Optimal approximate designs for estimating treatment contrasts resistant to nuisance effects

Samuel Rosa and Radoslav Harman

Faculty of Mathematics, Physics and Informatics, Comenius University,
Bratislava, Slovakia

April 23, 2015

Abstract

Suppose that we intend to perform an experiment consisting of a set of independent trials. The mean value of the response of each trial is assumed to be equal to the sum of the effect of the treatment selected for the trial, and some nuisance effects, e.g., the effect of a time trend, or blocking. In this model, we examine optimal approximate designs for the estimation of a system of treatment contrasts, with respect to a wide range of optimality criteria.

We show that it is necessary for any optimal design to attain the optimal treatment proportions, which may be obtained from the marginal model that excludes the nuisance effects. Moreover, we prove that for a design to be optimal, it is sufficient that it attains the optimal treatment proportions and satisfies some conditions of resistance to nuisance effects. For selected natural choices of treatment contrasts and optimality criteria, we calculate the optimal treatment proportions and give an explicit form of optimal designs. As we show, the obtained results can be used to calculate optimal approximate designs with a small support by means of linear programming. As a consequence, we can construct efficient exact designs by a simple heuristic.

Key words and phrases: approximate design, optimal design, treatment contrasts, resistance to nuisance effects, designs with small support
1 Introduction

The results of an experiment may be affected by conditions with effects that we aim to estimate and by other conditions with nuisance effects. For example, any experiment that consists of multiple trials performed in a time sequence may be subject to a nuisance time trend caused, for instance, by the ageing of the material used for the experiment, wearing down of the experimental devices or changes in the temperature. Exact designs of experiments that are, in some sense, resistant to time trend, have been studied for a long time, e.g., in [6], [5], [1] and [14]. Many of the agricultural experiments are subject to a two-dimensional nuisance trend, resulting from the arrangement of the trials in a two-dimensional field, see, e.g., [14] and [2]. The objective of the experimental design in such cases is to eliminate the nuisance effects, or to provide as much information as possible on the effects of interest.

The aim of this paper is to provide the $\Phi$-optimal approximate designs for estimating a system of contrasts of treatment effects under the presence of some nuisance effects, where $\Phi$ is a given optimality criterion. We show that a $\Phi$-optimal approximate design may be obtained in two steps: (i) Calculate $\Phi$-optimal proportions of treatment replications (treatment weights). These optimal proportions depend on the choice of contrasts of interest and on the optimality criterion $\Phi$; however, they do not depend on the nuisance effects. (ii) Subject to keeping the optimal proportions of treatment replications, distribute the treatments to nuisance conditions such that the resulting design is resistant to nuisance effects. The designs resistant to nuisance effects are an extension of the designs orthogonal to the time trend (balanced for trend, or trend-free, cf. [6], [15]) to a more general class of models and treatment contrasts.

For selected systems of treatment contrasts and a wide class of optimality criteria $\Phi$, we calculate $\Phi$-optimal treatment weights and thus obtain a class of $\Phi$-optimal designs. Specifically, for the estimation of contrasts for comparing treatments with a control, we provide optimal designs for Kiefer’s $\Phi_p$-optimality criteria, $p \in [-\infty, 0]$, including $A$-optimality ($p = -1$) and $E$-optimality ($p = -\infty$). In the particular case of $A$-optimality, similar results were given by [8] for exact designs, when the number of treatments is a square. Moreover, for any maximal system of orthonormal contrasts and for a system of centered contrasts, we show that the uniform design is $\Phi$-optimal for any orthogonally invariant information function $\Phi$. The results on centered contrasts generalize the results given by [21] for an additive blocking experiment.

The obtained results may be used to analytically construct optimal approximate designs. A special case of $\Phi$-optimal designs resistant to nuisance effects are the product designs with $\Phi$-optimal treatment proportions (cf., e.g., [23]), but the approximate product designs have a large support, which makes the transition to exact designs difficult. However, the set of
optimal approximate designs is typically large and both the conditions of optimal treatment weights and the conditions of resistance to nuisance effects are linear. Therefore, we can employ the simplex method of linear programming to obtain optimal approximate designs with a small support. This allows us to construct efficient exact design using a simple heuristic.

In the rest of Section 1, our notation and the statistical model is established. The main theoretical results are proved in Section 2. In Section 3 we provide optimal designs for estimating particular sets of contrasts, namely for contrasts corresponding to the comparison with a control, maximal orthonormal contrasts, and centered contrasts. Examples of experiments under the presence of nuisance effects are provided in Section 4. The theoretical results are applied in Section 5 to obtain optimal approximate designs with small support and efficient exact designs.

1.1 Notation

The symbols $1_n$ and $0_n$ denote the column vectors of length $n$ of ones and zeroes, respectively. The symbol $J_n$ denotes the $n \times n$ matrix $J_n = 1_n 1_n^T$ of ones and $e_u$ is the $u$-th standard unit vector (the $u$-th column of the identity matrix $I_n$, where $n$ is the dimension of $e_u$). By the symbol $0_{m \times n}$, or by $0$ if the dimensions are clear from the context, we denote the $m \times n$ matrix of zeroes. We denote the null space and the column space of a matrix $A$ by $\mathcal{N}(A)$ and $\mathcal{C}(A)$, respectively. By the symbol $\mathbb{S}_+^s$ we denote the set of $s \times s$ non-negative definite matrices and by $\preceq$ we denote the Loewner ordering of matrices in $\mathbb{S}_+^s$, i.e., $A \preceq B$ if $B - A$ is non-negative definite. Let $x = (x_1, \ldots, x_n)^T$ be a vector with nonzero components, then by $x^{-1}$ we denote the vector $x^{-1} := (x_1^{-1}, \ldots, x_n^{-1})^T$. By $\text{diag}(v_1, \ldots, v_k)$, where $v_1, \ldots, v_k$ are column or row vectors, we denote the diagonal matrix with diagonal elements corresponding to the elements of $v_1, \ldots, v_k$.

1.2 Statistical Model

Consider an experiment consisting of $N$ trials, where in each trial we choose one of $v$ treatments ($v \geq 2$). The response of the $i$-th trial is determined by the effect $\tau_{u(i)}$ of the chosen treatment $u(i)$ and by the effects of nuisance experimental conditions $t(i)$ from a finite set $\mathfrak{T}$, $|\mathfrak{T}| := n < \infty$.

We assume that the model is additive in the treatment and nuisance effects and that it can be expressed as

$$Y_i = \tau_{u(i)} + h^T(t(i))\theta + \varepsilon_i, \quad i = 1, \ldots, N,$$

where $Y_1, \ldots, Y_N$ are the observations, $\theta$ is a $d \times 1$ vector of nuisance parameters, $h : \mathfrak{T} \to \mathbb{R}^d$
is the regressor of the nuisance experimental conditions, and \( \varepsilon_1, \ldots, \varepsilon_N \) are independent and identically distributed random errors with zero mean and variance \( \sigma^2 < \infty \). Suppose that we aim to estimate a system of \( s \) contrasts \( Q^T \tau \), where \( \tau = (\tau_1, \ldots, \tau_v)^T \) and \( Q \) is a \( v \times s \) matrix satisfying \( Q^T 1_v = 0 \). We will assume that \( Q \) has full rank \( s \), unless stated otherwise. Moreover, we will assume that we are interested in all treatments \( 1, \ldots, v \), i.e., each treatment is present in \( Q \) (no row of \( Q \) is \( 0^T \)). We consider \( \theta \) to be a vector of nuisance parameters.

The model (1) can be expressed in the linear regression form

\[
Y_i = f^T(x_i) \beta + \varepsilon_i, \quad i = 1, \ldots, N,
\]

where \( x_i = (u(i), t(i)) \in \mathcal{X} \), \( \mathcal{X} = \{1, \ldots, v\} \times \mathcal{S} \), \( f(u, t) = (e_u^T, h(t))^T \), \( \beta = (\tau^T, \theta^T)^T \). The objective of the experiment is to estimate a system of contrasts \( K^T \beta \), where \( K^T = (Q^T, 0_{s \times d}) \).

Let the approximate design of experiment (or, in short, design) be a function \( \xi : \mathcal{X} \to [0, 1] \), such that \( \sum_{x \in \mathcal{X}} \xi(x) = 1 \), where \( \xi(x) \) represents the proportion of trials to be performed in \( x \in \mathcal{X} \). Hence, an exact design of experiment of size \( N \) is represented by a function \( \xi : \mathcal{X} \to \{0, 1/N, 2/N, \ldots, 1\} \), such that \( \sum_{x \in \mathcal{X}} \xi(x) = 1 \), where \( N\xi(x) \) is the number of trials in the design point \( x \in \mathcal{X} \).

The information matrix of the design \( \xi \) for estimating \( K^T \beta \) is the non-negative definite matrix (see [20])

\[
N_K(\xi) = \min_{L \in \mathbb{R}^{s \times m}, \sum L = I} LM(\xi) L^T,
\]

where \( M(\xi) = \sum_{x \in \mathcal{X}} \xi(x)f(x)f^T(x) \) is the moment matrix of the design \( \xi \) and the minimization is taken with respect to the Loewner ordering \( \preceq \). It is well known that the system \( K^T \beta \) is estimable if and only if \( C(K) \subseteq C(M(\xi)) \). When \( K^T \beta \) is estimable under \( \xi \), we say that \( \xi \) is feasible for \( K^T \beta \). In such a case, the information matrix of \( \xi \) is \( N_K(\xi) = (K^T M^{-1}(\xi) K)^{-1} \), where \( M^{-1}(\xi) \) is a generalized inverse of \( M(\xi) \).

Let \( \Phi : \mathcal{G}^s_+ \to \mathbb{R} \) be an optimality criterion. Then, a design \( \xi^* \) is said to be \( \Phi \)-optimal if it maximizes \( \Phi(N_K(\xi)) \) among all feasible designs \( \xi \). A widely used class of optimality criteria are the Kiefer’s \( \Phi_p \) criteria. Let \( H \) be a positive definite \( s \times s \) matrix with eigenvalues \( \lambda_1(H), \ldots, \lambda_s(H) \), and let \( \lambda_{\min}(H) \) be the smallest eigenvalue of \( H \). Then,

\[
\Phi_p(H) = \begin{cases} 
\left( \frac{1}{s} \sum_{j=1}^s \lambda_j^p(H) \right)^{1/p}, & p \in (-\infty, 0), \\
\left( \prod_{j=1}^s \lambda_j(H) \right)^{1/s}, & p = 0, \\
\lambda_{\min}(H), & p = -\infty.
\end{cases}
\]

If \( H \) is singular, we set \( \Phi_p(H) = 0 \). For \( p = 0, -1 \) and \( -\infty \), we obtain the \( D \)-, \( A \)- and \( E \)-optimality criterion, respectively. Note that \( \Phi_p \) criteria are information functions (see [20]).
in particular they are Loewner isotonic, positively homogeneous and concave.

We will investigate further the properties of experimental designs in model (1). The moment matrix of a design $\xi$ may be expressed in the form

$$M(\xi) = \begin{bmatrix} M_{11}(\xi) & M_{12}(\xi) \\ M_{T12}(\xi) & M_{22}(\xi) \end{bmatrix},$$

where

$$M_{11}(\xi) = \text{diag} \left( \sum_{t \in \mathcal{T}} \xi(1, t), \ldots, \sum_{t \in \mathcal{T}} \xi(v, t) \right),$$

$$M_{12}(\xi) = \left( \sum_{t \in \mathcal{T}} \xi(1, t) h(t), \ldots, \sum_{t \in \mathcal{T}} \xi(v, t) h(t) \right)^T,$$

$$M_{22}(\xi) = \sum_{t \in \mathcal{T}} \left( \sum_{u=1}^v \xi(u, t) \right) h(t) h^T(t).$$

Let us denote the Schur complement of the moment matrix $M(\xi)$ as $M_{T}(\xi) = M_{11}(\xi) - M_{12}(\xi)M_{T22}(\xi)M_{21}(\xi)$. It is simple to show that the system $K^T\beta$ is estimable under a design $\xi$ if and only if $C(M_{T}(\xi)) \subseteq C(Q)$. If $K^T\beta$ is estimable under $\xi$, the information matrix of $\xi$ is $N_K(\xi) = (Q^T M_{T}(\xi) Q)^{-1}$.

2 Optimal Approximate Designs

2.1 Preliminaries

We say that $w$ is a treatment proportions design if it is a design in the marginal model without nuisance effects

$$Y_i = \tau_{u(i)} + \epsilon_i, \quad i = 1, \ldots, N. \quad (3)$$

That is, $w$ is a function from $\{1, \ldots, v\}$ to $[0, 1]$ satisfying $\sum_u w(u) = 1$. For a design $\xi$ of (1), the marginal design defined by $w(u) = \sum_t \xi(u, t)$ for all $u$ represents the total weights of individual treatments in $\xi$, and it will be called the treatment proportions design of $\xi$. Since a design $w$ always provides $v$ weights $w(1), \ldots, w(v)$, we will often equivalently denote $w$ as a $v \times 1$ vector of weights $w = (w_1, \ldots, w_v)^T$. Note that if $\xi$ is an exact design of size $N$ and $w$ is its treatment proportions design, then $Nw$ is the vector of replications of treatments in $\xi$.

The properties of a treatment design $w$ in model (3) are generally very simple to analyze. For instance, it is straightforward to show that the moment matrix of $w$ is $M(w) = \text{diag}(w)$. 

5
Moreover, the set of contrasts $Q^T \tau$ is estimable in (3) under $w$ if and only if $w_u > 0$ for all $u$. In such a case, the information matrix of $w$ is evidently $N_Q(w) = (Q^T \text{diag}(w^{-1})Q)^{-1}$.

Similarly to the treatment replications design, we define *nuisance conditions design* $\alpha$ to be a design in the marginal model without treatments

$$Y_i = h^T(t(i))\theta + \varepsilon_i, \quad i = 1, \ldots, N,$$

i.e., $\alpha$ is a function from $\mathcal{T}$ to $[0,1]$ that satisfies $\sum_t \alpha(t) = 1$. For a design $\xi$ of (1), the marginal design $\alpha(t) = \sum_u \xi(u,t)$ for all $t$ defines the proportions of trials to be performed under particular nuisance conditions, and it will be called the *nuisance conditions design of* $\xi$.

**Proposition 1.** Let $\xi$ be a design in model (1) and let $w$ be its treatment proportions design. Then, $N_K(\xi) \preceq N_Q(w)$.

**Proof.** Let us partition the matrix $L$ in (2) as $L = (L_1, L_2)$, where $L_1$ is an $s \times v$ and $L_2$ is an $s \times d$ matrix. Then,

$$N_K(\xi) = \min_{L_K = I_s} LM(\xi)L^T = \min_{(L_1, L_2)(Q^T, 0)^T = I_s} (L_1, L_2)M(\xi)(L_1, L_2)^T$$

$$\leq \min_{L_1 = I_s} L_1 M_{11}(\xi)L_1^T = N_Q(w).$$

The previous proposition shows that by introducing nuisance effects, the information about the contrasts of interests can not increase. However, for a large class of designs, the information is exactly retained.

We say that a design $\xi$ with its treatment design $w$ is *resistant to nuisance effects*, or *nuisance resistant* for a given system of contrasts $Q$, if it satisfies

$$\left[ \frac{1}{w_1} \sum_{t \in \mathcal{T}} \xi(1,t)h(t), \ldots, \frac{1}{w_v} \sum_{t \in \mathcal{T}} \xi(v,t)h(t) \right] Q = 0. \quad (5)$$

The following proposition justifies this definition. The proof of Proposition 2 and other more technical proofs are deferred to the appendix.

**Proposition 2.** Let $\xi$ be a nuisance resistant design with its treatment proportions design $w > 0$, then (i) $\xi$ is feasible for $K^T \beta$, (ii) $K^T M^{-1}(\xi)K = Q^T M^{-1}(w)Q$ and (iii) $\xi$ has the same information matrix as $w$, i.e., $N_K(\xi) = N_Q(w)$. 


Note that the conditions of resistance to nuisance effects have also another desirable property: they are invariant with respect to a regular reparametrization of the nuisance regressors. That is, a design is resistant to nuisance effects with respect to nuisance regressors $h$ if and only if it is resistant to nuisance effects with respect to nuisance regressors $\tilde{h} = Rh$, where $R$ is any non-singular $d \times d$ matrix.

In general, the class of designs resistant to nuisance effects depends on the chosen system of contrasts $Q$. Nevertheless, as we show, there is a large subclass of nuisance resistant designs that is invariant to the choice of $Q$, i.e., these designs satisfy (5) for any system of contrasts.

We say that a design $\xi$ of (1) with its treatment design $w > 0$ is balanced if it satisfies

$$\frac{1}{w_1} \sum_{t \in \mathcal{T}} \xi(1, t) h(t) = \frac{1}{w_2} \sum_{t \in \mathcal{T}} \xi(2, t) h(t) = \ldots = \frac{1}{w_v} \sum_{t \in \mathcal{T}} \xi(v, t) h(t).$$

(6)

If $\xi$ is balanced, then for any $k \in \{1, \ldots, d\}$ the vector

$$s_k := \left(\frac{1}{w_1} \sum_{t \in \mathcal{T}} \xi(1, t) h_k(t), \ldots, \frac{1}{w_v} \sum_{t \in \mathcal{T}} \xi(v, t) h_k(t)\right)^T$$

satisfies $s_k = a_k 1_v$ for some $a_k \in \mathbb{R}$. Since $Q$ is a matrix of contrasts, we have $1_v^T Q = 0_v^T$ and hence $s_k^T Q = 0_v^T$. It follows that a balanced design $\xi$ is indeed nuisance resistant.

When the matrix of contrasts $Q$ attains the maximum rank, $v - 1$, the null space $\mathcal{N}(Q^T)$ has dimension 1 and it consists of vectors of the form $a 1_v$ for $a \in \mathbb{R}$. Hence, for such $Q$, the balanced designs are the only nuisance resistant designs, that is, in this specific but frequent case, the notions of nuisance resistance and balancedness coincide. One consequence of this observation is that for given nuisance regressors $h$, the class of balanced designs is the intersection of the sets of nuisance resistant designs with respect to all possible choices of contrast matrices $Q$.

We remark that the conditions (6) mean that a design $\xi$ is balanced with respect to the nuisance effects. That is, for each regressor $h_k$, the weighted average of the values $h_k(t)$ with weights $\xi(u, t)/w_u$, $t \in \mathcal{T}$, is the same for each treatment $u$. Balancedness can also be understood geometrically: assume that for each $u$ we calculate the barycentre of the $n$ points $h(t) \in \mathbb{R}^d$ with weights $\xi(u, t)/w_u$, $t \in \mathcal{T}$. Then, these barycentres must be the same for all treatments $u$.

A typical experimental situation is that we need to perform the same number of trials, usually one, under each nuisance condition $t \in \mathcal{T}$. In this case, it is straightforward to show that the conditions (6) may be expressed in a more compact form as follows.
Proposition 3. Let $\xi$ be a design which assigns the same weight to each nuisance condition, i.e., the nuisance conditions design of $\xi$ is $\alpha = 1_n/n$. Then, $\xi$ satisfies (6) if and only if it satisfies

$$\frac{1}{w_u} \sum_{t \in \mathcal{T}} \xi(u, t) h(t) = \frac{1}{n} \sum_{t \in \mathcal{T}} h(t) \text{ for all } u \in \{1, \ldots, v\}. \tag{7}$$

In the case of an exact design $\xi$ assigning one trial to each nuisance condition, the balancedness of $\xi$ has a straightforward interpretation. Suppose, for instance, that the nuisance conditions represent time and $h_1(t)$ is proportional to the room temperature at time $t$. For each treatment $u$, let $T_u$ be the average temperature at the times of trials with the treatment $u$. Then, the balance conditions for $h_1(t)$ mean that the temperature conditions are “fair” for all treatments in the sense that the average temperatures $T_u$ are the same: $T_u \equiv T$ for all $u$.

Let $w$ be a treatment proportions design and $\alpha$ be a nuisance conditions design. Then, a design $\xi$ is the product design of $w$ and $\alpha$ if it satisfies

$$\xi(u, t) = w(u) \alpha(t) \text{ for all } u \in \{1, \ldots, v\}, t \in \mathcal{T},$$

which we denote $\xi = w \otimes \alpha$. Note that any product design $w \otimes \alpha$ satisfies $\frac{1}{w_u} \sum_{t \in \mathcal{T}} \xi(u, t) h(t) = \sum_{t} \alpha(t) h(t)$ for all $u$, therefore the product design is balanced and consequently, it is also resistant to nuisance effects.

2.2 Conditions of Optimality

There are many results on the optimal exact designs in models that are specific cases of model (1) (e.g., [12], [4], [19]). However, we show that the approximate theory gives simple and general conditions of optimality, which provide an insight into the qualitative behaviour of optimal designs. In Section 5 we demonstrate that these conditions can be employed to construct efficient exact designs.

The following theorem shows that the optimality of treatment proportions is a necessary condition of the optimality of a design in model (1).

Theorem 1. Let $\Phi$ be an information function, let $\xi^*$ be a $\Phi$-optimal design in model (1) and let $w^*$ be its treatment proportions design. Then, $w^*$ is $\Phi$-optimal in (3).

Proof. Let $\xi$ be a design in (1). Using Proposition 1 we obtain that $N_K(\xi) \leq N_Q(w)$, where $w$ is the treatment proportions design of $\xi$. Moreover, part (iii) of Proposition 2 implies that $N_Q(w) = N_K(w \otimes \alpha)$ for any nuisance conditions design $\alpha$. Therefore, $N_K(\xi) \leq N_K(w \otimes \alpha)$.

Suppose that $w^*$ is not a $\Phi$-optimal design. Then, there exists a design $w_b$ under model (3) such that $\Phi(N_Q(w^*)) < \Phi(N_Q(w_b))$. Then, $\Phi(N_K(\xi^*)) \leq \Phi(N_Q(w^*)) < \Phi(N_Q(w_b))$. 

\( \Phi(N_K(w_b \otimes \alpha)) \) for any nuisance conditions design \( \alpha \). That is a contradiction with \( \xi^* \) being \( \Phi \)-optimal.

From Theorem 1 it follows that in order to find an optimal approximate design, we need to break up this process into two steps: obtain the optimal treatment weights and then optimally allocate these weights to nuisance conditions. Note that finding a \( \Phi \)-optimal treatment design is a convex \( v \)-dimensional optimization problem

\[
\max_{w>0, \mathbf{1}^T w = 1} \Phi((Q\text{diag}(w^{-1})Q^T)^{-1}),
\]

which can usually be easily solved numerically, and often analytically, as we demonstrate in Section 3.

Once the optimal treatment weights are obtained, we may allocate these weights to nuisance conditions using the following theorem, i.e., by choosing a nuisance resistant design.

**Theorem 2.** Let \( w^* \) be a \( \Phi \)-optimal treatment proportions design. Let \( \xi^* \) be a nuisance resistant design with its treatment proportions design \( w^* \). Then, \( \xi^* \) is \( \Phi \)-optimal and it has the same information matrix as \( w^* \), i.e., \( N_K(\xi^*) = (Q^T\text{diag}((w^*)^{-1})Q)^{-1} \).

**Proof.** Let \( \xi \) be a design in model (1) and \( w \) be its treatment proportions design. Since \( \Phi \) is isotonic, from Proposition 1 it follows that \( \Phi(N_Q(w)) \geq \Phi(N_Q(\xi)) \). Since \( w^* \) is \( \Phi \)-optimal, \( \Phi(N_Q(w^*)) \geq \Phi(N_Q(w)) \) and it is feasible, thus \( w^* > 0 \). Using Proposition 2 we get that \( \Phi(N_K(\xi^*)) = \Phi(N_Q(w^*)) \geq \Phi(N_Q(w)) \geq \Phi(N_K(\xi)) \), i.e., \( \xi^* \) is \( \Phi \)-optimal.

The balanced designs (and, as a special case, product designs \( w^* \otimes \alpha \) with any \( \alpha \)) are nuisance resistant, therefore, the balanced designs with \( \Phi \)-optimal treatment weights \( w^* \) are \( \Phi \)-optimal. Moreover, they have the same information matrix as \( w^* \). Since the product designs do not depend on the nuisance regressors, we may easily construct a \( \Phi \)-optimal design in model (1) with any nuisance effects, by taking \( w^* \otimes \alpha \) with any \( \alpha \). Therefore, the class of \( \Phi \)-optimal designs for model (1) is very large (unless \( n = 1 \)).

Note that the approach of first finding a design in a simpler model without nuisance effects and then assuring that the information is retained in the model with nuisance effects was used in [17], but for exact designs and for the entire vector of parameters of interest. We also note that similar results on product designs are given by [23] (cf. Theorem 3.2) in an additive model \( Y_i = \beta_0 + f_1^T(u_1(i))\beta_1 + f_2^T(u_2(i))\beta_2 + \varepsilon_i \). Their limitation is the need for the constant term \( \beta_0 \) in both the main model as well as the marginal models, which is not the case in Theorem 2.
Theorem 1 provides necessary conditions of optimality and Theorem 2 provides sufficient conditions of optimality. It turns out that for the wide class of strictly concave optimality criteria, we can provide conditions that are both necessary and sufficient for optimality of a design $\xi$ in model (1).

**Theorem 3.** Let $\Phi$ be a strictly concave function. Then, a design $\xi$ is $\Phi$-optimal if and only if (i) its treatment proportions design $w$ is $\Phi$-optimal in model (3) and (ii) $\xi$ is resistant to nuisance effects.

Since the balanced designs are the only nuisance resistant designs for a system of contrasts of maximum rank, $v - 1$, we obtain the following corollary.

**Corollary 1.** Let $\Phi$ be a strictly concave function, and let $Q$ be a matrix of contrasts of rank $v - 1$. Then, a design $\xi$ is $\Phi$-optimal for estimating $Q^T\tau$ if and only if its treatment proportions design is $\Phi$-optimal in (3) and $\xi$ is balanced.

### 2.3 Rank Deficient Subsystems

Until now, we always assumed that the $v \times s$ matrix $Q$ has full rank. However, there are some frequently used sets of contrasts that do not satisfy this assumption. Such subsystems of interest are called rank deficient subsystems; for a detailed study of such systems, see [20].

An example of a rank deficient subsystem is the set of contrasts determined by the matrix $Q = I_v - \frac{1}{v}J_v$, which aims at estimating the centered effects of treatments (see [21]).

In the rank deficient subsystems, the information matrix $N_K(\xi)$ is not well defined. Instead, following [20], for a feasible design we define the matrix $C_K(\xi) := (K^T M^-(\xi) K)^+,$

where the superscript $+$ denotes the Moore-Penrose inverse. For $K = (Q^T, 0)^T$, we get

$$C_K(\xi) = (Q^T M^-(\xi) Q)^+.$$ Then, instead of maximizing $\Phi$ defined on all eigenvalues of $N_K(\xi)$, we maximize $\Phi$ defined on the positive eigenvalues of $C_K(\xi)$.

For the full rank subsystem, the eigenvalues of the information matrix $N_K(\xi)$ are the inverses of the eigenvalues of $K^T M^-(\xi) K$. Similarly, the matrix $C_K(\xi)$ satisfies that its non-zero eigenvalues are inverses of the non-zero eigenvalues of the matrix $K^T M^-(\xi) K$. Thus, at least in the sense of eigenvalues, the matrices $C_K(\xi)$ are an analogue to the information matrices for full rank subsystems.

For rank deficient subsystems, we will consider only optimality criteria $\Phi$ that depend on the eigenvalues of $C_K(\xi)$, such as the $\Phi_p$ criteria. Note that an information function $\Phi(C)$ depends only on the eigenvalues of $C$ if and only if it is orthogonally invariant, i.e., $\Phi(UCUT^T) = \Phi(C)$ for any orthogonal matrix $U$ (e.g., [9]).
In the rank deficient case, we will provide results analogous to the full rank case. We will show that by introducing the nuisance effects, we cannot increase information about the treatment contrasts, as measured by \( C_K(\xi) \). The ordering of matrices \( C_K(\xi) \) is induced by the inverse ordering of the matrices \( K^T M^{-}(\xi) K \). For any design \( \xi \), we obtain \( K^T M^{-}(\xi) K = Q^T M^{-}(\xi) Q \) and for its treatment proportions design \( Q^T M^{-}(w) Q = Q^T M_{11}^{-}(\xi) Q \). Moreover, \( M_\tau(\xi) = M_{11}(\xi) - M_{12}(\xi) M_{22}(\xi) M_{22}^T(\xi) \leq M_{11}(\xi) \), therefore there exist generalized inverses that satisfy \( M_\tau(\xi) \geq M_{11}(\xi) \) (see [24]) and it follows that \( K^T M^{-}(\xi) K \geq Q^T M^{-}(w) Q \). As \( \Phi(N) \) depends only on the eigenvalues of \( N \) and the Moore-Penrose inverse \( X^+ \) has inverse non-zero eigenvalues of \( X \), it implies that \( \Phi((K^T M^{-}(\xi) K)^+) \geq \Phi((Q^T M^{-}(w) Q)^+) \), i.e., \( \Phi(C_K(\xi)) \geq \Phi(C_Q(w)) \).

From part (ii) of Proposition 2 it follows that a balanced design (as well as a product design) has the same matrix \( C_K(\xi) \) as its treatment proportions design, i.e., \( C_K(\xi) = C_Q(w) \). Hence, Theorems 1 and 2 hold even in the rank deficient case.

**Theorem 4.** Let \( \Phi \) be an information function and let \( Q \) be a \( v \times s \) matrix of contrasts with \( \text{rank}(Q) < s \). Let \( w^* \) be a \( \Phi \)-optimal design for estimating \( Q^T \tau \) in model (3). Then, the following holds

(i) Any nuisance resistant design \( \xi^* \), whose treatment proportions design is \( w^* \), is \( \Phi \)-optimal for estimating \( Q^T \tau \) and \( C_K(\xi^*) = (Q^T \text{diag}((w^*)^{-1}) Q)^+ \).

(ii) If \( \xi^* \) is a \( \Phi \)-optimal design in model (1) and \( w^* \) is its treatment proportions design, then \( w^* \) is \( \Phi \)-optimal for estimating \( Q^T \tau \) in model (3).

In particular, we obtain optimality of balanced and product designs with optimal treatment weights.

### 3 Systems of Contrasts

#### 3.1 Comparison With Control

Consider an experiment, where the first treatment is a control, and the aim of the experiment is to estimate the effects of the other treatments with respect to the effect of the control, i.e., \( \tau_2 - \tau_1, \ldots, \tau_v - \tau_1 \) and \( Q = (-1_{v-1}, I_{v-1})^T \). There has been a steady interest in the comparison of treatments with a control, see, e.g. [11] or [18]. Note that the matrix \( Q \) has rank \( v - 1 \) and thus the nuisance resistant designs and the balanced designs coincide.
We note that the set of contrasts is symmetric in treatments $2, \ldots, v$. This suggests that $\Phi_p$-optimal treatment weights should satisfy $w_2 = \ldots = w_v$. Such weights may be characterized by a single value, $\gamma \in (0, 1)$, the weight of the first treatment. By $w_\gamma$ we denote a treatment proportions design that satisfies

$$w_\gamma(1) = \gamma \quad \text{and} \quad w_\gamma(u) = \frac{1 - \gamma}{v - 1} \text{ for } u > 1.$$

For every $p \in [-\infty, 0]$, we will provide $\Phi_p$-optimal balanced designs, using Theorem 5 and the Equivalence Theorem (Theorem 7.20 in [20]).

**Theorem 5.** Let $p \in [-\infty, 0]$. If $p > -\infty$, let $\gamma_p$ be the unique solution of the equation

$$(v - 2)\gamma^{1-p} + 2\gamma - 1 = 0 \quad (9)$$

in the interval $(0, 1/2]$ and let $\gamma_{-\infty} = 1/2$. Then, any balanced design $\xi$ with its treatment proportions design $w_{\gamma_p}$ is $\Phi_p$-optimal for the estimation of $(-1_{v-1}, I_{v-1})^T$, with its information matrix $N_K(\xi) = \frac{1-\gamma_p}{v-1}I_{v-1} - \left(\frac{1-\gamma_p}{v-1}\right)^2I_{v-1}$.

We note that for any $p \in (-\infty, 0]$ and $v > 2$ there exists a unique solution $\gamma_p$ of the equation (9) in the interval $(0, 1/2)$. It is numerically easy to calculate the optimal $\gamma_p$, because the function $g(\gamma) := (v - 2)\gamma^{1-p} + 2\gamma - 1$ is an increasing convex function for $\gamma \in (0, 1/2)$. Furthermore $\gamma_p$ is a decreasing function, which satisfies $\lim_{p \to -\infty} \gamma_p = 1/2 = \gamma_{-\infty}$.

Using Theorem 5 we may calculate $\Phi_p$-optimal criterial values.

**Corollary 2.** Let $Q = (-1_{v-1}, I_{v-1})^T$. Then, for $p \in (-\infty, 0)$, the criterial value $\Phi_p(\xi^*)$ of any $\Phi_p$-optimal design $\xi^*$ is given by the equation

$$\Phi_p(\xi^*) = \frac{1 - \gamma_p}{v - 1} \left(1 - \frac{1 - \gamma_p}{v - 1}\right)^{1/p}, \quad (10)$$

where $\gamma_p$ is the solution of (9).

For $v > 2$, the values of $\gamma_p$ and the optimal criterial values for $D$, $A$- and $E$- optimality are

$$\gamma_0 = 1/v, \quad \Phi_0(\xi^*) = v^{-v/(v-1)} \quad (D\text{-optimality}),$$

$$\gamma_{-1} = \sqrt{v-1} - 1 \quad \frac{v-1}{v-2}, \quad \Phi_{-1}(\xi^*) = \left(\frac{\sqrt{v-1} - 1}{v-2}\right)^2 \quad (A\text{-optimality}),$$

$$\gamma_{-\infty} = 1/2, \quad \Phi_{-\infty}(\xi^*) = \frac{1}{4(v-1)} \quad (E\text{-optimality}).$$
3.2 Orthonormal Contrasts

By a maximal system of orthonormal contrasts, we mean a set of \( v - 1 \) contrasts that are orthogonal to each other and have norm 1, i.e., \( q_1, \ldots, q_{v-1} \) satisfy \( q_i^T q_j = 0 \) for \( i \neq j \) and \( q_i^T q_i = 1 \) for all \( i \). Note that a special case of the maximal system of orthonormal contrasts are the Helmert contrasts (see, e.g., [7], Appendix C). As in comparison with control, the matrix \( Q = (q_1, \ldots, q_{v-1}) \) has rank \( v - 1 \) and thus the nuisance resistant designs and the balanced designs coincide.

Since \( Q \) is a \( v \times (v-1) \) matrix of orthonormal contrasts, the matrix \( [Q, 1/v\sqrt{v}] \) is orthogonal. It follows that \( QQ^T = I_{v-1} \) and \( Q^T Q = I_{v-1} \).

In the following theorem, we show that a balanced design with its treatment proportions design \( \hat{w} = 1/v \) is \( \Phi \)-optimal for any orthogonally invariant information function \( \Phi \). In particular, we obtain the optimality of the uniform design \( \xi(u,t) = 1/(vn) \) for all \( u, t \), and of the product designs \( (1/v) \otimes \alpha \) for any nuisance conditions design \( \alpha \).

The information matrix of a balanced design with its treatment proportions design \( \hat{w} = 1/v \) is \( N_K(\hat{\xi}) = Q^T v^{-1} I_v Q - Q^T v^{-1} I_v J_v v^{-1} I_v Q = v^{-1} Q^T Q - 0 = v^{-1} I_{v-1} \).

Theorem 6. Let \( Q^T \tau \) be a maximal system of orthonormal contrasts and let \( \Phi \) be an orthogonally invariant information function. Then, any balanced design \( \xi^* \) with its treatment proportions design \( \hat{w} = 1/v \) is \( \Phi \)-optimal for \( Q^T \tau \), with its information matrix \( N_K(\xi^*) = v^{-1} I_{v-1} \).

3.3 Centered Contrasts

Let us assume that we are interested in estimating the centered treatment effects, i.e., the contrasts \( \tau_1 - \bar{\tau}, \ldots, \tau_v - \bar{\tau} \), where \( \bar{\tau} \) is the mean of the treatment effects. That is, \( Q = I_v - J_v/v \), which is again a matrix of rank \( v - 1 \). However, \( Q \) is a \( v \times v \) matrix and thus \( Q^T \tau \) is a rank deficient system of treatment contrasts. In Section 5 of the paper [21], this system of contrasts was analyzed in great detail for a special case of model [11], the block designs.
Analogously to Theorem 6, we obtain the optimality of product designs and balanced designs with uniform treatment weights with respect to any orthogonally invariant information function $\Phi$. In particular, we obtain the optimality of the uniform design $\bar{\xi}$.

The matrix $C_K(\xi)$ of a balanced design $\xi$ with uniform treatment weights $\bar{w} = 1_v/v$ satisfies $C_K(\xi) = (Q^T \text{diag}(v_1^T v)) Q = v Q^T Q = v^{-1} Q^+$. It is easy to verify that $Q^+ = Q$ and hence $C_K(\xi) = I_v/v - J_v/v^2$.

**Theorem 7.** Let $Q = I_v - J_v/v$ and let $\Phi$ be an orthogonally invariant information function. Let $\xi$ be a balanced design with treatment proportions design $\bar{w} = 1_v/v$. Then, $\xi$ is $\Phi$-optimal for $Q^T \tau$, with $C_K(\xi) = Q/v = I_v/v - J_v/v^2$.

### 4 Examples

#### 4.1 Trend Resistant Designs

Let us consider a model where we perform the trials in a time sequence, in each time exactly one trial, and the nuisance effect is the effect of some time trend

\[ Y_i = \tau_{u(i)} + h_1(t(i))\theta_1 + \ldots + h_d(t(i))\theta_d + \varepsilon_i, i \in \{1, \ldots, n\}, \tag{11} \]

where $u(i) \in \{1, \ldots, v\}$ represents the chosen treatment and $t(i) \in \{1, \ldots, n\}$ denotes in which time the treatment is to be applied in trial $i$. The functions $h_1, \ldots, h_d : \mathbb{R} \to \mathbb{R}$ are the regressors of the time trend, often chosen to be polynomials of degrees $0, \ldots, d-1$ respectively.

The interest in designs that perform well under model (11) dates back to the mid-20th century, e.g., in paper [6]. The research focus is usually on combinatorial construction of exact designs orthogonal to time trend (or trend free). These are designs that satisfy that no information is lost due to the time trend (see, e.g., [14], [3]). Usually, the focus is on all parameters of interest, not on a system of contrasts $Q$, resulting in the condition that a design is trend free with respect to $h_k$ in model (11) if \( \sum_i \xi(u, t) h_k(t) = 0 \), see, e.g. [6]. Such trend free designs satisfy $M_{12}(\xi) = 0$ and thus $M_v(\xi) = M_{11}(\xi)$.

The drawback of the combinatorial approach is that it is usually tailored for a very specific model. For example, the theoretical results on orthogonal designs require the number of design points to be a multiple of the number of treatments, the time points to be evenly spaced and the time trend needs to be represented by a polynomial. However, these conditions often do not hold. The reader may find a survey of the literature on the trend resistant experimental designs in the papers [5] or [1].

Note that the orthogonal designs satisfy [6] and thus they are balanced. However, since we aim at estimating a set of treatment contrasts $Q$, the stringent conditions of orthogonality
need not hold for the information to be retained. If \( \xi \) is resistant to nuisance effects, the equality \( M(\xi) = M_{11}(\xi) \) in general does not hold, but such \( \xi \) satisfies \( N_K(\xi) = N_Q(w) \), i.e., the designs resistant to nuisance effects eliminate the effects of the time trend. We remark that when \( \sum h(t) = 0 \), the conditions of orthogonality and the conditions of balancedness coincide.

We will examine the model with trigonometric time trend of degree \( D \in \mathbb{N} \), which can be used to model, for instance, circadian rhythms (cf. [16]). For simplicity, let \( \phi_n = 2\pi/n \) and consider the model

\[
Y_t = \tau_u(t) + \theta_0 + \theta_1 \cos(\phi_n t) + \theta_2 \sin(\phi_n t) + \ldots + \theta_{2D-1} \cos(D\phi_n t) + \theta_{2D} \sin(D\phi_n t) + \varepsilon_t,
\]

where \( t = 1, 2, \ldots, n \).

An exact design \( \xi \) will be represented by a sequence of treatments determining which treatments are to be chosen in which times. Note that the regression functions satisfy \( \sum_{t} h_k(t) = 0 \) for \( k > 0 \), i.e., the notions of orthogonal and balanced designs for this model coincide.

Theorem 2 and Lemma 6 (in the Appendix) yield that by repeating a sequence of treatments with \( \Phi \)-optimal treatment weights, we may obtain a \( \Phi \)-optimal design for model (12) of high degree.

**Proposition 5.** Let \( \Phi \) be an information function. Let \( l \in \mathbb{N} \) and let \( \xi_p \) be an exact design of size \( l \) with \( \Phi \)-optimal treatment proportions for estimating contrasts \( Q^T \tau \). Let \( m \in \mathbb{N} \). Then, the exact design \( \xi = \xi_p \xi_p \ldots \xi_p \) of size \( n = lm \) formed by an \( m \)-fold replication of \( \xi_p \) is \( \Phi \)-optimal for all trigonometric models (12) of degrees \( D < m \).

It is in fact possible to show that the design \( \xi \) from Proposition 5 is \( \Phi \)-optimal for models of the type (12) of any degree, but they cannot include the terms \( \cos(a\phi_n t) \) and \( \sin(a\phi_n t) \), where \( a \) is an integer multiple of \( m \).

We demonstrate the results given by Proposition 5 on a simple example.

**Example 1.** Consider the model

\[
Y_t = \tau_u + \theta_0 + \theta_1 \sin(\phi_n t) + \theta_2 \cos(\phi_n t) + \theta_3 \sin(2\phi_n t) + \theta_4 \cos(2\phi_n t) + \theta_5 \sin(3\phi_n t) + \theta_6 \cos(3\phi_n t) + \varepsilon_t,
\]

where \( r = \frac{2\pi}{n} t \) and \( t = 1, 2, \ldots, n \). Let \( n = 16 \), \( v = 3 \) and \( \xi_p = 2113 \). Then, the design \( \xi_1 = 2113, 2113, 2113, 2113 \) is \( E \)-optimal for estimating \( (-1_{v-1}, I_{v-1})^T \). Let \( n = 12 \), \( v = 3 \) and \( \xi_q = 321 \). Then, the design \( \xi_2 = 321, 321, 321, 321 \) is \( D \)-optimal for estimating \( (-1_{v-1}, I_{v-1})^T \). Moreover, let \( \Phi \) be an orthogonally invariant information function. Then, \( \xi_2 \) is \( \Phi \)-optimal for estimating \( (I_v - J_v/v)^T \tau \) or a maximal system of orthonormal contrasts \( Q^T \tau \).
4.2 Block Designs, Row-Column Designs

Consider an experiment, where the treatment units are arranged in $b$ blocks. As usual, for each of the $N$ treatment units, we choose one of $v$ treatments. The response is then determined by the treatment effects and block effects. We assume that the treatment and block effects do not interact, i.e., we obtain an additive blocking experiment

$$Y_i = \tau_{u(i)} + \eta_{t(i)} + \varepsilon_i, \quad i = 1, \ldots, N,$$

where $u(i) \in \{1, \ldots, v\}$ and $t(i) \in \{1, \ldots, b\}$. The designs of blocking experiments are called block designs. There is a large amount of literature on this topic, in particular the papers that consider treatment contrasts in block designs are, e.g., [12], [21].

Note that model (13) may be expressed as a special case of model (1), where $\mathcal{X} = \{1, \ldots, b\}$, $n = b$, $\theta = (\eta_1, \ldots, \eta_v)^T$ and $h(t) = e_t \in \mathbb{R}^b$ is the $t$-th elementary unit vector. For block designs, in the balance conditions (6) we obtain $\xi(1, t)/w_1 = \ldots = \xi(v, t)/w_v$ for all $t \in \{1, \ldots, b\}$, which leads to a product design $\xi = w \otimes \alpha$. That is, all balanced designs in model (13) are product designs. Therefore, for a system of contrasts of rank $v - 1$ and a strictly concave information function $\Phi$, from Theorem 3 it follows that all $\Phi$-optimal designs are product designs. Note that, in general, the balanced incomplete block designs and the balanced treatment incomplete block designs (see, e.g., [12]) are not balanced in the sense of conditions [6].

Block designs are often used for eliminating heterogeneity in one direction, e.g., caused by a nuisance time trend. If the position of a unit within a block affects the response as well, or in general, the heterogeneity needs to be eliminated in two directions, we may use the row-column designs (see [13]). Here, $N$ experimental units are arranged in $b_1$ rows and $b_2$ columns. The mean response is determined by the sum of the treatment, row and column effect, modelled as

$$Y_i = \tau_{u(i)} + \eta_{k(i)} + \varphi_{l(i)} + \varepsilon_i, \quad i = 1, \ldots, N,$$

where $u(i) \in \{1, \ldots, v\}$, $k(i) \in \{1, \ldots, b_1\}$ and $l(i) \in \{1, \ldots, b_2\}$ represent the row and column chosen for the $i$-th trial, respectively, and $\eta_{k(i)}, \varphi_{l(i)}$ are the row and column effects.

This model can also be expressed as a special case of model (1), where $\mathcal{X} = \{1, \ldots, b_1\} \times \{1, \ldots, b_2\}$, $n = b_1 b_2$, $\theta = (\eta_1, \ldots, \eta_v, \phi_1, \ldots, \phi_{b_2})^T$ and $h(k, l) = (e_k^T, e_l^T)^T \in \mathbb{R}^{b_1 + b_2}$. The balance conditions for the row-column model become $w_1^{-1} \sum \xi(1, k, l) = \ldots = w_v^{-1} \sum \xi(v, k, l)$ for all $k = 1, \ldots, b_1$ and $w_1^{-1} \sum \xi(1, k, l) = \ldots = w_v^{-1} \sum \xi(v, k, l)$ for all $l = 1, \ldots, b_2$. That is, for any row (column) the ratio of the total weights of any two treatments $i$, $j$ in the particular row (column) is given by the ratio of the treatment weights $w_i/w_j$. In other words, for
the design \( \xi \) to be balanced (and hence optimal, if \( \xi \) attains optimal treatment weights), the functions \( \xi(u, \cdot, \cdot)/w_u \) need to have the same row and column marginals for all \( u = 1, \ldots, v \).

The block and row-column designs are called the designs for the one-way and two-way elimination of heterogeneity, respectively (see [13]). By combining the models (13) and (11), we get the blocking experiment under the presence of a nuisance time trend, see, e.g., [4] or [14], which we will examine further in Example 4.

5 Constructing Efficient Exact Designs

By constructing product designs with optimal treatment weights, and calculating their criterial values (or by analytically deriving optimal criterial values, see Corollary 2), we may assess the quality of the exact designs. More precisely, we can compute lower bounds on the efficiency of any given exact design by calculating its approximate efficiency with respect to the criterion \( \Phi; \text{ eff}(\xi) = \frac{\Phi(\xi)}{\Phi(\xi^*)} \), where \( \xi^* \) is a \( \Phi \)-optimal approximate design. Moreover, as we demonstrate in this section, the balance conditions provide a tool for obtaining optimal approximate designs with small support and these designs can be used to construct efficient exact designs.

We will focus on exact designs of experiments in which exactly one trial is to be performed under each nuisance condition. The problem of finding such optimal designs is in general a difficult discrete optimization problem, see, e.g., [1] or [10].

Note that both the balance conditions (and, in general, the conditions of resistance to nuisance effects) and the conditions on \( \Phi \)-optimal weights are linear. Hence, results provided in the previous sections can be used to calculate a balanced approximate design with \( \Phi \)-optimal weights employing linear programming, solving the problem

\[
\min \{ c^T x | Ax = b, x \geq 0 \},
\]

where \( x \in \mathbb{R}^{vn} \) represents a design \( \xi \) in the vector form, \( A \) consists of sufficient conditions of optimality and we are free to choose the the vector \( c \) of the coefficients of the objective function. Let us denote the set of all feasible solutions of (15) as \( \mathcal{P} \).

The matrix \( A \) consists of

(i) \( v \) equalities \( \sum_t \xi(u,t) = w_u, u = 1, \ldots, v \), i.e., \( \xi \) attains the \( \Phi \)-optimal treatment weights,

(ii) \( d(v - 1) \) equalities \( w_1^{-1} \sum_t \xi(1,t)h(t) = w_u^{-1} \sum_t \xi(u,t)h(t), u = 2, \ldots, v \), i.e., \( \xi \) is a balanced design,
(iii) $n$ equalities $\sum_u \xi(u,t) = 1/n$, i.e., under each nuisance condition exactly one trial is performed.

Once the $\Phi$-optimal treatment weights $w^*$ are obtained, a $\Phi$-optimal design can be constructed as a product $w^* \otimes \alpha$ for any nuisance conditions design $\alpha$. However, in general, it is difficult to construct exact designs from the product designs, due to their regular structure and large support. To obtain an optimal design with small support, it is beneficial to employ the simplex method of linear programming, whose output is an optimal design $\xi^*$ that represents a vertex in $P$, the set of feasible solutions of (15).

**Proposition 6.** Let $\xi$ represent a vertex in $P$. Then, $\xi$ contains at most $v + (v - 1)k + n - 1$ support points, where $k$ is the affine dimension of the set $\{h(t)\}_{t \in T}$.

From Proposition 6 it follows that by employing the simplex method, we can obtain a $\Phi$-optimal design $\xi^*$ with at most $(v - 1)(k + 1) + n$ support points. As a special case, when a constant term $\theta_0$ is present in the time trend, it may be ignored in the conditions in (15), because it does not increase the affine dimension of $\{h(t)\}_{t \in T}$; reducing thus the upper bound on the number of support points by $v - 1$.

Suppose that $\xi$ satisfying (iii) has support of size $n$, the number of nuisance conditions. Then, $\xi$ uniquely determines an exact design of size $n$. The number of support points in designs obtained by the simplex method is only slightly larger than $n$; it exceeds this minimum support size by $(v - 1)(k + 1)$. Note that the number of exceeding support points does not depend on $n$, thus, even for increasing number of nuisance conditions, it remains small.

We note that using the Carathéodory Theorem (cf. Theorem 8.2. in [20]), it is possible to obtain results similar to Proposition 6, but the Carathéodory Theorem does not provide an actual method of constructing a design with small support, unlike the simplex method.

From an optimal approximate design with small support, an efficient exact design can be constructed by rounding, or often even by a complete enumeration of treatments in a small number of nuisance conditions.

**Example 2.** Consider an experiment of performing trials in a time sequence

$$Y_i = \tau u(i) + \theta_0 + \theta_1 h_1(t(i)) + \varepsilon_i, \quad i = 1, \ldots, n,$$

where $h_1(t) = e^t / \sum_j e^j$ represents an exponential time trend (e.g., the decay of wool in the experiment of wool processing, as suggested by [1]). Assume that $n = 8, v = 3$ and the objective is to find an $A$-optimal design for estimating $(-1_{v-1}, I_{v-1}) \tau$. The optimal weight of the first treatment is $\gamma^* = \sqrt{2} - 1$ and the optimal weights of the other two are $1 - \sqrt{2}/2$. 

18
First, we will provide an $A$-optimal balanced design by employing the simplex method (\texttt{linprog} function of Matlab, using the simplex algorithm). Since $\theta_0$ is the constant term, from Proposition 6 it follows that there are at most $n - 1 + v + (v - 1)D$ linearly independent rows of $A$ in (15), where $D = d - 1 = 1$. We remark that although we are free to choose the vector $c$ in the linear program, the support size of the design obtained by the simplex method does not seem to depend on the choice of $c$. Therefore, we chose each of the elements of $c$ uniformly randomly from $(0, 1)$.

We obtained a design $\xi_1$ that has the support of size 12 (and the minimum support size is 8) and is “fixed” in 5 times (i.e., in each of these times $\xi_1$ has only one non-zero element), see Table 1. The support size corresponds to the bound given by $n - 1 + v + (v - 1)D = 12$.

| $u \setminus t$ | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   |
|-----------------|-----|-----|-----|-----|-----|-----|-----|-----|
| 1               | 0   | 0.1250 | 0.0855 | 0.1250 | 0   | 0   | 0   | 0.0787 |
| 2               | 0.1250 | 0   | 0   | 0   | 0.0360 | 0.1250 | 0.0069 |
| 3               | 0   | 0   | 0.0395 | 0   | 0.1250 | 0.0890 | 0   | 0.0394 |

Table 1: $A$-optimal balanced approximate design obtained by the simplex method

By a complete enumeration of the possible treatment combinations in the remaining 3 non-fixed times, we chose the design $\hat{\xi}_1 = 21113321$ that maximizes the criterial value. Using Corollary 2 we calculated that $\hat{\xi}_1$ has approximate efficiency 0.946. For $v = 3$ and $n = 8$ it is possible to find the $A$-optimal exact design by a complete enumeration, $\xi^* = 11123321$. It turns out that the design $\hat{\xi}_1$ has efficiency 0.997 relative to $\xi^*$.

For $n = 150$ and the same model assumptions, we obtained a design $\xi_2$ with support of size 154, that has 296 zeroes, out of the maximal 300. That is, the number of support points of $\xi_2$ exceeds the minimum support size again by 4; moreover $\xi_2$ has again only three non-fixed times. Therefore, even for $n = 150$, an efficient exact design may be obtained by a complete enumeration of treatments in the non-fixed times. The resulting design $\hat{\xi}_2$ has efficiency 0.995. The efficiency of $\hat{\xi}_2$ relative to the optimal exact design would be even higher, but for the problem of this size, it is infeasible to compute the optimal exact design by a complete enumeration.

In the following example, we demonstrate for various values of $v$, $n$, $d$ that the simplex method provides optimal approximate designs with small support.

**Example 3.** Consider an experiment of performing trials in a time sequence which aims at comparing treatments with control and the observed values are subject to a polynomial
time trend
\[ Y_i = \tau_{u(i)} + \theta_0 p_0(t(i)) + \theta_1 p_1(t(i)) + \ldots + \theta_D p_D(t(i)) + \varepsilon_i, \quad i = 1, \ldots, n, \]
where \( p_0, \ldots, p_D \) are discrete orthogonal polynomials of degrees 0, \ldots, \( D \), respectively, i.e.,
\[ \sum_t p_i(t)p_j(t) = 0 \text{ for } i \neq j. \]
Furthermore, we set \( p_0 \equiv 1 \) and \( p_i(1) = 1 \) for all \( i \). Note that although the total number of time trend parameters is \( d = D + 1 \), the term \( \theta_0 p_0(t) = \theta_0 \) represents the constant term and thus, from Proposition 6 it follows that there are at most \( n + (v-1)(D+1) \) linearly independent rows of \( A \) in (15).

For varying \( v, n \) and \( D \), we calculated an A-optimal design for estimating \((-v-1, I_{v-1})\tau\) using the simplex method and we compared the size of its support with the minimum size of the support and with the theoretically derived bounds given by Proposition 6 (see Table 2).

| \( v \) | \( n \) | \( D \) | Simplex | Max. Simplex |
|---|---|---|---|---|
| 3 | 120 | 1 | 124 (4) | 124 |
| 3 | 150 | 1 | 154 (4) | 154 |
| 3 | 200 | 1 | 204 (4) | 204 |
| 4 | 120 | 1 | 126 (6) | 126 |
| 5 | 120 | 1 | 128 (8) | 128 |
| 8 | 120 | 1 | 134 (14) | 134 |
| 3 | 120 | 2 | 126 (6) | 126 |
| 3 | 120 | 3 | 128 (8) | 128 |
| 3 | 120 | 4 | 130 (10) | 130 |
| 3 | 120 | 5 | 132 (12) | 132 |

Table 2: The size of the support. For a given number of treatments \( v \), number of times \( n \) and degree of the time trend \( D \), the column Simplex contains the size of the support of the design calculated using the simplex method (and the number of support points over the minimum size of the support, \( n \), in parentheses); the column Max. Simplex contains the theoretical bound on the maximum number of support points given by Proposition 6. Note that for each of the studied cases the theoretical bound on the support has been exactly achieved.

Example 4. Consider the model given by [4]. We have a blocking experiment of \( b \) blocks, each of size \( l \), where the response of a trial is also influenced by a common trend effect determined by the position of the unit within the block. In each block, there is exactly one trial performed on each position. Moreover, the trend effect in position \( t_2(i) \) does not depend on the particular block \( t_1(i) \). We have
\[ Y_i = \tau_{u(i)} + \eta_{t_1(i)} + p^T(t_2(i))\varphi + \varepsilon_i, \quad i = 1, \ldots, n, \tag{16} \]
where \( t_1(i) \in \{1, \ldots, b\} \) is the block in which trial \( i \) is performed, \( \eta_{t_1} \) is the effect of the \( t_1 \)-th block, \( t_2 \in \{1, \ldots, l\} \) denotes the position of the unit within the block, \( n = bl \), \( \varphi \) is a \((D + 1) \times 1\) vector of nuisance trend effects and \( p : \mathbb{R} \rightarrow \mathbb{R}^{D+1} \) is a regression function of the nuisance trend.

Assume that \( v = 3 \), \( b = 3 \) and \( l = 8 \), \( n = 3 \times 8 = 24 \) and that the time trend is modelled by discrete orthogonal polynomials \( p_0, p_1, p_2 \) of degrees 0, 1, 2, i.e., \( D = 2 \). We aim to find an \( E \)-optimal design for comparing treatments with control, i.e., for estimating \((-1, I_{v-1})\tau\).

The optimal weight of the first treatment is \( \gamma^* = \frac{1}{2} \) and the optimal weights of the other two are \( \frac{1}{4} \).

The conditions (ii) in \( A \) can be expressed as two sets of conditions: (ii.a) \((v - 1)b\) conditions \( w_0^{-1} \sum_{t_2} \xi(1, t_1, t_2) = w_0^{-1} \sum_{t_2} \xi(u, t_1, t_2) \) for \( u = 2, \ldots, v \) and \( t_1 = 1, \ldots, b \), and (ii.b) \((v - 1)(D + 1)\) conditions \( w_0^{-1} \sum_{t_1, t_2} \xi(1, t_1, t_2)p(t_2) = w_0^{-1} \sum_{t_1, t_2} \xi(u, t_1, t_2)p(t_2), \ u = 2, \ldots, v. \)

By summing (ii.a) over all \( t_1 \), and using the fact that \( \sum \xi(u, t) = 1 \), we obtain (i), which reduces the number of linearly independent rows in \( A \) by \( v \). Similarly to Proposition 6, using (i), it follows that there are at most \((v - 1)(b + r) + n - 1\) linearly independent rows in \( A \), where \( r \) is the affine dimension of the set \( \{p(t_2)\}_{t_2} \). Since \( p_0\varphi_0 \) represents the constant term, the number of linearly independent rows in \( A \) is at most \((v - 1)(b + D) + n - 1 = 33 \). The minimum number of support points is \( n = 24 \).

Using the simplex method, we obtained an \( E \)-optimal balanced approximate design \( \xi^* \), see Table 3. The design \( \xi^* \) has the support of size 30, which exceeds the minimum support size by 6, and it is fixed in 18 out of the 24 positions.

| block | \( u \setminus t \) | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|-------|----------------|---|---|---|---|---|---|---|---|
| 1     | 1              | 0.0417 | 0 | 0.0417 | 0 | 0.0417 | 0 | 0.0417 | 0 |
| 2     | 0              | 0.0417 | 0 | 0 | 0 | 0 | 0.0417 | 0 | 0 |
| 3     | 0              | 0 | 0 | 0 | 0.0417 | 0 | 0 | 0 | 0.0417 |
| 2     | 1              | 0.0417 | 0.0417 | 0 | 0.0324 | 0 | 0.0417 | 0.0093 | 0 |
| 2     | 0 | 0 | 0 | 0 | 0.0417 | 0 | 0 | 0 | 0.0417 |
| 3     | 0 | 0 | 0.0417 | 0.0093 | 0 | 0 | 0.0324 | 0 | 0 |
| 3     | 1 | 0.0046 | 0 | 0.0083 | 0 | 0.0417 | 0.0417 | 0.0370 | 0.0333 |
| 2     | 0 | 0.0417 | 0.0333 | 0 | 0 | 0 | 0 | 0.0083 |
| 3     | 0.0370 | 0 | 0 | 0.0417 | 0 | 0 | 0.0046 | 0 | 0 |

Table 3: \( E \)-optimal balanced approximate design obtained by a simplex method for an experiment with 3 blocks, each of size 8, and a common trend effect.

By a complete enumeration of treatments in the 8 non-fixed positions, we obtained an exact design \( \xi : b_1 = 12131213, b_2 = 11312132, b_3 = 32231111, \) where the sequence \( b_j \) determines
the treatments and their positions in block \( j \). Using Corollary \([2]\) we get that \( \xi \) has efficiency 0.9987.

### Appendix

**Lemma 1.** Let \( \tilde{M} \) be a non-negative definite matrix. If a design \( \xi \) satisfies \( M(\xi)\tilde{M}^{-1}K = K \) for some generalized inverse \( \tilde{M}^{-1} \) of \( \tilde{M} \), then (i) \( \xi \) is feasible for \( K^T \beta \) and (ii) \( K^T\tilde{M}^{-1}(\xi)K = K^T\tilde{M}^{-1}K \).

**Proof.** The steps of the proof follow the proof of Theorem 8.13 from \([20]\). We denote \( G := \tilde{M}^{-1} \). Since \( M(\xi)GK = K \), we obtain \( M(\xi)X = K \), where \( X = GK \). Therefore \( C(K) \subseteq C(M(\xi)) \) and hence \( \xi \) is feasible. Let us premultiply the equation \( M(\xi)GK = K \) by \( K^{-T}\tilde{M}^{-1}(\xi) \) so that we obtain on the right-hand side \( K^{-T}\tilde{M}^{-1}(\xi)K \). The left-hand side is then equal to \( K^T\tilde{M}^{-1}(\xi)M(\xi)GK \). Note that \( K^T = X^T M^T(\xi) = X^T M(\xi) \) and hence the following holds

\[
K^T\tilde{M}^{-1}(\xi)M(\xi)GK = X^T M(\xi)\tilde{M}^{-1}(\xi)M(\xi)GK = X^T M(\xi)GK = K^T G K.
\]

It follows that \( K^T \tilde{M}^{-1}(\xi)K = K^T \tilde{M}^{-1}K \).

**Lemma 2.** Let \( w > 0 \) be a treatment proportions design and let \( G := \text{diag}(w^{-1}, 0_d) \). Let \( \xi \) be a design in model \([7]\), then \( \xi \) satisfies \( M(\xi)GK = K \) if and only if (i) \( w \) is a treatment proportions design of \( \xi \) and (ii) \( \xi \) is resistant to nuisance effects.

**Proof.** We may express \( MGK = K \) as \( M_{11}\text{diag}(w^{-1})Q = Q \) and \( M_{12}\text{diag}(w^{-1})Q = 0 \). Since both \( M_{11} \) and \( \text{diag}(w^{-1}) \) are diagonal matrices, the first equation is equivalent to \( \frac{1}{w_u} \sum_u \xi(u) = 1 \) for all \( u \), which is (i). From the second equation, we obtain that every row of \( M_{12}\text{diag}(w^{-1}) \) needs to be in \( \mathcal{N}(Q^T) \), which is (ii).

**Proof of Proposition \([2]\)**

Let \( M^* := \text{diag}(w, 0^T_d) \). Then, \( G := \text{diag}(w^{-1}, 0^T_d) \) is a generalized inverse of \( M^* \). From Lemma \([2]\) it follows that \( M(\xi)GK = K \) and from Lemma \([1]\) it follows that (i) and (ii) hold. The statement (iii) is a direct consequence of (ii).

**Lemma 3 (Theorem 8.13 from \([20]\)).** Let \( \Phi \) be a strictly concave information function and let \( \xi^* \) be \( \Phi \)-optimal for \( K^T \beta \). Let \( G \) be a generalized inverse of \( M(\xi^*) \) that satisfies the normality inequality of the General Equivalence Theorem (Theorem 7.14 from \([20]\)), i.e., there exists a non-negative definite matrix \( D \) that solves the polarity equation

\[
\Phi(N_K(\xi^*))\Phi^\infty(D) = \text{tr}(CD) = 1,
\]

as required.

22
where $\Phi^\infty$ is the polar information function of $\Phi$ (see [20]), and $G$ satisfies the normality inequality

$$\text{tr}(M(\xi)B) \leq 1 \quad \text{for all feasible designs } \xi,$$

where $B = GKN_K(\xi^*)DN_K(\xi^*)K^TG^T$. Then, a design $\xi$ is $\Phi$-optimal if and only if $M(\xi)GK = K$.

In order to use Lemma 3 we need to obtain a matrix $G$ that satisfies the normality inequality of the General Equivalence Theorem.

**Lemma 4.** Let $w^*$ be a $\Phi$-optimal treatment proportions design and let $G := \text{diag}((w^*)^{-1}, 0_d)$. Then, $G$ satisfies the normality inequality of the General Equivalence Theorem for estimating $K^T\beta$ in model (1).

**Proof.** Let us denote $N^* := N_Q(w^*)$ and $G_{11} := \text{diag}((w^*)^{-1})$. Since $w^*$ is optimal in (3), the matrix $G_{11}$ that is the unique generalized inverse of $M(w^*)$, satisfies normality inequality of the General Equivalence Theorem for model (3), i.e. there exists a matrix $D$ which satisfies the polarity equality $\Phi(N^*)\Phi^\infty(D) = \text{tr}(N^*D) = 1$ and the matrix $B_w = G_{11}Q N^* D N^* Q^T G_{11}$ satisfies the normality inequality $\text{tr}(M(\tilde{w})B_w) \leq 1$ for all $\tilde{w}$.

There exists a unique $\Phi$-optimal information matrix $N_K(\xi^*)$, because $\Phi$ is strictly concave. Since $N_K(w^* \otimes \alpha) = N_Q(w^*) = N^*$ is $\Phi$-optimal, we have $N_K(\xi^*) = N^*$. Thus, the polarity equality holds in model (1) for the same matrix $D$. Let $\tilde{\xi}$ be a feasible design. Then, the left-hand side of the normality inequality in model (1) is $\text{tr}(M(\tilde{\xi})B_w)$, where

$$B = \begin{bmatrix} G_{11} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} Q \\ 0 \end{bmatrix} N^* D N^* \begin{bmatrix} Q^T & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} G_{11} & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} B_w & 0 \\ 0 & 0 \end{bmatrix}.$$

Then, because $B_w$ satisfies the normality inequality in model (3), we obtain $\text{tr}(M(\tilde{\xi})B_w) = \text{tr}(M_{11}(\tilde{\xi})B_w) = \text{tr}(M(\tilde{\xi})B_w) \leq 1$, where $\tilde{w}$ is the treatment proportions design of $\tilde{\xi}$. □

**Proof of Theorem 3**

Let $G = \text{diag}((w^*)^{-1}, 0_d)$. From Lemma 4 it follows that $G$ satisfies the normality inequality of the General Equivalence Theorem. Lemma 4 yields that a design $\xi$ is $\Phi$-optimal if and only if $M(\xi)GK = K$. The equality $M(\xi)GK = K$ holds if and only if $\xi$ satisfies (i) and (ii) from Lemma 2. □

**Proof of Theorem 5**

For clarity, we will write $\gamma$ instead of $\gamma_p$. Using Theorem 4 it is sufficient to prove the optimality of $w_\gamma$ in model (3). The optimality may be proven using Equivalence Theorem for
\( \Phi_p \) criteria (see Sections 7.20 and 7.22 in [20]), i.e., for \( p \in (\mathbb{R}, 0] \), we will prove that there exists a generalized inverse \( G \) of \( M(w_\gamma) \) such that it satisfies the normality inequality

\[
f^T(u, t)GQN_Q^{p+1}(w_\gamma)Q^TGf(u, t) \leq \text{tr}(N_Q^p(w_\gamma)) \quad \text{for all } u, t.
\]

For \( p = -\infty \), we will find a generalized inverse \( G \) of \( M(w_\gamma) \) and a non-negative definite matrix \( E \) that satisfies \( \text{tr}(E) = 1 \) such that they satisfy the normality inequality

\[
f^T(u, t)GQ\mathcal{N}_Q(w_\gamma)EN_Q(w_\gamma)Q^TGf(u, t) \leq \lambda_{\min}(N_Q^p(w_\gamma)) \quad \text{for all } u, t.
\]

The moment matrix of \( w_\gamma \) is \( M(w_\gamma) = \text{diag}(\gamma, \frac{1-\gamma}{v}1_{v-1}^T) \) and we set \( G = \text{diag}(1/\gamma, \frac{v-1}{1-\gamma}1_{v-1}^T) \). By direct calculation, we obtain that the information matrix of \( p \)

\[
\gamma = 1/2, \quad \lambda_1 = \frac{1}{v-2}, \quad \text{and } \lambda_2 = \gamma \frac{v-2}{v-1} \text{ with multiplicity } v-2.
\]

Furthermore, it is possible to show that

\[
N_Q^{p+1} = \lambda_1^{p+1}I_{v-1} + \frac{-\lambda_1^{p+1} + \lambda_2^{p+1}}{v-1}J_{v-1}.
\]

Let \( p \in (\mathbb{R}, 0] \). Since \( \gamma \) satisfies (6), it also satisfies \( \gamma^{p-1} = \frac{v-2}{1-2\gamma} \). Hence, the right hand side of the normality inequality is

\[
R := \text{trace}(N_Q^p) = (v-2)\lambda_1^p + \lambda_2^p = \left(\frac{1-\gamma}{v-1}\right)^p(v-2 + \gamma^p) = \left(\frac{1-\gamma}{v-1}\right)^p(v-2)(1-\gamma)\frac{1-\gamma}{1-2\gamma}.
\]

For \( u \in \{1, \ldots, v\} \), the left hand side of the normality inequality is \( L_u := e_u^T GQN_Q^{p+1}Q^TG e_u \), the \( u \)-th diagonal element of \( GQN_Q^{p+1}Q^TG \). Therefore, using (9), we obtain

\[
L_u = \frac{1}{\gamma^2(v-1)}\left(\frac{\gamma(1-\gamma)}{v-1}\right)^{p+1} = \left(\frac{1-\gamma}{v-1}\right)^p(1-\gamma)\gamma^{p-1} = R
\]

for \( u = 1 \) and

\[
L_u = \left(\frac{1-\gamma}{v-1}\right)^{p-1}v-2 + \gamma^{p+1} \frac{1}{v-1} = \left(\frac{1-\gamma}{v-1}\right)^p \frac{1-\gamma}{1-\gamma} \frac{1-\gamma}{1-2\gamma}(v-2 + \gamma^{p+1}) \]

\[
eq \left(\frac{1-\gamma}{v-1}\right)^p \frac{v-2}{1-\gamma} \frac{(1-\gamma)^2}{(1-\gamma)(1-2\gamma)} = R
\]

for \( u > 1 \). That is, we obtained equality in the normality inequalities, which was to be expected, because some optimal designs (product designs with optimal weights) have support points in all design points \((u, t)\). This only proves the optimality for \( v > 2 \). For \( v = 2 \) we have from (9) the optimal \( \gamma = 1/2 \) and the proof is analogous.

For \( p = -\infty \), we have \( \gamma = 1/2 \) and we set \( E = \frac{1}{v-1}J_{v-1} \). The left hand side of the normality inequality is then equal to \( \frac{1}{2(v-1)} \) for both \( u = 1 \) and \( u > 1 \), which is equal to the right hand side. Again, as expected, the inequality is always attained as an equality. \( \square \)
Lemma 5. Let \( Q \) be a maximal system of orthonormal contrasts, \( w > 0 \) be a design for model \([3]\) and let \( P \) be a \( v \times v \) permutation matrix. Then, the matrices \( Q^T M^{-1}(w)Q \) and \( Q^T P M^{-1}(w)P^T Q \) are orthogonally similar.

**Proof.** We will use the well-known fact that if \( X \) is any matrix, the non-zero eigenvalues of the matrices \( X^T X \) and \( XX^T \) are the same (see \([22]\)), including multiplicities; therefore, \( X^T X \) and \( XX^T \) are orthogonally similar. Define \( Y = Q^T M^{-1/2}(w) \) and \( Z = Q^T P M^{-1/2}(w) \). Clearly,

\[
Y^T Y = M^{-1/2}(w) Q Q^T M^{-1/2}(w) = M^{-1/2}(w) (I_v - J_v / v) M^{-1/2}(w) = M^{-1/2}(w) P^T (I_v - J_v / v) P M^{-1/2}(w) = M^{-1/2}(w) P^T Q Q^T P M^{-1/2}(w) = Z^T Z.
\]

We can conclude the proof by observing that \( YY^T = Q^T M^{-1}(w)Q \) and \( ZZ^T = Q^T P M^{-1}(w)P^T Q \).

**Proof of Theorem 6**

For any treatment proportions design \( w \) and a \( v \times v \) permutation matrix \( P \), we define \( Pw \) to be a design given by the \( P \)-permutation of treatments in \( w \), i.e., \( Pw(u) = w(\pi_P(u)) \) for \( u \in \{1, \ldots, v\} \), where \( \pi_P \) is the permutation of elements \( \{1, \ldots, v\} \) corresponding to the matrix \( P \). Let \( w > 0 \) be a feasible treatment proportions design. Then, \( Pw > 0 \) is feasible and it has information matrix \( N_Q(Pw) = (Q^T M^{-1}(Pw)Q)^{-1} = (Q^T P M^{-1}(w)P^T Q)^{-1} \). From Lemma 5 it follows that \( N_Q(Pw) \) is orthogonally similar to \( (Q^T M^{-1}(w)Q)^{-1} = N_Q(w) \). Hence, \( \Phi(Pw) = \Phi(w) \).

The uniform treatment proportions design satisfies

\[
\Phi(\bar{w}) = \Phi \left( \frac{1}{v!} \sum_{P-\text{perm.}} Pw \right) \geq \frac{1}{v!} \sum_{P-\text{perm.}} \Phi(Pw) = \frac{1}{v!} \sum_{P-\text{perm.}} \Phi(w) = \frac{1}{v!} v! \Phi(w) = \Phi(w),
\]

where the inequality follows from the concavity of \( \Phi \). Thus, \( \bar{w} \) is \( \Phi \)-optimal. From Theorem 2 it follows that any balanced design \( \xi \) with treatment weights \( \bar{w} \) is \( \Phi \)-optimal.

**Proof of Theorem 7**

The matrix \( Q = I_v - J_v / v \) satisfies \( QP = PQ \) for \( v \times v \) permutation matrix \( P \). Let \( w > 0 \) be a feasible treatment proportions design. Then, the design \( Pw > 0 \) has the matrix \( C_Q(Pw) = (Q^T M^{-1}(Pw)Q)^+ = (Q^T P M^{-1}(w)P^T Q)^+ = (PQ^T M^{-1}(w)Q P^T)^+ = P(Q^T M^{-1}(w)Q)^+ P^T = P C_Q(w) P^T \). Thus, \( \Phi(Pw) = \Phi(w) \). Analogously to the proof of
Theorem 6, we obtain the optimality of $\bar{w}$ and from Theorem 2 it follows that any balanced design $\xi$ with treatment weights $\bar{w}$ is $\Phi$-optimal.

Lemma 6. Let $l, m \in \mathbb{N}$, let $\xi_p$ be an exact design of size $l$ and let $\xi = \xi_p \xi_p \ldots \xi_p$ be the exact design of size $n = lm$ formed by an $m$-fold replication of $\xi_p$. Assume that $a \in \mathbb{N}$ is not an integer multiple of $m$. Then, $\xi$ is balanced for the nuisance regressors of the form $\cos(a \phi_n t)$ and $\sin(a \phi_n t)$, $t = 1, \ldots, n$.

Proof. Let $u \in \{1, \ldots, v\}$. Using the fact that $\xi(u, k + lj) = \xi_p(u, k)$ for all $k \in \{1, \ldots, l\}$ and $j \in \{0, \ldots, m-1\}$, we obtain

$$\sum_{t=1}^{n} \xi(u, t) \cos(a \phi_n t) + i \sum_{t=1}^{n} \xi(u, t) \sin(a \phi_n t) = \sum_{t=1}^{n} \xi(u, t) e^{a \phi_n t i}$$

$$= \sum_{j=0}^{m-1} \sum_{k=1}^{l} \xi(u, k + lj) e^{a \phi_n (k + lj) i} = \left( \sum_{k=1}^{l} \xi_p(u, k) e^{a \phi_n k i} \right) \left( \sum_{j=0}^{m-1} e^{a \phi_n (lj) i} \right).$$

Note that if $a$ is not an integer multiple of $m$ then $a \phi_n l = 2\pi (a/m)$ is not an integer multiple of $2\pi$, which implies $e^{a \phi_n t i} \neq 1$. In that case

$$\sum_{j=0}^{m-1} e^{a \phi_n (lj) i} = \frac{1 - e^{a 2\pi i}}{1 - e^{a \phi_n t i}} = 0.$$ 

Proof of Proposition 6

It is well known that a point $x$ is a vertex of the set $\{x | Ax = b, x \geq 0\}$ if and only if the system $\{A_j | x_j > 0\}$, where $A_j$ is the $j$-th column of $A$, has full rank.

The matrix $A$ consists of $v + (v - 1)d + n$ rows, but they are linearly dependent. Let $k$ be the affine dimension of $\{h(t)\}_{t \in \mathbb{F}}$ and, without the loss of generality, let $\mathbb{F} = \{1, \ldots, n\}$. Then, the matrix $[h(2) - h(1), \ldots, h(n) - h(1)]$ has rank $k$ and thus its row space has dimension $k$.

That is, without the loss of generality, we obtain that $h_i(t) - h_i(1) = \sum_{j=1}^{k} c_j^{(i)} (h_j(t) - h_j(1))$ for some $c_1^{(i)}, \ldots, c_k^{(i)} \in \mathbb{R}$, for $i > k$ and $t \in \{1, \ldots, n\}$ (for $t = 1$, we formally get $0 = 0$). Let $u \in \{1, \ldots, v\}$. Then, if (ii) is satisfied in the first $k$ coordinates of $h$, i.e., for $h_1, \ldots, h_k$, we
have for all \( i > k \) and \( u \in \{1, \ldots, v\} \)

\[
\begin{align*}
    w_1^{-1} \sum_t \xi(1,t)h_i(t) &= w_1^{-1} \left( h_i(1) - \sum_{j=1}^k c_j^{(i)} h_j(1) \right) \sum_t \xi(1,t) + \sum_{j=1}^k c_j^{(i)} w_1^{-1} \sum_t \xi(1,t) h_j(t) \\
    &= h_i(1) - \sum_{j=1}^k c_j^{(i)} h_j(1) + \sum_{j=1}^k c_j^{(i)} w_1^{-1} \sum_t \xi(u,t) h_j(t) \\
    &= w_u^{-1} \sum_t \xi(u,t) \left( h_i(1) - \sum_{j=1}^k c_j^{(i)} h_j(1) \right) + \sum_{j=1}^k c_j^{(i)} w_u^{-1} \sum_t \xi(u,t) h_j(t) \\
    &= w_u^{-1} \sum_t \xi(u,t) \left[ \left( h_i(1) - \sum_{j=1}^k c_j^{(i)} h_j(1) \right) + \sum_{j=1}^k c_j^{(i)} h_j(t) \right] \\
    &= w_u^{-1} \sum_t \xi(u,t) h_i(t),
\end{align*}
\]

where the second and the third equality hold because of (i). It follows that (ii) provides at most \( k(v-1) \) additional linearly independent equalities.

If \( \xi \) satisfies (i), it holds that \( \sum_{u,t} \xi(u,t) = 1 \). Thus, if \( \xi \) satisfies (iii) for \( t = 1, \ldots, n-1 \), we have \( 1 = \sum_{t=1}^{n-1} \sum_u \xi(u,t) + \sum_u \xi(u,n) = \frac{n-1}{n} + \sum_u \xi(u,n) \) and therefore (iii) holds also for \( t = n \). That is, (iii) provides only \( n-1 \) additional linearly independent equalities. Hence, the rank of \( A \) is at most \( v + (v-1)k + n-1 \) and a vertex \( x \) contains at most \( v + (v-1)k + n-1 \) support points.

References

[1] Atkinson, A. C., Donev, A. N.: Experimental design optimally balanced for trend, Technometrics 38(4) (1996), pp. 333-341

[2] Bailey, R.A., Williams E.R.: Optimal nested row-column designs with specified components, Biometrika 94 (2007), pp. 459 – 468

[3] Bailey, R.A., Cheng, C.-S., Kipnis, P.: Construction of Trend-Resistant Factorial Designs, Statistica Sinica 2 (1992), 393-411

[4] Bradley, R.A., Yeh C.M.: Trend-Free Block Designs: Theory, The Annals of Statistics 8 (1980), pp. 883-893

[5] Cheng, C.-S.: Construction of Run Orders of Factorial Designs, Statistical Design and Analysis of Industrial Experiments (1990), Marcel-Dekker, New York, pp. 423-439
[6] Cox, D.R.: Some systematic experimental designs, *Biometrika* 38(3/4) (1951), pp. 312-323

[7] Cox, D.R., Reid, N.: *Theory of the Design of Experiments*, Chapman and Hall, London, 2000

[8] Fieller, E. C.: Some remarks on the statistical background in bioassay, *Analyst* 72 (1947), pp. 37-43.

[9] Harman, R.: Minimal efficiency of designs under the class of orthogonally invariant information criteria, *Metrika* 60 (2004), pp. 137-153

[10] Harman, R., Sagnol, G.: Computing D-Optimal Experimental Designs for Estimating Treatment Contrasts Under the Presence of a Nuisance Time Trend, *Stochastic Models, Statistics and Their Applications*, Springer Proceedings in Mathematics & Statistics 122 (2015), pp. 83-91

[11] Majumdar, D.: Optimal and efficient treatment-control designs, *Handbook of statistics 13: Design and Analysis of Experiments* (1996), pp. 1007-1053.

[12] Majumdar, D., Notz, W.I.: Optimal Incomplete Block Designs for Comparing Treatments with a Control, *The Annals of Statistics* 11 (1983), pp. 258-266

[13] Jacroux, M.: Some E-Optimal Designs for the One-way and Two-way Elimination of Heterogeneity, *Journal of the Royal Statistical Society* 44 (1982), pp. 253-261

[14] Jacroux, M., Majumdar, D., Shah, K.R.: On the Determination and Construction of Optimal Block Designs in the Presence of Linear Trends, *Journal of the American Statistical Association* 92 (1997), pp. 375–382

[15] Jacroux, M., Ray, R. S.: On the construction of trend-free run orders of treatments, *Biometrika* 77 (1990), pp. 187-191

[16] Kitsos, C. P., Titterington, D. M., Torsney, B.: An optimal design problem in rhythmometry, *Biometrics* 44 (1988), pp. 657-671.

[17] Kunert, J.: Optimal Design and Refinement of the Linear Model with Applications to Repeated Measurements Designs, *The Annals of Statistics* 11 (1983), pp. 247-257

[18] Kunert, J., Martin R. J., Eccleston J.: Optimal block designs comparing treatments with a control when the errors are correlated *Journal of Statistical Planning and Inference* 140 (2010), pp. 2719-2738

28
[19] Morgan, J. P., Wang, X.: E-optimality in treatment versus control experiments, *Journal of Statistical Theory and Practice* 5(1) (2011), pp. 99-107

[20] Pukelsheim, F.: *Optimal design of experiments*, Classics in Applied Mathematics, SIAM, 2006

[21] Pukelsheim, F.: On optimality properties of simple block designs in the approximate design theory, *Journal of statistical planning and inference* 8 (1983), pp. 193-208

[22] Seber, G. A.: *A Matrix Handbook for Statisticians*, John Wiley & Sons, 2008.

[23] Schwabe, R.: Optimal Designs for Additive Linear Models, *Statistics* 27 (1996), pp. 267-278

[24] Wu, C. F.: On Some Ordering Properties of the Generalized Inverses of non-negative Definite Matrices, *Linear Algebra and its Applications* 32 (1980), pp. 49-60