boldsymbol{D}_i\boldsymbol{D}_j) \\ &= \frac{N}{1-\rho^2} \end{aligned} \tag{A.5}$$

and

$$(\boldsymbol{X}'\boldsymbol{H}_j^{-1}\boldsymbol{X}) = \frac{1}{1-\rho^2}\,(N\boldsymbol{I}_{n+1} - \rho\boldsymbol{Z}_j) = \frac{N}{1-\rho^2}\left(\boldsymbol{I}_{n+1} - \frac{\rho}{N}\boldsymbol{Z}_j\right).$$

Thus, using the fact that $\boldsymbol{Z}_j^3 = N^2\boldsymbol{Z}_j$, we get

$$\begin{aligned}(\boldsymbol{X}'\boldsymbol{H}_j^{-1}\boldsymbol{X})^{-1} &= \frac{1-\rho^2}{N}\left[\boldsymbol{I}_{n+1} + \sum_{u=1}^{\infty}\left(\frac{\rho}{N}\right)^u(\boldsymbol{Z}_j)^u\right] \\ &= \frac{1-\rho^2}{N}\left[\boldsymbol{I}_{n+1} + \sum_{u=1}^{\infty}\frac{\rho^{2u-1}}{N}\boldsymbol{Z}_j + \sum_{u=1}^{\infty}\frac{\rho^{2u}}{N^2}\boldsymbol{Z}_j^2\right] \\ &= \frac{1-\rho^2}{N}\left[\boldsymbol{I}_{n+1} + \frac{\rho}{(1-\rho^2)N}\boldsymbol{Z}_j + \frac{\rho^2}{(1-\rho^2)N^2}\boldsymbol{Z}_j^2\right]. \end{aligned} \tag{A.6}$$

Moreover,

$$(\boldsymbol{X}'\boldsymbol{H}_j^{-1}\boldsymbol{H}_i\boldsymbol{H}_j^{-1}\boldsymbol{X}) = \frac{N}{(1-\rho^2)^2}\left[(1+\rho^2)\boldsymbol{I}_{n+1} + \frac{\rho(1+\rho^2)}{N}\boldsymbol{Z}_i - \frac{2\rho}{N}\boldsymbol{Z}_j - \frac{2\rho^2}{N}\boldsymbol{Z}_{ij}\right].$$

By using the results of Lemma A.2, we have

$$\mathrm{Tr}(\boldsymbol{X}'\boldsymbol{H}_j^{-1}\boldsymbol{X})^{-1}(\boldsymbol{X}'\boldsymbol{H}_j^{-1}\boldsymbol{H}_i\boldsymbol{H}_j^{-1}\boldsymbol{X}) = \frac{1+\rho^2}{1-\rho^2}\,(n+1) - \frac{2\rho^2}{1-\rho^2}\,(a_j+1). \tag{A.7}$$

Substitute (A.5) and (A.7) into (A.4), we have

$$\mathrm{Tr}(\boldsymbol{A}_j\boldsymbol{H}_i) = \frac{N}{1-\rho^2} - \frac{1+\rho^2}{1-\rho^2}\,(n+1) + \frac{2\rho^2}{1-\rho^2}\,(a_j+1). \tag{A.8}$$

Eq. (4.1) follows directly from substituting (A.2), (A.3) and (A.8) into (A.1).

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