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OPTIMAL DESIGNS FOR THE PROPORTIONAL INTERFERENCE MODEL

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The interference model has been widely used and studied in block experiments where the treatment for a particular plot has effects on its neighbor plots. In this paper, we study optimal circular designs for the proportional interference model, in which the neighbor effects of a treatment are proportional to its direct effect. Kiefer's equivalence theorems for estimating both the direct and total treatment effects are developed with respect to the criteria of A, D, E and T. Parallel studies are carried out for the undirectional model, where the neighbor effects do not depend on whether they are from the left or right. Moreover, the connection between optimal designs for the directional and undiretional models is built. Importantly, one can easily develop a computer program for finding optimal designs based on these theorems.

1. Introduction. In many agricultural experiments, the treatment assigned to a particular plot could also have effects on its neighbor plots. This is well recognized in literature. See Draper and Guttman (1980), Kempton (1982), Besag and Kempton (1986), Langton (1990), Gill (1993) and Goldringer, Brabant and Kempton (1994), for examples. To adjust the biases caused by these neighbor effects, the interference model is widely adopted. In a block design with n blocks of size k and t treatments, the response, y_{dij}, observed from the jth plot of block i is decomposed into the following items:

$$y_{dij} = \mu + \beta_i + \tau_{d(i,j)} + \gamma_{d(i,j-1)} + \rho_{d(i,j+1)} + \varepsilon_{ij}, \tag{1}$$

where the subscript $d(i, j)$ denotes the treatment assigned to the jth plot of block i by the design $d:\{1, 2, \ldots, n\} \times \{1, 2, \ldots, k\} \to \{1, 2, \ldots, t\}$. Furthermore, μ is the general mean, β_i is the effect of block i, $\tau_{d(i,j)}$ is the direct effect of treatment $d(i, j)$, $\lambda_{d(i,j-1)}$ is the neighbor effect of treatment $d(i, j-1)$ from the left and $\rho_{d(i,j+1)}$ is the neighbor effect of treatment $d(i, j+1)$ from the right. At last, ε_{ij} is the error term.

Kunert and Martin (2000) studied optimal designs under model (1) for estimating the direct treatment effect when $k = 3$ or 4. The latter was extended to

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$5 \le k \le t$ by Kunert and Mersmann (2011). Zheng (2015) recently provided a unified framework in deriving optimal designs for general values of k and t, with an arbitrary structure of the within-block covariance matrix. On the other hand, Bailey and Druilhet (2004) studied the optimal designs under the same model, however, for estimating the total treatment effect which is the summation of the direct and neighbor effects. This line of research was extended by Ai, Ge and Chan (2007), Ai, Yu and He (2009) and Druilhet and Tinsson (2012). See also Gill (1993), Druilhet (1999), Filipiak and Markiewicz (2003, 2005, 2007) and Filipiak (2012) among others for relevant works on optimal designs.

In this paper, we shall consider the proportional interference model, where the neighbor effects are proportional to the direct treatment effect, that is, $\gamma_i = \lambda_1 \tau_i$ and $\rho_i = \lambda_2 \tau_i$, $1 \le i \le t$, for unknown constants λ_1 and λ_2. This is reasonable for many applications since an effective treatment typically has large impacts on its neighbor plots. In fact, Draper and Guttman (1980) has proposed such model with $\lambda_1 = \lambda_2$. A model with this restriction is said to be undirectional; otherwise, it is directional. Yet, there is no literature on optimal designs under either of these two models according to the best knowledge of the authors. Meanwhile, optimal crossover designs under a similar proportional model have been studied by Kempton, Ferris and David (2001), Bailey and Kunert (2006), Bose and Stufken (2007) and Zheng (2013a). By their enlightenment, the nonlinear terms $\lambda_1 \tau_i$ and $\lambda_2 \tau_i$ in the proportional interference model can be handled in the same fashion. We are interested in finding the optimal designs for estimating the direct and total treatment effects, respectively, under either of the directional and undirectional models.

Let Y_d be the vector of responses organized block by block. Now we can write the proportional interference model as follows:

$$Y_d = 1_{nk}\mu + U\beta + (T_d + \lambda_1 L_d + \lambda_2 R_d)\tau + \varepsilon, \tag{2}$$

where 1_{nk} represents a vector of ones with length nk, $\beta = (\beta_1, \ldots, \beta_n)'$, $\tau = (\tau_1, \ldots, \tau_t)'$ and $U = I_n \otimes 1_k$. Here, I_n is the identity matrix of order n; $\otimes$ denotes the Kronecker product and $'$ means the transposition. Also, T_d, L_d and R_d represent the design matrices for the direct, left neighbor and right neighbor effects, respectively. Throughout the paper, we consider circular designs, for which $d(i, 0) = d(i, k)$ and $d(i, k + 1) = d(i, 1)$, $1 \le i \le n$. Hence we have $L_d = (I_n \otimes H)T_d$ and $R_d = (I_n \otimes H')T_d$, where $H = (\mathbb{I}_{i=j+1 (\mathrm{mod}\ k)})_{1 \le i,j \le k}$ with the indicator function $\mathbb{I}$. For the random error term ε, we assume that $\mathbb{E}(\varepsilon) = 0$ and $\mathrm{Var}(\varepsilon) = I_n \otimes \Sigma$, where Σ is an arbitrary $k \times k$ positive definite within-block covariance matrix.

The rest of the paper is organized as follows. Sections 2 and 3 investigate the optimal designs for estimating the direct and total treatment effects, respectively, under the proportional interference model. Kiefer's equivalence theorems are given with respect to A, D, E and T criteria therein. Section 4 carries out parallel studies for the undirectional model. Moreover, the connection between optimal designs for the two models is built. Section 5 illustrates these theorems through several examples. Section 6 concludes the paper with some discussions.

2. Optimal designs for direct treatment effect. For any matrix G, define G^- as a generalized inverse of G and the projection operator $\mathrm{pr}^\perp G = I - G(G'G)^- G'$. Let $\tilde{U} = (I_n \otimes \Sigma^{-1/2})U$, $\tilde{T}_d = (I_n \otimes \Sigma^{-1/2})T_d$, $\tilde{L}_d = (I_n \otimes \Sigma^{-1/2})L_d$ and $\tilde{R}_d = (I_n \otimes \Sigma^{-1/2})R_d$. The Fisher information matrix for the direct treatment effect τ under model (2) is

$$C_d(\tau) = (\tilde{T}_d + \lambda_1 \tilde{L}_d + \lambda_2 \tilde{R}_d)' \,\mathrm{pr}^\perp(\tilde{U}|\tilde{L}_d\tau|\tilde{R}_d\tau)(\tilde{T}_d + \lambda_1 \tilde{L}_d + \lambda_2 \tilde{R}_d).$$

For notational convenience, let $M_{x,y,z} = x\tilde{T}_d + y\tilde{L}_d + z\tilde{R}_d$ for any values of x, y and z. By setting $\lambda_0 = 1$, we have

$$\begin{aligned}
C_d(\tau) &= M'_{1,\lambda_1,\lambda_2} \,\mathrm{pr}^\perp(\tilde{U}|\tilde{L}_d\tau|\tilde{R}_d\tau) M_{1,\lambda_1,\lambda_2} \\
&= M'_{1,\lambda_1,\lambda_2} \,\mathrm{pr}^\perp(\tilde{U}) M_{1,\lambda_1,\lambda_2} - M'_{1,\lambda_1,\lambda_2} \,\mathrm{pr}^\perp(\tilde{U})(\tilde{L}_d\tau|\tilde{R}_d\tau) \\
&\quad \times \bigl[(\tilde{L}_d\tau|\tilde{R}_d\tau)' \,\mathrm{pr}^\perp(\tilde{U})(\tilde{L}_d\tau|\tilde{R}_d\tau)\bigr]^- (\tilde{L}_d\tau|\tilde{R}_d\tau)' \,\mathrm{pr}^\perp(\tilde{U}) M_{1,\lambda_1,\lambda_2} \qquad (3)\\
&= \sum_{i=0}^{2}\sum_{j=0}^{2} \lambda_i\lambda_j C_{dij} - A'_d \bigl(\tau' C_{dij}\tau\bigr)^-_{1\le i,j\le 2} A_d, \\
A_d &= \Biggl(\sum_{i=0}^{2} \lambda_i C_{di1}\tau \Bigg| \sum_{i=0}^{2} \lambda_i C_{di2}\tau\Biggr)',
\end{aligned}$$

where $C_{dij} = G'_i(I_n \otimes \tilde{B})G_j$, $0 \le i, j \le 2$, with $G_0 = T_d$, $G_1 = L_d$, $G_2 = R_d$ and $\tilde{B} = \Sigma^{-1} - \Sigma^{-1}1_k 1'_k \Sigma^{-1}/1'_k \Sigma^{-1} 1_k$. In particular, if Σ is a matrix of *type-H*, that is, $\Sigma = I_k + \eta 1'_k + 1_k \eta'$ with a vector η of length k, we have $\tilde{B} = \mathrm{pr}^\perp(1_k) := B_k$ [Kushner (1997)]. Examples of type-H matrices include the identity matrices and completely symmetric matrices.

One major objective of design theorists is to find a design with maximum information matrix. Following Kiefer (1975), we shall try to find the designs which maximize $\Phi(C_d(\tau))$, where Φ satisfies the following three conditions:

(C.1) Φ is concave;
(C.2) $\Phi(S'CS) = \Phi(C)$ for any permutation matrix S;
(C.3) $\Phi(bC)$ is nondecreasing in the scalar $b > 0$.

Note that $C_d(\tau)$ depends on the true value of τ itself, and thus the choice of optimal designs. Following Kempton, Ferris and David (2001), Bailey and Kunert (2006) and Zheng (2013a), we adopt the Bayesian type criterion

$$\phi_g(d) = \int \Phi\bigl(C_d(\tau)\bigr) g(\tau)\,\mathrm{d}(\tau) = \mathbb{E}_g\bigl(\Phi\bigl(C_d(\tau)\bigr)\bigr), \qquad (4)$$

where g is the prior distribution of τ and is assumed to be exchangeable throughout the paper. A design is said to be optimal if and only if it achieves the maximum of $\phi_g(d)$ among all designs for given g, Φ, λ_1 and λ_2. Furthermore, if a design maximizes $\phi_g(d)$ for any Φ, it is also said to be *universally optimal*.

In this paper we consider four popular criteria for finding optimal designs. For a $t \times t$ matrix C with eigenvalues $0 = a_0 \le a_1 \le a_2 \le \cdots \le a_{t-1}$, define the criterion functions as

$$\Phi_A(C) = (t-1)\left(\sum_{i=1}^{t-1} a_i^{-1}\right)^{-1},$$

$$\Phi_D(C) = \left(\prod_{i=1}^{t-1} a_i\right)^{1/(t-1)},$$

$$\Phi_E(C) = a_1,$$

$$\Phi_T(C) = (t-1)^{-1}\sum_{i=1}^{t-1} a_i.$$

A design is said to be $\mathcal{A}_g$-optimal if it maximizes $\phi_g(d)$ with $\Phi = \Phi_A$ in (4). The $\mathcal{D}_g$-, $\mathcal{E}_g$- and $\mathcal{T}_g$-optimality of a design are similarly defined.

Let $\Omega_{n,k,t}$ denote the set of all possible block designs with n blocks of size k and t treatments. A design in $\Omega_{n,k,t}$ could be considered as a result of selecting n elements from the set, $\mathcal{S}$, of all possible t^k block sequences with replacement. For each $s \in \mathcal{S}$, we define the sequence proportion $p_s = n_s/n$, where n_s is the number of replications of s in the design. For given n, a design is determined by the measure $\xi = (p_s, s \in \mathcal{S})$. If $p_s > 0$, then s is a supporting sequence of ξ. In approximate design theory, we search for optimal measures in the space of $\mathcal{P} = \{\xi : \sum_{s\in\mathcal{S}} p_s = 1, p_s \ge 0\}$. If such a measure happens to fall within the subset $\mathcal{P}_n = \{\xi \in \mathcal{P} : n\xi$ is a vector of integers$\}$, then we derive an exact design which is optimal among $\Omega_{n,k,t}$.

Let C_{sij} be the matrix C_{dij} when the design d is degenerated to a single sequence s for $0 \le i, j \le 2$. Then we have $C_{dij} = n\sum_{s\in\mathcal{S}} p_s C_{sij}$. By equation (3), we have

$$\begin{aligned}
&C_d(\tau) = nC_\xi(\tau),\\
&C_\xi(\tau) = \sum_{i=0}^{2}\sum_{j=0}^{2}\lambda_i\lambda_j C_{\xi ij} - A'_\xi\left(\tau' C_{\xi ij}\tau\right)^-_{1\le i,j\le 2} A_\xi,\\
&C_{\xi ij} = \sum_{s\in\mathcal{S}} p_s C_{sij},\\
&A_\xi = \left(\sum_{i=0}^{2}\lambda_i C_{\xi i1}\tau \,\middle|\, \sum_{i=0}^{2}\lambda_i C_{\xi i2}\tau\right)'.
\end{aligned} \tag{5}$$

Note that $C_\xi(\tau)$ is independent of n. Here we call $C_\xi(\tau)$ the information matrix of the measure ξ. Furthermore, by noting that the four criterion functions satisfy $\Phi(nC) = n\Phi(C)$, we have

$$\begin{aligned} \phi_g(d) &= n\phi_g(\xi), \\ \phi_g(\xi) &= \int \Phi\big(C_\xi(\tau)\big)g(\tau)\,\mathrm{d}(\tau). \end{aligned} \tag{6}$$

Equation (6) indicates that the number of blocks n is irrelevant to the search of approximate optimal designs. In the sequel, we shall focus on finding the optimal measures which maximize $\phi_g(\xi)$ among $\mathcal{P}$.

Let $\mathcal{O}$ denote the set of all $t!$ permutation operators on $\{1, 2, \dots, t\}$. For any $\sigma \in \mathcal{O}$ and $s = (t_1, \dots, t_k)$ with $1 \le t_i \le t$, define $\sigma s = (\sigma(t_1), \dots, \sigma(t_k))$. A measure is said to be *symmetric* if it is invariant under treatment relabeling, that is, $\sigma\xi = \xi$ for all $\sigma \in \mathcal{O}$, where $\sigma\xi = (p_{\sigma^{-1}s}, s \in \mathcal{S})$. By adopting similar arguments to Corollary 1 in Zheng (2013a), we get the following result.

PROPOSITION 1. *In approximate design theory, given any values of* λ_1 *and* λ_2, *and the exchangeable prior distribution* g *of* τ, *for any measure* ξ *there exists a symmetric measure, say* ξ^*, *such that*

$$\phi_g(\xi) \le \phi_g(\xi^*).$$

Proposition 1 indicates that an optimal measure in the subclass of symmetric measures is automatically optimal among $\mathcal{P}$. The merit of such a result is that the form of the information matrix for a symmetric measure is usually feasible to be calculated explicitly. In fact there is a larger subclass of measures with the same convenience. We say a measure is *pseudo symmetric* if $C_{\xi ij}$, $0 \le i, j \le 2$ are all completely symmetric. A symmetric measure is also pseudo symmetric [Kushner (1997)]. It is easy to verify that the column and row sums of $C_{\xi ij}$'s are all zero. Hence, for any pseudo symmetric measure we have $C_{\xi ij} = c_{\xi ij} B_t/(t-1)$, $0 \le i, j \le 2$, where $c_{\xi ij} = \operatorname{tr}(C_{\xi ij})$. Now let $\ell = (1, \lambda_1, \lambda_2)'$, $V_\xi = (c_{\xi ij})_{0 \le i, j \le 2}$, $Q_\xi = (c_{\xi ij})_{1 \le i, j \le 2}$ and

$$q_\xi^* = c_{\xi 00} - (\,c_{\xi 01} \quad c_{\xi 02}\,)\, Q_\xi^- \begin{pmatrix} c_{\xi 10} \\ c_{\xi 20} \end{pmatrix}. \tag{7}$$

PROPOSITION 2. *For a pseudo symmetric measure* ξ, *the information matrix* $C_\xi(\tau)$ *has eigenvalues of* 0, $(t-1)^{-1}q_\xi^*$ *and* $(t-1)^{-1}\ell' V_\xi \ell$ *with multiplicities of* 1, 1 *and* $t-2$, *respectively. Moreover we have* $q_\xi^* \le \ell' V_\xi \ell$.

PROOF. Due to $1_t'\tau = 0$, we have $B_t\tau = \tau$ and $\tau' C_{\xi ij}\tau = c_{\xi ij}\tau'\tau/(t-1)$. In view of (5), we obtain

$$(t-1)C_\xi(\tau) = \sum_{i=0}^{2}\sum_{j=0}^{2} \lambda_i\lambda_j c_{\xi ij} B_t - a\big(\tau'\tau\big)^{-1}\tau\tau',$$

$$a = \left(\sum_{i=0}^{2} \lambda_i c_{\xi i1} \middle| \sum_{i=0}^{2} \lambda_i c_{\xi i2}\right) Q_\xi^- \begin{pmatrix} \sum_{j=0}^{2} \lambda_j c_{\xi 1j} \\ \sum_{j=0}^{2} \lambda_j c_{\xi 2j} \end{pmatrix}.$$

Let $\{x_1, \dots, x_{t-2}\}$ be the orthogonal basis that is orthogonal to both 1_t and τ. Then $\{1_t, \tau, x_1, \dots, x_{t-2}\}$ forms the eigenvectors of $C_\xi(\tau)$. The corresponding eigenvalues are 0, $(t-1)^{-1}(\sum_{i=0}^{2}\sum_{j=0}^{2}\lambda_i\lambda_j c_{\xi ij} - a)$ and $(t-1)^{-1}\sum_{i=0}^{2}\sum_{j=0}^{2}\lambda_i\lambda_j c_{\xi ij}$ with multiplicities of 1, 1 and $t-2$, respectively. The proof is concluded in view of

$$\ell' V_\xi \ell = \sum_{i=0}^{2}\sum_{j=0}^{2} \lambda_i \lambda_j c_{\xi ij},$$

$$a = \ell' \begin{pmatrix} c_{\xi 01} & c_{\xi 02} \\ c_{\xi 11} & c_{\xi 12} \\ c_{\xi 21} & c_{\xi 22} \end{pmatrix} Q_\xi^- \begin{pmatrix} c_{\xi 01} & c_{\xi 11} & c_{\xi 21} \\ c_{\xi 02} & c_{\xi 12} & c_{\xi 22} \end{pmatrix} \ell \geq 0$$

and (7). $\square$

By Proposition 2, it is seen that $\phi_g(\xi) = \Phi(C_\xi(\tau))$ for any pseudo symmetric measure under the four criterion functions. Hence g is irrelevant to the determination of optimal pseudo symmetric measures for the four criteria.

LEMMA 1. *Except for measures with each supporting sequence consisting of only one treatment, we have* $c_{\xi ii} > 0$ *for* $i = 0, 1, 2$. *If* $\det(Q_\xi) > 0$, *then* $q_\xi^* = \det(V_\xi)/\det(Q_\xi)$, *where* $\det(\cdot)$ *means the determinant of a matrix. Otherwise,* $q_\xi^* = c_{\xi 00} - c_{\xi 01}^2/c_{\xi 11} = c_{\xi 00} - c_{\xi 02}^2/c_{\xi 22}$.

PROOF. Note that $\tilde{B}$ is nonnegative definite. So $c_{\xi 00} = \sum_{s\in\mathcal{S}} p_s \operatorname{tr}(T_s'\tilde{B}T_s) \geq 0$, where T_s is the matrix T_d when d is degenerated to a single sequence s. If $c_{\xi 00} = 0$, we have $T_s'\tilde{B}T_s = 0$ and thus $\tilde{B}T_s = 0$ for any supporting sequence s. It is known that $\tilde{B}x = 0$ if and only if x is a multiple of 1_k [Kushner (1997)]. This is only possible when each supporting sequence repeats the same treatment throughout the k plots. For $c_{\xi 11}$ and $c_{\xi 22}$, we have the similar arguments. The rest of the lemma follows by straightforward calculations. $\square$

From the proof of Lemma 1, we know $V_\xi = 0$ if each supporting sequence of ξ consists of only one treatment. There is no information gathered from such measures regarding τ, and hence it is impossible to be optimal. In the subsequent arguments, we neglect such measures by default.

Define the quadratic functions $q_\xi(x) = c_{\xi 00} + 2c_{\xi 01}x + c_{\xi 11}x^2$ and $x_\xi = -c_{\xi 01}/c_{\xi 11}$. Then we have $q_\xi(x_\xi) = c_{\xi 00} - c_{\xi 01}^2/c_{\xi 11}$. Let $c_{sij} = \operatorname{tr}(C_{sij})$,

$V_s = (c_{sij})_{0\le i,j\le 2}$, $Q_s = (c_{sij})_{1\le i,j\le 2}$ and $q_s(x) = c_{s00} + 2c_{s01}x + c_{s11}x^2$. Clearly, $c_{\xi ij} = \sum_{s\in\mathcal{S}} p_s c_s$, $V_\xi = \sum_{s\in\mathcal{S}} p_s V_s$, $Q_\xi = \sum_{s\in\mathcal{S}} p_s Q_s$ and $q_\xi(x) = \sum_{s\in\mathcal{S}} p_s q_s(x)$.

THEOREM 1. *In estimating τ under model* (2), *a pseudo symmetric measure ξ is optimal in the following cases. In each case*, *the p_s in ξ is positive only if s reaches the maximum therein.*

(i) *If* $\det(Q_\xi) = 0$, *then ξ is $\mathcal{A}_g$-optimal if and only if*

$$\max_{s\in\mathcal{S}} \frac{q_\xi(x_\xi)^{-2} q_s(x_\xi) + (t-2)(\ell' V_\xi \ell)^{-2}\ell' V_s \ell}{q_\xi(x_\xi)^{-1} + (t-2)(\ell' V_\xi \ell)^{-1}} = 1.$$

If $\det(V_\xi) > 0$, *then ξ is $\mathcal{A}_g$-optimal if and only if*

$$\max_{s\in\mathcal{S}} \frac{r_s \det(Q_\xi)/\det(V_\xi) + (t-2)(\ell' V_\xi \ell)^{-2}\ell' V_s \ell}{\det(Q_\xi)/\det(V_\xi) + (t-2)(\ell' V_\xi \ell)^{-1}} = 1.$$

(ii) *If* $\det(Q_\xi) = 0$, *then ξ is $\mathcal{D}_g$-optimal if and only if*

$$\max_{s\in\mathcal{S}} \left(\frac{1}{t-1} \frac{q_s(x_\xi)}{q_\xi(x_\xi)} + \frac{t-2}{t-1} \frac{\ell' V_s \ell}{\ell' V_\xi \ell} \right) = 1. \tag{8}$$

If $\det(V_\xi) > 0$, *then ξ is $\mathcal{D}_g$-optimal if and only if*

$$\max_{s\in\mathcal{S}} \left(\frac{r_s}{t-1} + \frac{t-2}{t-1} \frac{\ell' V_s \ell}{\ell' V_\xi \ell} \right) = 1. \tag{9}$$

(iii) *If* $\det(Q_\xi) = 0$, *then ξ is $\mathcal{E}_g$-optimal if and only if*

$$\max_{s\in\mathcal{S}} \frac{q_s(x_\xi)}{q_\xi(x_\xi)} = 1.$$

If $\det(V_\xi) > 0$, *then ξ is $\mathcal{E}_g$-optimal if and only if*

$$\max_{s\in\mathcal{S}} r_s = 1.$$

(iv) *If* $\det(Q_\xi) = 0$, *then ξ is $\mathcal{T}_g$-optimal if and only if*

$$\max_{s\in\mathcal{S}} \frac{q_s(x_\xi) + (t-2)\ell' V_s \ell}{q_\xi(x_\xi) + (t-2)\ell' V_\xi \ell} = 1.$$

If $\det(V_\xi) > 0$, *then ξ is $\mathcal{T}_g$-optimal if and only if*

$$\max_{s\in\mathcal{S}} \frac{r_s \det(V_\xi)/\det(Q_\xi) + (t-2)\ell' V_s \ell}{\det(V_\xi)/\det(Q_\xi) + (t-2)\ell' V_\xi \ell} = 1.$$

Here $r_s = \mathrm{tr}(V_s V_\xi^{-1}) - \mathrm{tr}(Q_s Q_\xi^{-1})$.

PROOF. Here we give only the proof for (ii) and the other three cases follow similarly. First we would like to show that

$$\det(V_\xi)/\det(Q_\xi) \le c_{\xi 00} - c_{\xi 01}^2/c_{\xi 11} \tag{10}$$

whenever $\det(Q_\xi) > 0$. To see this, consider the following inequality:

$$\begin{pmatrix} c_{\xi 00} & c_{\xi 01} \\ c_{\xi 10} & c_{\xi 11} \end{pmatrix} - \frac{1}{c_{\xi 22}} \begin{pmatrix} c_{\xi 02} \\ c_{\xi 12} \end{pmatrix} (c_{\xi 20} \quad c_{\xi 21}) \le \begin{pmatrix} c_{\xi 00} & c_{\xi 01} \\ c_{\xi 10} & c_{\xi 11} \end{pmatrix}. \tag{11}$$

The left (resp., right) hand side of (10) is the Schur complement of the left (resp., right) hand side of (11), and hence (10) follows by the nondecreasing property of Schur complement.

By the definition of $\mathcal{D}_g$-optimality, Propositions 1 and 2, Lemma 1 and inequality (10), a pseudo symmetric measure ξ with $\det(Q_\xi) = 0$ is $\mathcal{D}_g$-optimal if and only if

$$\lim_{\delta \to 0} \frac{\psi[(1-\delta)\xi + \delta\xi_0] - \psi(\xi)}{\delta} \le 0 \tag{12}$$

for any measure ξ_0, where $\psi(\xi) = \log(q_\xi(x_\xi)) + (t-2)\log(\ell' V_\xi \ell)$. Here we used the fact that $V_{\xi_0^*} = V_{\xi_0}$ and hence $\psi(\xi_0^*) = \psi(\xi_0)$, where ξ_0^* is a symmetric measure defined by $\xi_0^* = \sum_{\sigma \in \mathcal{O}} \sigma\xi_0/t!$. Direct calculations show that (12) is equivalent to

$$\frac{1}{t-1}\frac{q_{\xi_0}(x_\xi)}{q_\xi(x_\xi)} + \frac{t-2}{t-1}\frac{\ell' V_{\xi_0}\ell}{\ell' V_\xi \ell} \le 1. \tag{13}$$

By reducing ξ_0 to a degenerate measure which puts all mass on a single sequence s, we have

$$\max_{s \in \mathcal{S}} \left(\frac{1}{t-1}\frac{q_s(x_\xi)}{q_\xi(x_\xi)} + \frac{t-2}{t-1}\frac{\ell' V_s \ell}{\ell' V_\xi \ell} \right) \le 1. \tag{14}$$

By letting $\xi_0 = \xi$, we have equality in (13) and hence

$$\max_{s \in \mathcal{S}} \left(\frac{1}{t-1}\frac{q_s(x_\xi)}{q_\xi(x_\xi)} + \frac{t-2}{t-1}\frac{\ell' V_s \ell}{\ell' V_\xi \ell} \right) \ge 1 \tag{15}$$

in view of $q_\xi(x) = \sum_{s \in \mathcal{S}} p_s q_s(x)$. Combining (14) and (15), we obtain (8).

For a pseudo symmetric measure ξ with $\det(V_\xi) > 0$ and any measure ξ_0, by the continuity of $\det(Q_{(1-\delta)\xi+\delta\xi_0})$ in δ, there exists a constant $\epsilon > 0$ such that $\det(Q_{(1-\delta)\xi+\delta\xi_0}) > 0$ for all $\delta \in (-\epsilon, \epsilon)$. Hence ξ is $\mathcal{D}_g$-optimal if and only if

$$\lim_{\delta \to 0} \frac{\varphi[(1-\delta)\xi + \delta\xi_0] - \varphi(\xi)}{\delta} \le 0, \tag{16}$$

where $\varphi(\xi) = \log(\det(V_\xi)/\det(Q_\xi)) + (t-2)\log(\ell' V_\xi \ell)$. It is well known that

$$\lim_{\delta \to 0} \frac{\log(\det(V_{(1-\delta)\xi+\delta\xi_0})) - \log(\det(V_\xi))}{\delta} = \operatorname{tr}\big(V_{\xi_0} V_\xi^{-1}\big) - 3. \tag{17}$$

The same result holds for Q_ξ except that the number 3 in (17) is replaced with 2. By applying (17) to (16) we have

$$\frac{\mathrm{tr}(V_{\xi_0}V_\xi^{-1}) - \mathrm{tr}(Q_{\xi_0}Q_\xi^{-1})}{t-1} + \frac{t-2}{t-1}\frac{\ell' V_{\xi_0}\ell}{\ell' V_\xi \ell} \le 1. \tag{18}$$

Hence, for single sequences we have

$$\max_{s\in\mathcal{S}}\left(\frac{\mathrm{tr}(V_s V_\xi^{-1}) - \mathrm{tr}(Q_s Q_\xi^{-1})}{t-1} + \frac{t-2}{t-1}\frac{\ell' V_s \ell}{\ell' V_\xi \ell}\right) \le 1.$$

By taking $\xi_0 = \xi$, we have equality in (18). Also observe that conditioning on fixed ξ, the left-hand side of (18) is a linear function of the proportions in ξ_0. Hence we have

$$\max_{s\in\mathcal{S}}\left(\frac{\mathrm{tr}(V_s V_\xi^{-1}) - \mathrm{tr}(Q_s Q_\xi^{-1})}{t-1} + \frac{t-2}{t-1}\frac{\ell' V_s \ell}{\ell' V_\xi \ell}\right) \ge 1.$$

Then equation (9) follows. □

REMARK 1. Theorem 1 neglected the pseudo symmetric measures with $\det(V_\xi) = 0$ and $\det(Q_\xi) > 0$, and Theorem 1(i)–(iii) neglected those with $\det(Q_\xi) = 0$ and $q_\xi(x_\xi) = 0$. However, all these measures yield $q_\xi^* = 0$, and thus they cannot be optimal under $\mathcal{A}_g$, $\mathcal{D}_g$ and $\mathcal{E}_g$ criteria. Actually, τ is not estimable for any measure with $q_\xi^* = 0$ and hence such measures should not be adopted [Pukelsheim (1993), Chapter 3]. Note also that $\det(Q_\xi) = 0$ implies $\det(V_\xi) = 0$. Theorem 1 gives a comprehensive list of conditions to judge the optimality of a pseudo symmetric measure for estimating τ.

REMARK 2. Since we also have $q_\xi^* = c_{\xi 00} - c_{\xi 02}^2/c_{\xi 22}$ by Lemma 1, if the function $q_\xi(x)$ is replaced with $c_{\xi 00} + 2c_{\xi 02}x + c_{\xi 22}x^2$, equivalent conditions for optimal pseudo symmetric measures with respect to the four criteria could be derived similarly.

REMARK 3. For the nonproportional model (1), the information matrix of a pseudo symmetric measure has $t-1$ eigenvalues of q_ξ^* and one of 0. The measure in Theorem 1(iii) should also be universally optimal under model (1).

REMARK 4. When there is only one neighbor effect, say left, we have $\det(Q_\xi) = 0$ for all $\xi \in \mathcal{P}$. Theorem 1 reduces to equivalent conditions for the optimal crossover measures where the pre-period treatment is equal to the treatment in the last period for each subject.

3. Optimal designs for total treatment effect. In this section we study optimal measures for estimating the total treatment effect, defined by $\theta = (1 + \lambda_1 + \lambda_2)\tau$. Bailey and Druilhet (2004) commented that the total treatment effect is more important when the experiment is aimed at finding a single treatment which is recommended for use in the whole field.

When $1 + \lambda_1 + \lambda_2 = 0$, θ takes the value of constant 0 regardless the value of τ, and there is no need to carryout the experiment. In the following we assume $1 + \lambda_1 + \lambda_2 \neq 0$. By plugging $\tau = \theta/(1 + \lambda_1 + \lambda_2)$ into model (2), we have

$$Y_d = 1_{nk}\mu + U\beta + (1 + \lambda_1 + \lambda_2)^{-1}(T_d + \lambda_1 L_d + \lambda_2 R_d)\theta + \varepsilon.$$

The information matrix for θ is

$$\begin{aligned} C_d(\theta) &= (1 + \lambda_1 + \lambda_2)^{-2} \\ &\quad \times M'_{1,\lambda_1,\lambda_2} \operatorname{pr}^{\perp}(\tilde{U}|M_{-1,1+\lambda_2,-\lambda_2}\theta|M_{-1,-\lambda_1,1+\lambda_1}\theta)M_{1,\lambda_1,\lambda_2}. \end{aligned}$$

Here we used the equation $\operatorname{pr}^{\perp} EF = \operatorname{pr}^{\perp} E$ for any nonsingular matrix F. Actually, it is seen that $1 + \lambda_1 + \lambda_2 = 0$ will yield infinite $C_d(\theta)$ for any d, which implies that the covariance matrix for θ is zero. Our previous comment on this special case is justified here. In the same way that we defined $C_\xi(\tau)$ in Section 2, the information matrix of a measure ξ for θ is given by $C_\xi(\theta) = n^{-1}C_d(\theta)$, which is independent of n and can be expressed in a similar fashion to equation (5). In the spirit of Proposition 1, we shall restrict our considerations to pseudo symmetric measures.

To precede, we define $\ell_0 = (-1, 1 + \lambda_2, -\lambda_2)'$, $\ell_1 = (-1, -\lambda_1, 1 + \lambda_1)'$, $L_0 = (\ell_0, \ell_1)$ and $L_1 = (\ell, \ell_0, \ell_1)$. Let $V_{\xi,1} = L'_1 V_\xi L_1$, $Q_{\xi,1} = L'_0 V_\xi L_0$ and $q^*_{\xi,1} = \ell' V_\xi \ell - \ell' V_\xi L_0 Q^-_{\xi,1} L'_0 V_\xi \ell$.

PROPOSITION 3. *For a pseudo symmetric measure ξ, the information matrix $C_\xi(\theta)$ has eigenvalues of* 0, $(1+\lambda_1+\lambda_2)^{-2}(t-1)^{-1}q^*_{\xi,1}$ *and* $(1+\lambda_1+\lambda_2)^{-2}(t-1)^{-1}\ell' V_\xi \ell$ *with multiplicities of* 1, 1 *and* $t-2$, *respectively. Moreover we have* $q^*_{\xi,1} \leq \ell' V_\xi \ell$.

PROOF. Denote $\tilde{A}_d = (M_{-1,1+\lambda_2,-\lambda_2}\theta|M_{-1,-\lambda_1,1+\lambda_1}\theta)$. Using $1'_t\theta = 0$ and $C_{\xi ij} = c_{\xi ij} B_t/(t-1)$, we have

$$\begin{aligned} C_\xi(\theta) &= n^{-1}(1 + \lambda_1 + \lambda_2)^{-2} \\ &\qquad \times \{M'_{1,\lambda_1,\lambda_2} \operatorname{pr}^{\perp}(\tilde{U})M_{1,\lambda_1,\lambda_2} \\ &\qquad\quad - M'_{1,\lambda_1,\lambda_2} \operatorname{pr}^{\perp}(\tilde{U})\tilde{A}_d[\tilde{A}'_d \operatorname{pr}^{\perp}(\tilde{U})\tilde{A}_d]^- \tilde{A}'_d \operatorname{pr}^{\perp}(\tilde{U})M_{1,\lambda_1,\lambda_2}\} \\ &= (1 + \lambda_1 + \lambda_2)^{-2}(t-1)^{-1}[\ell' V_\xi \ell B_t - a(\theta'\theta)^{-1}\theta\theta'], \end{aligned}$$

where $a = \ell' V_\xi L_0 Q^-_{\xi,1} L'_0 V_\xi \ell$. Let $\{x_1, \dots, x_{t-2}\}$ be the orthogonal basis which is orthogonal to both 1_t and θ. Then $\{1_t, \theta, x_1, \dots, x_{t-2}\}$ forms the eigenvectors of

$C_\xi(\theta)$. The corresponding eigenvalues are 0, $(1+\lambda_1+\lambda_2)^{-2}(t-1)^{-1}q^*_{\xi,1}$ and $(1+\lambda_1+\lambda_2)^{-2}(t-1)^{-1}\ell' V_\xi \ell$ with multiplicities of 1, 1 and $t-2$, respectively. The proof is completed in view of $a \geq 0$. $\square$

Since $V_\xi = 0$ implies $V_{\xi,1} = 0$, we neglect the measures with each supporting sequence consisting of only one treatment. Note that $q^*_{\xi,1}$ is the same Schur complement of $V_{\xi,1}$ as q^*_ξ is that of V_ξ. Define $V_{s,1} = L_1' V_s L_1$ and $Q_{s,1} = L_0' V_s L_0$. Let $q_{\xi,1}(x)$ be the same function of $V_{\xi,1}$ as $q_\xi(x)$ is that of V_ξ, and $q_{s,1}(x)$ be the same function of $V_{s,1}$ as $q_s(x)$ is that of V_s. Similar arguments for Theorem 1 yield the following theorem.

THEOREM 2. *In estimating θ under model* (2), *a pseudo symmetric measure ξ with $\ell_0' V_\xi \ell_0 > 0$ is optimal in the following cases. In each case, the p_s in ξ is positive only if s reaches the maximum therein.*

(i) *If* $\det(Q_{\xi,1}) = 0$, *then ξ is $\mathcal{A}_g$-optimal if and only if*

$$\max_{s\in\mathcal{S}} \frac{q_{\xi,1}(x_{\xi,1})^{-2} q_{s,1}(x_{\xi,1}) + (t-2)(\ell' V_\xi \ell)^{-2}\ell' V_s \ell}{q_{\xi,1}(x_{\xi,1})^{-1} + (t-2)(\ell' V_\xi \ell)^{-1}} = 1.$$

If $\det(V_{\xi,1}) > 0$, *then ξ is $\mathcal{A}_g$-optimal if and only if*

$$\max_{s\in\mathcal{S}} \frac{r_{s,1}\det(Q_{\xi,1})/\det(V_{\xi,1}) + (t-2)(\ell' V_\xi \ell)^{-2}\ell' V_s \ell}{\det(Q_{\xi,1})/\det(V_{\xi,1}) + (t-2)(\ell' V_\xi \ell)^{-1}} = 1.$$

(ii) *If* $\det(Q_{\xi,1}) = 0$, *then ξ is $\mathcal{D}_g$-optimal if and only if*

$$\max_{s\in\mathcal{S}} \left(\frac{1}{t-1}\frac{q_{s,1}(x_{\xi,1})}{q_{\xi,1}(x_{\xi,1})} + \frac{t-2}{t-1}\frac{\ell' V_s \ell}{\ell' V_\xi \ell}\right) = 1.$$

If $\det(V_{\xi,1}) > 0$, *then ξ is $\mathcal{D}_g$-optimal if and only if*

$$\max_{s\in\mathcal{S}} \left(\frac{r_{s,1}}{t-1} + \frac{t-2}{t-1}\frac{\ell' V_s \ell}{\ell' V_\xi \ell}\right) = 1.$$

(iii) *If* $\det(Q_{\xi,1}) = 0$, *then ξ is $\mathcal{E}_g$-optimal if and only if*

$$\max_{s\in\mathcal{S}} \frac{q_{s,1}(x_{\xi,1})}{q_{\xi,1}(x_{\xi,1})} = 1.$$

If $\det(V_{\xi,1}) > 0$, *then ξ is $\mathcal{E}_g$-optimal if and only if*

$$\max_{s\in\mathcal{S}} r_{s,1} = 1.$$

(iv) *If* $\det(Q_{\xi,1}) = 0$, *then ξ is $\mathcal{T}_g$-optimal if and only if*

$$\max_{s\in\mathcal{S}} \frac{q_{s,1}(x_{\xi,1}) + (t-2)\ell' V_s \ell}{q_{\xi,1}(x_{\xi,1}) + (t-2)\ell' V_\xi \ell} = 1.$$

If $\det(V_{\xi,1}) > 0$, *then* ξ *is* $\mathcal{E}_g$*-optimal if and only if*

$$\max_{s\in\mathcal{S}} \frac{r_{s,1}\det(V_{\xi,1})/\det(Q_{\xi,1}) + (t-2)\ell' V_s \ell}{\det(V_{\xi,1})/\det(Q_{\xi,1}) + (t-2)\ell' V_\xi \ell} = 1.$$

Here $r_{s,1} = \operatorname{tr}(V_{s,1}V_{\xi,1}^{-1}) - \operatorname{tr}(Q_{s,1}Q_{\xi,1}^{-1})$ *and* $x_{\xi,1} = -\ell' V_\xi \ell_0/\ell_0' V_\xi \ell_0$.

REMARK 5. With arguments similar to those in Remark 1, Theorem 2 gives a comprehensive list of conditions to judge the optimality of pseudo symmetric measures with $\ell_0' V_\xi \ell_0 > 0$ for estimating θ. Equivalence conditions for the four criteria could be easily derived when $\ell_0' V_\xi \ell_0 = 0$, where we need to consider whether the cases of $\ell_1' V_\xi \ell_1$ are equal to 0 or not, separately. We omit the details due to limit of space.

REMARK 6. If the within-block covariance matrix Σ is of type-H, $\ell_0' V_\xi \ell_0 = 0$ implies $V_\xi \ell_0 = 0$, and thus $V_\xi = 0$ in view of equation (22) below. Similarly, $\ell_1' V_\xi \ell_1 = 0$ also results in $V_\xi = 0$. Therefore, except for measures with each supporting sequence consisting of only one treatment, we have $\ell_0' V_\xi \ell_0 > 0$ and $\ell_1' V_\xi \ell_1 > 0$ for any type-H matrix Σ.

The following proposition shows that the values of λ_1 and λ_2 are irrelevant to the determination of the $\mathcal{E}_g$-optimal pseudo symmetric measures for estimating θ.

PROPOSITION 4. *For any measure*, *we have*

$$q_{\xi,1}^* = (1+\lambda_1+\lambda_2)^2 \min_{x,y}\bigl[(1,x,y)\Gamma' V_\xi \Gamma(1,x,y)'\bigr],$$

where

$$\Gamma = \begin{pmatrix} 1 & -1 & -1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

PROOF. Let

$$\Lambda = (1+\lambda_1+\lambda_2)^{-1}\begin{pmatrix} 1+\lambda_1+\lambda_2 & 0 & 0 \\ \lambda_1 & 1+\lambda_2 & -\lambda_1 \\ \lambda_2 & -\lambda_2 & 1+\lambda_1 \end{pmatrix}.$$

Note that $L_1 = (\ell, \ell_0, \ell_1) = (1+\lambda_1+\lambda_2)\Gamma\Lambda$. From Proposition 3 in Kunert and Martin (2000), we have

$$\begin{aligned} q_{\xi,1}^* &= \min_{x,y}\bigl[(1,x,y)V_{\xi,1}(1,x,y)'\bigr] \\ &= (1+\lambda_1+\lambda_2)^2 \min_{x,y}\bigl[(1,x,y)\Lambda'\Gamma' V_\xi \Gamma\Lambda(1,x,y)'\bigr] \\ &= (1+\lambda_1+\lambda_2)^2 \min_{x,y}\bigl[(1,x,y)\Gamma' V_\xi \Gamma(1,x,y)'\bigr]. \end{aligned}$$

The last equality uses the fact that for all possible values of x and y, $\Lambda(1,x,y)'$ and $(1,x,y)'$ share the same vector space. □

4. Optimal designs for the undirectional model. In many applications, it is reasonable to assume $\lambda_1 = \lambda_2 := \lambda$; that is, the neighbor effects do not depend on whether they are from the left or right. See Draper and Guttman (1980), Besag and Kempton (1986) and Filipiak (2012), for examples. Under this condition, model (2) reduces to

$$Y_d = 1_{nk}\mu + U\beta + (T_d + \lambda L_d + \lambda R_d)\tau + \varepsilon. \tag{19}$$

The information matrix for τ under model (19) is

$$\tilde{C}_d(\tau) = M'_{1,\lambda,\lambda}\,\mathrm{pr}^{\perp}(\tilde{U}|M_{0,1,1}\tau)M_{1,\lambda,\lambda}.$$

The information matrix of a measure ξ for τ is $\tilde{C}_\xi(\tau) = n^{-1}\tilde{C}_d(\tau)$. Also we consider only optimal measures in the pseudo symmetric format.

Define $\ell_2 = (0, 1, 1)'$ and $L_2 = (\ell, \ell_2)$, where ℓ is defined in Section 2 with the value of $(1, \lambda, \lambda)'$ here. Let $V_{\xi,2} = L_2' V_\xi L_2$, $Q_{\xi,2} = \ell_2' V_\xi \ell_2$, $V_{s,2} = L_2' V_s L_2$, $Q_{s,2} = \ell_2' V_s \ell_2$ and $q^*_{\xi,2} = \ell' V_\xi \ell - \ell' V_\xi \ell_2 Q^-_{\xi,2} \ell_2' V_\xi \ell$. Similar to Proposition 3, we have the following.

PROPOSITION 5. *For a pseudo symmetric measure ξ, the information matrix $\tilde{C}_\xi(\tau)$ has eigenvalues of* 0, $(t-1)^{-1}q^*_{\xi,2}$ *and* $(t-1)^{-1}\ell' V_\xi \ell$ *with multiplicities of* 1, 1 *and* $t-2$, *respectively. Moreover we have* $q^*_{\xi,2} \le \ell' V_\xi \ell$.

Note that if $Q_{\xi,2} = 0$, then $q^*_{\xi,2} = \ell' V_\xi \ell = c_{\xi 00}$ and hence $\tilde{C}_\xi(\tau) = c_{\xi 00} B_t/(t-1)$. By arguments similar to those in Theorem 1, we obtain the following result.

THEOREM 3. *In estimating τ under model* (19), *a pseudo symmetric measure ξ is optimal in the following cases. In each case, the p_s in ξ is positive only if s reaches the maximum therein.*

(i) *If $Q_{\xi,2} = 0$, then ξ is universally optimal if and only if*

$$\max_{s\in\mathcal{S}} \frac{c_{s00}}{c_{\xi 00}} = 1.$$

(ii) *If* $\det(V_{\xi,2}) > 0$, *then ξ is $\mathcal{A}_g$-optimal if and only if*

$$\max_{s\in\mathcal{S}} \frac{r_{s,2} Q_{\xi,2}/\det(V_{\xi,2}) + (t-2)(\ell' V_\xi \ell)^{-2} \ell' V_s \ell}{Q_{\xi,2}/\det(V_{\xi,2}) + (t-2)(\ell' V_\xi \ell)^{-1}} = 1.$$

ξ is $\mathcal{D}_g$-optimal if and only if

$$\max_{s\in\mathcal{S}} \left(\frac{r_{s,2}}{t-1} + \frac{t-2}{t-1}\frac{\ell' V_s \ell}{\ell' V_\xi \ell}\right) = 1.$$

ξ is $\mathcal{E}_g$-optimal if and only if

$$\max_{s\in\mathcal{S}} r_{s,2} = 1.$$

ξ is $\mathcal{T}_g$-optimal if and only if

$$\max_{s\in\mathcal{S}} \frac{r_{s,2}\det(V_{\xi,2})/Q_{\xi,2} + (t-2)\ell' V_s \ell}{\det(V_{\xi,2})/Q_{\xi,2} + (t-2)\ell' V_\xi \ell} = 1.$$

(iii) *Otherwise*, *ξ is not optimal.*
Here $r_{s,2} = \operatorname{tr}(V_{s,2}V_{\xi,2}^{-1}) - Q_{s,2}Q_{\xi,2}^{-1}$.

It is easy to verify that for any measure,

$$q^*_{\xi,2} = \min_x\bigl[(1,x)V_{\xi,2}(1,x)'\bigr] = \min_x\bigl[(1,x,x)V_\xi(1,x,x)'\bigr]. \tag{20}$$

Therefore, the value of λ is irrelevant to the search of $\mathcal{E}_g$-optimal pseudo symmetric measures for estimating τ.

Next, we consider the total treatment effect θ. With the reason we explained earlier, we shall assume $1+2\lambda \neq 0$. The information matrix for θ under model (19) is

$$\tilde{C}_d(\theta) = (1+2\lambda)^{-2} M'_{1,\lambda,\lambda} \operatorname{pr}^\perp(\tilde{U}|M_{2,-1,-1}\theta) M_{1,\lambda,\lambda}.$$

For a measure ξ, its information matrix for θ is given by $\tilde{C}_\xi(\theta) = n^{-1}\tilde{C}_d(\theta)$. Now we define $\ell_3 = (2,-1,-1)'$ and $L_3 = (\ell, \ell_3)$. Let $V_{\xi,3} = L_3' V_\xi L_3$, $Q_{\xi,3} = \ell_3' V_\xi \ell_3$, $V_{s,3} = L_3' V_s L_3$, $Q_{s,3} = \ell_3' V_s \ell_3$ and $q^*_{\xi,3} = \ell' V_\xi \ell - \ell' V_\xi \ell_3 Q^-_{\xi,3} \ell_3' V_\xi \ell$. Also we have the following.

PROPOSITION 6. *For a pseudo symmetric measure ξ, the information matrix $\tilde{C}_\xi(\theta)$ has eigenvalues of* 0, $(1+2\lambda)^{-2}(t-1)^{-1}q^*_{\xi,3}$ *and* $(1+2\lambda)^{-2}(t-1)^{-1}\ell' V_\xi \ell$ *with multiplicities of* 1, 1 *and* $t-2$, *respectively. Moreover we have* $q^*_{\xi,3} \le \ell' V_\xi \ell$.

Note that if $Q_{\xi,3} = 0$, then $q^*_{\xi,3} = \ell' V_\xi \ell = (1+2\lambda)^2 c_{\xi 00}$ and hence $\tilde{C}_\xi(\theta) = c_{\xi 00} B_t/(t-1)$. Similar to Theorem 3, we obtain the following theorem.

THEOREM 4. *In estimating θ under model* (19), *a pseudo symmetric measure ξ is optimal in the following cases. In each case*, *the p_s in ξ is positive only if s reaches the maximum therein.*

(i) *If $Q_{\xi,3} = 0$, then ξ is universally optimal if and only if*

$$\max_{s\in\mathcal{S}} \frac{c_{s00}}{c_{\xi 00}} = 1.$$

(ii) *If* $\det(V_{\xi,3}) > 0$, *then ξ is $\mathcal{A}_g$-optimal if and only if*

$$\max_{s\in\mathcal{S}} \frac{r_{s,3}Q_{\xi,3}/\det(V_{\xi,3}) + (t-2)(\ell' V_\xi \ell)^{-2}\ell' V_s \ell}{Q_{\xi,3}/\det(V_{\xi,3}) + (t-2)(\ell' V_\xi \ell)^{-1}} = 1.$$

ξ is $\mathcal{D}_g$-optimal if and only if

$$\max_{s\in\mathcal{S}}\left(\frac{r_{s,3}}{t-1}+\frac{t-2}{t-1}\frac{\ell' V_s\ell}{\ell' V_\xi\ell}\right)=1.$$

ξ is $\mathcal{E}_g$-optimal if and only if

$$\max_{s\in\mathcal{S}} r_{s,3}=1.$$

ξ is $\mathcal{T}_g$-optimal if and only if

$$\max_{s\in\mathcal{S}}\frac{r_{s,3}\det(V_{\xi,3})/Q_{\xi,3}+(t-2)\ell' V_s\ell}{\det(V_{\xi,3})/Q_{\xi,3}+(t-2)\ell' V_\xi\ell}=1.$$

(iii) *Otherwise*, ξ *is not optimal.*
Here $r_{s,3}=\operatorname{tr}(V_{s,3}V_{\xi,3}^{-1})-Q_{s,3}Q_{\xi,3}^{-1}$.

It is easy to verify that for any measure,

$$q^*_{\xi,3}=\min_x\big[(1,x)V_{\xi,3}(1,x)'\big]=(1+2\lambda)^2\min_x\big[(1,x,x)\Gamma' V_\xi\Gamma(1,x,x)'\big]. \tag{21}$$

Therefore, the value of λ is also irrelevant in the search of $\mathcal{E}_g$-optimal pseudo symmetric measures for estimating θ.

Finally, we establish the connection between optimal measures for the directional and undirectional models if the within-block covariance matrix Σ is of type-H.

LEMMA 2. *If Σ is of type-H, we have $q^*_{\xi,2}=q^*_\xi$ and $(1+2\lambda)^{-2}q^*_{\xi,3}=(1+\lambda_1+\lambda_2)^{-2}q^*_{\xi,1}$.*

PROOF. Note that $\tilde{B}=B_k$ if Σ is of type-H. For a sequence $s=(t_1,\dots,t_k)$, define $t_0=t_k$ and $t_{k+1}=t_1$. Let k_j be the frequency of treatment i appearing in s. Clearly, $\sum_{i=1}^t k_i=k$. Let $m_s=k^{-1}\sum_{i=1}^t k_i^2$, $f_s=\sum_{i=1}^k \mathbb{I}_{t_i=t_{i-1}}$, $g_s=\sum_{i=1}^k \mathbb{I}_{t_i=t_{i+1}}$ and $h_s=\sum_{i=1}^k \mathbb{I}_{t_{i-1}=t_{i+1}}$. By straightforward calculations, we have $c_{s00}=c_{s11}=c_{s22}=k-m_s$, $c_{s01}=f_s-m_s$, $c_{s02}=g_s-m_s$ and $c_{s12}=h_s-m_s$. Since $f_s=g_s$, we have

$$V_s=(c_{sij})_{0\le i,j\le 2}=\begin{pmatrix} k-m_s & f_s-m_s & f_s-m_s\\ f_s-m_s & k-m_s & h_s-m_s\\ f_s-m_s & h_s-m_s & k-m_s\end{pmatrix}. \tag{22}$$

Note that $V_s=0$ if and only if s consists of only one treatment. From Proposition 3 in Kunert and Martin (2000), we have $q^*_\xi=\min_{x,y}[(1,x,y)V_\xi(1,x,y)']$. Since $(1,x,y)V_\xi(1,x,y)'$ is convex and exchangeable in x and y by equation (22) and $V_\xi=\sum_{s\in\mathcal{S}}p_sV_s$, it can achieve the minimum at some point of $x=y$. Therefore, $q^*_\xi=\min_x(1,x,x)V_\xi(1,x,x)'=q^*_{\xi,2}$ in view of equation (20).

From Proposition 4, $q^*_{\xi,1} = (1 + \lambda_1 + \lambda_2)^2 \min_{x,y}[(1, x, y)\Gamma' V_\xi \Gamma(1, x, y)']$. By equation (22) and $V_\xi = \sum_{s\in\mathcal{S}} p_s V_s$, we know $(1, x, y)\Gamma' V_\xi \Gamma(1, x, y)'$ is convex and exchangeable in x and y. Thus it can achieve the minimum at some point of $x = y$. Then $(1 + \lambda_1 + \lambda_2)^{-2} q^*_{\xi,1} = \min_x[(1, x, x)\Gamma' V_\xi \Gamma(1, x, x)'] = (1 + 2\lambda)^{-2} q^*_{\xi,3}$ in view of equation (21). □

THEOREM 5. *If Σ is of type-H, a pseudo symmetric measure is $\mathcal{E}_g$-optimal for τ (resp., θ) under model (19) if and only if it is $\mathcal{E}_g$-optimal for τ (resp., θ) under model (2). Furthermore, if $\lambda_1 = \lambda_2 = \lambda$, the same result holds for $\mathcal{A}_g$-, $\mathcal{D}_g$- and $\mathcal{T}_g$-optimal pseudo symmetric measures.*

This theorem is readily proved by using Lemma 2 and Propositions 2, 3, 5 and 6.

5. Examples. For a sequence $s = (t_1, \dots, t_k)$, define the symmetric block of s as $\langle s\rangle = \{\sigma s : \sigma \in \mathcal{O}\}$. A symmetric block is an equivalence class, and hence $\mathcal{S}$ is partitioned into $m+1$ symmetric blocks, say $\langle s_0\rangle, \langle s_1\rangle, \dots, \langle s_m\rangle$, where s_i's are the representative sequences in their own blocks. Without loss of generality, let $\langle s_0\rangle$ be the symmetric block of sequences with identical elements. For a measure $\xi = (p_s, s \in \mathcal{S})$, let $p_{\langle s_i\rangle} = \sum_{s\in\langle s_i\rangle} p_s$ and $P_\xi = (p_{\langle s_1\rangle}, \dots, p_{\langle s_m\rangle})$. Since V_s is invariant for sequences in the same symmetric block, two pseudo symmetric measures with the same P_ξ will share the same value of $\phi_g(\xi)$. By Remark 2 in Zheng (2013a), one can derive an exact optimal design in two steps: First, find the optimal P_ξ, and then construct an exact pseudo symmetric design with that P_ξ by using some combinatory structures, such as type I orthogonal arrays [Rao (1961)]. See Azaïs, Bailey and Monod (1993) and Bailey and Druilhet (2014) for more techniques to construct exact pseudo symmetric designs.

Note that $C_{sij} = 0, 0 \le i, j \le 2$, for any $s \in \langle s_0\rangle$. Given a measure ξ with $p_{\langle s_0\rangle} > 0$, one can always obtain a measure superior to ξ by replacing all sequences in $\langle s_0\rangle$ with sequences not in the set. Therefore, the symmetric block $\langle s_0\rangle$ will be ignored in the following discusssion.

In the sequel, we will determine the optimal P_ξ under model (2) through computer search based on Theorems 1 and 2. The one for the undirectional model (19) can be determined in a similar way by using Theorems 3, 4 and 5. The general algorithm for deriving the optimal P_ξ can be obtained by small modifications of the algorithm in Zheng (2013b). For ease of illustration, we consider only $2 \le t, k \le 5$ and use the within-block covariance matrix to be of the form $\Sigma = (\mathbb{I}_{i=j} + \rho\mathbb{I}_{i-j=\pm1(\text{mod } k)})_{1\le i,j\le k}$. In the following examples, we take ρ in $\{0, -0.3, 0.3\}$. Note that $\rho = 0$ implies $\Sigma = I_k$; that is, the errors are uncorrelated. First, let λ_1 and λ_2 be nonnegative values from $[0, 1]$, and the negative case will be discussed later. All measures given below are pseudo symmetric measures.

Cases $k = 2$ and 3. When $k = 2$, the symmetric block is $\langle 12\rangle$. When $k = 3$, the symmetric block is $\langle 112\rangle$ for $t = 2$, and those are $\langle 112\rangle$ and $\langle 123\rangle$ for $t \ge 3$. By straightforward calculations, it can be verified that the second smallest eigenvalues of $C_\xi(\tau)$ and $C_\xi(\theta)$ are both zero for any measure when $k=2$ and 3. Therefore, neither τ nor θ is estimable, and the optimal measures do not exist in these cases. This phenomenon is also observed by Bailey and Druilhet (2004) and Druilhet and Tinsson (2012) for the nonproportional interference model.

Case of $k=4$. When $t=2$, the four criteria become the same one. From Propositions 2, 3 and 4, it is known that the optimality of a measure for τ or θ does not depend on the values of λ_1 and λ_2. For τ, we find that the measure with $p_{\langle 1122\rangle}=1$ is optimal for the three values of ρ. Next, consider the optimal measures for θ. If $\rho=0$, the measure with $p_{\langle 1122\rangle}=2/3$ and $p_{\langle 1212\rangle}=1/3$ is optimal. An exact pseudo symmetric design with three blocks based on it is given by

$$\begin{pmatrix} 1 & 1 & 2 & 2 \\ 1 & 1 & 2 & 2 \\ 1 & 2 & 1 & 2 \end{pmatrix}.$$

In order to implement this design in practice, one has to adopt the randomization procedure as suggested by Azaïs, Bailey and Monod (1993). If $\rho=-0.3$, the measure with $p_{\langle 1122\rangle}=0.61$ and $p_{\langle 1212\rangle}=0.39$ is optimal. If $\rho=0.3$, the measure with $p_{\langle 1122\rangle}=0.76$ and $p_{\langle 1212\rangle}=0.24$ is optimal.

When $t=3$, the measure with $p_{\langle 1123\rangle}=1$ is optimal for τ under the four criteria given all the values of λ_1, λ_2 and ρ. Consider the optimal measures for θ. If $\rho=0$, the $\mathcal{A}_g$-, $\mathcal{D}_g$- and $\mathcal{T}_g$-optimal measures vary for different values of λ_1 and λ_2. For all of them, there are two supporting symmetric blocks, that is, $\langle 1123\rangle$ and $\langle 1213\rangle$. Meanwhile, the former symmetric block dominates. The measure with $p_{\langle 1123\rangle}=2/3$ and $p_{\langle 1213\rangle}=1/3$ is $\mathcal{E}_g$-optimal. If $\rho=-0.3$ and 0.3, we observe that the supporting symmetric blocks are the same as those for $\rho=0$, except for the proportions of the supporting symmetric blocks.

When $t=4$ and 5, we find that the measure with $p_{\langle 1234\rangle}=1$ is optimal for both τ and θ under the four criteria, given all the values of λ_1, λ_2 and ρ.

Case of $k=5$. When $t=2$, for both τ and θ we have the following. The measure with $p_{\langle 11122\rangle}=0.8$ and $p_{\langle 11212\rangle}=0.2$ is optimal for $\rho=0$, the measure with $p_{\langle 11122\rangle}=0.71$ and $p_{\langle 11212\rangle}=0.29$ is optimal for $\rho=-0.3$ and the measure with $p_{\langle 11122\rangle}=0.90$ and $p_{\langle 11212\rangle}=0.10$ is optimal for $\rho=0.3$.

When $t=3$, first consider optimal measures for τ. If $\rho=0$, the optimal measures vary for different values of λ_1 and λ_2 while the supporting symmetric blocks are always $\langle 11223\rangle$ and $\langle 12123\rangle$. The proportion of $\langle 11223\rangle$ is almost one for $\mathcal{A}_g$-, $\mathcal{D}_g$- and $\mathcal{T}_g$-optimal measures and is 0.90 for the $\mathcal{E}_g$-optimal measure. If $\rho=-0.3$, the supporting symmetric blocks remain the same as those for $\rho=0$ and $\langle 11223\rangle$ still dominates. If $\rho=0.3$, the measure with $p_{\langle 11223\rangle}=1$ is optimal under the four criteria for $\lambda_1, \lambda_2 \in [0, 1]$. For θ, we have observations similar to those for τ.

When $t=4$, the supporting symmetric blocks are $\langle 11234\rangle$ and $\langle 11223\rangle$. When $t=5$, the supporting symmetric blocks are $\langle 11234\rangle$, $\langle 11223\rangle$ and $\langle 12345\rangle$. The

TABLE 1
Efficiencies of optimal measures for τ at $(k, t, \rho, \lambda_1, \lambda_2) = (5, 3, 0, 0.1, 0.2)$

$p_{\langle 11223 \rangle}$	**A**	**D**	**E**	**T**
0.98	1	0.99997	0.98817	0.99988
0.99	0.99998	1	0.98670	0.99996
0.90	0.99265	0.99213	1	0.99156
1	0.99988	0.99997	0.98496	1

optimal proportions and the dominating block may change for different values of λ_1, λ_2 and ρ.

From Theorems 1 and 2, it is seen that as t increases, the equivalent conditions for optimal measures under $\mathcal{A}_g$, $\mathcal{D}_g$ and $\mathcal{T}_g$ criteria tend to agree with each other. For example, take $k = 5$, $\rho = 0$, $\lambda_1 = 0.1$ and $\lambda_2 = 0.2$. The measure with $p_{\langle 12345 \rangle} = 1$ is optimal under the three criteria for both τ and θ when $t \geq 12$. Meanwhile, the measure with $p_{\langle 11234 \rangle} = 0.955$ and $p_{\langle 12345 \rangle} = 0.045$ is $\mathcal{E}_g$-optimal for both τ and θ as long as $t \geq 5$.

Though the four criteria do not lead to the same optimal measure in general, the optimal measure under one criterion is typically highly efficient under the other three. Here the efficiency of a measure under a criterion is defined as the ratio of $\phi_g(\xi)$ to the maximum value among all measures. For the case of $k = 5$, $t = 3$, $\rho = 0$, $\lambda_1 = 0.1$ and $\lambda_2 = 0.2$, the efficiencies of optimal measures for τ are shown in Table 1 and those for θ under the four criteria are shown in Table 2. They all have efficiencies higher than 0.97. Furthermore, from the two tables we observe that the optimal measures for τ also have high efficiencies in estimating θ since they are almost the same as those for θ.

From a practical viewpoint, the optimal proportions are sometimes too harsh for deriving exact designs. However, since the four criterion functions are continuous in the proportions, we could get a measure with good proportions in the neighborhood of the optimal one at the cost of a little efficiency. For example,

TABLE 2
Efficiencies of optimal measures for θ at $(k, t, \rho, \lambda_1, \lambda_2) = (5, 3, 0, 0.1, 0.2)$

$p_{\langle 11223 \rangle}$	**A**	**D**	**E**	**T**
0.93	1	0.99676	0.98828	0.98702
0.99	0.99556	1	0.98671	0.99787
0.90	0.99859	0.99213	1	0.97925
1	0.99307	0.99981	0.98215	1

when $k = t = 5$, $\rho = 0$, $\lambda_1 = 0.1$ and $\lambda_2 = 0.2$, the $\mathcal{A}_g$-optimal measure for τ is given by $p_{\langle 11223\rangle} = 0.06$ and $p_{\langle 12345\rangle} = 0.94$, which requires n to be a multiple of 50 at least. By rounding the proportions, we obtain a measure with $p_{\langle 12345\rangle} = 1$, which has efficiency higher than 0.99. An exact pseudo symmetric design with four blocks based on it is given by Azaïs, Bailey and Monod (1993) as

$$\begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 1 & 3 & 5 & 2 & 4 \\ 1 & 4 & 2 & 5 & 3 \\ 1 & 5 & 4 & 3 & 2 \end{pmatrix}.$$

In some occasions, the values of λ_1 and λ_2 could be negative. For example, a good fertilizer will possibly make a plant grow well so that the plant will compete with its neighbors for the sunlight, water and other resources in the soil. Suppose $\lambda_1, \lambda_2 \in [-1, 0)$. The $\mathcal{A}_g$-, $\mathcal{D}_g$- and $\mathcal{T}_g$-optimal measures found by the computer program are different from the preceding ones for $\lambda_1, \lambda_2 \in [0, 1]$ in some cases. In estimating both τ and θ, we observe the following. When $(k, t) = (4, 3)$, the supporting symmetric blocks are $\langle 1123\rangle$ and $\langle 1213\rangle$ for $\mathcal{A}_g$- and $\mathcal{D}_g$-optimal measures, and are $\langle 1212\rangle$ and $\langle 1213\rangle$ for $\mathcal{T}_g$-optimal measures. Contrarily, for $\lambda_1, \lambda_2 \in [0, 1]$, there is only one supporting symmetric block $\langle 1123\rangle$ for optimal measures in estimating τ, and the $\mathcal{T}_g$-optimal measure in estimating θ has two supporting symmetric blocks as $\langle 1123\rangle$ and $\langle 1213\rangle$. When $(k, t) = (4, 4)$, the $\mathcal{A}_g$-optimal measure is still given by $p_{\langle 1234\rangle} = 1$. The supporting symmetric blocks are $\langle 1212\rangle$, $\langle 1213\rangle$ and $\langle 1234\rangle$ for $\mathcal{D}_g$-optimal measures, and are $\langle 1212\rangle$ and $\langle 1213\rangle$ for $\mathcal{T}_g$-optimal measures. But for $\lambda_1, \lambda_2 \in [0, 1]$, there is only one supporting symmetric block $\langle 1234\rangle$ for optimal measures under the three criteria. The details for other combinations of parameters are omitted due to the limit of space.

6. Discussions. In this article, two proportional interference models are considered, in which the neighbor effects of a treatment are proportional to its direct effect. We investigate the optimal circular designs for the direct and total treatment effects. Kiefer's equivalence theorems with respect to A, D, E and T criteria are established, based on which the search of optimal designs is easy to perform. Moreover, the connection between optimal designs for the two models is built. Examples are given to illustrate these theorems for several combinations of parameters.

We now remark on directions for future work. Note that the number of distinct symmetric blocks will increase, at least geometrically, as the block size k grows. In such circumstance, it is unlikely that we could find the optimal proportions within a reasonable amount of time by using the current algorithm. Therefore, determining the forms of supporting symmetric blocks theoretically is vital to solving this problem. As a design theorist, the ultimate goal is to provide efficient or even optimal exact designs for any number of blocks. One way to achieve this is to further explore the constructions of exact pseudo symmetric designs. The other is to develop methods to build up efficient exact designs by modifying existing designs of smaller or larger size.

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