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IDENTIFICATION OF UNIVERSALLY OPTIMAL CIRCULAR DESIGNS FOR THE INTERFERENCE MODEL

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Many applications of block designs exhibit neighbor and edge effects. A popular remedy is to use the circular design coupled with the interference model. The search for optimal or efficient designs has been intensively studied in recent years. The circular neighbor balanced designs at distances 1 and 2 (CNBD2), including orthogonal array of type I (OA_I) of strength 2, are the two major designs proposed in literature for the purpose of estimating the direct treatment effects. They are shown to be optimal within some reasonable subclasses of designs. By using benchmark designs in approximate design theory, we show that CNBD2 is highly efficient among all possible designs when the error terms are homoscedastic and uncorrelated. However, when the error terms are correlated, these designs will be outperformed significantly by other designs. Note that CNBD2 fall into the special catalog of pseudo symmetric designs, and they only exist when the number of treatments is larger than the block size and the number of blocks is multiple of some constants. In this paper, we elaborate equivalent conditions for any design, pseudo symmetric or not, to be universally optimal for any size of experiment and any covariance structure of the error terms. This result is novel for circular designs and sheds light on other similar models in the search for optimal or efficient asymmetric designs.

1. Introduction. In many applications of block designs, the treatments applied to the plots exhibit neighbor effects. Relevant examples can be found in Rees (1967), Dyke and Shelley (1976), Draper and Guttman (1980), Kempton (1982), Besag and Kempton (1986), Azaïs, Onillon and Lefort-Buson (1986), Speckel et al. (1987), Bailey and Payne (1990), Hide and Read (1990), Gill (1993), Goldringer, Brabant and Kempton (1994), Connolly et al. (1995), Clarke, Baker and DePauw (2000) and David et al. (2001) among others. When each block is a single line of plots and blocks are well separated, the following interference model has been typically used for data analysis:

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

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Here, Y_{dij} is the response observed from the jth plot of block i and the subscript $d(i, j)$ denotes the treatment assigned in the same plot by the design $d \in \Omega_{k,t,n}$, where $\Omega_{k,t,n}$ represents the set of all possible designs with n blocks of size k and t treatments, and hence d is essentially a mapping: $\{1, 2, \dots, n\} \times \{1, 2, \dots, k\} \to \{1, 2, \dots, t\}$. Furthermore, μ is the general mean, β_i is the ith block effect, $\tau_{d(i,j)}$ is the direct treatment effect of treatment $d(i, j)$, $\lambda_{d(i,j-1)}$ is the neighbor effect of treatment $d(i, j-1)$ from the left neighbor and $\rho_{d(i,j+1)}$ is the neighbor effect of treatment $d(i, j+1)$ from the right neighbor. Finally, ε_{ij} is the error term with mean zero. Our interest is to find plausible designs for the purpose of estimating the direct treatment effects.

For Model (1), the terms $d(i, 0)$ and $d(i, k+1)$ have to be particularly dealt with since $1 \le j \le k$. In many practical situations, even though there are no treatments applied to the outside plots, the responses in the two ends of the block are still affected by these outside plots, for example, Bhalli et al. (1964), MacDonald and Peck (1976), Langton (1990). Such effects are said to be *edge effects*. When the edge effects are not negligible, Azaïs, Bailey and Monod (1993) adopted the idea of using guarding plots, for which treatments are applied, however, no measurement is taken. They proposed to use circular designs, that is, $d(i, 0) = d(i, k)$ and $d(i, k+1) = d(i, 1)$, and studied the construction of relevant designs and discussed their statistical properties. One type of the designs therein was defined to be circular neighbor balanced designs at distances 1 and 2 (CNBD2) by Druilhet (1999), who showed the universal optimality of CNBD2 within different subclasses of designs for different cases. Filipiak and Markiewicz (2004) showed universal optimality of type I orthogonal arrays (OA_I) of strength 2, a special type of CNBD2, among binary designs for arbitrary within-block covariance matrix. Filipiak et al. (2008) studied alternative designs for E-optimality. Circular designs for other similar models have been studied by Filipiak and Markiewicz (2003, 2005, 2007, 2012, 2014), Filipiak and Różański (2013) and Li, Zheng and Ai (2015). For the purpose of estimating the total effects, namely the summation of the direct and neighbor effects from two sides, circular designs are studied by Bailey and Druilhet (2004), Ai, Ge and Chan (2007), Ai, Yu and He (2009), Druilhet and Tinsson (2012) and Jeevitha and Santharam (2013). In particular, Filipiak and Markiewicz (2005, 2012, 2014) and Filipiak and Różański (2013) focused on the model with one side neighbour effects, while Druilhet (1999), Filipiak and Markiewicz (2003, 2004, 2007), Bailey and Druilhet (2004), Ai, Ge and Chan (2007), Ai, Yu and He (2009) and Jeevitha and Santharam (2013) considered both models with one side and two sides neighbour effects. Aldred et al. (2014) considered the construction of relevant designs.

Note that CNBD2 only exists when $t \ge k$ and n should be multiple of some particular numbers depending on t and k. Further, their optimality is conditional. In this paper, we establish the approximate design theory so as to find the optimal or highly efficient circular designs for any feasible values of k, t, n and any structure of the within-block covariance matrix. By using the optimal approximate

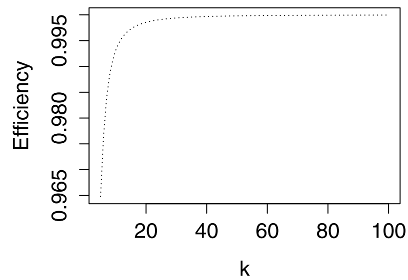

FIG. 1. *The efficiency of CNBD*2 *for* $5 \leq k \leq 100$.

designs as the benchmark, we verified that CNBD2 is highly efficient among $\Omega_{k,t,n}$ in the homoscedastic and uncorrelated case. Their performance only depends on the value of k. Particularly, when $k = 4$ or ∞, they are universally optimal. See Figure 1 for $5 \leq k \leq 100$. Yet, for the general within-block covariance matrix, their efficiency could be quite low. The theorems developed in this paper provide a powerful device for finding optimal or efficient designs in all scenarios.

In the case of the no edge effect, where $\lambda_{d(i,0)} = \rho_{d(i,k+1)} = 0$ by convention, the approximate design theory has been provided by Kunert and Martin (2000), Kunert and Mersmann (2011) and Zheng (2015). Particularly, a class of pseudo symmetric design is studied by Kunert and Martin (2000) when k is 3 or 4, which is extended by Kunert and Mersmann (2011) to $t \geq k \geq 5$. The general conditions for the optimality of designs given arbitrary k, t and the within-block covariance matrix is provided by Zheng (2015). However, the arguments of Zheng (2015) do not apply here, as detailed in Remark 1. Novel ideas are needed to tackle with this new challenge.

The rest of the paper is organized as follows. Section 2 formulates the problem into a mathematical form. Section 3 gives a necessary and sufficient condition for a pseudo symmetric measure to be universally optimal. Meanwhile, it provides some preliminary results which lay a foundation for the theorems in Section 4. The latter provides a necessary and sufficient condition for a general measure to be universally optimal. Section 5 further enhances the theoretical results to facilitate the identification of optimal designs. Section 6 investigates the performance of existing designs proposed in the literature and also provides extra examples of optimal or efficient designs for various combinations of k, t, n and within-block covariance matrix.

2. Formulation of the problem.

First, we would like to rewrite Model (1) in the following matrix form:

$$Y_d = 1_{nk}\mu + U\beta + T_d\tau + L_d\lambda + R_d\rho + \varepsilon. \tag{2}$$

Here, Y_d is the vector of responses organized block by block, while $\beta = (\beta_1, \ldots, \beta_n)'$, $\tau = (\tau_1, \ldots, \tau_t)'$, $\lambda = (\lambda_1, \ldots, \lambda_t)'$ and $\rho = (\rho_1, \ldots, \rho_t)'$. The notation $'$ means the transpose of a vector or a matrix. By observation, we have

$U = I_n \otimes 1_k$ with $\otimes$ as the Kronecker product, I_n as the identity matrix of order n, and 1_k as the vector of ones with length k. Moreover, we observe $L_d = (I_n \otimes H)T_d$ and $R_d = (I_n \otimes H')T_d$, where $H(i, j) = \mathbb{I}_{\{i-j=1 \pmod{k}\}}$ with $\mathbb{I}$ being the indicator function. We call T_d, L_d and R_d the design matrices for the direct, left neighbor and right neighbor effects, respectively.

For the error term, we would like to adopt a very general setup, that is, $\mathrm{Var}(\varepsilon) = I_n \otimes \Sigma$, with Σ being an arbitrary $k \times k$ positive definite within-block covariance matrix. The information matrix for the direct treatment effect τ in Model (2) is

$$C_d = T_d' V \mathrm{pr}^{\perp}(VU|VL_d|VR_d)VT_d, \tag{3}$$

where V is a symmetric matrix such that $V^2 = I_n \otimes \Sigma^{-1}$. The projection operator $\mathrm{pr}^{\perp}$ is defined as $\mathrm{pr}^{\perp}G = I - G(G'G)^{-}G'$ for a generic matrix G. To this end, we conclude from the following lemma that no circular design provides any information regarding the direct treatment effect when $k \leq 3$, and hence we shall assume $k \geq 4$ in the rest of the paper.

LEMMA 1. *We have $C_d = 0$ when $k \leq 3$.*

PROOF. Let N be the $n \times t$ block-treatment incident matrix so that its (i, j)th entry is given by the number of times that treatment j appears in block i. When $k = 3$, one can verify that $T_d = UN - (L_d + R_d)$. When $k = 2$, we have $T_d = UN - (L_d + R_d)/2$. The lemma is concluded by (3) and the definition of the projection operator. $\square$

For the purpose of finding optimal designs, we would like to give another representation of the information matrix:

$$\begin{aligned} C_d &= E_{d00} - E_{d01}E_{d11}^{-}E_{d10}, \\ E_{d00} &= C_{d00}, \\ E_{d10}' = E_{d01} &= \begin{pmatrix} C_{d01} & C_{d02} \end{pmatrix}, \\ E_{d11} &= \begin{pmatrix} C_{d11} & C_{d12} \\ C_{d21} & C_{d22} \end{pmatrix}, \end{aligned}$$

where $C_{dij} = G_i'(I_n \otimes \tilde{B})G_j, 0 \leq i, j \leq 2$ with $G_0 = T_d$, $G_1 = L_d$, $G_2 = R_d$ and $\tilde{B} = \Sigma^{-1} - \Sigma^{-1}J_k\Sigma^{-1}/1_k'\Sigma^{-1}1_k$ with $J_k = 1_k1_k'$. Note that $\Sigma = I_k$ implies $\tilde{B} = I_k - k^{-1}J_k = \mathrm{pr}^{\perp}(1_k)$. We denote this special matrix by B_k throughout the paper. Kushner (1997) pointed out that when Σ is of *type-H*, that is, $aI_k + b1_k' + 1_kb'$ with $a \in \mathbb{R}^+$ and $b \in \mathbb{R}^k$, we have

$$\tilde{B} = B_k/a. \tag{4}$$

Hence, the choices of designs agree with that for $\Sigma = I_k$. This special case will be particularly dealt with in Section 5.3. We allow Σ to be an arbitrary covariance matrix throughout the rest of the paper.

Note that a design in $\Omega_{k,t,n}$ can be considered as a result of selecting n elements from the set, $\mathcal{S}$, of all possible t^k block sequences with replacement. For sequence $s \in \mathcal{S}$, define the sequence proportion $p_s = n_s/n$, where n_s is the number of replications of s in the design. A design is determined by $n_s, s \in \mathcal{S}$, which is in turn determined by the *measure* $\xi = (p_s, s \in \mathcal{S})$ for any fixed n. For $0 \le i, j \le 2$, define C_{sij} to be C_{dij} and E_{sij} to be E_{dij} when the design consists of the single sequence s, and let $C_{\xi ij} = \sum_{s\in\mathcal{S}} p_s C_{sij}$ and $E_{\xi ij} = \sum_{s\in\mathcal{S}} p_s E_{sij}$. Then we have $C_{dij} = nC_{\xi ij}$ and $E_{dij} = nE_{\xi ij}$, $0 \le i, j \le 1$, $0 \le i, j \le 2$. By direct calculations, we have

$$C_d = nC_\xi, \tag{5}$$

where

$$C_\xi = E_{\xi 00} - E_{\xi 01} E_{\xi 11}^{-} E_{\xi 10}.$$

The significance of (5) is to justify the approach of the approximate design theory, where we try to find the optimal measure ξ among the set $\mathcal{P} = \{(p_s, s \in \mathcal{S}) : \sum_{s\in\mathcal{S}} p_s = 1, p_s \ge 0\}$. Following Kiefer (1975), we call a measure *universally optimal* if it maximizes $\Phi(C_\xi)$ among $\mathcal{P}$ for any function, say Φ, which 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 $b > 0$.

Such measure is optimal under criteria of A, D, E, T, etc. See Section 6 for the formal definitions of these criteria. An exact design can be constructed from ξ if and only if $\xi \in \mathcal{P}_n = \{\xi \in \mathcal{P} : n\xi \text{ is a vector of integers}\}$. If for a measure, there is at least one sequence with p_s being an irrational number, then the corresponding measure does not belong to $\mathcal{P}_n$ for any n. Hence, there is no exact design corresponding to such measure. However, by the continuity of the criterion functions with respect to the measure, a measure in $\mathcal{P}_n$ *close* enough to the optimal measure will surely be highly efficient. The distance between two measures could be defined based on (11) and (12). More specifically, we did the following: Vectorise the matrices on the two sides of (11) and (12) so that we have two vectors and then solve for measure in $\mathcal{P}_n$ which minimises the Euclidean distance of these two vectors. There could be other particular ways of doing this.

3. Pseudo symmetric measure. Let $\mathcal{G}$ be the set of all $t!$ permutations on symbols $\{1, 2, \dots, t\}$. For permutation $\sigma \in \mathcal{G}$ and sequence $s = (t_1, t_2, \dots, t_k)$ with $1 \le t_i \le t$ and $1 \le i \le k$, we define $\sigma s = (\sigma(t_1), \sigma(t_2), \dots, \sigma(t_k))$. For measure $\xi = (p_s, s \in \mathcal{S})$, we define $\sigma\xi = (p_{\sigma^{-1}s}, s \in \mathcal{S})$. A measure is said to be *symmetric* if $\sigma\xi = \xi$ for all $\sigma \in \mathcal{G}$. For sequence s, denote by $\langle s\rangle = \{\sigma s : \sigma \in \mathcal{G}\}$ the *symmetric block* generated by s. Due to the group structure of permutation, we have the partition of $\mathcal{S} = \bigcup_{i=0}^{m} \langle s_i \rangle$, where $m+1$ is the number of partitions of a set of k elements and called the Bell number in literature. For a symmetric measure, we have

$$p_s = p_{\langle s_i \rangle} / \big|\langle s_i \rangle\big| \qquad \text{for } s \in \langle s_i \rangle, 0 \le i \le m, \tag{6}$$

where $p_{\langle s_i \rangle} = \sum_{s \in \langle s_i \rangle} p_s$ and $|\langle s_i \rangle|$ is the cardinality of $\langle s_i \rangle$. By the same arguments in Kushner (1997), we have the following lemma.

LEMMA 2. *There exists a symmetric measure which is universally optimal among $\mathcal{P}$.*

Define a measure to be *pseudo symmetric* if $C_{\xi ij}, 0 \le i, j \le 2$ are all completely symmetric. It is easy to verify that a symmetric measure is also pseudo symmetric. The difference is that equation (6) does not have to hold for a general pseudo symmetric measure. Lemma 2 indicates that an optimal measure in the subclass of (pseudo) symmetric measures is automatically optimal among $\mathcal{P}$. For a pseudo symmetric measure, we have $C_{\xi ij} = c_{\xi ij} B_t/(t-1)$, $0 \le i, j \le 2$, where $c_{\xi ij} = \operatorname{tr}(C_{\xi ij})$. Correspondingly, we have the representations $E_{\xi 11} = Q_\xi \otimes B_t/(t-1)$ with $Q_\xi = (c_{\xi ij})_{1 \le i,j \le 2}$ and $E_{\xi 10} = \ell_\xi \otimes B_t/(t-1)$ with $\ell_\xi = (c_{\xi 01}, c_{\xi 02})'$. By replacing the subscript ξ in these notation by s, then the notation c_{sij}, Q_s and ℓ_s can be similarly defined for sequence s. Meanwhile, we have $c_{\xi ij} = \sum_{s \in \mathcal{S}} p_s c_{sij}$, $Q_\xi = \sum_{s \in \mathcal{S}} p_s Q_s$, $\ell_\xi = \sum_{s \in \mathcal{S}} p_s \ell_s$, $E_{s11} = Q_s \otimes B_t/(t-1)$ with $Q_s = (c_{sij})_{1 \le i,j \le 2}$ and $E_{s10} = \ell_s \otimes B_t/(t-1)$ with $\ell_s = (c_{s01}, c_{s02})'$. For a pseudo symmetric measure, one has

$$C_\xi = q_\xi^* B_t/(t-1), \tag{7}$$

where

$$q_\xi^* = c_{\xi 00} - \ell_\xi' Q_\xi^- \ell_\xi. \tag{8}$$

By Lemma 2 and (7), we have the following.

LEMMA 3. *Let $y^* = \max_{\xi \in \mathcal{P}} q_\xi^*$.* (i) *A pseudo symmetric measure is universally optimal if and only if $q_\xi^* = y^*$.* (ii) *A measure is universally optimal if and only if $C_\xi = y^* B_t/(t-1)$.*

Define the quadratic functions $q_s(x) = c_{s00} + 2\ell_s' x + x' Q_s x$ and $q_\xi(x) = c_{\xi 00} + 2\ell_\xi' x + x' Q_\xi x$ so that $q_\xi(x) = \sum_{s \in \mathcal{S}} p_s q_s(x)$, $x \in \mathbb{R}^2$. One can verify that $q_\xi^* = \min_{x \in \mathbb{R}^2} q_\xi(x)$ and the minimum is achieved if and only if $Q_\xi x + \ell_\xi = 0$. When Q_ξ is nonsingular, we have the unique solution $x^* = -Q_\xi^{-1} \ell_\xi$. Lemma 3 indicates that it is critical to find the measure whose q_ξ^* reaches the maximum of $y^* = \max_{\xi \in \mathcal{P}} \min_{x \in \mathbb{R}^2} q_\xi(x)$. Define $r(x) = \max_{s \in \mathcal{S}} q_s(x)$, which is convex due to the convexity of $q_s(x)$. Hence, it has an attainable minimum point, namely $y_* :=$

$\min_{x\in\mathbb{R}^2} r(x)$. For this purpose, we define $\mathcal{T} = \{s \in \mathcal{S} : q_s(x) = y_* \text{ for all } x \in \mathcal{X}\}$, where $\mathcal{X} = r^{-1}(y_*)$ is the collection of minimum points of $r(x)$. Let $\nabla q_s(x)$ [resp., $\nabla q_\xi(x)$] be the gradient of the bivariate function $q_s(\cdot)$ [resp. $q_\xi(\cdot)$] evaluated at point x and $\mathcal{V}_\xi = \{s : p_s > 0, s \in \mathcal{S}\}$ be the support of ξ. To facilitate the proofs in Lemma 4 and Theorem 2, we define $\mathcal{C}_{x,\mathcal{H}} = \{\sum_{s\in\mathcal{H}} w_s \nabla q_s(x) : w_s \geq 0, \sum_{s\in\mathcal{H}} w_s > 0\}$. For the empty set, $\varnothing$, we have the convention $\mathcal{C}_{x,\varnothing} = \varnothing$ for all x.

LEMMA 4. (i) $y^* = y_*$. (ii) $q_\xi^* = y^*$ *implies* $q_\xi(x) = y^*$ *for all* $x \in \mathcal{X}$ *and* $\mathcal{V}_\xi \subset \mathcal{T}$.

PROOF. Since $\max_{\xi\in\mathcal{P}} q_\xi(x) = r(x)$, we have $q_\xi^* = \min_{x\in\mathbb{R}^2} q_\xi(x) \leq \min_{x\in\mathbb{R}^2} \max_{\xi\in\mathcal{P}} q_\xi(x) = y_*$, which implies $y^* = \max_{\xi\in\mathcal{P}} q_\xi^* \leq y_*$. For $x \in \mathcal{X}$, define $\mathcal{T}_x = \{s \in \mathcal{S} : q_s(x) = y_*\}$. Now we claim $0 \in \mathcal{C}_{x,\mathcal{T}_x}$. Otherwise, there exists a vector $c \in \mathbb{R}^2$ such that $c'\nabla q_s(x) < 0$ for all $s \in \mathcal{T}_x$, which implies that $r(x)$ decreases in the direction c at point x, a contradiction to the condition of $r(x) = y_*$. As a result, there exists a measure, say ξ_0, satisfying $\nabla q_{\xi_0}(x) = 0$ and $q_{\xi_0}(x) = y_*$. Then $y^* \geq q_{\xi 0}^* = q_{\xi_0}(x) = y_*$. Hence, part (i) is concluded.

Now suppose $q_\xi^* = y^*$. For $x \in \mathcal{X}$, we have $y_* = r(x) \geq q_\xi(x) \geq q_\xi^* = y^*$, which implies $q_\xi(x) = y^*$. Suppose there exists a sequence $s \in \mathcal{V}_\xi$ and $s \notin \mathcal{T}$, then there will exist at least a point $x_0 \in \mathcal{X}$ such that $y^* = y_* > q_\xi(x_0) \geq q_\xi^*$, a contradiction. $\square$

THEOREM 1. (i) *For any measure* $\xi = (p_s : s \in \mathcal{S})$ *with* (10), *if* (9) *holds for a single point* $x \in \mathcal{X}$, *then* (9) *also holds for all* $x \in \mathcal{X}$:

$$\sum_{s\in\mathcal{T}} p_s \nabla q_s(x) = 0, \tag{9}$$

$$\sum_{s\in\mathcal{T}} p_s = 1. \tag{10}$$

Particularly, (10) *is equivalent to* $\mathcal{V}_\xi \subset \mathcal{T}$. (ii) *A pseudo symmetric measure is universally optimal if and only if* (9) *holds for an arbitrary* $x \in \mathcal{X}$ *and* (10) *holds*.

PROOF. Suppose (9) holds for an $x \in \mathcal{X}$ and (10) holds, then $q_\xi(x)$ reaches its minimum at x, and hence $q_\xi^* = q_\xi(x) = \sum_{s\in\mathcal{T}} p_s q_s(x) = \sum_{s\in\mathcal{T}} p_s y_* = y_* = y^*$. So ξ is universally optimal due to Lemma 3(i), and hence the sufficiency of part (ii). Now suppose ξ is universally optimal, then by Lemma 3(i) and Lemma 4(ii), (9) must hold for all $x \in \mathcal{X}$ and (10) must hold, in view of $\nabla q_\xi(x) = \sum_{s\in\mathcal{S}} p_s \nabla q_s(x)$. This leads to the necessity of part (ii) and hence the conclusion of part (i). $\square$

4. Linear equations. Note that $\mathcal{X}$ is determined by the values of k, t as well as the covariance matrix Σ, which motivates us to discuss optimal designs based on given forms of $\mathcal{X}$. By Corollary 1, $\mathcal{X}$ is impossible to be a two-dimensional region under any circumstance. Hence, we will derive equivalence theorems for universally optimal measures when $\mathcal{X}$ is a singleton (Theorem 2) or assembles a segment of line in $\mathbb{R}^2$ (Theorem 3). To accomplish this, we have to introduce the following two technical lemmas. For a square matrix Q, the inequality $Q > 0$ means that Q is positive definite. Let $\mathcal{X}_\xi$ be the set of minimum points of $q_\xi(x)$.

LEMMA 5. (i) *For any measure, say* ξ, *we have* $\operatorname{tr}(C_\xi) \le q_\xi^*$, *with the equality obtained by pseudo symmetric measures*. (ii) *If* ξ *is universally optimal, we have* $\mathcal{X} \subset \mathcal{X}_\xi$ *and* $q_\xi^* = y^*$.

PROOF. Part (i) follows from the same arguments as in proof of Theorem 3 in Zheng (2015). Now suppose ξ is universally optimal, from Lemma 3(ii), we have $y^* = \operatorname{tr}(C_\xi) \le q_\xi^* \le y^*$. Hence, we have $q_\xi^* = y^*$ and $q_\xi(x) \ge y^* = y_*$ for any $x \in \mathbb{R}^2$. Meanwhile we have $q_\xi(x) \le y_*$ for $x \in \mathcal{X}$ by definition. Hence, we have $q_\xi(x) = y_* = y^*$ for $x \in \mathcal{X}$. To this end, we have shown $\mathcal{X} \subset \mathcal{X}_\xi$. $\square$

LEMMA 6. $\mathcal{X}_\xi$ *can only be one of the following three types*: (i) $\mathcal{X}_\xi$ *consists of a single point as given by* $-Q_\xi^{-1}\ell_\xi$ *if* $Q_\xi > 0$; (ii) $\mathcal{X}_\xi$ *represents a straight line in* $\mathbb{R}^2$ *if* Q_ξ *is of rank* 1 *and* (iii) $\mathcal{X}_\xi = \mathbb{R}^2$ *if* $Q_\xi = 0$.

PROOF. If $Q_\xi > 0$, the minimum is reached at the unique point of $x = -Q_\xi^{-1}\ell_\xi$. By Pukelsheim (1993), ℓ_ξ belongs to the column space of Q_ξ. If Q_ξ is of rank 1, then Q_ξ is proportional to $\ell_\xi\ell_\xi'$. As a result, the minimum of $q_\xi(x)$ is obtained at point x if and only if $\ell_\xi' x$ is a constant, which defines a straight line in $\mathbb{R}^2$. If $Q_\xi = 0$, we have $\ell_\xi = 0$, and hence $\mathcal{X}_\xi = \mathbb{R}^2$. $\square$

LEMMA 7. *A universally optimal measure satisfies* (10).

This lemma is a direct result of Lemma 4(ii) and Lemma 5(ii).

COROLLARY 1. $\mathcal{X}$ *is impossible to be a two-dimensional region*.

PROOF. Now suppose $\mathcal{X}$ represents a two-dimensional region and let ξ be a universally optimal measure. By Lemma 5(ii) and Lemma 6, we end up with $Q_\xi = 0$. This equation is only possible when all sequences in ξ consist of a single treatment. This further leads to $C_\xi = 0$ and such measure is impossible to be universally optimal; hence a contradiction. $\square$

THEOREM 2. *Suppose $\mathcal{X}$ consists of a single point, say $\mathcal{X} = \{x^*\}$. A measure $\xi = (p_s, s \in \mathcal{S})$ is universally optimal among $\mathcal{P}$ if and only if*

$$\sum_{s\in\mathcal{T}} p_s\big[E_{s00} + E_{s01}\big(x^* \otimes B_t\big)\big] = y^* B_t/(t-1), \tag{11}$$

$$\sum_{s\in\mathcal{T}} p_s\big[E_{s10} + E_{s11}\big(x^* \otimes B_t\big)\big] = 0, \tag{12}$$

and (10) *hold.*

PROOF. First, we show that there exists a symmetric measure, say ξ_1, such that $Q_{\xi_1} > 0$ and the measure is universally optimal. This is obvious when $\mathcal{T}$ consists of a single symmetric block. We exclude this case in the following discussion. In the proof of Lemma 4, we have shown that $0 \in \mathcal{C}_{x^*,\mathcal{T}}$. Let $\mathcal{T}_0 = \{s \in \mathcal{T} : -\nabla q_s(x^*) \in \mathcal{C}_{x^*,\mathcal{T}\setminus\langle s\rangle}\}$. By definition, we have $0 \notin \mathcal{C}_{x^*,\mathcal{T}\setminus\mathcal{T}_0}$. Then for any $s \in \mathcal{T}_0$, there exists a universally optimal symmetric measure with $p_s > 0$. Since the convex combination of universally optimal measures should also be universally optimal. Hence, there exists a universally optimal symmetric measure which includes all sequences in $\mathcal{T}_0$. We let ξ_1 be such a measure. Now we further the discussion in three cases. *Case One*—there exists a sequence with $Q_s > 0$, then trivially we have $Q_{\xi_1} > 0$. *Case Two*—there exist two sequences $s_1, s_2 \in \mathcal{T}_0$ such that Q_{s_1} and Q_{s_2} are both of rank 1 and meanwhile ℓ_{s_1} and ℓ_{s_2} are linearly independent. Since Q_{s_1} and Q_{s_2} are proportional to $\ell_{s_1}\ell'_{s_1}$ and $\ell_{s_2}\ell'_{s_2}$, respectively, hence any convex combination of Q_{s_1} and Q_{s_2} is positive definite, so is Q_{ξ_1}. *Case Three*—for any $s \in \mathcal{T}_0$, Q_s is either equal to 0 or of rank 1. For the latter case, all ℓ_s's are proportional to each other. For all $s \in \mathcal{T}_0$, we have $q_s(x) = y_*$ for all points on the straight line pass through x^* as given by $\ell'_s(x - x^*) = 0$. If $\mathcal{T} \setminus \mathcal{T}_0$ is empty, then we come to a contradiction with the fact that $\mathcal{X}$ consists of a single value. If it is not empty, we can always find a point $x_0 \neq x^*$ on the line as given above such that for all $s \in \mathcal{T} \setminus \mathcal{T}_0$ we have $\nabla q_s(x^*)'(x_0 - x^*) < 0$ by the definition of $\mathcal{T}_0$. Then one can find small enough $\epsilon > 0$ such that $(1-\epsilon)x^* + \epsilon x_0 \in \mathcal{X}$. This leads to a contradiction with the fact that $\mathcal{X}$ consists of a single element.

Note that (10)–(12) are equivalent to (10) and

$$E_{\xi 00} + E_{\xi 01}\big(x^* \otimes B_t\big) = y^* B_t/(t-1), \tag{13}$$

$$E_{\xi 10} + E_{\xi 11}\big(x^* \otimes B_t\big) = 0. \tag{14}$$

Now we try to show the necessity of (13), (14) and (10). Suppose ξ is universally optimal; we have (10) by Lemma 7. Also, we have $C_\xi = C_{\xi_1} = y^* B_t/(t-1)$. Define $\xi_2 = (\xi + \xi_1)/2$. With $A_\xi = (E_{\xi ij})_{0\le i,j\le 1}$, we have $A_{\xi_2} = (A_\xi + A_{\xi_1})/2$, which indicates $C_{\xi_2} \ge (C_\xi + C_{\xi_1})/2 = y^* B_t/(t-1)$. The latter combined with Lemma 3(ii) yields $C_{\xi_2} = y^* B_t/(t-1)$. Hence, by similar arguments as in Kushner (1997), we have

$$E_{\xi 11}\big(E^+_{\xi 11} E_{\xi 10} - E^+_{\xi_2 11} E_{\xi_2 10}\big) = 0, \tag{15}$$

$$E_{\xi_1 11}\big(E^+_{\xi_1 11} E_{\xi_1 10} - E^+_{\xi_2 11} E_{\xi_2 10}\big) = 0, \tag{16}$$

where $^+$ means the Moore–Penrose generalized inverse. Since ξ_1 is a symmetric measure, we have $E_{\xi_1 11} = Q_{\xi_1} \otimes B_t/(t-1)$. Since $B_t C_{\xi_2 ij} = C_{\xi_2 ij}$, $0 \le i, j \le 2$, (16) is equivalent to $(Q_{\xi_1} \otimes I_t)(E^+_{\xi_1 11} E_{\xi_1 10} - E^+_{\xi_2 11} E_{\xi_2 10}) = 0$. Now due to the positive definiteness of Q_{ξ_1}, we have

$$\begin{aligned} E^+_{\xi_2 11} E_{\xi_2 10} &= E^+_{\xi_1 11} E_{\xi_1 10} \\ &= Q^{-1}_{\xi_1} \ell_{\xi_1} \otimes B_t \\ &= -x^* \otimes B_t. \end{aligned} \tag{17}$$

Here, the last equality in (17) is given by Lemma 5(ii) and Lemma 6(i). Now (14) is derived from (15) and (17). By (14), we have

$$y^* B_t/(t-1) = C_\xi = E_{\xi 00} - E_{\xi 01} E^-_{\xi 11} E_{\xi 10} \tag{18}$$

$$= E_{\xi 00} + E_{\xi 01} E^-_{\xi 11} E_{\xi 11} (x^* \otimes B_t) \tag{19}$$

$$= E_{\xi 00} + E_{\xi 01} (x^* \otimes B_t), \tag{20}$$

which is essentially (13).

The sufficiency of (13), (14) and (10) follows from (18)–(20). □

REMARK 1. In identifying optimal designs for the model with no edge effects, Zheng (2015) had the same representation of C_ξ as in (7) and (8), except that the term Q_ξ therein is guaranteed to be positive definite. Hence, the discussions of Corollary 1 and Theorem 3 are not needed in Zheng (2015).

THEOREM 3. *Suppose $\mathcal{X}$ is a segment of a line and let w be a vector parallel to the segment. Then for all $s \in \mathcal{T}$, we have*

$$E_{s01}(w \otimes I_t) = (w' \otimes I_t) E_{s10} = E_{s11}(w \otimes I_t) = (w' \otimes I_t) E_{s11} = 0. \tag{21}$$

Let x^* be an arbitrary point in $\mathcal{X}$, a measure is universally optimal if and only if (10)–(12) *hold.*

PROOF. Given an arbitrary sequence $s \in \mathcal{T}$, it can be seen that $\nabla q_s(x) = 2w'(\ell_s + Q_s x) = 0$ for all x on the segment, which indicates that Q_s is either a zero matrix or of rank 1. For the former case, we have $\ell_s = 0$ and for the latter case Q_s will be proportional to $\ell_s \ell_s'$, and thus $\nabla q_s(x)$ is proportional to ℓ_s for x on the segment. To this end, we have shown that for any $s \in \mathcal{T}$,

$$w' \ell_s = 0. \tag{22}$$

Now suppose ξ is universally optimal; we try to show (13), (14) and (10) since they are equivalent to (10)–(12). We have (10) by Lemma 7, which indicates that Q_ξ is of rank at most 1. Now we try to show

$$w' Q_\xi = 0. \tag{23}$$

To see this, $Q_\xi = 0$ automatically implies (23). Now suppose that Q_ξ is of rank 1, and hence $Q_\xi = a_\xi \ell_\xi \ell'_\xi$, where $a_\xi = \mathrm{tr}(Q_\xi)/\ell'_\xi \ell_\xi$. The latter together with (10) and (22) implies (23). Since $w' Q_\xi w = \mathrm{tr}[(w' \otimes I_t) E_{\xi 11}(w \otimes I_t)]$, then we have $(w' \otimes I_t) E_{\xi 11}(w \otimes I_t) = 0$, and hence

$$(w' \otimes I_t) E_{\xi 11} = 0. \tag{24}$$

By nonnegative definiteness of $(E_{\xi ij})_{0 \le i, j \le 1}$, we have

$$E_{\xi 01}(w \otimes I_t) = (w' \otimes I_t) E_{\xi 10} = E_{\xi 11}(w \otimes I_t) = (w' \otimes I_t) E_{\xi 11} = 0, \tag{25}$$

which is equivalent to (21) in view of (10). Now we claim that there exists a symmetric universally optimal measure, say ξ_1, with $Q_{\xi_1} \neq 0$. Otherwise, we will have $Q_s = 0$ for all $s \in \mathcal{T}$, which leads to a contradiction with the fact that $\mathcal{X}$ is a segment of a line.

Let $\xi_2 = (\xi + \xi_1)/2$. As in Theorem 2, we can derive (15) and (16). Since ξ_1 is a symmetric measure, we have $E_{\xi_1 11} = a_{\xi_1} \ell_{\xi_1} \ell'_{\xi_1} \otimes B_t/(t-1)$ with $a_{\xi_1} > 0$. Since $B_t C_{\xi_2 ij} = C_{\xi_2 ij}$, $0 \le i, j \le 2$, (16) is equivalent to $(a_{\xi_1} \ell_{\xi_1} \ell'_{\xi_1} \otimes I_t)(E^+_{\xi_1 11} E_{\xi_1 10} - E^+_{\xi_2 11} E_{\xi_2 10}) = 0$. By (23), we have $M(E^+_{\xi_1 11} E_{\xi_1 10} - E^+_{\xi_2 11} E_{\xi_2 10}) = 0$, where $M = (a_{\xi_1} \ell_{\xi_1} \ell'_{\xi_1} + w w') \otimes I_t > 0$. As a result, we have $E^+_{\xi_1 11} E_{\xi_1 10} - E^+_{\xi_2 11} E_{\xi_2 10} = 0$. By direct calculations, we have $E_{\xi_1 10} = \ell_{\xi_1} \otimes B_t/(t-1)$,

$$E^+_{\xi_1 11} = Q^+_{\xi_1} \otimes (t-1) B_t = \frac{\ell_{\xi_1} \ell'_{\xi_1}}{\mathrm{tr}(Q_{\xi_1}) \ell'_{\xi_1} \ell_{\xi_1}} \otimes (t-1) B_t,$$

and thus

$$\begin{aligned} E^+_{\xi_2 11} E_{\xi_2 10} &= E^+_{\xi_1 11} E_{\xi_1 10} \\ &= \frac{\ell_{\xi_1}}{\mathrm{tr}(Q_{\xi_1})} \otimes B_t. \end{aligned} \tag{26}$$

Now we have $q_\xi(x) = c_{\xi 00} + 2\ell'_\xi x + a_\xi (\ell'_\xi x)^2$. The minimum of $q_\xi(x)$ is attained whenever $\ell'_\xi x = -1/a_\xi$. By Lemma 5(ii), we have

$$\ell'_\xi x = -1/a_\xi \tag{27}$$

for all $x \in \mathcal{X}$. Notice that $x = -\ell_{\xi_1}/\mathrm{tr}(Q_{\xi_1})$ is a solution for (27). With $x^* \in \mathcal{X}$, we have

$$\ell_{\xi_1}/\mathrm{tr}(Q_{\xi_1}) = -x^* + bw, \tag{28}$$

where b is a scaler determined by x^*, w and ξ_1. Equation (14) is now a direct result of (15), (25), (26) and (28). Equation (13) can be shown exactly the same way as in (18)–(20). The latter shows the sufficiency of (13), (14) and (10), and hence the sufficiency of (10)–(12). $\square$

5. Identification of optimal measures. Built upon Theorems 2 and 3, here we elaborate two approaches for the identification of optimal measures. Section 5.1 provides a general strategy for the general structure of Σ. Section 5.2 is of independent interest itself in building the connection between the current interference model with a reduced one where the left and right neighbor effects are equal. More importantly, it paves the way to Section 5.3 where we give a more ready-to-use solution when Σ is of type-H.

5.1. *A direct approach.* Theorems 1–3 indicate that the identification of a universally optimal measures, either symmetric or not, boils down to that of $\mathcal{X}$ and y^*. They can be derived by applying a regular Newton–Raphson method to the convex bivariate function $r(x)$. See Bailey and Druilhet (2014) for an example where x is 5-dimensional. Alternatively, we can build an efficient algorithm based on Theorem 4 to derive an optimal pseudo symmetric measure, which further induces x^* and y^*. The proof of Theorem 4 is similar to that of Theorem 1 in Li, Zheng and Ai (2015). By Corollary 1, we only need to consider two forms of $\mathcal{X}$.

THEOREM 4. (i) *When $\mathcal{X}$ is a singleton, there exists a universally optimal pseudo symmetric measure, say ξ, with* $\det(V_\xi) > 0$, *where* $V_\xi = (c_{\xi ij})_{0\le i,j\le 2}$. *A pseudo symmetric measure with this inequality is universally optimal if and only if*

$$\max_{s\in\mathcal{S}}\bigl[\operatorname{tr}\bigl(V_s V_\xi^{-1}\bigr) - \operatorname{tr}\bigl(Q_s Q_\xi^{-1}\bigr)\bigr] = 1, \tag{29}$$

where $V_s = (c_{sij})_{0\le i,j\le 2}$. *Moreover, each sequence in $\mathcal{V}_\xi$ reaches the maximum in* (29).

(ii) *When $\mathcal{X}$ is a segment of a line, there exists a universally optimal pseudo symmetric measure, say ξ, with $c_{\xi 11} > 0$. A pseudo symmetric measure with this inequality is universally optimal if and only if*

$$\max_{s\in\mathcal{S}} \frac{\bar{q}_s(x_\xi)}{\bar{q}_\xi(x_\xi)} = 1, \tag{30}$$

where $x_\xi = -c_{\xi 01}/c_{\xi 11}$, $\bar{q}_\xi(z) = c_{\xi 00} + 2c_{\xi 01}z + c_{\xi 11}z^2$ *and* $\bar{q}_s(z) = c_{s00} + 2c_{s01}z + c_{s11}z^2$. *Moreover, each sequence in $\mathcal{V}_\xi$ reaches the maximum in* (30).

REMARK 2. Theorem 4 provides a tool to derive special types of universally optimal measures, based on which we can recover $\mathcal{X}$, y^* and $\mathcal{T}$, and hence have access to all possible universally optimal measures through Theorems 2 and 3.

5.2. *The connection with the equal neighbor effects model.* In assuming equal neighbor effects, Model (31) is also frequently adopted in many applications and the optimality results are given by Theorem 5 and Corollary 2. Interestingly, Theorem 6 elaborates its connection with Model (2), which facilitates the identification for universally optimal measures substantially when Σ is bisymmetric or even of type-H. Note that a bisymmetric matrix is a square matrix that is symmetric about both of its main diagonals. See Theorem 6, Corollary 2 and Section 5.3 for more details.

$$Y_d = 1_{nk}\mu + U\beta + T_d\tau + (L_d + R_d)\lambda + \varepsilon. \tag{31}$$

The information matrix, $\tilde{C}_d$, for τ under Model (31) is given by

$$\begin{aligned}\tilde{C}_d &= C_{d00} - \tilde{C}_{d01}\tilde{C}_{d11}^{-}\tilde{C}_{d10},\\ \tilde{C}_{d10}' &= \tilde{C}_{d01} = T_d'(I_n \otimes \tilde{B})(L_d + R_d),\\ \tilde{C}_{d11} &= (L_d + R_d)'(I_n \otimes \tilde{B})(L_d + R_d).\end{aligned}$$

It is obvious that $\tilde{C}_d/n$ only depends on the measure $\xi = (p_s, s \in \mathcal{S})$, and we denote such matrix by $\tilde{C}_\xi$. Let $\tilde{q}_s(z) = q_s((z,z)')$, $\tilde{r}(z) = \max_{s\in\mathcal{S}} \tilde{q}_s(z)$ for $z \in \mathbb{R}$, $y_0 = \min_{z\in\mathbb{R}} \tilde{r}(z)$, and $\mathcal{Z} = \{z : \tilde{r}(z) = y_0\}$ be the set of minimum points of $\tilde{r}(z)$. Note that $\tilde{r}(z)$ is convex due to the convexity of $r(x)$. Hence, $\tilde{r}(z)$ is a compact set, namely either an interval or a single point set. It can be shown that $\mathcal{T}_1 = \{s \in \mathcal{S} : \tilde{q}_s(z) = y_0 \text{ for all } z \in \mathcal{Z}\}$ contains the support set of sequences for any universally optimal measure. The proofs for the results in this section can be derived by slight modifications of the proofs in Section 4 and Section 4 of Zheng (2015), and hence will be omitted for the sake of brevity.

THEOREM 5. *For measure $\xi = (p_s, s \in \mathcal{S})$*, (i) *$\xi$ is universally optimal under Model* (31) *if and only if $\tilde{C}_\xi = y_0 B_t/(t-1)$*. (ii) *If $\mathcal{Z} = \{z^*\}$, ξ is universally optimal under Model* (31) *if and only if*

$$\sum_{s\in\mathcal{T}_1} p_s\big[C_{s00} + z^*\tilde{C}_{s01}B_t\big] = y_0 B_t/(t-1), \tag{32}$$

$$\sum_{s\in\mathcal{T}_1} p_s\big[\tilde{C}_{s10} + z^*\tilde{C}_{s11}B_t\big] = 0, \tag{33}$$

$$\sum_{s\in\mathcal{T}_1} p_s = 1. \tag{34}$$

(iii) *If $\mathcal{Z}$ is an interval, ξ is universally optimal under Model* (31) *if and only if*

$$\sum_{s\in\mathcal{T}_1} p_s C_{s00} = y_0 B_t/(t-1), \tag{35}$$

and (34) *hold.*

LEMMA 8. *Suppose Σ is bisymmetric and let $\mathcal{L} = \{z1_2 : z \in \mathbb{R}\}$ be the set of points on the line which pass through the origin with slope* 1. (i) *$\mathcal{X}$ is symmetric about $\mathcal{L}$ and $\mathcal{X} \cap \mathcal{L} = \{z1_2 : z \in \mathcal{Z}\}$. Moreover, if $\mathcal{X} = \{x^*\}$, we have $\mathcal{Z} = \{z^*\}$ and $x^* = (z^*, z^*)'$.* (ii) *$y^* = y_0$.* (iii) *$\mathcal{T} = \mathcal{T}_1$.*

REMARK 3. There is a wide range of covariance matrices which are bisymmetric. Examples include the identity matrix, the completely symmetric matrix, the AR(1) type covariance matrix, symmetric circulant matrice, etc. By Corollary 2.2 of Kushner (1997), Lemma 8 still holds if $\Sigma = \Sigma_0 + \gamma 1_k' + 1_k \gamma'$ with Σ_0 being bisymmetric. In fact, the lemma holds as long as $\tilde{B}$ is bisymmetric. When $\tilde{B}$ is not bisymmetric, empirical evidence indicates that we typically have $y^* < y_0$ and part (i) is violated. Even though we observe $\mathcal{T} = \mathcal{T}_1$ very often, however, the optimal proportions for sequences in the support would be different for the two models.

Now we are ready to illustrate the connection between the two models. In view of (5) and Lemma 3, we define the efficiencies of a design under Model (2) and criteria of A, D, E and T as follows:

$$\mathcal{E}_{\mathrm{A}}(d) = \frac{(t-1)^2}{ny^*(\sum_{i=1}^{t-1} a_i^{-1})},$$

$$\mathcal{E}_{\mathrm{D}}(d) = \frac{t-1}{ny^*}\left(\prod_{i=1}^{t-1} a_i\right)^{1/(t-1)},$$

$$\mathcal{E}_{\mathrm{E}}(d) = \frac{(t-1)a_1}{ny^*},$$

$$\mathcal{E}_{\mathrm{T}}(d) = \frac{1}{ny^*}\sum_{i=1}^{t-1} a_i,$$

where $0 = a_0 \le a_1 \le \cdots \le a_{t-1}$ are the t eigenvalues of C_d. If we replace y^* by y_0 and a_i, $0 \le i \le t-1$ by the eigenvalues of $\tilde{C}_d$, these qualities will be the definition of the efficiency of a design under Model (31) and criteria of A, D, E and T. For a sequence $s = (t_1, t_2, \ldots, t_k)$, define its dual as $s' = (t_k, t_{k-1}, \ldots, t_1)$. We also call a measure $\xi = (p_s, s \in \mathcal{S})$ to be *self-dual* if $p_{\langle s \rangle} = p_{\langle s' \rangle}$, $s \in \mathcal{S}$. Then we have the following result.

THEOREM 6. *If Σ is bisymmetric, we have the following.* (i) *For any measure, its universal optimality under Model* (2) *implies its universal optimality under Model* (31). (ii) *For a pseudo symmetric self-dual measure, its universal optimality under Model* (31) *implies its universal optimality under Model* (2). (iii) *Given any criterion function satisfying Conditions* (C.1)–(C.3), *the efficiency of any measure under Model* (31) *is at least its efficiency under Model* (2).

COROLLARY 2. (i) *If $\mathcal{Z} = \{z^*\}$, a measure with $C_{\xi 00}$, $\tilde{C}_{\xi 01}$ and $\tilde{C}_{\xi 11}$ being completely symmetric is universally optimal under Model* (31) *if and only if*

$$\sum_{s \in \mathcal{T}} p_s \frac{\partial \tilde{q}_s(z)}{\partial z}\bigg|_{z=z^*} = 0, \tag{36}$$

and (10) *hold. If* $\mathcal{Z}$ *is an interval, a measure with* $C_{\xi 00}$, $\tilde{C}_{\xi 01}$ *and* $\tilde{C}_{\xi 11}$ *being completely symmetric is universally optimal under Model* (31) *if and only if* (10) *holds.* (ii) *When* Σ *is bisymmetric, a pseudo symmetric self-dual measure is universally optimal under Model* (2) *if and only if* (36) *and* (10) *hold.*

REMARK 4. Since $\tilde{q}_s(z)$ is a univariate function, the identification of optimal measures is a lot simpler than the procedure as laid out in the first two paragraphs of this section.

5.3. *Type-H covariance matrix.* Here, we try to provide stronger results when the covariance matrix Σ is of type-H. Two such covariance matrices are the identity matrix and a completely symmetric matrix. Under this condition, recall that we have $y^* = y_0$, $\mathcal{T} = \mathcal{T}_1$ and $\{(z, z) : z \in \mathcal{Z}\} \subset \mathcal{X}$ by Lemma 8. We shall be able to apply Theorems 1–3 to find universally optimal measure under Model (2) once we know y^*, $\mathcal{T}$ and $\mathcal{Z}$. Here, we derive theoretical results of them for all $t \geq 2$ and $k \geq 4$.

For a sequence $s = (t_1, t_2, \dots, t_k)$, a shift operator δ results in $\delta s = (t_2, t_3, \dots, t_k, t_1)$. It can be verified that $C_{sij} = C_{\delta sij}$, $0 \leq i, j \leq 2$ for all $s \in \mathcal{S}$. This indicates that the two sequences contribute to the information matrix C_ξ in exactly the same way. Hence in this section or the context where Σ is of type-H, we shall redefine the symmetric block as $\langle s \rangle = \{\sigma \delta^l s : \sigma \in \mathcal{G}, 0 \leq l \leq k-1\}$. For example, $\langle (1, 1, 2, 2) \rangle = \langle (1, 2, 2, 1) \rangle$. For sequence $s = (t_1, \dots, t_k)$, define $f_{s,i} = \sum_{j=1}^k \mathbb{I}_{t_j = i}$, $\chi_s = \sum_{i=1}^t f_{s,i}^2$, $\psi_s = \sum_{i=1}^k \mathbb{I}_{t_i = t_{i-1}}$, $\kappa_s = \sum_{i=1}^k \mathbb{I}_{t_{i-1} = t_{i+1}}$ by the convention of $t_0 = t_k$ and $t_{k+1} = t_1$. By direct calculations, we have

$$
\begin{aligned}
(c_{sij})_{0 \leq i,j \leq 2} &= \begin{pmatrix} c_{s00} & \ell_\xi' \\ \ell_\xi & Q_s \end{pmatrix} \\
&= \begin{pmatrix} k - \chi_s/k & \psi_s - \chi_s/k & \psi_s - \chi_s/k \\ \psi_s - \chi_s/k & k - \chi_s/k & \kappa_s - \chi_s/k \\ \psi_s - \chi_s/k & \kappa_s - \chi_s/k & k - \chi_s/k \end{pmatrix}.
\end{aligned} \tag{37}
$$

Let $s_0 = (1_k')$, $s_1 = (1_{k/2}' \otimes (1, 2))$ and $s_2 = (1_{k/4}' \otimes (1, 1, 2, 2))$. Note that s_1 (*resp.*, s_2) only exists when k is even (*resp.*, a multiple of 4). By convention, the symmetric blocks $\langle s_1 \rangle$ and $\langle s_2 \rangle$ reduce to the empty set when they do not exist. Under this convention, the total number of distinct symmetric blocks no longer m, but $\tilde{m} = m + 1 - \mathbb{I}_{2|k} - \mathbb{I}_{4|k}$. It is indicated by Lemma 9 that $Q_s > 0$ if and only if $s \notin \langle s_0 \rangle \cup \langle s_1 \rangle \cup \langle s_2 \rangle$. Since $c_{sij} = 0$, $0 \leq i, j \leq 2$, for $s \in \langle s_0 \rangle$, such sequences make no contribution to the information of the treatment. On the other hand, the sequences in $\langle s_1 \rangle \cup \langle s_2 \rangle$ play a crucial rule in constructing optimal measures as indicated by Theorem 7(i) and (ii).

LEMMA 9. *When* Σ *is of type-H*, Q_s *is positive definite if and only if* $s \notin \langle s_0 \rangle \cup \langle s_1 \rangle \cup \langle s_2 \rangle$.

PROOF. The nonnegative definiteness of Q_s indicates $\det(Q_s) = (k-\kappa_s)(k+\kappa_s - 2\chi_s/k) \geq 0$. Further, for a sequence $s = (t_1, \ldots, t_k)$, the equality of $k - \kappa_s = 0$ implies $t_{i-1} = t_{i+1}$, $i = 1, \ldots, k$, which is only possible when $s \in \langle s_0 \rangle$ or $\langle s_1 \rangle$. The proof will be complete if one can show that the equality of

$$k + \kappa_s - 2\chi_s/k = 0 \tag{38}$$

is equivalent to $s \in \langle s_0 \rangle \cup \langle s_2 \rangle$. Note that this equality is obviously satisfied by sequences in $\langle s_0 \rangle$. In the following, we consider sequence $s \notin \langle s_0 \rangle$ which satisfies (38). It is sufficient for us to prove $s \in \langle s_2 \rangle$.

Note that (38) is equivalent to $c_{s11} + c_{s12} = 0$, which indicates $\det(V_s) = -4c_{s01}^2 c_{s00} \geq 0$. Meanwhile, since $c_{s00} > 0$ for any $s \notin \langle s_0 \rangle$, one has

$$c_{s01} = \psi_s - \chi_s/k = 0. \tag{39}$$

Now we continue the discussion in the following two cases, namely $\kappa_s = 0$ and $\kappa_s > 0$:

(i) Suppose $\kappa_s = 0$. The equality in (38) and (39) yields $\psi_s = \chi_s/k = k/2$. By the value of ψ_s, s has to be of the form $(a \otimes 1_2')$, where $a = (a_1, \ldots, a_{k/2})$ and $a_i \neq a_{i+1}$, $i = 1, \ldots, k/2$. This indicates $f_{s,i} \leq k/2$ for $i = 1, \ldots, t$ and hence $\chi_s \leq k^2/2$. The only possibility for $\chi_s = k^2/2$, that is, $\chi_s/k = k/2$, to hold is when $f_{s,i} = f_{s,j} = k/2$ for some $i \neq j$, which means $s \in \langle s_2 \rangle$.

(ii) Suppose $\kappa_s > 0$. Let $\nu_s = \sum_{i=1}^k \mathbb{I}_{t_i \neq t_{i-1}}$. Clearly, $\psi_s = k - \nu_s$. The equality in (38) and (39) yields $\psi_s = \chi_s/k$ and $\kappa_s = k - 2\nu_s > 0$. The latter indicates that $\nu_s < k/2$, which further implies $\chi_s = k\psi_s = k(k - \nu_s) > k^2/2$. If $f_{s,i} \leq k/2$ for all $i = 1, \ldots, t$, then $\chi_s \leq (k/2)^2 + (k/2)^2 = k^2/2$, which leads to a contradiction. Without loss of generality, we assume $f_{s,1} > k/2$ in the sequel.

Define $\nu_{s1} = \sum_{i=1}^k \mathbb{I}_{t_i \neq t_{i-1}, t_i = t_{i+1}}$, $\nu_{s2} = \sum_{i=1}^k \mathbb{I}_{t_i \neq t_{i-1}, t_i \neq t_{i+1}}$, $\kappa_{s1} = \sum_{i=1}^k \mathbb{I}_{t_{i-1} = t_{i+1} = t_i}$ and $\kappa_{s2} = \sum_{i=1}^k \mathbb{I}_{t_{i-1} = t_{i+1} \neq t_i}$. We have $\nu_s = \nu_{s1} + \nu_{s2}$ and $\kappa_s = \kappa_{s1} + \kappa_{s2}$. We know $\kappa_{s1} = k - \sum_{i=1}^k \mathbb{I}_{t_i \neq t_{i-1}, t_i = t_{i+1}} - \sum_{i=1}^k \mathbb{I}_{t_i = t_{i-1}, t_i \neq t_{i+1}} - \sum_{i=1}^k \mathbb{I}_{t_i \neq t_{i-1}, t_i \neq t_{i+1}}$. Moreover, it can be verified that $\sum_{i=1}^k \mathbb{I}_{t_i \neq t_{i-1}, t_i = t_{i+1}} = \sum_{i=1}^k \mathbb{I}_{t_i = t_{i-1}, t_i \neq t_{i+1}}$. So we have $\kappa_{s1} = k - 2\nu_{s1} - \nu_{s2}$. This together with $\kappa_s = k - 2\nu_s$ yields $\kappa_{s2} = -\nu_{s2} = 0$. By the latter equation, we know for every i, it holds that $t_i = t_{i-1}$ or $t_i = t_{i+1}$. This indicates that $f_{s,1} \leq k - \nu_s = \chi_s/k \leq (f_{s,1}^2 + (k - f_{s,1})^2)/k = k - 2f_{s,1} + 2f_{s,1}^2/k$, which is not possible when $k > f_{s,1} > k/2$. □

THEOREM 7. *Assume Σ is of type-H.* (i) *If $k = 4$ and $t = 2$, then $y^* = 2$, $\mathcal{Z} = [0, 1]$ and $\mathcal{T} = \langle (1, 1, 2, 2) \rangle$.*

(ii) *If $k = 4$ and $t = 3$, then $y^* = 2$, $\mathcal{Z} = \{1/2\}$ and $\mathcal{T} = \langle (1, 1, 2, 2) \rangle \cup \langle (1, 1, 2, 3) \rangle$.*

(iii) *If $k > 4$ and $2 \leq t \leq k - 2$, then $y^* = k - k/t - v(t - v)/(kt)$, $\mathcal{Z} = \{0\}$ and $\mathcal{T} = \{s : f_{s,i} = u$ or $u + 1, i = 1, \ldots, t\}$, where $k = ut + v$ and $0 \leq v < t$.*

(iv) *If* $k > 4$ *and* $t = k-1$, *then* $y^* = k - 1 - 2/k - 8/(k^3 - 2k^2 - 4k)$, $\mathcal{Z} = \{2/(k^2 - 2k - 4)\}$ *and* $\mathcal{T} = \langle(1, 1, 2, 3, \ldots, t)\rangle$.

(v) *If* $t \ge k \ge 4$, *then* $y^* = k/2 + (k^2 - 4k)(k - 2 - \sqrt{k^2 - 4k})/4$, $\mathcal{Z} = \{(k - 2 - \sqrt{k^2 - 4k})/4\}$ *and* $\mathcal{T} = \bigcup_{f_{s,i} \le 2, 1 \le i \le h \le t} \langle(1'_{f_{s,1}}, 21'_{f_{s,2}}, \ldots, h1'_{f_{s,h}})\rangle$.

PROOF. Due to (4), here we assume $\Sigma = I_k$ throughout the proof without loss of generality. By (37), we have

$$\tilde{q}_s(z) = q_{s,0} + 2q_{s,1}z + q_{s,2}z^2, \tag{40}$$

$$q_{s,0} = c_{s00} = k - \chi_s/k, \tag{41}$$

$$q_{s,1} = c_{s01} + c_{s02} = 2(\psi_s - \chi_s/k), \tag{42}$$

$$q_{s,2} = c_{s11} + 2c_{s12} + c_{s22} = 2(k + \kappa_s - 2\chi_s/k). \tag{43}$$

Parts (i) and (ii) can be obtained by exhaust enumeration of all possible symmetric blocks. For the rest three cases, let z^* be the single value in $\mathcal{Z}$, it will be sufficient to show the maximum of $\max_{s \in \mathcal{S}} \tilde{q}_s(z^*)$ is attained if and only if $s \in \mathcal{T}$ and the minimum of $\min_{z \in \mathbb{R}} \max_{s \in \mathcal{T}} \tilde{q}_s(z)$ is attained at $z = z^*$.

For part (iii), we have $\tilde{q}_s(0) = k - \chi_s/k$, which is maximized by sequence s if and only if $f_{s,i} = u$ or $u+1$, $1 \le i \le t$. Now we consider $\tilde{q}'_s(0) = 4(\psi_s - \chi_s/k)$. Let $s_3 = ((1, 2, \ldots, t - v) \otimes 1'_u, (t - v + 1, \ldots, t) \otimes 1'_{u+1})$. Then $\tilde{q}'_{s_3}(0)/4 = k - t - (k^2 + v(t - v))/(tk)$, which is trivially positive when $v = 1$ and $t = 2$ or $v = 0$ and $t \ge 2$. When $v > 0$ and $t > 2$, we have $(kt)\tilde{q}'_{s_3}(0)/4 = k(t-1)(k-t-1) - k - v(t - v) \ge k(t-2) - v(t-v) \ge (t+v)(t-2) - v(t-v) = t(t-2) + v(v-2) > 0$. Here, the first inequality relied on the condition that $t \le k-2$. To this end, we have shown $\tilde{q}'_{s_3}(0) > 0$. Now let $s_4 = (1'_u \otimes (1, 2, \ldots, t), 1, \ldots, v)$. We have $\tilde{q}'_{s_4}(0) = \mathbb{I}_{v=1} - \chi_{s_4}/k \le 1 - k/t < 0$.

For part (iv), let $s_5 = (1, 1, 2, 3, \ldots, t)$. Then $\tilde{q}_{s_5}(z) = (k - 1 - 2/k) - 8z/k + 2(k - 2 - 4/k)z^2$ and the minimum is attained at $z^* = 2/(k^2 - 2k - 4)$. Now it is sufficient to prove that $\tilde{q}_{s_5}(z^*) > \tilde{q}_s(z^*)$ for any $s \notin \langle(1, 1, 2, 3, \ldots, t)\rangle$. Note that $\tilde{q}_s(z^*) = k + 2kz^{*2} - (1 + 2z^*)^2\chi_s/k + 2z^*(2\psi_s + z^*\kappa_s)$. For given values of $f_{s,i}$, $1 \le i \le t$, χ_s is fixed and $\tilde{q}_s(z^*)$ will be an increasing function in the quantity $2\psi_s + z^*\kappa_s$. Let $\psi_{s,j} = \sum_{i=1}^k \mathbb{I}_{t_i = t_{i-1} = j}$, $\kappa_{s,j} = \sum_{i=1}^k \mathbb{I}_{t_{i-1} = t_{i+1} = j}$ for $1 \le j \le t$. Then we have $2\psi_s + z^*\kappa_s = \sum_{j=1}^t 2\psi_{s,j} + z^*\kappa_{s,j}$. Throughout all sequences with a fixed value of $f_{s,j} \ge 2$, the maximum of $\kappa_{s,j}$ is $f_{s,j} - 1$, which enforces $\psi_{s,j}$ to be zero. In this case, we have $2\psi_{s,j} + z^*\kappa_{s,j} = z^*(f_{s,j} - 1)$. On the other hand, we can attain the maximum of $\psi_{s,j}$ as $f_{s,j} - 1$ while having $\kappa_{s,j} = f_{s,j} - 2$ only one less than its maximum. As a result, we have $2\psi_{s,j} + z^*\kappa_{s,j} > f_{s,j} - 1$. To achieve the latter case, we have to place all replications of treatment j next to each other in the sequence. Hence, for fixed value of $f_{s,i}$, $1 \le i \le t$, $\tilde{q}_s(z^*)$ is maximized by sequences of the format $s = (1'_{f_{s,1}}, 21'_{f_{s,2}}, \ldots, h1'_{f_{s,h}})$, without loss of generality. Here, $h := h(s)$ is the number of distinct treatments in sequence s and $\sum_{i=1}^h f_{s,i} = k$. Among sequences of this particular format, the sequence which maximizes $\tilde{q}_s(z^*)$ should satisfy $\max_{1\le i\le h} f_{s,i} \le 2$. To see this, suppose $f_{s,1} \ge 3$, which indicates $h < t$. By decreasing $f_{s,1}$ by one and changing $f_{s,h+1}$ from 0 to 1, the quantity $\tilde{q}_s(z^*)$ is increased by the amount of

$$\begin{aligned}\Delta_s &= \frac{2(f_{s,1}-1)(1+2z^*)^2}{k} - 2z^*(2+z^*)\\ &> \frac{4}{k} - 4z^* = \frac{4(k^2-4k-4)}{k(k^2-2k-4)} > 0.\end{aligned}$$

Furthermore, suppose $f_{s,1} = f_{s,2} = 2$. By similar calculations, we can also increase the quantity $\tilde{q}_s(z^*)$ by decreasing $f_{s,2}$ by one and changing $f_{s,h+1}$ from 0 to 1, which leads to conclusion of part (iv).

For part (v), consider two sequences $s_6 = (1, 2, \dots, k)$ and $s_7 = (1, 1, 2, \dots, k-1)$. We have

$$\begin{aligned}\tilde{q}_{s_6}(z) &= k - 1 - 4z + 2(k-2)z^2,\\ \tilde{q}_{s_7}(z) &= k - \frac{k+2}{k} - \frac{8}{k}z + 2\left(k - 2\frac{k+2}{k}\right)z^2.\end{aligned}$$

Let $G(z) = 1 + (4-2k)z + 4z^2$. Observe that $\tilde{q}_{s_7}(z) = \tilde{q}_{s_6}(z) - \frac{2}{k}G(z)$ and hence $\tilde{q}_{s_6}(z)$ and $\tilde{q}_{s_7}(z)$ intersect at the two roots of $G(z)$. Note that $z^* = (k - 2 - \sqrt{k^2-4k})/4$ is the left root of $G(z)$. We are ready to prove that $\tilde{q}_{s_6}(z^*) = \max_{s\in\mathcal{S}} \tilde{q}_s(z^*)$. Obversely, $\tilde{q}_{s_6}(z^*) > \tilde{q}_{s_0}(z^*) = 0$. For any $s \notin \langle s_6\rangle \cup \langle s_0\rangle$, there must be a treatment, say 1, appearing more than once in s and another treatment, say 2, not appearing in s. Obtain a new sequence $\tilde{s}$ by replacing one appearance of 1 in s with 2, and for this plot to be relabeled, at least one of its neighbors should not be 1. In view of (37), we have

$$\begin{aligned}\tilde{q}_{\tilde{s}}(z^*) - \tilde{q}_s(z^*) = \frac{2(f_{s,1}-1)}{k} &+ 4\left[\psi_{\tilde{s}} - \psi_s + \frac{2(f_{s,1}-1)}{k}\right]z^*\\ &+ 2\left[\kappa_{\tilde{s}} - \kappa_s + \frac{4(f_{s,1}-1)}{k}\right]z^{*2}.\end{aligned}$$

First, we know that $0 \ge \psi_{\tilde{s}} - \psi_s \ge -1$ and $0 \ge \kappa_{\tilde{s}} - \kappa_s \ge -2$. In the following, we consider three cases. (a) $\psi_{\tilde{s}} = \psi_s$. Note that $z^* > z^{*2}$. We get $\tilde{q}_{\tilde{s}}(z^*) - \tilde{q}_s(z^*) \ge \frac{2}{k} + \frac{8}{k}z^* + (\frac{8}{k} - 4)z^{*2} > \frac{2}{k}G(z^*) = 0$. (b) $\psi_{\tilde{s}} = \psi_s - 1$ and $\kappa_{\tilde{s}} - \kappa_s \le -1$. This implies $f_{s,1} \ge 3$, and hence $\tilde{q}_{\tilde{s}}(z^*) - \tilde{q}_s(z^*) \ge \frac{4}{k} + (\frac{16}{k} - 4)z^* + (\frac{16}{k} - 4)z^{*2} = 4(z^* - z^{*2}) > 0$. (c) $\psi_{\tilde{s}} = \psi_s - 1$ and $\kappa_{\tilde{s}} = \kappa_s$. Note that $z^* > 0$ and $f_{s,1} \ge 2$. We get $\tilde{q}_{\tilde{s}}(z^*) - \tilde{q}_s(z^*) \ge \frac{2}{k} + 4(-1 + \frac{2}{k})z^* + \frac{8}{k}z^{*2} = \frac{2}{k}G(z^*) = 0$ with the equality attained when $f_{s,1} = 2$. Therefore, we always have $\tilde{q}_{\tilde{s}}(z^*) \ge \tilde{q}_s(z^*)$ and the equality holds if and only if $\kappa_{\tilde{s}} = \kappa_s$, $f_{s,1} = 2$ and $\psi_{\tilde{s}} - \psi_s = -1$. By replacing the repeated treatments in s with nonappearing treatments iteratively, we end up with a sequence in $\langle s_6\rangle$. Hence, we conclude that $\tilde{q}_{s_6}(z^*) \ge \tilde{q}_s(z^*)$ and the equality achieves if and only if s has the format $s = (1'_{f_{s,1}}, 21'_{f_{s,2}}, \dots, h1'_{f_{s,h}})$ with $f_{s,i} \le 2$,

$i = 1, \ldots, h$. For $k = 4$, we have $\tilde{q}'_{s_6}(z^*) = 0$. For $k \geq 5$, we have $\tilde{q}'_{s_6}(z^*) < 0$ and $\tilde{q}'_{s_7}(z^*) > 0$. The result in part (v) follows. □

REMARK 5. One of our referees has brought to our attention one important design for case (iii) of the theorem. A de Bruijn sequence, denoted by $B(t,l)$, is a cyclic sequence with t symbols for which every possible subsequence of length l appears as a sequence of consecutive characters exactly once. As a result, the length of $B(t,l)$ is $k = t^l$. Let sequence s be a $B(t,2)$ of length $k = t^2$, we have $C_{s00} = tB_t = y^* B_t/(t-1)$ and $C_{s01} = C_{s02} = 0$. Hence, a design consisting of arbitrary numbers of copies of such sequence will be universally optimal under Model (2) when Σ is of type-H. In particular, $(1,1,2,2)$ is a $B(2,2)$ and $(1,1,2,3,2,2,1,3,3)$ is a $B(3,2)$. See relevant studies in Finney and Outhwaite (1956), Magda (1980) and Aldred et al. (2014).

6. Examples. The benefit of the approximate design theory is that solutions can be provided for arbitrary structures of Σ and arbitrary configurations of k, t, n. In this section, we construct exact designs based on the theoretical results in approximate design theory as derived in this paper. Theorem 6(iii) indicates that the efficiencies of any design will be the same or higher under Model (31) than under Model (2) when Σ is bisymmetric. Hence, our focus will be Model (2). The idea of converting a measure to a design is as follows. If a measure happens to fall in $\mathcal{P}_n = \{\xi \in \mathcal{P} : n\xi \text{ is a vector of integers}\}$, we get an exact design. The universal optimality (resp., high efficiency) of the measure will imply the universal optimality (resp., high efficiency) of the design. Otherwise, we can derive efficient exact designs through the procedure of integer programming: multiply both sides of (11) and (12) by n so that the left side becomes linear combinations of n_s while the right side is irrelevant to n_s. Then minimize the Euclidean distance between the two sides of the equations with respect to n_s under practical constraints. Since the treatment labels in all the examples are single digits, we will abbreviate the representation of a sequence $s = (t_1, t_2, \ldots, t_k)$ by $s = (t_1 t_2, \ldots, t_k)$ by omitting the commas.

If d is pseudo symmetric, its efficiency under the A, D, E and T criteria are identical. The statistical performance of CNBD2 has been studied in literature. Section 6.1 enhances the relevant knowledge. Note that these designs do not exist in most cases and they are not highly efficient when Σ is not of type-H. Section 6.2 provides more examples of exact designs for various situations.

6.1. *The performance of CNBD2 and* OA_I *of strength* 2. For completeness, we give the formal definitions of CNBD2 and OA_I of strength 2. A *circular neighbour balanced design at distances 1 and 2* (CNBD2) is a design such that:

1. It is a balanced block design (in the usual sense), where each treatment is replicated for no more than once in any block.

2. For each ordered pair of distinct treatments, there exist the same number of inner plots which receive the first chosen treatment and which has the second chosen treatment as right neighbour in the circular sense.

3. For each ordered pair of distinct treatments, there exist the same number of inner plots which receive the first chosen treatment as left neighbour and which has the second chosen treatment as right neighbour in the circular sense.

A $k \times n$ array of t symbols is an *Orthogonal Array of Type I* (OA_I) of strength 2 if every set of 2 rows contains all $t(t-1)$ ordered distinct pairs of symbols for the same number of times. It can be observed that an OA_I of strength 2 is a CNBD2.

When Σ is of type-H, Druilhet (1999) showed that: (i) for $3 \le k \le t$, CNBD2 is universally optimal among designs with no treatment preceded by itself. (ii) For $t = 5$ and $t \ge 7$, a CNBD2 is universally optimal over the class of equireplicated designs in $\Omega_{t,t,t-1}$. (iii) For $t \ge 13$, a CNBD2 is universally optimal over the class of equi-replicated designs in $\Omega_{t-1,t,t}$. The catalog and the methods of constructing CNBD2s in $\Omega_{t,t,t-1}$ and $\Omega_{t-1,t,t}$ are given by Azaïs, Bailey and Monod (1993). Under Model (31), Filipiak (2012) gave a sufficient condition for a design to be universally optimal among designs with no treatment preceded by itself and showed that some designs in Rees (1967), Azaïs, Bailey and Monod (1993) and Druilhet (1999) satisfy this condition.

Note that CNBD2 is pseudo symmetric with binary sequences, that is, a sequence with $f_{s,i} \in \{0, 1\}$, $1 \le i \le t$. By Theorem 7(v), their efficiency under all four criteria as defined are given by

$$e_k = \frac{4(k^2 - 3k)/(k-2)}{2k + (k^2 - 4k)(k - 2 - \sqrt{k^2 - 4k})}$$

when Σ is of type-H. Note that the efficiency does not depend on t and $e_4 = e_\infty = 1$. it drops immediately to its minimum at $e_5 = 0.9648$, and then gradually rises up with values of $e_6 = 0.9766$, $e_7 = 0.9839$, $e_8 = 0.9884$, $e_9 = 0.9912$, etc. This pattern is visualised by Figure 1. Note that e_k is defined in the approximate design theory, so with the exact design under consideration, e_k only serves as the lower bound of the actual efficiency. For $t \ge k \ge 5$, the optimal measure as a benchmark for evaluating efficiencies involves irrational proportions, and hence the actually efficiency should be surely higher. Figure 1 indicates that CNBD2 should be highly efficient, if not optimal, when Σ is of type-H.

Filipiak and Markiewicz (2004) showed the universal optimality of OA_I of strength 2 among binary designs with arbitrary Σ. This result is actually a direct result of Lemma 2 due to the fact that OA_I of strength 2 is a pseudo symmetric design and all binary pseudo symmetric design have the same information matrix. The following example shows that the restriction to the subclass of binary designs is quite sever when Σ is not of type-H. Consider the form $\Sigma = (\mathbb{I}_{i=j} + \eta \mathbb{I}_{i-j=\pm 1 (\mathrm{mod}\ k)})_{1 \le i,j \le k}$. When $t = k = 5$ and $\eta = 0$, the efficiency of OA_I of strength 2 is 0.9648 under criteria A, D, E and T. When $\eta = 0.3$, its

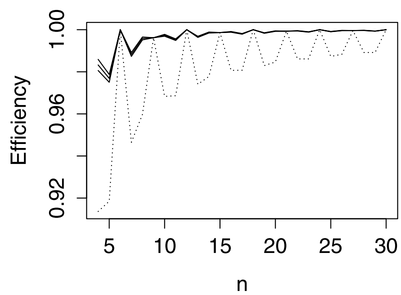

FIG. 2. *The efficiencies of exact designs for* $4 \le n \le 30$ *when* $k = 5$, $t = 3$ *and* $\eta = 0.3$. *The E-efficiency is plotted by the dashed line, while A-, D- and T-efficiencies are plotted by the solid lines.*

efficiency reduces to 0.9087. Note that OA_I of strength 2 adopted sequences from $\langle(12345)\rangle$. In fact, the dominating symmetric blocks for universally optimal measures is $\langle(11223)\rangle$ in this case. A pseudo symmetric design based on $\langle(11223)\rangle$ has the efficiency of 0.9846. For $\eta = 0.6$, the efficiency of OA_I of strength 2 further reduces to 0.8081. While the pseudo symmetric design based on $\langle(11223)\rangle$ becomes universally optimal. When η takes negative values, the efficiency of OA_I of strength 2 may become higher. For example, its efficiencies for $\eta = -0.3$ and -0.4 are 0.9940 and 0.9985, respectively. Figure 2 shows that integer programming is powerful in deriving efficient exact designs for arbitrary n. Note that the four criteria are evaluated on the same exact design for a given n.

6.2. *More examples.* Here, we mainly focus on the most interesting case when Σ is of type-H unless otherwise noticed. For type-H Σ, cases (i)–(v) below corresponds exactly to the five cases in Theorem 7. We added case (vi) to deal with Σ not of type-H. Recall for cases (i)–(v), a symmetric block is enlarged to be of form $\langle s\rangle = \{\sigma\delta^l s : \sigma \in \mathcal{G}, 0 \le l \le k-1\}$ as explained by Section 5.3.

Case (i): $(k,t) = (4,2)$. We have $\mathcal{T} = \langle(1122)\rangle$. Since $\langle(1122)\rangle = \{\delta^l(1122) : 0 \le l \le 3\}$, a design with arbitrary combinations of sequences from $\langle(1122)\rangle$ will be universally optimal, for example, $p_{(1122)} = 1$. See Remark 5 for more general results.

Case (ii): $(k,t) = (4,3)$. We have $\mathcal{T} = \langle(1123)\rangle \cup \langle(1122)\rangle$. Since $\tilde{q}_s'(z^*) = 0$ for all $s \in \mathcal{T}$, any proportion of the two symmetric blocks will yield a universally optimal design as long as it is pseudo symmetric. Particularly with $p_{\langle(1122)\rangle} = 1$, a pseudo symmetric measure is universally optimal if and only if $p_{(1122)} = p_{(2233)} = p_{(1133)} = 1/3$. An exact universally optimal design exists as long as n is a multiple of three. Let $p_1, \dots, p_6$ denote the proportions of (1123), (1132), (2213), (2231), (3312), (3321), respectively. Now for $p_{\langle(1123)\rangle} = 1$, a pseudo symmetric measure is universally optimal if and only if $p_1 = 1/6 + p_6 - p_4$, $p_2 = 1/6 + p_4 - p_6$, $p_3 = 1/3 - p_4$ and $p_5 = 1/3 - p_6$. Two such designs are given as below when $n = 6$. Here, the columns of the design present the blocks for purpose of saving space:

$$d_1 = \begin{pmatrix} 1 & 1 & 2 & 2 & 3 & 3 \\ 1 & 1 & 2 & 2 & 3 & 3 \\ 2 & 3 & 1 & 3 & 1 & 2 \\ 3 & 2 & 3 & 1 & 2 & 1 \end{pmatrix}, \qquad d_2 = \begin{pmatrix} 1 & 1 & 2 & 2 & 3 & 3 \\ 1 & 1 & 2 & 2 & 3 & 3 \\ 2 & 3 & 1 & 1 & 1 & 1 \\ 3 & 2 & 3 & 3 & 2 & 2 \end{pmatrix}.$$

Moreover, any juxtaposition of the designs as proposed so far for this case is also universally optimal. Here, we also give d_3, a universally optimal design which is not pseudo symmetric. This design is a result of the integer programming:

$$d_3 = \begin{pmatrix} 1 & 1 & 1 & 2 & 2 & 2 \\ 1 & 1 & 1 & 2 & 2 & 2 \\ 2 & 3 & 3 & 3 & 3 & 1 \\ 2 & 3 & 3 & 3 & 1 & 3 \end{pmatrix}.$$

Case (iii): $k > 4$ and $2 \le t \le k - 2$. The number of symmetric blocks in $\mathcal{T}$ may be very large for big k. To save the space, we only illustrate the case of $k = 6$ and $t = 2$. First, we have $\mathcal{T} = \langle(111222)\rangle \cup \langle(112122)\rangle \cup \langle(121212)\rangle$. For each of these blocks, sequences therein could be derived from each other by shifting. This fact coupled with Corollary 2 indicate that any design with $p_{(111222)} - p_{(112122)} - 3p_{(121212)} = 0$ is universally optimal, for example, $p_{(111222)} = p_{(112122)} = 1/2$. That means we could construct a universally optimal design with only two blocks. As pointed out by one of our referees, when $t \ge 3$ and t divides k, it is possible to construct such small size designs by using methods for building Williams squares. Examples include

$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \\ 3 & 1 & 2 \\ 3 & 1 & 2 \\ 2 & 3 & 1 \\ 1 & 2 & 3 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 1 & 2 \\ 4 & 1 \\ 2 & 3 \\ 3 & 4 \\ 3 & 4 \\ 2 & 3 \\ 4 & 1 \\ 1 & 2 \end{pmatrix}$$

for $(k, t, n) = (6, 3, 3)$ and $(k, t, n) = (8, 4, 2)$, respectively.

Case (iv): $k > 4$ and $t = k - 1$. We have $\mathcal{T} = \langle(112 \cdots t)\rangle$. One easy way is to start with an OA_I of strength 2 and duplicate the first or the last row. See d_4, for example, when $k = 5$, $t = 4$ and $n = 12$:

$$d_4 = \begin{pmatrix} 1 & 1 & 1 & 2 & 2 & 2 & 3 & 3 & 3 & 4 & 4 & 4 \\ 1 & 1 & 1 & 2 & 2 & 2 & 3 & 3 & 3 & 4 & 4 & 4 \\ 2 & 3 & 3 & 3 & 3 & 1 & 4 & 2 & 1 & 1 & 1 & 2 \\ 4 & 4 & 4 & 4 & 1 & 4 & 1 & 1 & 2 & 3 & 3 & 3 \\ 3 & 2 & 2 & 1 & 4 & 3 & 2 & 4 & 4 & 2 & 2 & 1 \end{pmatrix}.$$

Case (v)(i): $t \geq k = 4$. We have $\mathcal{T} = \langle(1122)\rangle \cup \langle(1123)\rangle \cup \langle(1234)\rangle$. Since $\tilde{q}_s'(z^*) = 0$ for all $s \in \mathcal{T}$, any proportion of the three symmetric blocks will yield a universally optimal design as long as it is pseudo symmetric. Particularly with $p_{\langle(1234)\rangle} = 1$, we see that CNBD2 is always universally optimal, which echoes the equation $e_4 = 1$ in Section 6.1. When $t = 5$ and $n = 5$, Druilhet (1999) and Filipiak (2012) only claimed that the CNBD2, d_5, is universal optimality among the designs with no treatment preceded by itself. Here, we show that d_5 is actually universally optimal among all possible designs:

$$d_5 = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 2 & 3 & 4 & 5 & 1 \\ 4 & 5 & 1 & 2 & 3 \\ 3 & 4 & 5 & 1 & 2 \end{pmatrix}.$$

By Theorems 2 and 3, we can sometimes find all possible designs, either pseudo symmetric or not. Take $(k, t) = (4, 4)$, for example. With $p_{\langle(1122)\rangle} = 1$, a design is universally optimal if and only if $p_{(1122)} = p_{(1133)} = p_{(1144)} = p_{(2233)} = p_{(2244)} = p_{(3344)} = 1/6$. The case of $p_{\langle(1123)\rangle} = 1$ is complicated. To save the space, we here give one sufficient condition: $p_{(1123)} = p_{(4421)} = p_{(4413)} = p_{(4432)} = 1/6$ and $p_{(2213)} = p_{(2231)} = p_{(3312)} = p_{(3321)} = 1/12$. With $p_{\langle(1234)\rangle} = 1$, a design is universally optimal if and only if $p_{(1234)} = p_{(1243)} = p_{(1324)} = p_{(1342)} = p_{(1423)} = p_{(1432)} = 1/6$.

Case (v)(ii): $t \geq k \geq 5$. The unique value in $\mathcal{Z}$ is irrational, and thus the optimal proportions of the support sequences are irrational numbers. An exact universally optimal design doesn't exist in this case. However, efficient exact designs can be derived through the integer programming for any n. For example, when $t = k = 5$, we have $\mathcal{T} = \langle(11223)\rangle \cup \langle(11234)\rangle \cup \langle(12345)\rangle$. When $n = 4$, our integer programming leads to the solution of d_6, which is known as 2-perfect cycle system in literature. It also appeared in Druilhet (1999) and Filipiak (2012) as CNBD2. Here, we show that this design has the efficiency of 0.9648 under all four criteria. Note that d_6 only uses sequences from $\langle(12345)\rangle$. With $n = 5$, we derive d_7 which has the efficiencies of $\mathcal{E}_{\mathrm{A}} = 0.9812$, $\mathcal{E}_{\mathrm{D}} = 0.9853$, $\mathcal{E}_{\mathrm{E}} = 0.8952$, $\mathcal{E}_{\mathrm{T}} = 0.9894$. The E-efficiency is lower due to the asymmetry of d_7:

$$d_6 = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 2 & 3 & 4 & 5 \\ 3 & 5 & 2 & 4 \\ 4 & 2 & 5 & 3 \\ 5 & 4 & 3 & 2 \end{pmatrix}, \qquad d_7 = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 1 & 2 & 3 & 4 & 5 \\ 4 & 4 & 4 & 1 & 2 \\ 3 & 5 & 5 & 3 & 3 \\ 2 & 1 & 2 & 5 & 1 \end{pmatrix}.$$

Case (vi): Σ is not of type-H. Section 6.1 shows the impact of Σ on the choice of designs. It also showcases the ability of Theorems 2 and 3 for deriving exact designs for arbitrary configurations of k, t, n and Σ. To this end, we give an efficient design when Σ is not bisymmetric. Consider $t = k = 5$, and

$$\Sigma = \begin{pmatrix} 1 & 0.2 & 0.1 & 0 & 0 \\ 0.2 & 1 & 0.2 & 0.1 & 0.1 \\ 0.1 & 0.2 & 1 & 0.2 & 0.2 \\ 0 & 0.1 & 0.2 & 1 & 0.3 \\ 0 & 0.1 & 0.2 & 0.3 & 1 \end{pmatrix}.$$

We find that the pseudo symmetric measure with $p_{\langle(12231)\rangle} = 0.245$ and $p_{\langle(12341)\rangle} = 0.755$ is universally optimal under Model (2), while the efficiency of OA_I of strength 2 based on $\langle(12345)\rangle$ is 0.8838. With $n = 5$, the integer programming leads to d_8 with efficiencies of $\mathcal{E}_{\mathrm{A}} = 0.9625$, $\mathcal{E}_{\mathrm{D}} = 0.9698$, $\mathcal{E}_{\mathrm{E}} = 0.8334$ and $\mathcal{E}_{\mathrm{T}} = 0.9772$. Since Σ is not bisymmetric, Model (31) leads to a different measure, namely $p_{\langle(12231)\rangle} = 0.264$ and $p_{\langle(12341)\rangle} = 0.736$:

$$d_8 = \begin{pmatrix} 1 & 2 & 5 & 3 & 4 \\ 3 & 4 & 4 & 1 & 1 \\ 5 & 5 & 3 & 4 & 5 \\ 2 & 1 & 2 & 2 & 3 \\ 1 & 2 & 5 & 3 & 4 \end{pmatrix}.$$

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