On the equivalence of three estimators for dispersion effects in unreplicated two-level factorial designs

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Abstract: Box and Meyer were the first to consider identifying both location and dispersion effects from unreplicated two-level fractional factorial designs. Since the publication of their paper a number of different procedures (both iterative and non-iterative) have been proposed for estimating the location and dispersion effects. Under a linear structure for the dispersion effects, non-iterative estimation methods for the dispersion effects were proposed by Brenneman and Nair, Liao and Iyer and Wiklander. We prove that for two-level factorial designs the proposed estimators are different representations of a single estimator. The proof uses the framework of Seely, in which quadratic estimators are expressed as inner products of symmetric matrices.

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1 Introduction

Box and Meyer (1986) were the first to consider identifying both location and dispersion effects from unreplicated two-level fractional factorial designs. Since the publication of their paper a number of different procedures (both iterative and non-iterative) have been proposed for estimating the location and dispersion effects (Wang (1989); Nelder and Lee (1991); Engel and Huele (1996); Bergman and Hynén (1997); Wiklander (1998); Liao and Iyer (2000); McGrath and Lin (2001); Brenneman and Nair (2001); Wiklander and Holm (2003)). An overview and a critical analysis of most of these procedures is given by Brenneman and Nair (2001). In their paper they note that the analysis of location and dispersion effects is an intrinsically difficult problem and show that all methods proposed so far suffer from bias to some extent.

   Most of the papers consider a log-linear model for the dispersion effects. However, several estimation methods have been proposed for cases in which a linear structure for the dispersion effects is more applicable. Under a linear structure for dispersion effects, non-iterative estimation methods were proposed by Brenneman and Nair (2001), Liao and Iyer (2000) and Wiklander (1998) (see also Wiklander and Holm (2003)). In these papers the following general mixed linear model is assumed for the random vector Y of observations

$$\mathrm{E}\left(Y\right) = X\theta$$

$$\mathrm{Var}\left(Y\right) = \sum_{i=1}^{m} \alpha_i \Gamma_i{}' \tag{1}$$

where X is a known $N \times p$ full rank matrix and $\Gamma_1, \Gamma_2, \ldots, \Gamma_m$ are known matrices, but parameters $\alpha_1, \alpha_2, \ldots, \alpha_m$ and $\theta = (\theta_1, \theta_2, \ldots, \theta_p)^T$ are unknown. Brenneman and Nair (2001) suggest a linear regression of the squared residuals. This method can be applied for any design and the model in (1) provided that the matrices $\Gamma_i, i \in \{1, 2, \ldots, m\}$, are diagonal. Liao and Iyer (2000) describe a general method for finding quadratic forms in the vector of observations that estimate the dispersion parameters $\alpha_1, \alpha_2, \ldots, \alpha_m$ in model (1). Although their method for estimation applies to any design, the content of their paper is mainly restricted to estimation in two-level factorial designs. They present a method to construct two-level fractional factorial designs that are A-optimal for this method of estimation when there is only one factor responsible for the dispersion effects. The estimators proposed by Wiklander (1998) and Wiklander and Holm (2003) are sums of products of specific pairs of linear estimators of negligible (higher order) location effects. The use of this method is restricted to two-level factorial designs and regular fractions of such designs.

   Surprisingly, the three proposed methods for estimation are equivalent when the design is a two-level factorial design. In this paper a proof for the equivalence of these estimation methods is given. The proof uses the framework of Seely (1970a) and Seely (1970b). Within this framework quadratic estimators are expressed as inner products of symmetric matrices. The paper is organized as follows. First the notation of the article is described in Section 2. In Section 3 we present the framework for quadratic estimators proposed in Seely (1970a) and Seely (1970b). The estimation methods of Wiklander (1998) (see also Wiklander and Holm (2003)), Liao and Iyer (2000) and Brenneman and Nair (2001) are described in Section 4. Equivalence of these estimation methods for two-level full factorial designs and regular fractions of these designs is shown in Section 5.

2 Preliminaries

The following notation will be used for two-level factorial designs. We let $N = 2^n$ (for some $n \in \mathbb{N}$) denote the total number of runs in the experiment. We denote by Y the length N random vector of observations and for this vector the model given in (1) is assumed. The design matrix X is an $N \times p$ matrix, the columns of which will be denoted by $x_1, x_2, \ldots, x_p$. We let the column x_1 correspond to the constant term in the model, *i.e.*, all entries in this column be equal to 1. The other columns of X each correspond to a main-effect or interaction-effect. The jth entry in these columns equals 1 when the corresponding factor is at its high level and -1 when it is at its lower level in run j. The matrices $\Gamma_i, i \in \{1, 2, \ldots, m\}$, are diagonal matrices. We let $\Gamma_1 = I$ and let the other matrices correspond to main-effects or interaction-effects. The jth diagonal element of Γ_k is 1 if the corresponding factor or interaction is at its higher level and -1 otherwise. Note that we do not assume that the location model and the dispersion model involve the same factors and interactions.

In this paper both full two-level factorial designs and balanced orthogonal fractions of these designs are considered. Throughout the paper we will use the term regular to refer to a balanced orthogonal fraction. When considering a fraction we assume that the effects to which the columns of X correspond are not confounded. Furthermore, we assume that there is no confounding of the effects to which the matrices $\Gamma_j, 1 \leq j \leq m$, correspond. By $\widetilde{X}$ we denote the extended design matrix. In case of the full factorial design this is the $N \times N$ matrix that comes from extending the design matrix X with all columns that correspond to location effects that are not in the model. In the case of a regular fraction the matrix $\widetilde{X}$ is defined as any non-unique matrix that results from extending the matrix X to an $N \times N$ matrix for which the columns correspond to a maximum set of unconfounded effects. This will be illustrated in Section 5.2.

Throughout the paper the operator $\circ$ denotes the Hadamard product for vectors. For $a = (a_1, a_2, \ldots, a_N)^T$ and $b = (b_1, b_2, \ldots, b_N)^T$ the product $a \circ b$ is given by $(a_1 b_1, a_2 b_2, \ldots, a_N b_N)^T$. The columns of the extended design matrix $\widetilde{X}$ for a full factorial design form a group under this operation. Finally, by diag (A) we denote the diagonal of the matrix A as a column vector.

3 Framework for quadratic estimators

In this section we describe the framework for quadratic estimators proposed by Seely (1970a) (see also Seely (1970b)), in which quadratic estimators are expressed as inner products of symmetric matrices. A specific orthonormal basis for the vector space of symmetric matrices is proposed. In proving equality of the estimators we use the unique Fourier-Bessel expansion with respect to this basis.

We let $\mathcal{M}$ denote the vector space of all symmetric $N \times N$ matrices endowed with the inner product $\langle \cdot, \cdot \rangle$, defined by $\langle A, B \rangle = \text{Tr}\,(AB)$. If we let $U = YY^T$ then the set of all quadratic estimators, *i.e.*, the set of all quadratic forms in the random vector Y, is given by $\{\langle A, U \rangle : A \in \mathcal{M}\}$.

We use a method from Seely (1970b) to construct an orthonormal basis for $\mathcal{M}$ from an orthonormal basis for $\mathbb{R}^N$. Let $\{q_1, q_2, \ldots, q_p\} \subset \mathbb{R}^N$ and define symmetric matrices

$Q_{ij}, 1 \leq i \leq j \leq p$, by

$$
\begin{aligned}
Q_{ii} &= q_i q_i^T & 1 \leq i \leq p \\
Q_{ij} &= \tfrac{1}{\sqrt{2}} \left(q_i q_j^T + q_j q_i^T \right) & 1 \leq i < j \leq p
\end{aligned} \tag{2}
$$

The following theorem tells us that if $\{q_1, q_2, \ldots, q_p\}$ is an orthonormal set in $\mathbb{R}^N$ then the matrices $Q_{ij}, 1 \leq i \leq j \leq p$, form an orthonormal set in $\mathcal{M}$. It also tells us how to construct an orthonormal basis for $\mathcal{M}$ given an orthonormal basis for $\mathbb{R}^N$.

Theorem 3.1 *Let $\{q_1, q_2, \ldots, q_p\}$ be an orthonormal set of vectors in $\mathbb{R}^N$. The set $\{Q_{ij} : 1 \leq i \leq j \leq p\}$ with Q_{ij} as defined in (2) is an orthonormal set of vectors in the inner product space $(\mathcal{M}, \langle \cdot, \cdot \rangle)$. In particular, if $\{q_1, q_2, \ldots, q_N\}$ is an orthonormal basis for $\mathbb{R}^N$, then the set $\{Q_{ij} : 1 \leq i \leq j \leq N\}$ is an orthonormal basis for $(\mathcal{M}, \langle \cdot, \cdot \rangle)$.*

Proof Let B_{ij} be defined as

$$
B_{ij} = q_i q_j^T + q_j q_i^T \quad 1 \leq i \leq j \leq p .
$$

Then we have

$$
\langle B_{ij}, B_{k\ell} \rangle = \text{Tr} \left(B_{ij} B_{k\ell} \right) = \text{Tr} \left(q_i q_j^T q_k q_\ell^T \right) + \text{Tr} \left(q_i q_j^T q_\ell q_k^T \right) + \text{Tr} \left(q_j q_i^T q_k q_\ell^T \right) + \text{Tr} \left(q_j q_i^T q_\ell q_k^T \right) =
$$

$$
\text{Tr} \left(q_j^T q_k q_\ell^T q_i \right) + \text{Tr} \left(q_j^T q_\ell q_k^T q_i \right) + \text{Tr} \left(q_i^T q_k q_\ell^T q_j \right) + \text{Tr} \left(q_i^T q_\ell q_k^T q_j \right) =
$$

$$
q_j^T q_k q_\ell^T q_i + q_j^T q_\ell q_k^T q_i + q_i^T q_k q_\ell^T q_j + q_i^T q_\ell q_k^T q_j.
$$

Let δ_{ij} denote the Kronecker delta. Since $\{q_1, q_2, \ldots, q_p\}$ is a orthonormal set we find that

$$
\langle B_{ij}, B_{k\ell} \rangle = \delta_{jk}\delta_{\ell i} + \delta_{j\ell}\delta_{ki} + \delta_{ik}\delta_{\ell j} + \delta_{i\ell}\delta_{kj} = \begin{cases} 4 & \text{if } i = j = k = l \\ 2 & \text{if } i = k < j = \ell \\ 0 & \text{otherwise} \end{cases} .
$$

Using this result we find that $\langle Q_{ij}, Q_{k\ell} \rangle = 0$ if $i \neq k$ or $j \neq \ell$ and $\langle Q_{ij}, Q_{ij} \rangle = 1$ for all i and j. The set $\{Q_{ij} : 1 \leq i \leq j \leq p\}$ is thus an orthonormal set of vectors in the inner product space $(\mathcal{M}, \langle \cdot, \cdot \rangle)$. If $p = N$ then $\{q_1, q_2, \ldots, q_N\}$ is an orthonormal basis for $\mathbb{R}^N$. The number of elements in the orthonormal set $\{Q_{ij} : 1 \leq i \leq j \leq N\}$ is in that case equal to $\frac{1}{2}N(N+1)$ which is $\dim(\mathcal{M})$. We have shown that the set $\{Q_{ij} : 1 \leq i \leq j \leq N\}$ is an orthonormal basis for $(\mathcal{M}, \langle \cdot, \cdot \rangle)$ $\qquad\square$

The next lemma tells us how any element in the span of an orthonormal set of vectors in an inner product space can be uniquely expressed in terms of this orthonormal set.

Lemma 3.2 *Consider a finite orthonormal set $\{e_1, e_2, \ldots, e_n\}$ in an inner product space. Then $\{e_1, e_2, \ldots, e_n\}$ is a basis for $\mathcal{S} = \text{span}\{e_1, e_2, \ldots, e_n\}$ and every $x \in \mathcal{S}$ has a unique representation of the form*

$$
x = \sum_{i=1}^{n} \langle x, e_i \rangle e_i.
$$

Proof Let $x \in \mathcal{S}$. Then there exist $\beta_1, \beta_2, \ldots, \beta_n$ such that $x = \beta_1 e_1 + \beta_2 e_2 + \ldots + \beta_n e_n$. Using orthonormality of $\{e_1, e_2, \ldots, e_n\}$ we find that $\langle x, e_i \rangle = \beta_i$ for all i. As a result $\{e_1, e_2, \ldots, e_n\}$ is linearly independent and a basis for $\mathcal{S}$. $\qquad\square$

The expansion given in Lemma 3.2 is called the Fourier-Bessel expansion. It tells us how any symmetric matrix in $\mathcal{M}$ can be expressed as a unique linear combination of the symmetric matrices $Q_{ij}, 1 \leq i \leq j \leq N$, defined in (2).

4 Estimation methods

Wiklander (1998) (see also Wiklander and Holm (2003)), Liao and Iyer (2000) and Brenneman and Nair (2001) proposed non-iterative methods for estimation of the dispersion effects in the model given in (1). All methods at first neglect the heterogeneity and use the ordinary least squares as a first step in the estimation of the location effects. The three methods for estimating the dispersion effects are described in this section.

4.1 Wiklander and Holm

Wiklander (1998) and Wiklander and Holm (2003) describe a method for finding estimators for the parameters $\alpha_1, \alpha_2, \ldots, \alpha_m$ when the design is a two-level full factorial design or a regular fraction of such a design. The method for a 2^n full factorial design can be described as follows. Let $\widetilde{X}$ denote the $N \times N$ matrix resulting from extending the design matrix $X = (x_1 : x_2 : \ldots : x_p)$ with columns corresponding to all effects that are not in the location model. The ith column of $\widetilde{X}$ is denoted by x_i. Wiklander (1998) and Wiklander and Holm (2003) propose a one-to-one transformation of the elements of Y into new random variables

$$Z_i = \frac{1}{N} x_i^T Y \text{ for } 1 \leq i \leq N.$$

Note that the random variables $Z_1, Z_2, \ldots, Z_p$ are unbiased estimators for the location effects. These estimators need not be independent. The estimators for the dispersion parameters are constructed using products of specific pairs of random variables in the set $\{Z_i : p+1 \leq i \leq N\}$. More precisely, for any pair (i, j) such that diag $(\Gamma_k) = x_i \circ x_j$ and $p+1 \leq i \leq j \leq N$ we have that $N Z_i Z_j$ is an unbiased estimator for α_k. The estimator for α_k proposed by Wiklander (1998) and Wiklander and Holm (2003) is the average of all such estimators with different i and j. This is the estimator that we consider in this paper. Wiklander (1998) and Wiklander and Holm (2003) also propose a reduced estimator consisting of the maximum number of independent estimators $N Z_i Z_j$. We do not consider this reduced estimator here.

For a regular fraction a slight modification is needed. Let $n = q - r$, then the extended design matrix of a regular 2^{q-r} fraction is equal to that of a 2^n full factorial design up to the signs of the columns. If for a certain pair (i, j) with $p + 1 \leq i \leq j \leq N$ and $k \in \{1, 2, \ldots, m\}$ we have diag $(\Gamma_k) = x_i \circ x_j$, then $E(N Z_i Z_j) = \alpha_k$. If, on the other hand, diag $(\Gamma_k) = -x_i \circ x_j$, then $E(-N Z_i Z_j) = \alpha_k$. The proposed unbiased estimator for α_k is the average of all estimators of these two types.

4.2 Liao and Iyer

Liao and Iyer (2000) propose a general method for finding estimators for the parameters $\alpha_1, \alpha_2, \ldots, \alpha_m$ in model (1). They define matrices $A_1, A_2, \ldots, A_m$ of the form

$$A_k = (I - P_X) \Gamma_k (I - P_X), \tag{3}$$

where P_X is the projection matrix onto the column space of X, i.e.

$$P_X = X \left(X^T X\right)^- X^T,$$

where $\left(X^T X\right)^-$ denotes the generalized inverse of $X^T X$. Note that $I - P_X$ is the projection on the orthoplement of the range of X, i.e, onto the space spanned by the columns in $\widetilde{X}$ that

are not in X. Define the vector $W = \left(Y^T A_1 Y, Y^T A_2 Y, \ldots, Y^T A_m Y\right)^T$ and the matrix K by

$$K = \begin{pmatrix} \text{Tr}\,(A_1 \Gamma_1) & \text{Tr}\,(A_1 \Gamma_2) & \ldots & \text{Tr}\,(A_1 \Gamma_m) \\ \text{Tr}\,(A_2 \Gamma_1) & \text{Tr}\,(A_2 \Gamma_2) & \ldots & \text{Tr}\,(A_2 \Gamma_m) \\ \vdots & \vdots & \ddots & \vdots \\ \text{Tr}\,(A_m \Gamma_1) & \text{Tr}\,(A_m \Gamma_2) & \ldots & \text{Tr}\,(A_m \Gamma_m) \end{pmatrix}.$$

If K is invertible then $K^{-1} W$ is an unbiased estimator for $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_m)^T$.

For the case $m = 2$ Liao and Iyer (2000) propose a method to determine regular two-level fractional factorial designs of resolution at least III that are A-optimal for estimating the parameters α_1 and α_2 using this method.

4.3 Brenneman and Nair

Under model (1), Brenneman and Nair (2001) propose using a linear regression of the squared residuals after estimating the location effects using ordinary least squares estimation. The covariance matrix of the vector R of residuals is given by

$$\text{Var}\,(R) = \text{Var}\,((I - P_X) Y) = (I - P_X)\,\text{Var}\,(Y)\,(I - P_X).$$

Given model (1) this matrix can be expressed in terms of the parameters $\alpha_1, \alpha_2, \ldots, \alpha_m$ by

$$\text{Var}\,(R) = \sum_{1 \leq k \leq m} \alpha_k (I - P_X) \Gamma_k (I - P_X) = \sum_{1 \leq k \leq m} \alpha_k A_k,$$

with A_k defined as in (3). Let $R^\star$ denote the vector of squared residuals. Since $E\,(R) = 0$ the model for the squared residuals is given by

$$E\,(R^\star) = \text{diag}\,(\text{Var}\,(R)) = B\alpha,$$

where

$$B = \left(\ \text{diag}\,(A_1)\ :\ \text{diag}\,(A_2)\ :\ \ldots\ :\ \text{diag}\,(A_m)\ \right).$$

If B is full rank then an unbiased estimator for α is $\left(B^T B\right)^{-1} B^T R^\star$.

For the case of a two-level full factorial design, let $p_k, 2 \leq k \leq m$, denote the number of pairs of columns x_i and x_j in X for which $\text{diag}\,(\Gamma_k) = x_i \circ x_j$. By R_i we denote the ith element of the vector R of residuals. Brenneman and Nair (2001) showed if $2 \leq k \leq m$ and $N > 2\,(p - p_k)$ then

$$\frac{1}{N - 2\,(p - p_k)} \left(\sum_{i:(\text{diag}\,(\Gamma_k))_i = 1} R_i^2 - \sum_{i:(\text{diag}\,(\Gamma_k))_i = -1} R_i^2\right) \tag{4}$$

is an unbiased estimator for α_k. Brenneman and Nair (2001) do not give an explicit expression for the estimator of α_1 that is obtained using their method. In Theorem A.1 we show that if $N > p$ the estimator for α_1 obtained using a linear regression of the squared residuals is

$$\frac{1}{N - p} \sum_{1 \leq i \leq N} R_i^2. \tag{5}$$

When the design is a regular fraction then (4) and (5) can still be used. However, p_k should then be defined as the number of pairs of columns x_i and x_j in X for which $\text{diag}\,(\Gamma_k) = \pm\, x_i \circ x_j$. This result is stated in Theorem A.1.

5 Proof of equivalence

In this section we show that the three methods of estimation described in Section 4 give the same estimates for the dispersion parameters in model (1) for two-level full factorial designs and regular fractions of these designs.

5.1 Two-level full factorial designs

Before we show equality of the estimators, we first give a lemma that we need in the proof. Recall that the extended design matrix $\widetilde{X}$ for a two-level full factorial design is the $N \times N$ matrix that comes from extending the design matrix X with all columns corresponding to the location effects that are not in the model. The columns in the extended design matrix $\widetilde{X}$ of a full factorial design form a group with the Hadamard product $\circ$. The identity element in this group is the vector of length $N = 2^n$ with each element equal to 1. We will denote this identity element by e. The proof of the next lemma uses the group property and orthogonality of the columns in $\widetilde{X}$.

Lemma 5.1 *Let x_i and x_j be columns in the extended design matrix $\widetilde{X}$ of a two-level full factorial design and let Γ denote a diagonal matrix with a column of $\widetilde{X}$ as its diagonal, then we have*

$$x_i^T \Gamma x_j = \left\{ \begin{array}{ll} N & \text{if } diag\,(\Gamma) = x_i \circ x_j \\ 0 & \text{otherwise} \end{array} \right. .$$

Proof If the diagonal of Γ equals the column x_k of $\widetilde{X}$, then

$$x_i^T \Gamma x_j = (x_i \circ x_k)^T x_j = \left\{ \begin{array}{ll} N & \text{if } x_j = (x_i \circ x_k) \\ 0 & \text{otherwise} \end{array} \right. .$$

Since all elements of x_i are non-zero we have

$$x_j = x_i \circ x_k \Leftrightarrow x_i \circ x_j = x_i \circ x_i \circ x_k = e \circ x_k = x_k = \text{diag}\,(\Gamma),$$

which completes the proof. $\square$

Our main theorem shows equivalence of the three estimation methods discussed in Section 4 when the design is a 2^n full factorial design.

Theorem 5.2 *Consider a full factorial design with design matrix and extended design matrix given by $X = (x_1 : x_2 : \ldots : x_p)$ and $\widetilde{X} = (x_1 : x_2 : \ldots : x_N)$, respectively. Let the matrices $\Gamma_1, \Gamma_2, \ldots, \Gamma_m$ be diagonal matrices with different columns of $\widetilde{X}$ as their diagonal. Assume that x_1 is a vector of ones and that $\Gamma_1 = I$. Then the estimation methods proposed by (i) Wiklander (1998) and Wiklander and Holm (2003), (ii) Liao and Iyer (2000) and (iii) Brenneman and Nair (2001) all give the same estimates for the parameters $\alpha_1, \alpha_2, \ldots, \alpha_m$ in (1).*

Proof We will first show equality of the estimators proposed by Wiklander (1998) and Liao and Iyer (2000). Let $q_1, q_2, \ldots, q_N$ denote the columns in the extended design matrix $\widetilde{X}$ after normalization, *i.e.*, $q_i = \frac{x_i}{\sqrt{N}}$ for all i, and let the matrices Q_{ij} be defined as in (2). Since $\{q_1, q_2, \ldots, q_N\}$ is an orthonormal basis for $\mathbb{R}^N$ it follows from Theorem 3.1 that $\{Q_{ij} \mid 1 \leq$

$i \le j \le N\}$ is an orthonormal basis for the inner product space $(\mathcal{M}, \langle \cdot, \cdot \rangle)$. By Lemma 3.2 we have that each matrix Γ_k has a unique representation of the form

$$\Gamma_k = \sum_{1 \le i \le j \le N} \langle \Gamma_k, Q_{ij} \rangle Q_{ij}.$$

The coefficient of the matrix $Q_{ii}, i = 1, \ldots, N$, in this representation equals

$$\langle \Gamma_k, Q_{ii} \rangle = \mathrm{Tr}\left(\Gamma_k q_i q_i^T\right) = q_i^T \Gamma_k q_i = \frac{1}{N} x_i^T \Gamma_k x_i = \delta_{k1}.$$

The coefficients of matrix Q_{ij} where $i \ne j$ are given by

$$\langle \Gamma_k, Q_{ij} \rangle = \frac{1}{\sqrt{2}} \mathrm{Tr}\left(\Gamma_k q_i q_j^T + \Gamma_k q_j q_i^T\right) = \sqrt{2} q_i^T \Gamma_k q_j.$$

Using $q_i = \frac{x_i}{\sqrt{N}}$ and Lemma 5.1 we find

$$\langle \Gamma_k, Q_{ij} \rangle = \frac{\sqrt{2}}{N} x_i^T \Gamma_k x_j = \begin{cases} \sqrt{2} & \text{if } \mathrm{diag}\,(\Gamma_k) = x_i \circ x_j \\ 0 & \text{otherwise} \end{cases}.$$

The matrix Γ_1 can be expressed in terms of the matrices Q_{ij} in the following way

$$\Gamma_1 = \sum_{1 \le i \le N} Q_{ii}. \tag{6}$$

The matrix $\Gamma_k, 2 \le k \le m$, are given in terms of the matrices Q_{ij} by

$$\Gamma_k = \sqrt{2} \sum Q_{ij}, \tag{7}$$

where the summation is over all different pairs (i, j) for which $1 \le i \le j \le N$ and $x_i \circ x_j = \mathrm{diag}\,(\Gamma_k)$. Note that since $x_1, x_2, \ldots, x_p$ are columns in X and the columns $x_{p+1}, x_{p+2}, \ldots, x_N$ of $\widetilde{X}$ are orthogonal to span $\{x_1, x_2, \ldots, x_p\}$ we have

$$(I - P_X) Q_{ij} (I - P_X) = \begin{cases} Q_{ij} & \text{if } p + 1 \le i \le j \le N \\ 0 & \text{otherwise} \end{cases}.$$

The matrix A_1 defined in (3) is uniquely represented in terms of the matrices Q_{ij} by

$$A_1 = \sum_{p+1 \le i \le N} Q_{ii}. \tag{8}$$

Let S_k denote the set of all pairs (i, j) with $p + 1 \le i \le j \le N$ for which $x_i \circ x_j = \mathrm{diag}\,(\Gamma_k)$. The matrices $A_k, 2 \le k \le m$, defined in (3) are uniquely represented by

$$A_k = \sqrt{2} \sum_{(i,j) \in S_k} Q_{ij}. \tag{9}$$

The elements of the matrix K are given by

$$\mathrm{Tr}\,(A_k \Gamma_j) = \langle A_k, \Gamma_j \rangle. \tag{10}$$

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Let n_k denote the number of elements in the set S_k. Substituting (6), (7), (8) and (9) into (10) and using that the matrices Q_{ij} form an orthonormal set we find

$$\text{Tr}\,(A_k\Gamma_j) = \begin{cases} N - p & \text{if } j = k = 1 \\ 2n_k & \text{if } 2 \leq j = k \leq m \\ 0 & \text{otherwise} \end{cases}.$$

Hence, the matrix K is a diagonal matrix with $(N - p, 2n_2, 2n_3, \ldots, 2n_m)^T$ as its diagonal. The estimator for α_1 proposed by Liao and Iyer (2000) is

$$\frac{1}{N - p} Y^T A_1 Y. \tag{11}$$

The estimator proposed for $\alpha_k, 2 \leq k \leq m$, is

$$\frac{1}{2n_k} Y^T A_k Y. \tag{12}$$

The equality of the estimators for α_1 proposed by Liao and Iyer (2000) and Wiklander (1998) follows from observing that

$$\begin{aligned}
\frac{1}{N - p} Y^T A_1 Y &= \frac{1}{N - p} \sum_{p+1 \leq i \leq N} Y^T Q_{ii} Y = \frac{1}{N - p} \sum_{p+1 \leq i \leq N} \frac{1}{N} x_i^T Y x_i^T Y \\
&= \frac{1}{N(N - p)} \sum_{p+1 \leq i \leq N} N Z_i N Z_i = \frac{1}{N - p} \sum_{p+1 \leq i \leq N} N Z_i Z_i.
\end{aligned} \tag{13}$$

The equality of estimators for $\alpha_k, 2 \leq k \leq m$, proposed follows from

$$\begin{aligned}
\frac{1}{2n_k} Y^T A_k Y &= \frac{1}{\sqrt{2}n_k} \sum_{(i,j)\in S_k} Y^T Q_{ij} Y = \frac{1}{Nn_k} \sum_{(i,j)\in S_k} x_i^T Y x_j^T Y \\
&= \frac{1}{Nn_k} \sum_{(i,j)\in S_k} N Z_i N Z_j = \frac{1}{n_k} \sum_{(i,j)\in S_k} N Z_i Z_j.
\end{aligned} \tag{14}$$

Recall that the estimator for α_k proposed by Wiklander (1998) and Wiklander and Holm (2003) was the average of $N Z_i Z_j$ over all (i,j) with $p + 1 \leq i \leq j \leq N$ and for which diag $(\Gamma_k) = x_i \circ x_j$, which is exactly the right-hand side of (13) and (14).

We will now show equality of the estimators proposed by Liao and Iyer (2000) and Brenneman and Nair (2001). The estimator for $\alpha_k, 2 \leq k \leq m$, proposed by Brenneman and Nair (2001) is given by

$$\frac{1}{N - 2(p - p_k)} \left(\sum_{i:(\text{diag}\,(\Gamma_k))_i = 1} R_i^2 - \sum_{i:(\text{diag}\,(\Gamma_k))_i = -1} R_i^2 \right), \tag{15}$$

where $p_k, 2 \leq k \leq m$, denotes the number of pairs of columns x_i and x_j in X for which diag $(\Gamma_k) = x_i \circ x_j$. By R_i we denote the ith element of the vector R of residuals. Note that since Γ_k is a diagonal matrix we have

$$\left(\sum_{i:(\text{diag}\,(\Gamma_k))_i = 1} R_i^2 - \sum_{i:(\text{diag}\,(\Gamma_k))_i = -1} R_i^2 \right) = R^T \Gamma_k R. \tag{16}$$

Since the location effects are estimated using ordinary least squares we have that

$$R = (I - P_X)Y. \tag{17}$$

Substituting (16) and (17) into (15) we find that the proposed estimator equals

$$\frac{1}{N - 2(p - p_k)} Y^T (I - P_X) \Gamma_k (I - P_X) Y = \frac{1}{N - 2(p - p_k)} Y^T A_k Y, \tag{18}$$

with A_k given in (3). Note that there are $\frac{N}{2}$ pairs of columns x_i and x_j in $\widetilde{X}$ such that $x_i \circ x_j = \text{diag}(\Gamma_k)$. For p_k of these pairs both x_i and x_j are in X (by the definition of p_k). For all other $p - 2p_k$ columns x_i in X there exists a column $x_j, p + 1 \le j \le N$, of $\widetilde{X}$ such that $x_i \circ x_j = \text{diag}(\Gamma_k)$. The number n_k of columns x_i and x_j with $p + 1 \le i \le j \le N$ for which $x_i \circ x_j = \text{diag}(\Gamma_k)$ is, hence, $\frac{N}{2} - p_k - (p - 2p_k) = \frac{N}{2} - (p - p_k)$. Substitution of $\frac{N}{2} - (p - p_k) = n_k$ into (18) gives

$$\frac{1}{2n_k} Y^T A_k Y,$$

which equals (12). The estimator for α_1 obtained using a linear regression of the squared residuals is

$$\frac{1}{N - p} \sum_{1 \le i \le N} R_i^2 = \frac{1}{N - p} R^T \Gamma_1 R = \frac{1}{N - p} Y^T A_1 Y,$$

which equals (11). Hence, also the estimators proposed by Brenneman and Nair (2001) and Liao and Iyer (2000) are equal for all k, $1 \le i \le k$. □

5.2 Regular fractions of two-level factorial designs

The equivalence of the estimation methods proposed by Wiklander (1998), Liao and Iyer (2000) and Brenneman and Nair (2001) can also be shown for regular fractions of two-level factorial designs. Recall that the extended design matrix for a regular fraction is defined as any non-unique matrix that results from extending the matrix X to a $N \times N$ matrix for which the columns correspond to a maximal set of unconfounded effects. In the full factorial case the columns in the extended design matrix form a group with respect to the Hadamard product. For regular fractions the columns of an extended design matrix do not always have this property. This is illustrated by the next example.

Example Consider the regular 2^{3-1} fractional factorial design given in Table 1. The matrix X consisting of the columns in the table is a $N \times N$ matrix with columns corresponding to a maximal set of unconfounded effects. Hence, $\widetilde{X} = X$ is an extended design matrix for the design. Let x_i denote the ith column in Table 1, then $\widetilde{X} = \begin{pmatrix} x_1 & : & x_2 & : & x_3 & : & x_4 \end{pmatrix}$. For this extended design matrix we have that $x_2 \circ x_3 = -x_4$. Since $-x_4$ is not a column in the extended design matrix $\widetilde{X}$, the columns x_1, x_2, x_3 and x_4 do not form a group with the Hadamard product $\circ$.

We have shown that the columns of the extended design matrix for regular fractions in general do not form a group with operation $\circ$. However, if $\widetilde{X}$ is an extended design matrix for a regular two-level fractional factorial design and x_i and x_j are columns in $\widetilde{X}$ then either $x_i \circ x_j$ or $-x_i \circ x_j$ is a column in $\widetilde{X}$. We will use this property to proof that the three methods also give the same estimators in regular fractions of two-level factorial designs. The next theorem states the equivalence for regular two-level fractional factorial designs.

Table 1: Fraction of the 2^3 factorial design with $I = -ABC$

Run	I	A	B	C
1	1	-1	-1	-1
2	1	1	-1	1
3	1	-1	1	1
4	1	1	1	-1

Theorem 5.3 *Consider a regular two-level fractional factorial design with design matrix and extended design matrix given by $X = (x_1 : x_2 : \ldots : x_p)$ and $\widetilde{X} = (x_1 : x_2 : \ldots : x_N)$, respectively. Let the matrices $\Gamma_1, \Gamma_2, \ldots, \Gamma_m$ be a set of linearly independent matrices with columns of $\widetilde{X}$, possibly multiplied by -1, as their diagonal. Assume that x_1 is a vector of ones and that $\Gamma_1 = I$. Then the estimation methods proposed by (i) Wiklander (1998) and Wiklander and Holm (2003), (ii) Liao and Iyer (2000) and (iii) Brenneman and Nair (2001) all give the same estimates for the parameters $\alpha_1, \alpha_2, \ldots, \alpha_m$ in (1).*

Proof We will first show that the methods proposed by Wiklander (1998) and Liao and Iyer (2000) yield the same estimates. Let $q_1, q_2, \ldots, q_N$ denote the columns in the extended design matrix $\widetilde{X}$ and let matrices Q_{ij} be defined as in (2). Then we have

$$\langle \Gamma_k, Q_{ij} \rangle = \begin{cases} -\sqrt{2} & \text{if diag} (\Gamma_k) = -x_i \circ x_j \\ \sqrt{2} & \text{if diag} (\Gamma_k) = x_i \circ x_j \\ 0 & \text{otherwise} \end{cases} .$$

The matrices Γ_k can be written in terms of matrices Q_{ij} as follows

$$\Gamma_k = \sqrt{2} \sum_+ Q_{ij} - \sqrt{2} \sum_- Q_{ij},$$

where $\sum_+$ and $\sum_-$ denote the sums over all pairs $(i, j), 1 \leq i \leq j \leq N$, for which $x_i \circ x_j = \text{diag} (\Gamma_k)$ and $x_i \circ x_j = -\text{diag} (\Gamma_k)$, respectively. The matrices A_k can be written in terms of the matrices Q_{ij} as follows

$$A_k = \sqrt{2} \sum_{+,p+1} Q_{ij} - \sqrt{2} \sum_{-,p+1} Q_{ij},$$

where $\sum_{+,p+1}$ and $\sum_{-,p+1}$ denote the sums over all pairs $(i, j), p + 1 \leq i \leq j \leq N$, for which $x_i \circ x_j = \text{diag} (\Gamma_k)$ and $x_i \circ x_j = -\text{diag} (\Gamma_k)$, respectively. Let n_k denote the number of pairs (i, j) for which $p + 1 \leq i \leq j \leq N$ and $x_i \circ x_j = \pm \text{diag} (\Gamma_k)$. The elements in the matrix K are given by

$$\text{Tr} (A_k \Gamma_j) = \begin{cases} N - p & \text{if } j = k = 1 \\ 2n_k & \text{if } j = k \in \{2, 3, \ldots, m\} \\ 0 & \text{otherwise} \end{cases} .$$

The estimator for $\alpha_k, 2 \leq k \leq m$, proposed by Liao and Iyer (2000) is

$$\frac{1}{2n_k} Y^T A_k Y.$$

This estimator is equal to

$$\frac{1}{n_k} \left(\sum_{+,p+1} NZ_iZ_j - \sum_{-,p+1} NZ_iZ_j \right),$$

which is the estimator proposed by Wiklander (1998). The estimator for α_1 proposed by Liao and Iyer (2000) is

$$\frac{1}{N-p} Y^T A_1 Y.$$

This estimator is equal to

$$\frac{1}{N-p} \sum_{p+1 \le i \le N} NZ_i^2,$$

which is the estimator proposed by Wiklander (1998).

We will now show that the estimation methods proposed by Liao and Iyer (2000) and Brenneman and Nair (2001) are equal. The estimator for $\alpha_k, k \in \{2, 3, \dots, m\}$, proposed by Brenneman and Nair (2001) is given by

$$\frac{1}{N-2(p-p_k)} \left(\sum_{i:(\text{diag}(\Gamma_k))_i=1} R_i^2 - \sum_{i:(\text{diag}(\Gamma_k))_i=-1} R_i^2 \right) = \frac{1}{N-2(p-p_k)} Y^T A_k Y, \quad (19)$$

where $p_k, k \in \{2, 3, \dots, m\}$, denotes the number of pairs of columns x_i and x_j in X for which $\text{diag}(\Gamma_k) = \pm x_i \circ x_j$. There are $\frac{N}{2}$ pairs of columns in $\widetilde{X}$ for which $x_i \circ x_j = \pm \text{diag}(\Gamma_k)$. For all other $p - 2p_k$ columns x_i in X there exists a column $x_j, p+1 \le j \le N$, of $\widetilde{X}$ such that $x_i \circ x_j = \pm \text{diag}(\Gamma_k)$. The number n_k of columns x_i and x_j with $p+1 \le i \le j \le N$ for which $x_i \circ x_j = \pm \text{diag}(\Gamma_k)$ is, hence, $\frac{N}{2} - p_k - (p - 2p_k) = \frac{N}{2} - (p - p_k)$. Substitution of $\frac{N}{2} - (p - p_k) = n_k$ into (19) gives

$$\frac{1}{2n_k} Y^T A_k Y,$$

which is the estimator proposed by Liao and Iyer (2000). The estimator for α_1 obtained using a linear regression of the squared residuals is given in Theorem A.1 and equals

$$\frac{1}{N-p} \sum_{1 \le i \le N} R_i^2 = \frac{1}{N-p} R^T \Gamma_1 R = \frac{1}{N-p} Y^T A_1 Y.$$

The expression on the right-hand side is the estimator for α_1 proposed by Liao and Iyer (2000). Hence, also the estimators proposed by Brenneman and Nair (2001) and Liao and Iyer (2000) are equal for all k, $1 \le i \le k$.

$\square$

6 Concluding remarks

In the previous section we showed equivalence of the estimation methods proposed by Wiklander (1998), Wiklander and Holm (2003), Liao and Iyer (2000) and Brenneman and Nair (2001) for estimating dispersion effects in two-level full factorial designs and regular fractions. The use of methods proposed by Liao and Iyer (2000) and Brenneman and Nair (2001) is not

Table 2: A non-regular fraction of the 2^4 factorial design

Run	A	B	C	D
1	-1	-1	-1	-1
2	1	-1	-1	-1
3	-1	-1	1	-1
4	1	1	1	-1
5	-1	1	-1	1
6	1	1	-1	1
7	1	-1	1	1
8	-1	1	1	1

limited to factorial designs and regular fractions of these designs. The equivalence, however, does not generalize to non-regular fractions of two-level factorial designs. This is shown by the next example.

Example To illustrate that the estimators for the dispersion effects obtained with methods proposed by Liao and Iyer (2000) and Brenneman and Nair (2001) may differ in non-regular two-level factorial designs, we consider the non-regular fraction of the 2^4 factorial design given in Table 2. We consider a main-effects model for the mean and assume that only the factor A has a possible dispersion effect. Using the method proposed by Liao and Iyer (2000) we find the following estimator for the dispersion effect associated with factor A

$$Y^T \begin{pmatrix} -0.125 & -0.125 & 0.221 & 0.029 & 0.183 & 0.067 & 0.029 & -0.279 \\ -0.125 & 0.221 & -0.067 & -0.029 & 0.067 & -0.163 & -0.029 & 0.125 \\ 0.221 & -0.067 & -0.125 & -0.029 & -0.279 & 0.125 & -0.029 & 0.183 \\ 0.029 & -0.029 & -0.029 & 0.029 & 0.029 & -0.029 & 0.029 & -0.029 \\ 0.183 & 0.067 & -0.279 & 0.029 & -0.125 & -0.125 & 0.029 & 0.221 \\ 0.067 & -0.163 & 0.125 & -0.029 & -0.125 & 0.221 & -0.029 & -0.067 \\ 0.029 & -0.029 & -0.029 & 0.029 & 0.029 & -0.029 & 0.029 & -0.029 \\ -0.279 & 0.125 & 0.183 & -0.029 & 0.221 & -0.067 & -0.029 & -0.125 \end{pmatrix} Y.$$

The method proposed by Brenneman and Nair (2001) gives the following estimator for the same dispersion effect

$$Y^T \begin{pmatrix} -0.125 & -0.125 & 0.246 & 0.004 & 0.134 & 0.116 & 0.004 & -0.254 \\ -0.125 & 0.246 & -0.116 & -0.004 & 0.116 & -0.237 & -0.004 & 0.125 \\ 0.246 & -0.116 & -0.125 & -0.004 & -0.254 & 0.125 & -0.004 & 0.134 \\ 0.004 & -0.004 & -0.004 & 0.004 & 0.004 & -0.004 & 0.004 & -0.004 \\ 0.134 & 0.116 & -0.254 & 0.004 & -0.125 & -0.125 & 0.004 & 0.246 \\ 0.116 & -0.237 & 0.125 & -0.004 & -0.125 & 0.246 & -0.004 & -0.116 \\ 0.004 & -0.004 & -0.004 & 0.004 & 0.004 & -0.004 & 0.004 & -0.004 \\ -0.254 & 0.125 & 0.134 & -0.004 & 0.246 & -0.116 & -0.004 & -0.125 \end{pmatrix} Y.$$

The entries of both matrices were first computed exactly and only replaced by numerical values in the end. Given symmetric matrices A and B we have that the statement $Y^T A Y = Y^T B Y$

is true for all $Y \in \mathbb{R}^N$ if and only if $A = B$. Since some of the entries in the matrices differ, the equality of the estimators obtained using the two methods does not hold for general $Y \in \mathbb{R}^N$.

A   Details of the Brenneman and Nair estimation method

Brenneman and Nair (2001) propose a linear regression of the squared residuals for estimating the dispersion effects in two-level factorial designs. In their paper they give an expression for the estimators for $\alpha_2, \alpha_3, \ldots, \alpha_m$ when the design is a two-level full factorial design. They do not give expressions for the estimator for α_1 in case of a full factorial design and the estimators for $\alpha_1, \alpha_2, \ldots, \alpha_m$ when the design is a regular two-level fractional factorial design. In this section we deduce expressions for the estimators of $\alpha_1, \alpha_2, \ldots, \alpha_m$ obtained using the method proposed by Brenneman and Nair (2001) for cases in which the design is a two-level full factorial design or a regular fraction of such a design.

Let for $1 \leq i \leq m$ the matrices A_i be defined by $A_i = (I - P_X)\Gamma_i(I - P_X)$. The unbiased estimator for $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_m)^T$ proposed by Brenneman and Nair (2001) is $\left(B^T B\right)^{-1} B^T R^\star$ where $R^\star$ denotes the vector of squared residuals and the matrix B is given by

$$B = \left(\ \text{diag}\,(A_1)\ :\ \text{diag}\,(A_2)\ :\ \ldots\ :\ \text{diag}\,(A_m)\ \right).$$

The expressions for the estimators in terms of the squared residuals are given in the next theorem.

Theorem A.1 *Consider a full two-level factorial design or a regular two-level fractional factorial design with design matrix and extended design matrix given by $X = (x_1 : x_2 : \ldots : x_p)$ and $\widetilde{X} = (x_1 : x_2 : \ldots : x_N)$, respectively. Let the matrices $\Gamma_1, \Gamma_2, \ldots, \Gamma_m$ be a set of linearly independent matrices with columns of $\widetilde{X}$, possibly multiplied by -1, as their diagonal. If $p < N$ and $2(p - p_k) < N$, for all $k, 2 \leq k \leq N$, then the estimators for the dispersion parameters in (1) proposed by Brenneman and Nair (2001) are given by*

$$
\begin{array}{ll}
\frac{1}{N-p} \sum_{1 \leq j \leq N} R_j^2 & \text{if } i = 1 \\[2mm]
\frac{1}{N-2(p-p_i)} \left(\sum_{j:(diag\,(\Gamma_i))_j=1} R_j^2 - \sum_{j:(diag\,(\Gamma_i))_j=-1} R_j^2 \right) & \text{if } 2 \leq i \leq m
\end{array}
,
$$

where p_k denotes the number of pairs of columns in the design matrix X for which $diag\,(\Gamma_i) = \pm\, x_j \circ x_k$

Proof Using that P_X and $\Gamma_k, 1 \leq k \leq m$, are symmetric matrices we find that

$$\text{diag}\,(A_k) = \text{diag}\,(\Gamma_k) - 2\text{diag}\,(\Gamma_k P_X) + \text{diag}\,(P_X \Gamma_k P_X).$$

Note that $\text{diag}\,(\Gamma_k P_X)$ can be written as

$$\text{diag}\,(\Gamma_k P_X) = \text{diag}\,(\Gamma_k) \circ \text{diag}\,(P_X) = \frac{1}{N}\text{diag}\,(\Gamma_k) \circ \text{diag}\,\left(X X^T\right) = \frac{p}{N}\text{diag}\,(\Gamma_k)$$

To find a different expression for $\text{diag}\,(P_X \Gamma_k P_X)$ observe that

$$
X^T \Gamma_k X = \begin{pmatrix}
(\text{diag}\,(\Gamma_k)\circ x_1)^T x_1 & (\text{diag}\,(\Gamma_k)\circ x_1)^T x_2 & \cdots & (\text{diag}\,(\Gamma_k)\circ x_1)^T x_p \\
(\text{diag}\,(\Gamma_k)\circ x_2)^T x_1 & (\text{diag}\,(\Gamma_k)\circ x_2)^T x_2 & \cdots & (\text{diag}\,(\Gamma_k)\circ x_2)^T x_p \\
\vdots & \vdots & \ddots & \vdots \\
(\text{diag}\,(\Gamma_k)\circ x_p)^T x_1 & (\text{diag}\,(\Gamma_k)\circ x_p)^T x_2 & \cdots & (\text{diag}\,(\Gamma_k)\circ x_p)^T x_p
\end{pmatrix}.
$$

The elements of $X^T \Gamma_k X$ are given by

$$\left(X^T \Gamma_k X\right)_{ij} = \left(\text{diag}\,(\Gamma_k) \circ x_i\right)^T x_j = \begin{cases} -N & \text{if } x_i \circ x_j = -\text{diag}\,(\Gamma_k) \\ N & \text{if } x_i \circ x_j = \text{diag}\,(\Gamma_k) \\ 0 & \text{otherwise} \end{cases}.$$

Note that each row and each column of M has at most one non-zero element. We find that $X\left(X^T \Gamma_i X\right) = (c_1 : c_2 : \ldots : c_p)$ where

$$c_j = \begin{cases} -N x_i & \text{if } x_i \circ x_j = -\text{diag}\,(\Gamma_k) \\ N x_i & \text{if } x_i \circ x_j = \text{diag}\,(\Gamma_k) \\ 0 & \text{otherwise} \end{cases}.$$

As a consequence,

$$\left(X\left(X^T \Gamma_k X\right) X^T\right)_{\ell\ell} = \sum (c_j)_\ell \, (x_j)_\ell, \tag{20}$$

where the summation is over all j for which there exits an $i, 1 \leq j \leq p$, such that $x_i \circ x_j = \pm \text{diag}\,(\Gamma_k)$. For j satisfying this condition and the corresponding i,

$$(c_j)_\ell \, (x_j)_\ell = N \left(x_j \circ \text{diag}\,(\Gamma_k)\right)_\ell (x_j)_\ell = N (x_j)_\ell \, \text{diag}\,(\Gamma_k)_\ell \, (x_j)_\ell = N \text{diag}\,(\Gamma_k)_\ell .$$

Since all p columns x_i in X satisfy $x_i \circ x_i = \text{diag}\,(\Gamma_1)$,

$$\left(X\left(X^T \Gamma_1 X\right) X^T\right)_{\ell\ell} = Np\left(\text{diag}\,(\Gamma_1)\right)_\ell .$$

The number of pairs x_i and x_j of columns in X that satisfy $\text{diag}\,(\Gamma_k) = x_i \circ x_j$ equals p_k and since each of these pairs appears twice in the sum in (20) we find for k such that $2 \leq k \leq m$,

$$\left(X\left(X^T \Gamma_k X\right) X^T\right)_{\ell\ell} = 2Np_k\left(\text{diag}\,(\Gamma_k)\right)_\ell .$$

Hence, we have found that

$$\text{diag}\,(P_X \Gamma_k P_X) = \frac{1}{N^2} \text{diag}\,\left(XX^T \Gamma_k XX^T\right) = \begin{cases} \frac{p}{N} \text{diag}\,(\Gamma_1) & \text{if } k = 1 \\ \frac{2p_k}{N} \text{diag}\,(\Gamma_k) & \text{if } 2 \leq k \leq m \end{cases}.$$

The diagonals of matrix A_k is a multiple of the diagonal of the matrix Γ_k, in particular,

$$\text{diag}\,(A_k) = \begin{cases} \frac{N-p}{N} \text{diag}\,(\Gamma_1) & \text{if } k = 1 \\ \frac{N - 2(p - p_k)}{N} \text{diag}\,(\Gamma_k) & \text{if } 2 \leq k \leq m \end{cases}.$$

The conditions $p < N$ and $2\,(p - p_k) < N$, imply that none of the columns $\text{diag}\,(A_k), 1 \leq k \leq m$, in B equals zero. Since the columns of this matrix B are all multiples of different diagonals of the matrices $\Gamma_i, 1 \leq i \leq m$, the matrix B is orthogonal. The matrix $\left(B^T B\right)^{-1} B^T$ is

$$\left(B^T B\right)^{-1} B^T = \begin{pmatrix} \frac{1}{N-p}\left(\text{diag}\,(\Gamma_1)^T\right) \\ \frac{1}{N - 2(p - p_2)}\left(\text{diag}\,(\Gamma_2)^T\right) \\ \vdots \\ \frac{1}{N - 2(p - p_m)}\left(\text{diag}\,(\Gamma_m)^T\right) \end{pmatrix}.$$

The estimator for α_1 proposed by Brenneman and Nair (2001) is the first element of $\left(B^T B\right)^{-1} B^T R^\star$ and is given by

$$\frac{1}{N-p} \sum_{1 \le i \le N} R_i^2.$$

The estimator for the dispersion effect $\alpha_k, 2 \le k \le m$, is given by

$$\frac{1}{N-2\left(p-p_k\right)}\left(\sum_{i:(\operatorname{diag}\left(\Gamma_k\right))_i=1} R_i^2 - \sum_{i:(\operatorname{diag}\left(\Gamma_k\right))_i=-1} R_i^2\right).$$

This completes the proof. $\qquad\square$

References

B. Bergman and A. Hynén. Dispersion effects from unreplicated designs in the 2^{k-p} series. *Technometrics*, 39(2):191–198, 1997.

G.E.P. Box and R.D. Meyer. Dispersion effects from fractional designs. *Technometrics*, 28 (1):19–27, 1986.

W.A. Brenneman and V.N. Nair. Methods for identifying dispersion effects in unreplicated factorial experiments: a critical analysis and proposed strategies. *Technometrics*, 43(4): 388–405, 2001.

J. Engel and A.F. Huele. A generalized linear modeling approach to robust design. *Technometrics*, 38:365–373, 1996.

C.T. Liao and H.K. Iyer. Optimal 2^{n-p} fractional factorial designs for dispersion effects under a location-dispersion model. *Comm. Statist. Theory Methods*, 29(4):823–835, 2000.

R.N. McGrath and D.K.J. Lin. Testing multiple dispersion effects in unreplicated fractional factorial designs. *Technometrics*, 43(4):406–414, 2001.

J.A. Nelder and Y. Lee. Generalized linear models for the analysis of Taguchi-type experiments. *Appl. Stoch. Models Bus. Ind.*, 7:107–120, 1991.

J. Seely. Linear spaces and unbiased estimation. *Ann. Math. Statist.*, 41:1725–1734, 1970.

J. Seely. Linear spaces and unbiased estimation—Application to the mixed linear model. *Ann. Math. Statist.*, 41:1735–1748, 1970.

P.C. Wang. Tests for dispersion effects from orthogonal arrays. *Comp. Stat. Data Anal.*, 8: 109–117, 1989.

K. Wiklander. A comparison of two estimators of dispersion effects. *Comm. Statist. Theory Methods*, 27(4):905–923, 1998.

K. Wiklander and S. Holm. Dispersion effects in unreplicated factorial designs. *Appl. Stoch. Models Bus. Ind.*, 19(1):13–30, 2003.