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Optimal Designs on Undirected Network Structures for Network-Based Models

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ABSTRACT

With the rapid growth of social network services, network-related studies have become a burgeoning research area. Allocating a treatment to a unit affects the unit as well as its neighbors, simultaneously resulting in a treatment effect and a network effect. In the literature of experimental designs, Parker, Gilmour, and Schormans (2017) and Chang, Phoa, and Huang (2021) both adopted a linear network effect model to design experiments on general networks. However, this model has not been heavily recognized yet. Kolaczyk and Csárdi (2014) reviewed statistical models for network graphs such as exponential random graph models and network block models. Zhang *et al.* (2020) considered a network-based logistic regression model to describe the network effect. In this article, we propose a new statistical model for networks in the same spirit as Kolaczyk and Csárdi (2014) and Zhang *et al.* (2020). Moreover, we derive conditions for selecting optimal designs and illustrate our theory through simulations and real examples.

Key words and phrases: Social network, Treatment effect, Network effect, Network modeling, Bipartite/Cycle/Path graph, D-optimality.

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1. Introduction

In the 21st century, with the rapid development of the Internet, it has been more common for people to meet a group of friends with common interests in virtual worlds such as Facebook, Twitter, or Instagram. Some people set up online shopping companies, making it easier for people to have different shopping options. These interpersonal relationships and user behaviors can be described through social networks and recommendation networks. In practice, examples of network structures are ubiquitous, such as in agricultural experiments, bioinformatics, medical experiments, machine learning, physics, social sciences, and many other scientific fields.

Most of the literature on networks focuses on modeling, parameter estimation, prediction and inference, but rarely discusses designing experiments. Moreover, many statistical theories for designing experiments have assumed that the experimental units are uncorrelated. Recently, some related works have been proposed. In the field of experimental design, the nodes in networks represent experimental units. The edges represent the connections between experimental units. If two experimental units (nodes) are connected, one is called a neighbor of the other. Besides, a treatment affects both the unit to which it is applied and the neighbors of that unit. These effects are called *treatment effects* and *network effects*, respectively. Parker, Gilmour, and Schormans (2017) and Chang, Phoa, and Huang (2021) both adopted a linear network effect model to design experiments with unstructured treatments on general undirected networks. The difference is that Parker, Gilmour, and Schormans (2017) regarded the network effects as fixed effects, while Chang, Phoa, and Huang (2021) modeled them as random effects. However, this model has not been heavily recognized yet. Therefore, we are devoted to proposing a new statistical model for networks in this article, which incorporates the concept of the network literature. Additionally, we discuss design issues under the new model.

The rest of this article is organized as follows. In Section 2, we review the literature of some popular network modeling methods as well as the experiments with network structures. In Section 3, we set up a novel statistical model, illustrate the optimality criterion, and present some results of theoretical conditions for optimal designs. In

Section 4, numerical examples for specific graphs and their real applications are given, such as bipartite graphs, path graphs, and cycle graphs. Three real networks are investigated in Section 5. At last, some concluding remarks are given in Section 6.

2. Literature Review

In the last century, researchers in different fields have been enthusiastic about network studies, so the literature about networks has been burgeoning. In the field of statistics, exponential random graph models (ERGMs) are one of the most popular network modeling methods. ERGMs are similar to generalized linear models, while ERGMs use many metrics, such as the degree, density, and centrality, to describe the structural features of a network.

ERGMs were first proposed by Holland and Leinhardt (1981) and further developed by Frank and Strauss (1986). Meanwhile, Frank and Strauss (1986) proposed Markov random graph models, which was the mainstay of ERGMs. However, the Markov random graph model had been rarely adopted by researchers until Wasserman and Pattison (1996) extended it to p^* *models*, which became the ERGMs applied for social networks. The log-linear form of the p^* models facilitated extensions of the original basic framework, resulting in models for different types of data, such as multivariate network data (Wasserman and Pattison, 1999), valued network data (Robins, Pattison, and Wasserman, 1999), and bipartite network data (Skvoretz and Faust, 1999).

Nowadays, ERGMs have become a powerful network modeling method and have been widely explored. Social selection (Robins, Elliott, and Pattison, 2001a) and social influence (Robins, Pattison, and Elliott, 2001b) models considered actor attributes in their models. Snijders (2002) offered a numerical method for estimating the parameters of the ERGM using the Markov chain Monte Carlo (MCMC) methods, such as the Gibbs sampling and the Metropolis-Hastings sampling. Almquist and Butts (2014) showed how to extend a logistic network regression approach to serve as a framework for modeling large networks with dynamic vertex sets. Jiao *et al.* (2017) used ERGMs to analyze the subjective well-being of teenagers under peer relationship networks and to draw the conclusion that there exist positive reciprocal effects, positive transitivity effects, and negative expansiveness effects.

In addition to ERGMs, *network block models* are also a type of popular network modelings with many applications. When the nodes are divided into subgroups based on their attributes, the density of ties from one subgroup to another could be quite different. It means that the graph contains communities, which are characterized by interconnected subsets with specific edge densities. For example, edges within communities may have a higher probability to be connected than those between communities. Thus, the notion of "blocking" appeared in social networks.

The first simple block model was proposed by Fienberg and Wasserman (1981). Wang and Wong (1987) modified it and then proposed a p_1 *block model* involving the nodal attributes as well as the individual nodes. Nowicki and Snijders (2001) initiated a statistical approach to a posteriori block modeling for digraphs and valued digraphs. They assumed that the probability distribution of the relation between two nodes only depends on the latent classes to which they belong and the relations are conditionally independent on these classes. Karrer and Newman (2011) demonstrated how to generalize the block model when missing elements exist, in order to improve the objective function for community detections. Kolaczyk and Csárdi (2014) provided an extensive review to different statistical analyses of network data (e.g., visualization, network modeling, static and dynamic network process, and so on), in use of the R programming language (R Core Team, 2020).

Different from the two network modeling methods mentioned above, which regard the edges of the network as responses, Zhang *et al.* (2020) initiated a *network-based logistic regression (NLR) model*. They mainly focused on how to bring the network structure into a traditional classification problem, i.e., the class label instead of the edges is the response. The NLR model assumed that whether two nodes are connected is affected by their responses and their similarity in predictors. Furthermore, attributes of each node were also used to predict class labels through the classical logistic regression model.

As mentioned above, the majority of literature about networks has focused on parameter estimation, prediction, and inference, while few discussed design experimentation. Moreover, most statistical theories for randomized experiments have assumed that experimental units are uncorrelated. Besag and Kempton (1986) described that the response of a plot is affected by the particular treatments on neighboring plots and discussed four distinct agricultural experimental applications. Druilhet (1999) investigated the optimality of circular neighbor-balanced block designs. They considered both neighbor (i.e., network) effects and treatment effects in the model.

Recently, Parker, Gilmour, and Schormans (2017) have initiated a new approach, using A_s-optimality, to design network experiments. They considered unstructured treatments and experimental units with a general network structure. They pointed out that the assumption of treatment effect additivity no longer holds because of the existence of network effects. Therefore, they proposed a *linear network effect model* in which both treatment effects and network effects were regarded as fixed effects.

Chang, Phoa, and Huang (2021) investigated a similar design problem to Parker, Gilmour, and Schormans (2017), but they assumed that network effects were random variables. They pointed out that when one experimental unit is transmitting an effect to another, this effect is possible to be perturbed by unknown noises. Besides, they provided theoretical conditions for efficiently estimating treatment effects and accurately predicting network effects. Therefore, they believed using stochastic mechanisms to model network effects is a reasonable choice even if the treatments are specified in advance.

We notice that in network modeling, the linear network effect model has been seldom applied and recognized yet. Therefore, we combine the concept of the NLR (Zhang *et al.*, 2020) and network block models in Kolaczyk and Csárdi (2014) into the design experimentation problem. As noted, the research of networks is important and beneficial to many fields, while existing research in experimental design paid little attention to general network structures. Hence, we are committed to designing experiments on networks and proposing a more appropriate statistical model.

3. Methodology

3.1 Model

Consider a network $\mathbf{G} = (\mathbf{V}, \mathbf{E})$, a collection of nodes $\mathbf{V}$ and edges $\mathbf{E} \subseteq (\mathbf{V} \times \mathbf{V})$.

The nodes represent experimental units to which some treatments are applied. The edges represent the relationships between the units. Suppose we have $|\mathbf{V}| = N$ units and m treatments. We assume that each unit receives exactly one treatment. Let $\mathbf{U} = (U_1, \ldots, U_N)^T$ be an $N \times m$ unit-treatment incidence matrix with $[\mathbf{U}]_{ij} = 1$ if the ith node receives the jth treatment and zero otherwise. In each row of $\mathbf{U}$, i.e., U_i^T, there is exactly one non-zero element.

Let $\mathbf{Y} = (y_1, \ldots, y_N)^T \in \mathbb{R}^N$ be the vector of responses, where y_i is the response of the ith node. Given the network and $\mathbf{U}$, the relationship between the treatments and the responses is modeled by

$$\mathbf{Y} = \mathbf{U}\boldsymbol{\alpha} + \boldsymbol{\varepsilon}, \tag{1}$$

where $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_m)^T$ is the m-dimensional vector of treatment effects and the error term $\boldsymbol{\varepsilon}$ is normally distributed with zero mean and covariance matrix $\sigma^2 \mathbf{I}_N$. We assume the treatment effects $\boldsymbol{\alpha}$ to be unknown constants. In addition to the treatment effects, we assume that there exist network effects due to the relationship between units, where their responses are correlated and depend on the treatments applied to them. To describe the network structure, the relationship between units is represented by an $N \times N$ adjacency matrix $\mathbf{A}$ where $[\mathbf{A}]_{ik} = 1$ if and only if unit i and unit k are connected, and zero otherwise. Following the convention, we set $[\mathbf{A}]_{ii} = 0$. For simplicity, we assume that edges are undirected. Therefore, $\mathbf{A}$ is a symmetric matrix, i.e., $[\mathbf{A}]_{ik} = [\mathbf{A}]_{ki}$.

Following Zhang *et al.* (2020), we express our network effects similar to the random graph logistic model, where the probability of a connection between pairs of vertices depends on their treatments, i.e., $[\mathbf{A}]_{ij}$s are random variables. In practical applications, the network structure is observed from the data; each $[\mathbf{A}]_{ij}$ is fixed at zero or one. Our model assumes that whether two nodes are connected is influenced by their similarity in treatments as well as the overall treatment-connection pattern of the network.

Let $L_{t(i)t(j)}$ be the number of observed edges in the network connecting pairs of vertices with treatment $t(i)$ and $t(j)$, where $t(i)$ and $t(j)$ are the treatments applied to unit i and unit j, and $L_{t(i)t(j)} = L_{t(j)t(i)}$. Given $\mathbf{U}$, we assume the edges are independent random variables, i.e., $[\mathbf{A}]_{ij}$s are independent, such that

$$P([\mathbf{A}]_{ij} = 1 | U_i, U_j) = \frac{\exp(s_{ij} + \phi L_{t(i)t(j)})}{1 + \exp(s_{ij} + \phi L_{t(i)t(j)})} \equiv \pi_{ij}, \tag{2}$$

where $s_{ij} = U_i^T U_j$ represents the similarity of the ith node and the jth node according to their predictors and ϕ indicates the strength of blocks on the link probability. The s_{ij} in the model describes the *local patterns* of the network because it only considers the similarity of treatments between two nodes. On the other hand, the $L_{t(i)t(j)}$ reflects the *global patterns* of the network. We note that $\sum_{i\leq j}^{m} L_{t(i)t(j)}$ is equal to the number of edges of an observed network.

The equation (2) implicitly assumes that receiving the same treatment, i.e., $s_{ij} = 1$, would result in a higher probability of connection. Similarly, when ϕ is positive, larger $L_{t(i)t(j)}$ will lead to a higher connection probability. By contrast, when ϕ is negative, larger $L_{t(i)t(j)}$ will have the opposite results. As ϕ approaches zero, the influence of $L_{t(i)t(j)}$ is getting small; that is, the connection probabilities are only determined by the local patterns of the network.

Our statistical model combines (1) and (2). Let $\boldsymbol{\theta} = (\boldsymbol{\alpha}^T, \sigma, \phi)^T$. We assume the marginal distribution of $[\mathbf{A}]_{ij}$ is irrelevant to $\boldsymbol{\theta}$, so the likelihood of $\boldsymbol{\theta}$ conditioned on $\mathbf{A}$ is proportional to

$$\begin{aligned}
\mathbb{L}(\boldsymbol{\theta}) &= P(\mathbf{Y}, \mathbf{A} | \mathbf{U}) = P(\mathbf{Y}|\mathbf{U}) P(\mathbf{A}|\mathbf{U}) \\
&= \prod_{i=1}^{N} P(y_i | U_i) \prod_{i \neq j}^{N} P([\mathbf{A}]_{ij} | U_i, U_j) \\
&= \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{1}{2\sigma^2} \left(y_i - U_i^T \boldsymbol{\alpha} \right)^2 \right] \prod_{i \neq j}^{N} \pi_{ij}^{[\mathbf{A}]_{ij}} \left(1 - \pi_{ij} \right)^{1 - [\mathbf{A}]_{ij}}.
\end{aligned}$$

3.2 Optimality Criterion

In this study, we strive for finding a design that can efficiently estimate $\boldsymbol{\theta}$ under the D-optimality (Kiefer and Wolfowitz, 1960), which is to maximize the determinant of the Fisher information matrix of $\boldsymbol{\theta}$. We begin with the log-likelihood of the parameters

$\boldsymbol{\theta}$:

$$\ell(\boldsymbol{\theta}) = -\frac{N}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}\sum_{i=1}^{N}\left(y_i - U_i^T\boldsymbol{\alpha}\right)^2$$
$$+\sum_{i=1}^{N}\sum_{j\neq i}\Big[[\mathbf{A}]_{ij}\log\pi_{ij} + (1-[\mathbf{A}]_{ij})\log(1-\pi_{ij})\Big].$$

Then we derive the Fisher information matrix. Note that $[\mathbf{A}]_{ij}$ are observed when the data is obtained. We plug in the observed $[\mathbf{A}]_{ij}$ in the computation of the information matrix. Therefore, the resulting information matrix is given as below:

$$\begin{aligned}
\mathbf{J}(\boldsymbol{\theta}) &= -\mathrm{E}\left[\nabla^2\ell(\boldsymbol{\theta})\right] \\
&= -\mathrm{E}\begin{bmatrix}
\frac{\partial^2\ell(\boldsymbol{\theta})}{\partial\alpha_1^2} & \frac{\partial^2\ell(\boldsymbol{\theta})}{\partial\alpha_1\partial\alpha_2} & \cdots & \frac{\partial^2\ell(\boldsymbol{\theta})}{\partial\alpha_1\partial\phi} \\
\frac{\partial^2\ell(\boldsymbol{\theta})}{\partial\alpha_2\partial\alpha_1} & \frac{\partial^2\ell(\boldsymbol{\theta})}{\partial\alpha_2^2} & \cdots & \frac{\partial^2\ell(\boldsymbol{\theta})}{\partial\alpha_2\partial\phi} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial^2\ell(\boldsymbol{\theta})}{\partial\phi\partial\alpha_1} & \frac{\partial^2\ell(\boldsymbol{\theta})}{\partial\phi\partial\alpha_2} & \cdots & \frac{\partial^2\ell(\boldsymbol{\theta})}{\partial\phi^2}
\end{bmatrix} \\
&= \begin{bmatrix}
\frac{n_1}{\sigma^2} & 0 & \cdots & 0 & 0 & 0 \\
0 & \frac{n_2}{\sigma^2} & \ddots & 0 & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & 0 & 0 \\
0 & 0 & \cdots & \frac{n_m}{\sigma^2} & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{2N}{\sigma^2} & 0 \\
0 & 0 & 0 & 0 & 0 & \sum_{i=1}^{N}\sum_{j\neq i}L_{t(i)t(j)}^2\pi_{ij}(1-\pi_{ij})
\end{bmatrix},
\end{aligned}$$

where n_i is the number of the experimental units which receive the ith treatments ($\sum_{i=1}^{m} n_i = N$). Thus, we have

$$\begin{aligned}
\det(\mathbf{J}(\boldsymbol{\theta})) &= \left(\prod_{i=1}^{m}\frac{n_i}{\sigma^2}\right)\times\frac{2N}{\sigma^2}\times\left[\sum_{i=1}^{N}\sum_{j\neq i}L_{t(i)t(j)}^2\pi_{ij}(1-\pi_{ij})\right] \\
&= \frac{2N}{\sigma^{2m+2}}\prod_{i=1}^{m}n_i\left[\sum_{i=1}^{N}\sum_{j\neq i}L_{t(i)t(j)}^2\pi_{ij}(1-\pi_{ij})\right]
\end{aligned}$$

$$= \frac{2N}{\sigma^{2m+2}} \prod_{i=1}^{m} n_i \left[\sum_{i=1}^{N} \sum_{j \neq i} L_{t(i)t(j)}^2 \frac{\exp(s_{ij} + \phi L_{t(i)t(j)})}{\left[1 + \exp(s_{ij} + \phi L_{t(i)t(j)})\right]^2} \right]$$

$$= \frac{2N}{\sigma^{2m+2}} \mathbf{I}_1(\boldsymbol{\theta}; \mathbf{n}) \mathbf{I}_2(\boldsymbol{\theta}),$$

where $\mathbf{n} = (n_1, \ldots, n_m)$,

$$\mathbf{I}_1(\boldsymbol{\theta}; \mathbf{n}) = \prod_{i=1}^{m} n_i,$$

and

$$\mathbf{I}_2(\boldsymbol{\theta}) = \sum_{i=1}^{N} \sum_{j \neq i} L_{t(i)t(j)}^2 \frac{\exp(s_{ij} + \phi L_{t(i)t(j)})}{\left[1 + \exp(s_{ij} + \phi L_{t(i)t(j)})\right]^2}.$$

A constraint on n_i is that $n_i > 0$; that is, every treatment must be assigned to at least one unit; otherwise $\det(\mathbf{J}(\boldsymbol{\theta})) = 0$. Since the graph has been observed, we can estimate ϕ by the maximum likelihood estimation. The likelihood equation of ϕ is given below:

$$\frac{\partial \ell(\boldsymbol{\theta})}{\partial \phi} = \sum_{i=1}^{N} \sum_{j \neq i} L_{t(i)t(j)} \left([\mathbf{A}]_{ij} - \frac{\exp(s_{ij} + \phi L_{t(i)t(j)})}{1 + \exp(s_{ij} + \phi L_{t(i)t(j)})} \right) = 0.$$

In general, $\mathbf{I}_2(\boldsymbol{\theta}) = \sum_{i=1}^{N} \sum_{j \neq i} L_{t(i)t(j)}^2 \pi_{ij}(1 - \pi_{ij})$ is not easily manageable since $\hat{\phi}$ depends on different designs.

We consider maximizing $\det(\mathbf{J}(\boldsymbol{\theta}))$ into two steps: maximizing $\mathbf{I}_1(\boldsymbol{\theta}; \mathbf{n})$ and maximizing $\mathbf{I}_2(\boldsymbol{\theta})$. Let $f(\mathbf{n}) = \mathbf{I}_1(\boldsymbol{\theta}; \mathbf{n}) = \prod_{i=1}^{m} n_i$. We show that $f(\mathbf{n})$ is *Schur-concave* by using the Schur-Ostrowski criterion (Ostrowski, 1952) as below:

$$\begin{aligned} (n_i - n_j) \left(\frac{\partial f}{n_i} - \frac{\partial f}{n_j} \right) &= (n_i - n_j) \prod_{p \neq i,j}^{m} n_p \, (n_j - n_i) \\ &= -\,(n_i - n_j)^2 \prod_{p \neq i,j}^{m} n_p \leq 0 \end{aligned}$$

for all $\mathbf{n} \in \mathbb{R}^m$ holds for all $1 \leq i \neq j \leq m$. Based on the theory of majorization, a function $f : \mathbb{R}^m \to \mathbb{R}$ is Schur-concave if for any two vectors $\mathbf{n}_a$ and $\mathbf{n}_b$, we have $f(\mathbf{n}_a) \leq f(\mathbf{n}_b)$ given that $\mathbf{n}_a$ majorizes $\mathbf{n}_b$. This indicates the components of $\mathbf{n}$ should spread more evenly to get a large $f(\mathbf{n})$. Consequently, we conclude that to maximize $\mathbf{I}_1(\boldsymbol{\theta}; \mathbf{n})$, one needs to evenly spread the components of $\mathbf{n}$, i.e., n_is should be as equal as possible, resulting in a (nearly) balanced design.

With regard to $\mathbf{I}_2(\boldsymbol{\theta})$, we derive the conditions according to the number of treatments, $m = 2$ and $m > 2$:

(1) $m = 2$: we classify π_{ij} into $\binom{m}{1} + \binom{m}{2} = 3$ groups, denoted by p_{kl}, where $k = \min(t(i), t(j))$ and $l = \max(t(i), t(j))$. Then the determinant $\det(\mathbf{J}(\boldsymbol{\theta}))$ is

$$\frac{2N}{\sigma^6} n_1 n_2 \cdot 2 \left[\sum_{k=1}^{2} \binom{n_k}{2} L_{kk}^2 \frac{\exp(1 + \hat{\phi} L_{kk})}{\left[1 + \exp(1 + \hat{\phi} L_{kk})\right]^2} + n_1 n_2 L_{12}^2 \frac{\exp(\hat{\phi} L_{12})}{\left[1 + \exp(\hat{\phi} L_{12})\right]^2} \right]$$

$$= \frac{4N}{\sigma^6} n_1 n_2 \left[\sum_{k=1}^{2} \binom{n_k}{2} L_{kk}^2 p_{kk} + n_1 n_2 L_{12}^2 p_{12} \right]$$

$$\propto \mathbf{I}_1(\boldsymbol{\theta}; \mathbf{n}) \mathbf{I}_2(\boldsymbol{\theta}),$$

where

$$\mathbf{I}_1(\boldsymbol{\theta}; \mathbf{n}) = n_1 n_2,$$

and

$$\mathbf{I}_2(\boldsymbol{\theta}) = \sum_{k=1}^{2} \binom{n_k}{2} L_{kk}^2 p_{kk} + n_1 n_2 L_{12}^2 p_{12}.$$

As previously noted, $\mathbf{I}_2(\boldsymbol{\theta})$ is not easily tractable due to the estimation of ϕ. We discuss a simplified case with ϕ approaching zero in order to establish sufficient conditions for optimal designs. In addition, we examine whether these conditions hold for the general case where ϕ is estimated from the data. As ϕ approaches zero, the determinant is

$$\begin{aligned}
\lim_{\phi \to 0} \det(\mathbf{J}(\boldsymbol{\theta})) &\propto \lim_{\phi \to 0} \mathbf{I}_1(\boldsymbol{\theta}; \mathbf{n}) \mathbf{I}_2(\boldsymbol{\theta}) \\
&= n_1 n_2 \left\{ \binom{n_1}{2} L_{11}^2 p_{11} + \binom{n_2}{2} L_{22}^2 p_{22} + n_1 n_2 L_{12}^2 p_{12} \right\} \\
&= n_1 n_2 \left\{ \frac{\exp(1)}{[1 + \exp(1)]^2} \left[\binom{n_1}{2} L_{11}^2 + \binom{n_2}{2} L_{22}^2 \right] + \frac{1}{4} n_1 n_2 L_{12}^2 \right\}.
\end{aligned}$$

We have the following results:

(i) Consider how to spread L_{11} and L_{22} to make $\mathbf{I}_2(\boldsymbol{\theta})$ large given n_1 and n_2.

We compare

$$(L_{11}, L_{22}, L_{12}) = \left(c, c, \frac{1}{2}tr(\mathbf{A}^T\mathbf{A}) - 2c\right) \tag{3}$$

and

$$(L_{11}, L_{22}, L_{12}) = \left(c+a, c-a, \frac{1}{2}tr(\mathbf{A}^T\mathbf{A}) - 2c\right), \tag{4}$$

where $a = -c, -(c-1), \ldots, -1, 1, \ldots, c-1, c$ and $c = 0, 1, \ldots, \frac{1}{4}tr(\mathbf{A}^T\mathbf{A})$. Substracting $\mathbf{I}_2(\boldsymbol{\theta})$ of (4) from that of (3) yields

$$\frac{\exp(1)}{[1+\exp(1)]^2}\left[\tbinom{n_1}{2}c^2 + \tbinom{n_2}{2}c^2 - \tbinom{n_1}{2}(c+a)^2 - \tbinom{n_2}{2}(c-a)^2\right]. \tag{5}$$

The condition that (5) is larger than zero is equivalent to

$$-a^2\left[\tbinom{n_1}{2} + \tbinom{n_2}{2}\right] + 2ac\left[\tbinom{n_2}{2} - \tbinom{n_1}{2}\right] = -z\left(a - \frac{cy}{z}\right)^2 + \frac{c^2y^2}{x} \geq 0,$$

where $y = \binom{n_2}{2} - \binom{n_1}{2}$ and $z = \binom{n_1}{2} + \binom{n_2}{2}$. Finally, we have

$$\left|\frac{cy}{z}\right| + \frac{cy}{z} \geq a \geq -\left|\frac{cy}{z}\right| + \frac{cy}{z}.$$

Hence, evenly spreading L_{11} and L_{22} leads to large $\mathbf{I}_2(\boldsymbol{\theta})$ when the following is satisfied:

$$\begin{cases} a \in (\frac{2cy}{z}, 0)\,, \text{if}\, y < 0\,, \text{i.e.}\, n_1 > n_2; \\ a \in (0, \frac{2cy}{z})\,, \text{if}\, y \geq 0\,, \text{i.e.}\, n_1 \leq n_2. \end{cases}$$

We conclude that given n_1, n_2, without calculating $\mathbf{I}_2(\boldsymbol{\theta})$, as long as the design satisfies the above condition, it would result in a larger $\mathbf{I}_2(\boldsymbol{\theta})$.

(ii) Consider how to spread L_{11} and L_{12} to make $\mathbf{I}_2(\boldsymbol{\theta})$ large given n_1 and n_2. We compare

$$(L_{11}, L_{22}, L_{12}) = \left(c, \frac{1}{2}tr(\mathbf{A}^T\mathbf{A}) - c, 0\right) \tag{6}$$

and

$$(L_{11}, L_{22}, L_{12}) = \left(c-a, \frac{1}{2}tr(\mathbf{A}^T\mathbf{A}) - c, a\right), \tag{7}$$

where $a = 1, 2, \ldots, c$ and $c = 1, 2, \ldots, \frac{1}{2}tr(\mathbf{A}^T\mathbf{A})$. Substracting $\mathbf{I}_2(\boldsymbol{\theta})$ of (7) from that of (6) yields

$$\frac{\exp(1)}{[1+\exp(1)]^2}\left[\binom{n_1}{2}c^2 - \binom{n_1}{2}(c-a)^2\right] - \frac{1}{4}n_1n_2a^2. \tag{8}$$

The condition that (8) is larger than zero is equivalent to

$$-y\left(a-\frac{z}{y}\right)^2 + \frac{z^2}{y} \geq 0,$$

where

$$y = \frac{\exp(1)}{[1+\exp(1)]^2}\binom{n_1}{2} + \frac{1}{4}n_1n_2$$

and

$$z = \frac{c\exp(1)}{[1+\exp(1)]^2}\binom{n_1}{2}.$$

Finally, we have

$$\frac{2z}{y} \geq a \geq 0.$$

Hence, largest L_{11} leads to large $\mathbf{I}_2(\boldsymbol{\theta})$ when it satisfies

$$\frac{2z}{y} \geq a \geq 0.$$

We conclude that given n_1, n_2, without calculating $\mathbf{I}_2(\boldsymbol{\theta})$, as long as the design satisfies the above condition, largest L_{11} would result in a larger $\mathbf{I}_2(\boldsymbol{\theta})$.

(2) $m > 2$: the determinant $\det(\mathbf{J}(\boldsymbol{\theta}))$ is proportional to

$$\prod_{i=1}^{m} n_i \left[\sum_{k=1}^{m}\binom{n_k}{2}L_{kk}^2\frac{\exp(1+\hat{\phi}L_{kk})}{\left[1+\exp(1+\hat{\phi}L_{kk})\right]^2} + \sum_{i=1}^{m-1}\sum_{j>i}^{m} n_in_jL_{ij}^2\frac{\exp(\hat{\phi}L_{ij})}{\left[1+\exp(\hat{\phi}L_{ij})\right]^2}\right]$$

$$= \prod_{i=1}^{m} n_i \left[\sum_{k=1}^{m}\binom{n_k}{2}L_{kk}^2p_{kk} + \sum_{i=1}^{m-1}\sum_{j>i}^{m} n_in_jL_{ij}^2p_{ij}\right] = \mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})\mathbf{I}_2(\boldsymbol{\theta}),$$

where

$$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n}) = \prod_{i=1}^{m} n_i,$$

and

$$\mathbf{I}_2(\boldsymbol{\theta}) = \sum_{k=1}^{m} \binom{n_k}{2} L_{kk}^2 p_{kk} + \sum_{i=1}^{m-1} \sum_{j>i}^{m} n_i n_j L_{ij}^2 p_{ij}.$$

Similarly, we discuss a case where ϕ approaches zero. As ϕ approaches zero, $p_{kk} = \frac{\exp(1)}{[1+\exp(1)]^2}$ and $p_{ij} = \frac{1}{4}$. We have

$$\lim_{\phi \to 0} \det(\mathbf{J}(\boldsymbol{\theta})) \propto \prod_{i=1}^{m} n_i \left\{ \frac{\exp(1)}{[1+\exp(1)]^2} \sum_{k=1}^{m} \binom{n_k}{2} L_{kk}^2 + \frac{1}{4} \sum_{i=1}^{m-1} \sum_{j>i}^{m} n_i n_j L_{ij}^2 \right\}.$$

We have the following results:

(i) Consider how to spread L_{kk}s to make $\mathbf{I}_2(\boldsymbol{\theta})$ largest given n_is. First, we consider

$$(L_{11}, L_{22}, \ldots, L_{mm}) = \left(c_1, c_2, \ldots, \frac{1}{2} tr(\mathbf{A}^T \mathbf{A}) - \sum_{i=1}^{m-1} c_i - a \right)$$

given L_{ij}s and $\sum_{i=1}^{m-1} \sum_{j>i}^{m} L_{ij} = a$. Then comparing $\mathbf{I}_2(\boldsymbol{\theta})$ can be simplified to only comparing

$$\sum_{k=1}^{m} \binom{n_k}{2} L_{kk}^2. \tag{9}$$

Let $g(L_{kk}) = \binom{n_k}{2} L_{kk}^2$. The $g(L_{kk})$ is a convex function defined on a real interval since $g''(L_{kk}) = 2\binom{n_k}{2} \geq 0$. By the theory of majorization, (9) is *Schur-convex*, and (9) reaches a maximum when L_{kk} attains the maximum, where $n_k = \max(n_1, \ldots, n_m)$. For example, if n_1 is the largest among n_is, then $(L_{11}, L_{22}, \ldots, L_{mm}) = \left(\frac{1}{2} tr(\mathbf{A}^T \mathbf{A}) - a, 0, \ldots, 0\right)$ makes $\mathbf{I}_2(\boldsymbol{\theta})$ largest.

(ii) Consider how to spread L_{ij}s to make $\mathbf{I}_2(\boldsymbol{\theta})$ largest given n_is. First, we consider

$$(L_{12}, L_{13}, \ldots, L_{m-1,m}) = \left(c_{12}, c_{13}, \ldots, \frac{1}{2} tr(\mathbf{A}^T \mathbf{A}) - \sum_{i=1}^{m-1} \sum_{j>i}^{m} c_{ij} - a \right)$$

given L_{kk}s and $\sum_{k=1}^{m} L_{kk} = a$. Then comparing $\mathbf{I}_2(\boldsymbol{\theta})$ can be simplified to only comparing

$$\sum_{i=1}^{m-1}\sum_{j>i}^{m} n_i n_j L_{ij}^2. \tag{10}$$

Let $g(L_{ij}) = n_i n_j L_{ij}^2$. Then $g(L_{ij})$ is a convex function defined on a real interval since $g''(L_{ij}) = 2n_i n_j \geq 0$. By the theory of majorization, (10) is Schur-convex, and (10) reaches a maximum when L_{ij} attains the maximum, where $n_i n_j = \max(n_1 n_2, \ldots, n_{m-1} n_m)$. For example, if n_1 and n_2 are the first two largest among n_is, then $(L_{12}, L_{13}, \ldots, L_{m-1m}) = \left(\frac{1}{2}tr(\mathbf{A}^T\mathbf{A}) - a, 0, \ldots, 0\right)$ makes $\mathbf{I}_2(\boldsymbol{\theta})$ largest.

We summarize the results above in a theroem as follows.

Theorem 1. *Given* $\det(\mathbf{J}(\boldsymbol{\theta})) = \mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})\mathbf{I}_2(\boldsymbol{\theta})$, *to maximize* $\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})$, *the treatments should be evenly spread; that is, n_is should be as equal as possible, resulting in a (nearly) balanced design. With respect to maximizing* $\mathbf{I}_2(\boldsymbol{\theta})$, *we provide two conditions:*

(i) Given n_is, L_{ij}s $(i \neq j)$ and $\sum_{i=1}^{m-1}\sum_{j>i}^{m} L_{ij}$ being fixed, $\mathbf{I}_2(\boldsymbol{\theta})$ reaches a maximum when L_{kk} attains the maximum with $k = \{1 \leq l \leq m : n_l = \max(n_1, n_2, \ldots, n_m)\}$.

(ii) Given n_is, L_{kk}s and $\sum_{k=1}^{m} L_{kk}$ being fixed, $\mathbf{I}_2(\boldsymbol{\theta})$ reaches a maximum when L_{ij} attains the maximum with $(i,j) = \{1 \leq l < s \leq m : n_l n_s = \max(n_1 n_2, n_1 n_3, \ldots, n_{m-1} n_m)\}$.

Calculating $\det(\mathbf{J}(\boldsymbol{\theta}))$ for all designs can be prohibitive. Theorem 1 provides a set of sufficient conditions for a design to be D-optimal. The computational cost of these conditions is much lower than computing the determinant of $\mathbf{J}(\boldsymbol{\theta})$. The numerical study in Section 4 shows that the designs satisfying these conditions tend to perform well.

4. Numerical Results with Real Applications

For an N-node graph and m treatments, there are m^N designs in total. For a small network, we can completely search for all designs and calculate the values of the design criteria. However, exhaustive search incurs a large computational cost. It becomes prohibitive for a large-scale network or numerous treatments. Parker, Gilmour, and

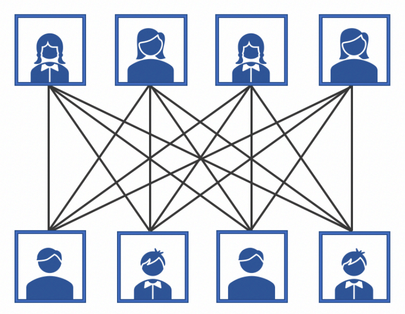


Figure 1: Network Structure for a Singles Mixer.

Schormans (2017) mentioned that we can reduce the size of the search area in two ways: the symmetry of the labels and the symmetry in the graph. Hence, we use these two techniques to reduce computation. In the following, we provide the results for $m = 2$, while those for $m = 3$ are given in the appendix. For each given network, the $L_{t(i)t(j)}$s can be computed once a treatment allocation is assigned.

4.1 $m = 2$ with $\phi \to 0$

In Section 3.2, we derive theoretical results for $m = 2$ as ϕ approaches zero. Here, we examine numerical results by four types of graphs: complete bipartite graph, cycle graph, path graph, and the second example in Parker, Gilmour, and Schormans (2017) (also in Chang, Phoa, and Huang (2021)). Except for the last graph, we also provide real applications.

Scenario 1. Complete Bipartite Graph

A complete bipartite graph is a special case of bipartite graphs where each unit in the first subset is connected to those in the other subset.

For instance, when people participate in the singles mixer, they will receive a list of basic contact information of the opposite gender from the marriage service corporation, including the name, occupation, horoscope, and blood type. The contact information will be exchanged between members according to their own wishes. Hence, these participants constitute a social network, which has a complete bipartite structure; see Figure 1. If the marriage service corporation wants to distribute advertisements for their social activities to those who are willing to socialize, the issue of treatment assignment

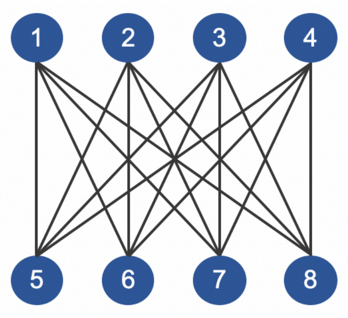


Figure 2: Complete Bipartite Graph with $N = 8$.

Table 1: Nonisomorphic Designs for Scenario 1 as $\phi \to 0$.

Treatment assignment	L_{11}	L_{22}	L_{12}	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})$	$\mathbf{I}_2(\boldsymbol{\theta})$	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})\mathbf{I}_2(\boldsymbol{\theta})$
$\{\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	16	0	0	2818.63	0.00
$\{1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	12	4	7	1245.11	8715.76
$\{1,1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	8	8	12	761.50	9137.94
$\{1,\mathbf{2},\mathbf{2},\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2}\}$	1	9	6	12	694.16	8329.92
$\{1,1,\mathbf{2},\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2}\}$	2	6	8	15	626.28	9394.19
$\{1,1,1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	4	12	15	1142.92	17143.74
$\{1,1,1,1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	0	16	16	2048.00	32768.00
$\{1,1,\mathbf{2},\mathbf{2},1,1,\mathbf{2},\mathbf{2}\}$	4	4	8	16	587.50	9399.98
$\{1,1,1,\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2}\}$	3	3	10	16	842.47	13479.49

matters. The treatments can be different kinds of advertisements, and the response can be the number of clicks on the advertisement page.

We illustrate this scenario via a simple example with eight units as in Figure 2.

Let $\{t(1), \ldots, t(N)\}$ be the set of treatments on units 1 to N. We find nine non-isomorphic designs shown in Table 1. The blue one corresponds to the largest $\mathbf{I}_2(\boldsymbol{\theta})$, but it does not involve the first treatment. The red one corresponds to the D-optimal design. The design with the largest L_{12} is D-optimal, which is supported by Theorem 1.

Scenario 2. Cycle Graph

A cycle graph is a graph that the vertices are connected in a closed chain, and the number of vertices equals the number of edges. All vertices have the degree two; that

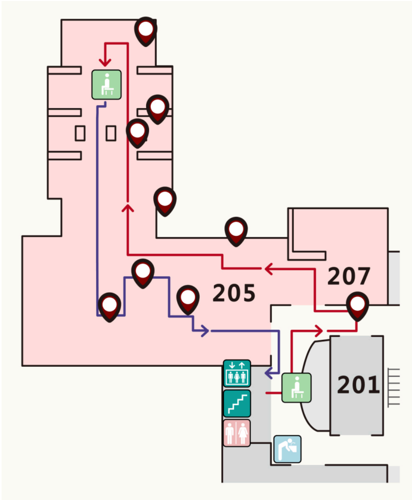


Figure 3: The Floor Plan of National Palace Museum.

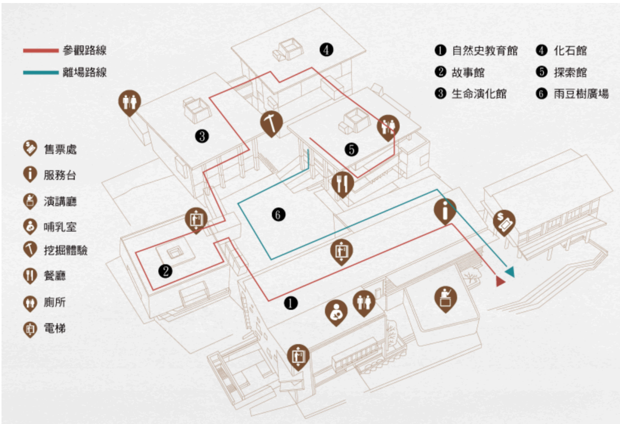


Figure 4: The Floor Plan of Tainan City Zuojhen Fossil Park.

is, every vertex has exactly two edges linked with it.

The floor plan of the museum can be realized as a cycle network. The museum attaches great importance to the layout of works to make the best use of storage space and allow visitors to enjoy the works as comfortably and completely as possible. Take National Palace Museum and Tainan City Zuojhen Fossil Park as examples. See Figure 3 and Figure 4 for illustration. They use a forced-route design to guide customers to travel the entire predetermined route. If people come here to see exhibitions, they will follow the same route most of the time. From a commercial point of view, the museum tries to solve the following problems: how to decide the position of the works or theme introductions in the route, so as to promote the activities to the maximum extent?

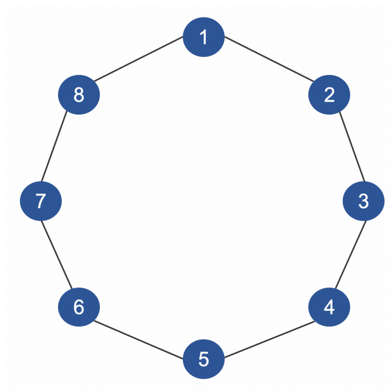


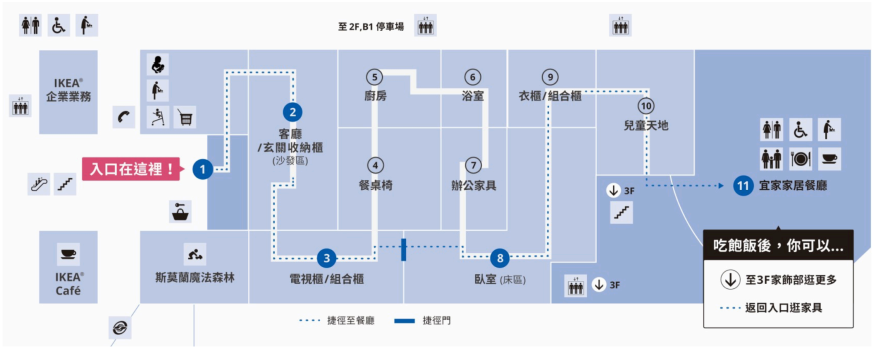
Figure 5: Cycle Graph with $N = 8$.

Table 2: Nonisomorphic Designs for Scenario 2 as $\phi \to 0$.

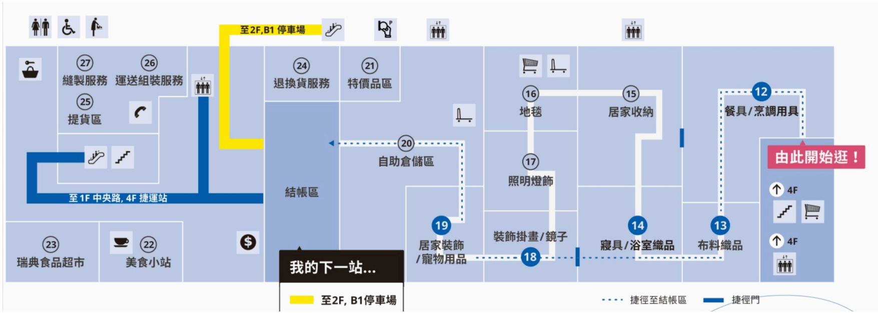
Treatment assignment	L_{11}	L_{22}	L_{12}	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})$	$\mathbf{I}_2(\boldsymbol{\theta})$	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})\mathbf{I}_2(\boldsymbol{\theta})$
$\{\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	8	0	0	704.66	0.00
$\{\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	6	2	7	311.28	2178.94
$\{\mathbf{1},\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	1	5	2	12	171.85	2062.23
$\{\mathbf{1},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	4	4	12	190.37	2284.49
$\{\mathbf{1},\mathbf{1},\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	2	4	2	15	97.64	1464.52
$\{\mathbf{1},\mathbf{1},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	1	3	4	15	156.57	2348.55
$\{\mathbf{1},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	2	6	15	285.73	4285.93
$\{\mathbf{1},\mathbf{1},\mathbf{1},\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	3	3	2	16	74.47	1191.49
$\{\mathbf{1},\mathbf{1},\mathbf{1},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{2}\}$	2	2	4	16	146.88	2350.00
$\{\mathbf{1},\mathbf{1},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{2}\}$	1	1	6	16	292.72	4683.50
$\{\mathbf{1},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{1},\mathbf{2}\}$	0	0	8	16	512.00	8192.00

The number of views by the customers can be used as a response. We regard each work/type of showroom as a node and connect adjacent works/showrooms based on a one-way path layout. We define the area in front of the entrance and exit as the same node, so this path is a cycle graph.

In this scenario, we illustrate a simple example with eight units as in Figure 5. We have eleven nonisomorphic designs shown in Table 2. The result is similar to that of Scenario 1. The design with the largest L_{12} is D-optimal, supported by Theorem 1.



(a)



(b)

Figure 6: The Floor Plans of IKEA.

Scenario 3. Path Graph

A path graph is a walk with all different units and edges. The difference between path graphs and cycle graphs is that the first unit is connected with the last unit in cycle graphs.

As we mentioned in the previous scenario, the layout of facilities plays an important role in operations for exhibitions. It also works for shopping malls, which may affect customer purchases. Traditional retail stores usually allow customers to navigate directly to any part, but some stores like IKEA use a path to guide customers to every area in the store; see Figure 6. IKEA's layout is a one-way path system that guides customers from the entrance to the checkout area through different parts. Suppose we have two posters about recruiting new members with two-dimensional QR codes attached, and each part of the store has one of them. The store owner may want to decide the placement of two different posters effectively and explore which version of the poster is more attractive.

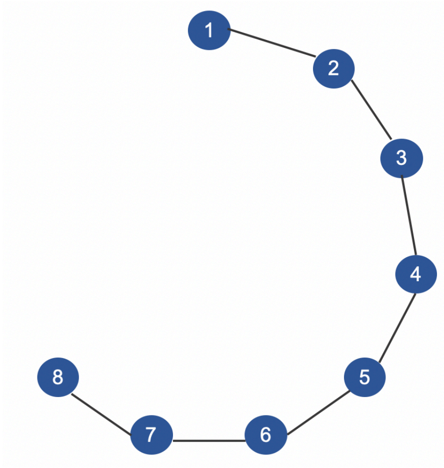


Figure 7: Path Graph with $N = 8$.

Table 3: Nonisomorphic Designs for Scenario 3 as $\phi \to 0$.

Treatment assignment	L_{11}	L_{22}	L_{12}	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})$	$\mathbf{I}_2(\boldsymbol{\theta})$	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})\mathbf{I}_2(\boldsymbol{\theta})$
$\{2,2,2,2,2,2,2,2\}$	0	7	0	0	539.50	0.00
$\{1,2,2,2,2,2,2,2\}$	6	0	1	7	300.78	2105.44
$\{2,1,2,2,2,2,2,2\}$	5	0	2	7	220.44	1543.10
$\{1,2,2,2,2,2,2,1\}$	0	5	2	12	171.46	2057.51
$\{1,1,2,2,2,2,2,2\}$	1	5	1	12	153.85	1846.23
$\{2,1,2,1,2,2,2,2\}$	0	3	4	12	149.09	1789.02
$\{1,2,1,2,2,2,2,2\}$	0	4	3	12	148.37	1780.49
$\{2,1,1,2,2,2,2,2\}$	1	4	2	12	118.77	1425.20
$\{2,1,2,1,2,1,2,2\}$	0	1	6	15	273.93	4108.98
$\{1,2,1,2,1,2,2,2\}$	0	2	5	15	203.23	3048.98
$\{1,2,1,2,2,2,2,1\}$	0	3	4	15	155.39	2330.85
$\{2,1,1,2,1,2,2,2\}$	1	2	4	15	136.91	2053.63
$\{1,1,2,1,2,2,2,2\}$	1	3	3	15	104.07	1561.05
$\{1,1,2,2,2,2,2,1\}$	1	4	2	15	94.10	1411.43
$\{1,1,1,2,2,2,2,2\}$	2	4	1	15	75.14	1127.02
$\{2,1,1,1,2,2,2,2\}$	2	3	2	15	70.11	1051.63
$\{1,2,1,2,1,2,1,2\}$	0	0	7	16	392.00	6762.00
$\{2,1,1,2,1,2,1,2\}$	1	0	6	16	290.36	4645.75
$\{1,1,2,1,2,1,2,2\}$	1	1	5	16	204.72	3275.50
$\{2,1,1,1,2,1,2,2\}$	2	1	4	16	139.80	2236.75
$\{1,1,1,2,1,2,2,2\}$	2	2	3	16	90.88	1454.08
$\{2,1,1,1,1,2,2,2\}$	3	2	2	16	62.67	1002.74
$\{1,1,1,1,2,2,2,2\}$	3	3	1	16	50.47	807.49

Similarly, we illustrate a path graph with eight units as in Figure 7. We have twenty-three nonisomorphic designs shown in Table 3. The D-optimal design has the largest L_{12}, supported by Theorem 1.

Scenario 4. Example 2 in Parker, Gilmour, and Schormans (2017)

The graph in Figure 8 is an example discussed in Parker, Gilmour, and Schormans (2017). This network has ten units connected by a relationship with the following adjacency matrix:

$$\mathbf{A} = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 0 \end{bmatrix}.$$

On account of the unsymmetry in the graph, we choose not to show all nonisomorphic designs in Table 4. We list the designs whose $\mathbf{I}_2(\boldsymbol{\theta})$ are larger than that of the D-optimal design. In Table 4, we observe the same results as the previous scenarios. On the other hand, we compare the results with Parker, Gilmour, and Schormans (2017) and Chang, Phoa, and Huang (2021). See Table 5 for details. With respect to the criterion we propose, the design chosen in this article is better.

4.2 $m = 2$ with estimated ϕ

In this section, ϕ is estimated by the maximum likelihood estimation. It leads to different p_{kl} and determinants for different designs. Through simulating the same scenarios as in Section 4.1, different results happen from those under ϕ approaching zero.

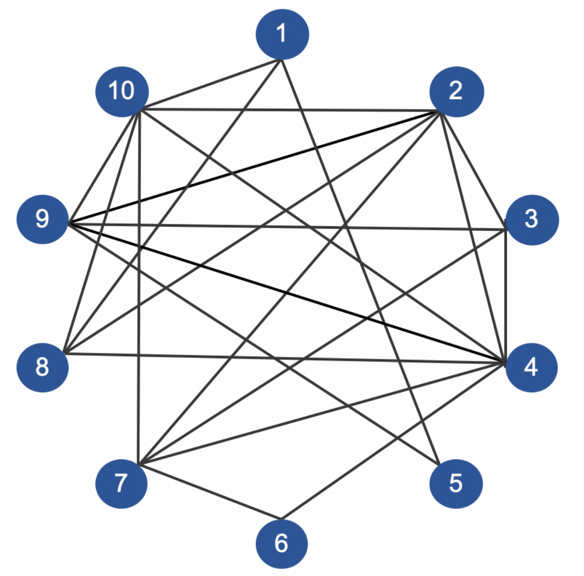


Figure 8: Example 2 in Parker, Gilmour, and Schormans (2017).

Table 4: Optimal Designs for Scenario 4 as $\phi \to 0$.

Treatment assignment	L_{11}	L_{22}	L_{12}	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})$	$\mathbf{I}_2(\boldsymbol{\theta})$	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})\mathbf{I}_2(\boldsymbol{\theta})$
$\{\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	22	0	0	8564.42	0.00
$\{\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	20	2	9	5680.42	51123.81
$\{\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	20	2	9	5680.42	51123.81
$\{\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	19	3	9	5150.84	46357.54
$\{\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{2}\}$	0	18	4	9	4658.56	41927.07
$\{\mathbf{2},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	18	4	9	4658.56	41927.07
$\{\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{1},\mathbf{2}\}$	0	17	5	9	4203.60	37832.41
$\{\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	17	5	9	4203.60	37832.41
$\{\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{1}\}$	0	16	6	9	3785.95	34073.56
$\{\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	16	6	9	3785.95	34073.56
$\{\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	15	7	9	3405.61	30650.52
$\{\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{1},\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	18	4	16	3695.33	59125.23
$\{\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	1	18	3	16	3639.72	58235.52
$\{\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	17	5	16	3381.97	54111.48
$\{\mathbf{2},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{1},\mathbf{1},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{1}\}$	1	5	16	25	3302.24	82555.96

Table 5: Comparison in Optimal Designs for Scenario 4 as $\phi \to 0$.

This article						
Treatment assignment	L_{11}	L_{22}	L_{12}	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})$	$\mathbf{I}_2(\boldsymbol{\theta})$	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})\mathbf{I}_2(\boldsymbol{\theta})$
$\{\mathbf{2},\mathbf{2},1,\mathbf{2},1,1,\mathbf{2},1,\mathbf{2},1\}$	1	5	16	25	3302.24	82555.96
Parker, Gilmour, and Schormans (2017)						
Treatment assignment	L_{11}	L_{22}	L_{12}	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})$	$\mathbf{I}_2(\boldsymbol{\theta})$	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})\mathbf{I}_2(\boldsymbol{\theta})$
$\{1,1,\mathbf{2},\mathbf{2},\mathbf{2},1,\mathbf{2},1,\mathbf{2},1\}$	5	6	11	25	1752.37	43809.16
$\{1,\mathbf{2},1,\mathbf{2},1,\mathbf{2},\mathbf{2},1,\mathbf{2},1\}$	4	7	11	25	1768.10	44202.39
Chang, Phoa, and Huang (2021)						
Treatment assignment	L_{11}	L_{22}	L_{12}	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})$	$\mathbf{I}_2(\boldsymbol{\theta})$	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})\mathbf{I}_2(\boldsymbol{\theta})$
$\{\mathbf{2},1,\mathbf{2},\mathbf{2},1,\mathbf{2},\mathbf{2},1,1,1\}$	6	5	11	25	1752.37	43809.16
$\{\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2},1,1,1,\mathbf{2},1\}$	6	5	11	25	1752.37	43809.16

Scenario 1. Complete Bipartite Graph

For the scenario of the complete bipartite graph, we show the nonisomorphic designs in Table 6. The red one represents the optimal design in Section 4.1. The orange one represents the optimal design for estimated ϕ. The range of $\hat{\phi}$ is from -0.055 to 1.223. We find that the optimal design under ϕ approaching zero is the worst in this condition; since $\hat{\phi} = 1.223$ causes $p_{12} = 1$, the determinant is zero.

Scenario 2. Cycle Graph

In this case, we present the results in Table 7. The range of $\hat{\phi}$ is from -0.505 to 0. The optimal design in Section 4.1 is also optimal here.

Scenario 3. Path Graph

In this scenario, we present the 23 nonisomorphic designs in Table 8. The range of $\hat{\phi}$ is from -0.649 to -0.036. Similar to Scenario 2, the optimal design for ϕ approaching zero is also optimal for estimated ϕ.

Table 6: Nonisomorphic Designs for Scenario 1 under $\hat{\phi}$ = MLE.

Treatment assignment	L_{11}	L_{22}	L_{12}	$\hat{\phi}$	p_{11}	p_{22}	p_{12}
$\{\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	16	0	−0.045	0.571	0.731	0.500
$\{1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	12	4	−0.055	0.731	0.585	0.446
$\{1,1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	8	8	−0.020	0.731	0.699	0.460
$\{1,\mathbf{2},\mathbf{2},\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2}\}$	1	9	6	−0.047	0.722	0.640	0.429
$\{1,1,\mathbf{2},\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2}\}$	2	6	8	−0.014	0.726	0.715	0.473
$\{1,1,1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	4	12	0.076	0.731	0.787	0.714
$\{1,1,1,1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	0	16	1.223	0.731	0.731	1.000
$\{1,1,\mathbf{2},\mathbf{2},1,1,\mathbf{2},\mathbf{2}\}$	4	4	8	−0.011	0.723	0.723	0.479
$\{1,1,1,\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2}\}$	3	3	10	0.028	0.747	0.747	0.569

Treatment assignment	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})$	$\mathbf{I}_2(\boldsymbol{\theta})$	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})\mathbf{I}_2(\boldsymbol{\theta})$
$\{\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	3510.86	0.00
$\{1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	7	1523.32	10662.56
$\{1,1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	12	785.89	9430.62
$\{1,\mathbf{2},\mathbf{2},\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2}\}$	12	722.19	9266.55
$\{1,1,\mathbf{2},\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2}\}$	15	630.15	9452.29
$\{1,1,1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	15	935.73	14035.98
$\{1,1,1,1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	16	0.00	0.00
$\{1,1,\mathbf{2},\mathbf{2},1,1,\mathbf{2},\mathbf{2}\}$	16	588.05	9408.79
$\{1,1,1,\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2}\}$	16	825.40	13206.36

Table 7: Nonisomorphic Designs for Scenario 2 under $\hat{\phi}$ = MLE.

Treatment assignment	L_{11}	L_{22}	L_{12}	$\hat{\phi}$	p_{11}	p_{22}	p_{12}
$\{\mathbf{2,2,2,2,2,2,2,2}\}$	0	8	0	−0.240	0.286	0.731	0.500
$\{\mathbf{1,2,2,2,2,2,2,2}\}$	0	6	2	−0.325	0.731	0.279	0.343
$\{\mathbf{1,1,2,2,2,2,2,2}\}$	1	5	2	−0.380	0.650	0.289	0.319
$\{\mathbf{1,2,1,2,2,2,2,2}\}$	0	4	4	−0.368	0.731	0.384	0.187
$\{\mathbf{1,1,1,2,2,2,2,2}\}$	2	4	2	−0.455	0.523	0.306	0.287
$\{\mathbf{1,1,2,1,2,2,2,2}\}$	1	3	4	−0.392	0.648	0.456	0.173
$\{\mathbf{1,2,1,2,1,2,2,2}\}$	0	2	6	−0.145	0.731	0.670	0.295
$\{\mathbf{1,1,1,1,2,2,2,2}\}$	3	3	2	−0.505	0.374	0.374	0.267
$\{\mathbf{1,1,1,2,1,2,2,2}\}$	2	2	4	−0.399	0.550	0.550	0.169
$\{\mathbf{1,1,2,1,2,1,2,2}\}$	1	1	6	−0.135	0.704	0.704	0.308
$\{\mathbf{1,2,1,2,1,2,1,2}\}$	0	0	8	0.000	0.731	0.731	0.500

Treatment assignment	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})$	$\mathbf{I}_2(\boldsymbol{\theta})$	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})\mathbf{I}_2(\boldsymbol{\theta})$
$\{\mathbf{2,2,2,2,2,2,2,2}\}$	0	731.43	0.00
$\{\mathbf{1,2,2,2,2,2,2,2}\}$	7	317.00	2218.98
$\{\mathbf{1,1,2,2,2,2,2,2}\}$	12	175.51	2106.17
$\{\mathbf{1,2,1,2,2,2,2,2}\}$	12	171.83	2061.95
$\{\mathbf{1,1,1,2,2,2,2,2}\}$	15	98.53	1478.00
$\{\mathbf{1,1,2,1,2,2,2,2}\}$	15	114.62	1719.31
$\{\mathbf{1,2,1,2,1,2,2,2}\}$	15	242.49	3637.32
$\{\mathbf{1,1,1,1,2,2,2,2}\}$	16	75.61	1209.74
$\{\mathbf{1,1,1,2,1,2,2,2}\}$	16	95.53	1528.44
$\{\mathbf{1,1,2,1,2,1,2,2}\}$	16	250.48	4007.67
$\{\mathbf{1,2,1,2,1,2,1,2}\}$	16	512.00	8192.00

Table 8: Nonisomorphic Designs for Scenario 3 under $\hat{\phi}$ = MLE.

Treatment assignment	L_{11}	L_{22}	L_{12}	$\hat{\phi}$	p_{11}	p_{22}	p_{12}
$\{\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	7	0	−0.300	0.250	0.731	0.500
$\{1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	6	0	1	−0.332	0.270	0.731	0.418
$\{\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	5	0	2	−0.434	0.237	0.731	0.296
$\{1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},1\}$	0	5	2	−0.384	0.731	0.285	0.317
$\{1,1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	1	5	1	−0.383	0.286	0.650	0.406
$\{\mathbf{2},1,\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	3	4	−0.457	0.408	0.731	0.138
$\{1,\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	4	3	−0.465	0.297	0.731	0.199
$\{\mathbf{2},1,1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	1	4	2	−0.540	0.238	0.613	0.253
$\{\mathbf{2},1,\mathbf{2},1,\mathbf{2},1,\mathbf{2},\mathbf{2}\}$	0	1	6	−0.116	0.708	0.731	0.332
$\{1,\mathbf{2},1,\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	2	5	−0.252	0.621	0.731	0.221
$\{1,\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},1\}$	0	3	4	−0.375	0.731	0.469	0.182
$\{\mathbf{2},1,1,\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2}\}$	1	2	4	−0.448	0.526	0.635	0.143
$\{1,1,\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	1	3	3	−0.560	0.337	0.608	0.157
$\{1,1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},1\}$	1	4	2	−0.493	0.624	0.274	0.272
$\{1,1,1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	2	4	1	−0.460	0.302	0.520	0.387
$\{\mathbf{2},1,1,1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	2	3	2	−0.661	0.272	0.420	0.210
$\{1,\mathbf{2},1,\mathbf{2},1,\mathbf{2},1,\mathbf{2}\}$	0	0	7	−0.036	0.731	0.731	0.438
$\{\mathbf{2},1,1,\mathbf{2},1,\mathbf{2},1,\mathbf{2}\}$	1	0	6	−0.110	0.731	0.709	0.341
$\{1,1,\mathbf{2},1,\mathbf{2},1,\mathbf{2},\mathbf{2}\}$	1	1	5	−0.236	0.682	0.682	0.235
$\{\mathbf{2},1,1,1,\mathbf{2},1,\mathbf{2},\mathbf{2}\}$	2	1	4	−0.405	0.644	0.547	0.165
$\{1,1,1,\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2}\}$	2	2	3	−0.621	0.440	0.440	0.134
$\{\mathbf{2},1,1,1,1,\mathbf{2},\mathbf{2},\mathbf{2}\}$	3	2	2	−0.649	0.426	0.279	0.214
$\{1,1,1,1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	3	3	1	−0.522	0.362	0.362	0.372

Treatment assignment	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})$	$\mathbf{I}_2(\boldsymbol{\theta})$	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})\mathbf{I}_2(\boldsymbol{\theta})$
$\{\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	0	514.50	0.00
$\{1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	7	301.73	2112.10
$\{\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	7	201.41	1409.86
$\{1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},1\}$	12	173.69	2084.25
$\{1,1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	12	159.54	1914.48
$\{\mathbf{2},1,\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	12	110.98	1331.75
$\{1,\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	12	134.70	1616.37
$\{\mathbf{2},1,1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	12	105.80	1269.54
$\{\mathbf{2},1,\mathbf{2},1,\mathbf{2},1,\mathbf{2},\mathbf{2}\}$	15	243.83	3657.49
$\{1,\mathbf{2},1,\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2}\}$	15	147.91	2218.66
$\{1,\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},1\}$	15	116.39	1745.77
$\{\mathbf{2},1,1,\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2}\}$	15	80.13	1201.98
$\{1,1,\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	15	77.41	1161.13
$\{1,1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},1\}$	15	88.87	1333.06
$\{1,1,1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	15	80.54	1208.10
$\{\mathbf{2},1,1,1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	15	61.45	921.68
$\{1,\mathbf{2},1,\mathbf{2},1,\mathbf{2},1,\mathbf{2}\}$	16	385.88	6174.00
$\{\mathbf{2},1,1,\mathbf{2},1,\mathbf{2},1,\mathbf{2}\}$	16	261.39	4182.27
$\{1,1,\mathbf{2},1,\mathbf{2},1,\mathbf{2},\mathbf{2}\}$	16	149.09	2385.47
$\{\mathbf{2},1,1,1,\mathbf{2},1,\mathbf{2},\mathbf{2}\}$	16	85.22	1363.45
$\{1,1,1,\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2}\}$	16	57.14	914.18
$\{\mathbf{2},1,1,1,1,\mathbf{2},\mathbf{2},\mathbf{2}\}$	16	55.04	880.60
$\{1,1,1,1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2}\}$	16	57.38	918.10

Table 9: Optimal Designs for Scenario 4 under $\hat{\phi}$ = MLE.

Treatment assignment	L_{11}	L_{22}	L_{12}	$\hat{\phi}$
{2, 2, 2, 2, 2, 2, 2, 2, 2, 2}	0	22	0	−0.047
{2, 2, 2, 2, 2, 1, 2, 2, 2, 2}	0	20	2	−0.040
{1, 2, 2, 2, 2, 2, 2, 2, 2, 2}	0	19	3	−0.048
{2, 2, 2, 2, 2, 2, 2, 1, 2, 2}; {2, 2, 1, 2, 2, 2, 2, 2, 2, 2}	0	18	4	−0.056
{2, 2, 2, 2, 2, 2, 2, 2, 1, 2}; {2, 2, 2, 2, 2, 2, 1, 2, 2, 2}	0	17	5	−0.063
{2, 2, 2, 2, 2, 2, 2, 2, 2, 1}; {2, 1, 2, 2, 2, 2, 2, 2, 2, 2}	0	16	6	−0.070
{2, 2, 2, 1, 2, 2, 2, 2, 2, 2}	0	15	7	−0.076
{2, 2, 2, 2, 1, 1, 2, 2, 2, 2}	0	18	4	−0.030
{1, 2, 2, 2, 1, 2, 2, 2, 2, 2}	1	18	3	−0.029
{1, 2, 2, 2, 2, 1, 2, 2, 2, 2}	0	17	5	−0.039
{2, 2, 2, 2, 2, 1, 2, 1, 2, 2}; {2, 2, 2, 2, 1, 2, 2, 1, 2, 2}; {2, 2, 1, 2, 2, 1, 2, 2, 2, 2}; {2, 2, 1, 2, 1, 2, 2, 2, 2, 2}	0	16	6	−0.047
{2, 2, 2, 2, 1, 2, 2, 2, 1, 2}; {1, 2, 2, 2, 2, 2, 2, 1, 2, 2}; {2, 2, 2, 2, 2, 1, 1, 2, 2, 2}	1	16	5	−0.050
{2, 2, 2, 2, 1, 2, 2, 2, 1, 2}; {2, 2, 2, 2, 1, 2, 1, 2, 2, 2}; {1, 2, 1, 2, 2, 2, 2, 2, 2, 2}	0	15	7	−0.055
{2, 2, 2, 2, 2, 1, 2, 2, 2, 1}; {2, 2, 2, 2, 1, 2, 2, 2, 2, 1}; {1, 2, 2, 2, 2, 2, 2, 2, 1, 2}; {2, 2, 1, 2, 2, 2, 2, 1, 2, 2}; {1, 2, 2, 2, 2, 2, 1, 2, 2, 2}; {2, 1, 2, 2, 2, 1, 2, 2, 2, 2}; {2, 1, 2, 2, 1, 2, 2, 2, 2, 2}	0	14	8	−0.060
{2, 1, 1, 2, 1, 1, 2, 2, 2, 1}	2	4	16	0.020
{2, 2, 1, 2, 1, 1, 2, 1, 2, 1}	1	5	16	0.023

Treatment assignment	p_{11}	p_{22}	p_{12}
$\{2,2,2,2,2,2,2,2,2,2\}$	0.731	0.489	0.500
$\{2,2,2,2,2,1,2,2,2,2\}$	0.731	0.549	0.480
$\{1,2,2,2,2,2,2,2,2,2\}$	0.731	0.523	0.464
$\{2,2,2,2,2,2,2,1,2,2\}$; $\{2,2,1,2,2,2,2,2,2,2\}$	0.731	0.500	0.445
$\{2,2,2,2,2,2,2,2,1,2\}$; $\{2,2,2,2,2,2,1,2,2,2\}$	0.731	0.482	0.422
$\{2,2,2,2,2,2,2,2,2,1\}$; $\{2,1,2,2,2,2,2,2,2,2\}$	0.731	0.470	0.396
$\{2,2,2,1,2,2,2,2,2,2\}$	0.731	0.464	0.37
$\{2,2,2,2,1,1,2,2,2,2\}$	0.731	0.615	0.470
$\{1,2,2,2,1,2,2,2,2,2\}$	0.725	0.616	0.478
$\{1,2,2,2,2,1,2,2,2,2\}$	0.731	0.584	0.451
$\{2,2,2,2,2,1,2,1,2,2\}$; $\{2,2,2,2,1,2,2,1,2,2\}$; $\{2,2,1,2,2,1,2,2,2,2\}$; $\{2,2,1,2,1,2,2,2,2,2\}$	0.731	0.560	0.429
$\{2,2,2,2,1,2,2,2,1,2\}$; $\{1,2,2,2,2,2,2,1,2,2\}$; $\{2,2,2,2,2,1,1,2,2,2\}$	0.721	0.550	0.438
$\{2,2,2,2,1,2,2,2,1,2\}$; $\{2,2,2,2,1,2,1,2,2,2\}$; $\{1,2,1,2,2,2,2,2,2,2\}$	0.731	0.544	0.405
$\{2,2,2,2,2,1,2,2,2,1\}$; $\{2,2,2,2,1,2,2,2,2,1\}$; $\{1,2,2,2,2,2,2,2,1,2\}$; $\{2,2,1,2,2,2,2,1,2,2\}$; $\{1,2,2,2,2,1,2,2,2,2\}$; $\{2,1,2,2,2,1,2,2,2,2\}$; $\{2,1,2,2,1,2,2,2,2,2\}$	0.731	0.539	0.382
$\{2,1,1,2,1,1,2,2,2,1\}$	0.746	0.739	0.578
$\{2,2,1,2,1,1,2,1,2,1\}$	0.736	0.753	0.592

Treatment assignment	$\mathbf{I}_1$	$\mathbf{I}_2$	$\mathbf{I}_1\mathbf{I}_2$
$\{\mathbf{2,2,2,2,2,2,2,2,2,2}\}$	0	10884.62	0.00
$\{\mathbf{2,2,2,2,2,1,2,2,2,2}\}$	9	7148.50	64336.53
$\{\mathbf{1,2,2,2,2,2,2,2,2,2}\}$	9	6525.00	58725.00
$\{\mathbf{2,2,2,2,2,2,2,1,2,2}\}$; $\{\mathbf{2,2,1,2,2,2,2,2,2,2}\}$	9	5903.12	53128.06
$\{\mathbf{2,2,2,2,2,2,2,2,1,2}\}$; $\{\mathbf{2,2,2,2,2,2,1,2,2,2}\}$	9	5305.05	47745.45
$\{\mathbf{2,2,2,2,2,2,2,2,2,1}\}$; $\{\mathbf{2,1,2,2,2,2,2,2,2,2}\}$	9	4746.21	42715.93
$\{\mathbf{2,2,2,1,2,2,2,2,2,2}\}$	9	4234.85	38113.66
$\{\mathbf{2,2,2,2,1,1,2,2,2,2}\}$	16	4424.18	70786.84
$\{\mathbf{1,2,2,2,1,2,2,2,2,2}\}$	16	4365.22	69843.55
$\{\mathbf{1,2,2,2,2,1,2,2,2,2}\}$	16	4130.52	66088.27
$\{\mathbf{2,2,2,2,2,1,2,1,2,2}\}$; $\{\mathbf{2,2,2,2,1,2,2,1,2,2}\}$; $\{\mathbf{2,2,1,2,2,1,2,2,2,2}\}$; $\{\mathbf{2,2,1,2,1,2,2,2,2,2}\}$	16	3814.97	61039.48
$\{\mathbf{2,2,2,2,1,2,2,2,1,2}\}$; $\{\mathbf{1,2,2,2,2,2,2,1,2,2}\}$; $\{\mathbf{2,2,2,2,2,1,1,2,2,2}\}$	16	3745.92	59934.74
$\{\mathbf{2,2,2,2,1,2,2,2,1,2}\}$; $\{\mathbf{2,2,2,2,1,2,1,2,2,2}\}$; $\{\mathbf{1,2,1,2,2,2,2,2,2,2}\}$	16	3503.17	56050.69
$\{\mathbf{2,2,2,2,2,1,2,2,2,1}\}$; $\{\mathbf{2,2,2,2,1,2,2,2,2,1}\}$; $\{\mathbf{1,2,2,2,2,2,2,2,1,2}\}$; $\{\mathbf{2,2,1,2,2,2,2,1,2,2}\}$; $\{\mathbf{1,2,2,2,2,2,1,2,2,2}\}$; $\{\mathbf{2,1,2,2,2,1,2,2,2,2}\}$; $\{\mathbf{2,1,2,2,1,2,2,2,2,2}\}$	16	3210.87	51373.85
$\{\mathbf{2,1,1,2,1,1,2,2,2,1}\}$	25	3197.29	79932.20
$\{\mathbf{2,2,1,2,1,1,2,1,2,1}\}$	25	3187.42	79685.50

Note. $\mathbf{I}_1 = \mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})$, $\mathbf{I}_2 = \mathbf{I}_2(\boldsymbol{\theta})$, and $\mathbf{I}_1\mathbf{I}_2 = \mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})\mathbf{I}_2(\boldsymbol{\theta})$.

Table 10: Comparison in Optimal Designs for Scenario 4 under $\hat{\phi}$ = MLE.

This article							
Treatment assignment	L_{11}	L_{22}	L_{12}	$\hat{\phi}$	p_{11}	p_{22}	p_{12}
$\{\mathbf{2},\mathbf{2},1,\mathbf{2},1,1,\mathbf{2},1,\mathbf{2},1\}$	1	5	16	0.023	0.736	0.753	0.592
Parker, Gilmour, and Schormans (2017)							
Treatment assignment	L_{11}	L_{22}	L_{12}	$\hat{\phi}$	p_{11}	p_{22}	p_{12}
$\{1,1,\mathbf{2},\mathbf{2},\mathbf{2},1,\mathbf{2},1,\mathbf{2},1\}$	5	6	11	−0.041	0.689	0.680	0.388
$\{1,\mathbf{2},1,\mathbf{2},1,\mathbf{2},\mathbf{2},1,\mathbf{2},1\}$	4	7	11	−0.036	0.702	0.678	0.402
Chang, Phoa, and Huang (2021)							
Treatment assignment	L_{11}	L_{22}	L_{12}	$\hat{\phi}$	p_{11}	p_{22}	p_{12}
$\{\mathbf{2},1,\mathbf{2},\mathbf{2},1,\mathbf{2},\mathbf{2},1,1,1\}$	6	5	11	−0.041	0.689	0.680	0.388
$\{\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2},1,1,1,\mathbf{2},1\}$	6	5	11	−0.041	0.689	0.680	0.388

This article			
Treatment assignment	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})$	$\mathbf{I}_2(\boldsymbol{\theta})$	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})\mathbf{I}_2(\boldsymbol{\theta})$
$\{\mathbf{2},\mathbf{2},1,\mathbf{2},1,1,\mathbf{2},1,\mathbf{2},1\}$	25	3187.42	79685.50
Parker, Gilmour, and Schormans (2017)			
Treatment assignment	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})$	$\mathbf{I}_2(\boldsymbol{\theta})$	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})\mathbf{I}_2(\boldsymbol{\theta})$
$\{1,1,\mathbf{2},\mathbf{2},\mathbf{2},1,\mathbf{2},1,\mathbf{2},1\}$	25	1701.04	42526.00
$\{1,\mathbf{2},1,\mathbf{2},1,\mathbf{2},\mathbf{2},1,\mathbf{2},1\}$	25	1734.77	43369.27
Chang, Phoa, and Huang (2021)			
Treatment assignment	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})$	$\mathbf{I}_2(\boldsymbol{\theta})$	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})\mathbf{I}_2(\boldsymbol{\theta})$
$\{\mathbf{2},1,\mathbf{2},\mathbf{2},1,\mathbf{2},\mathbf{2},1,1,1\}$	25	1701.04	42526.00
$\{\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2},1,1,1,\mathbf{2},1\}$	25	1701.04	42526.00

Scenario 4. Example 2 in Parker, Gilmour, and Schormans (2017)

In this case, the optimal design in Section 4.1 is not optimal here; see Table 9. However, we observe that via complete search, its determinant is very close to that of the optimal design. Likewise, we compare the results with Parker, Gilmour, and Schormans (2017) and Chang, Phoa, and Huang (2021) in Table 10. The design chosen in this article is better.

From the four scenarios we discussed, we know that the conclusion in Section 4.1 might be not applicable when ϕ is estimated by the MLE.

5. Real Networks

The real networks are from `https://sites.google.com/site/ucinetsoftware/datasets`. They are datasets in UCINET software Borgatti, Everett, and Freeman(2002). In this section, we apply our theory to real networks and give the corresponding optimal designs.

5.1 Teenage Friends and Lifestyle Study

This social network data were collected in the Teenage Friends and Lifestyle Study. Friendship networks and substance use were recorded for a group of students in a school in the West of Scotland. The data were recorded for three years, starting in 1995 and ending in 1997. A total of 160 students took part in the study. The friendship networks were formed by allowing the students to name twelve best friends.

Schools might be interested in the influence of different interventions for promoting a healthy life among a group of students that knew each other socially, according to their friendship network structure. Some students might be sent daily text messages about healthy eating information, and the others might be sent a weekly magazine of the disadvantage of consuming tobacco, alcohol and cannabis. In addition to the effectiveness of the interventions, researchers were also interested in whether the message/magazine sent to one student had an effect on other students that connected with the original student in the social network. The treatment could be different daily text

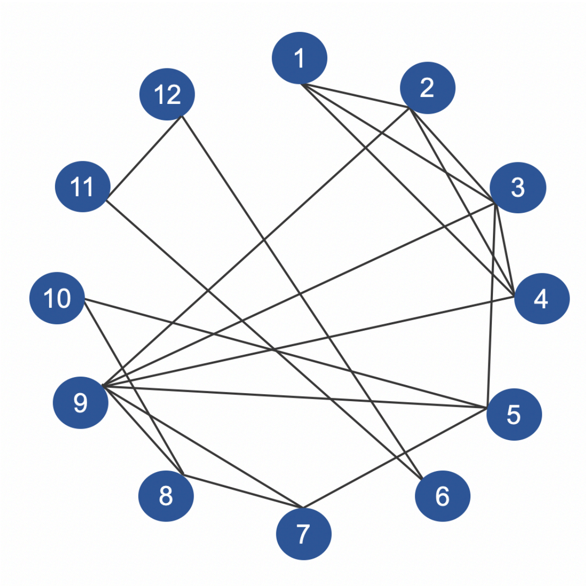


Figure 9: A Subset of the Friendship Network in a School in the West of Scotland.

messages about healthy eating information or weekly magazines of the disadvantage of consuming tobacco, alcohol and cannabis. The response could be sale volumes of tobacco, alcohol and cannabis.

The network shown in Figure 9 is a subset of the data. It has twelve units and twenty edges connected as the following adjacency matrix:

$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}.$$

We assume there are two different daily texts. Then we present the optimal designs in Table 11. The design with the largest L_{12} is D-optimal when ϕ approaches zero. However, when ϕ is estimated by the MLE, the optimal design is another one.

Table 11: Optimal Designs for Real Network 1 as $\phi \to 0$ and $\hat{\phi}$ = MLE.

Treatment assignment	L_{11}	L_{22}	L_{12}	$\hat{\phi}$	p_{11}	p_{22}	p_{12}
$\phi \to 0$							
$\{\mathbf{2},1,\mathbf{2},1,1,\mathbf{2},\mathbf{2},1,\mathbf{2},\mathbf{2},1,1\}$	2	3	15	0.00	0.731	0.731	0.500
$\{1,\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2},1,\mathbf{2},1,1,\mathbf{2},1\}$	3	2	15	0.00	0.731	0.731	0.500
$\{\mathbf{2},1,\mathbf{2},1,1,1,\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2},1\}$	2	3	15	0.00	0.731	0.731	0.500
$\hat{\phi}$ = MLE							
$\{\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},1,1\}$	3	17	0	−0.06	0.691	0.477	0.5

Treatment assignment	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})$	$\mathbf{I}_2(\boldsymbol{\theta})$	$\mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})\mathbf{I}_2(\boldsymbol{\theta})$
$\phi \to 0$			
$\{\mathbf{2},1,\mathbf{2},1,1,\mathbf{2},\mathbf{2},1,\mathbf{2},\mathbf{2},1,1\}$	36	4126.68	148560.43
$\{1,\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2},1,\mathbf{2},1,1,\mathbf{2},1\}$	36	4126.68	148560.43
$\{\mathbf{2},1,\mathbf{2},1,1,1,\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2},1\}$	36	4126.68	148560.43
$\hat{\phi}$ = MLE			
$\{\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},1,\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{2},1,1\}$	27	5202.28	140461.58

5.2 Friendship and Unionization in a Hi-tech Firm

The case is a small hi-tech computer firm that sells, installs, and maintains computer systems. The network contains the friendship ties between the employees, which were gathered by means of the question: Who do you consider to be a personal friend? A few months later, employees tried to organize a union in the firm: they sought support among the employees to let the union have a say in the firm. According to the friendship network structure, organizers want to know which slogan is more attractive to their colleagues to join the union. The subjects might be sent proposals about joining the union with different slogans. The response could be the number of clicks on

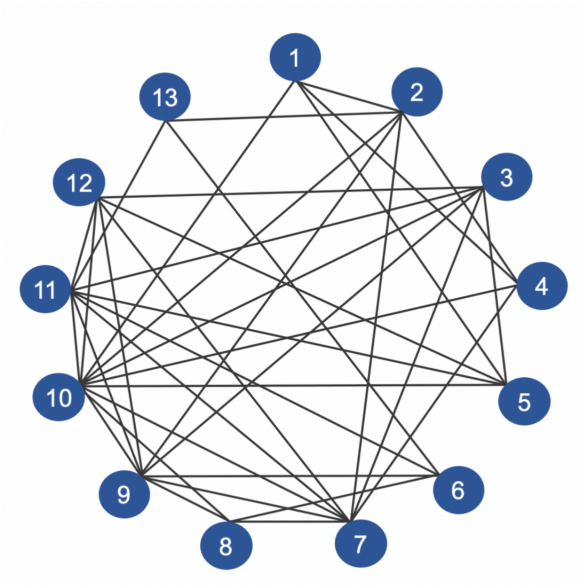


Figure 10: A Subset of the Friendship Nework in a Hi-tech Computer Firm.

proposal links.

The network shown in Figure 10 is a subset of the data, with thirteen nodes and thirty-eight edges connected as the following adjacency matrix:

$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 & 1 & 0 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 & 0 & 1 & 1 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix}.$$

We assume there are proposals about joining the union with two different slogans. Then we have the optimal designs under ϕ approaching zero and under ϕ estimated by the MLE in Table 12. The optimal designs are the same, which have the largest L_{12}.

Table 12: Optimal Designs for Real Network 2 as $\phi \to 0$ and $\hat{\phi}$ = MLE.

$\phi \to 0$							
Treatment assignment	L_{11}	L_{22}	L_{12}	$\hat{\phi}$	p_{11}	p_{22}	p_{12}
$\{\mathbf{2},\mathbf{2},\mathbf{2},1,1,1,1,\mathbf{2},1,1,\mathbf{2},\mathbf{2},1\}$	8	4	26	0.00	0.731	0.731	0.500
$\{1,\mathbf{2},\mathbf{2},\mathbf{2},1,1,1,\mathbf{2},1,1,\mathbf{2},\mathbf{2},1\}$	8	4	26	0.00	0.731	0.731	0.500
$\hat{\phi}$ = MLE							
Treatment assignment	L_{11}	L_{22}	L_{12}	$\hat{\phi}$	p_{11}	p_{22}	p_{12}
$\{\mathbf{2},\mathbf{2},\mathbf{2},1,1,1,1,\mathbf{2},1,1,\mathbf{2},\mathbf{2},1\}$	8	4	26	0.01	0.740	0.736	0.538
$\{1,\mathbf{2},\mathbf{2},\mathbf{2},1,1,1,\mathbf{2},1,1,\mathbf{2},\mathbf{2},1\}$	8	4	26	0.01	0.740	0.736	0.538

$\phi \to 0$			
Treatment assignment	$\mathbf{I}_1$	$\mathbf{I}_2$	$\mathbf{I}_1\mathbf{I}_2$
$\{\mathbf{2},\mathbf{2},\mathbf{2},1,1,1,1,\mathbf{2},1,1,\mathbf{2},\mathbf{2},1\}$	42	14818.87	622392.40
$\{1,\mathbf{2},\mathbf{2},\mathbf{2},1,1,1,\mathbf{2},1,1,\mathbf{2},\mathbf{2},1\}$	42	14818.87	622392.40
$\hat{\phi}$ = MLE			
Treatment assignment	$\mathbf{I}_1$	$\mathbf{I}_2$	$\mathbf{I}_1\mathbf{I}_2$
$\{\mathbf{2},\mathbf{2},\mathbf{2},1,1,1,1,\mathbf{2},1,1,\mathbf{2},\mathbf{2},1\}$	42	14724.23	618417.77
$\{1,\mathbf{2},\mathbf{2},\mathbf{2},1,1,1,\mathbf{2},1,1,\mathbf{2},\mathbf{2},1\}$	42	14724.23	618417.77

Note. $\mathbf{I}_1 = \mathbf{I}_1(\boldsymbol{\theta}; \mathbf{n})$, $\mathbf{I}_2 = \mathbf{I}_2(\boldsymbol{\theta})$, and $\mathbf{I}_1\mathbf{I}_2 = \mathbf{I}_1(\boldsymbol{\theta}; \mathbf{n})\mathbf{I}_2(\boldsymbol{\theta})$.

5.3 Discussion of Student Government

This network contains discussion relations among the eleven students who were members of the student government at the University of Ljubljana in Slovenia. The students were asked to point out with whom of their fellows they discussed matters concerning the administration of the university informally. Within the parliament, students have positions that convey official ranking: the prime minister, the ministers, and the advisors. The student government is responsible for legislating and supervising various administrative affairs of student associations, such as funding. A student

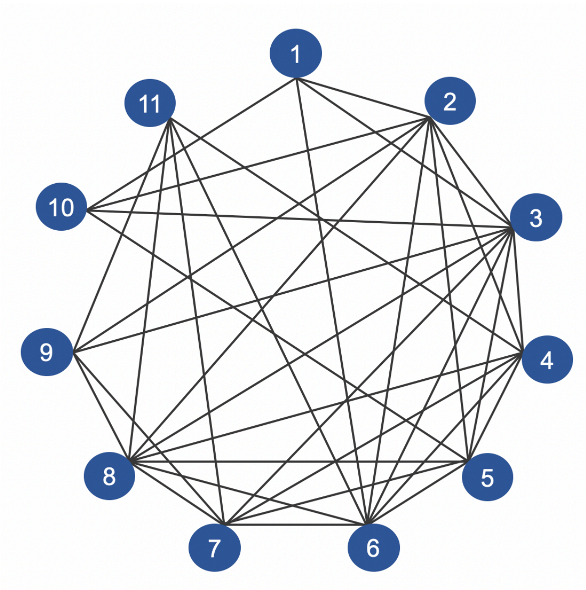


Figure 11: The Student Government Discussion Network.

wants to make the student government willing to provide more funds through distinct proposals. The treatments could be distinct proposals. The response could be funds.

The network shown in Figure 11 has eleven units and thirty-six edges connected as the following adjacency matrix:

$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 & 1 & 1 & 0 & 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 1 & 0 & 1 & 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 & 1 & 1 & 0 & 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 1 & 1 & 1 & 0 & 0 \end{bmatrix}.$$

We assume a student provides three different activity proposals. Then we present the optimal designs in Table 13. Similar to the previous examples, the design with the largest L_{12} is D-optimal under the condition that ϕ approaches zero. However, the optimal design is not suitable for the condition that ϕ is estimated by the MLE.

Table 13: Optimal Designs for Real Network 3 as $\phi \to 0$ and $\hat{\phi}$ = MLE.

Treatment assignment	L_{11}	L_{22}	L_{33}	L_{12}	L_{13}	L_{23}	$\hat{\phi}$
$\phi \to 0$							
$\{\mathbf{3},\mathbf{1},\mathbf{1},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{1}\}$	6	4	0	22	2	2	0.00
$\hat{\phi}$ = MLE							
$\{\mathbf{3},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{1},\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{1}\}$	6	6	0	20	2	2	0.05
$\{\mathbf{3},\mathbf{1},\mathbf{1},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{1}\}$	6	6	0	20	2	2	0.05
$\{\mathbf{3},\mathbf{3},\mathbf{1},\mathbf{3},\mathbf{1},\mathbf{1},\mathbf{3},\mathbf{3},\mathbf{1},\mathbf{2},\mathbf{1}\}$	6	0	6	2	20	2	0.05

Treatment assignment	p_{11}	p_{22}	p_{33}	p_{12}	p_{13}	p_{23}	$\mathbf{I}_1$	$\mathbf{I}_2$	$\mathbf{I}_1\mathbf{I}_2$
$\phi \to 0$									
$\{\mathbf{3},\mathbf{1},\mathbf{1},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{1}\}$	0.73	0.73	0.73	0.50	0.50	0.50	25	6274	156862
$\hat{\phi}$ = MLE									
$\{\mathbf{3},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{1},\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{1}\}$	0.79	0.79	0.73	0.75	0.53	0.53	25	4017	100415
$\{\mathbf{3},\mathbf{1},\mathbf{1},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{2},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{1}\}$	0.79	0.79	0.73	0.75	0.53	0.53	25	4017	100415
$\{\mathbf{3},\mathbf{3},\mathbf{1},\mathbf{3},\mathbf{1},\mathbf{1},\mathbf{3},\mathbf{3},\mathbf{1},\mathbf{2},\mathbf{1}\}$	0.79	0.73	0.79	0.53	0.75	0.53	25	4017	100415

Note. $\mathbf{I}_1 = \mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})$, $\mathbf{I}_2 = \mathbf{I}_2(\boldsymbol{\theta})$, and $\mathbf{I}_1\mathbf{I}_2 = \mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})\mathbf{I}_2(\boldsymbol{\theta})$.

6. Conclusion

This article studies optimal designs for experimental units with general network structures. Different from the linear network effect model proposed by Parker, Gilmour, and Schormans (2017) and Chang, Phoa, and Huang (2021), we propose a novel statistical network-based model, more easily justified by the network literature. Our model is an extension of network block models and NLR models, and incorporates the local and global patterns of a network. We derive a theoretical result under the condition ϕ approaching zero, and provide sufficient conditions for optimal designs. In the numerical study, we consider common classes of graphs, such as bipartite, path, and cycle networks, and a network in Parker, Gilmour, and Schormans (2017) and Chang, Phoa, and Huang (2021). By the comparison in the numerical study, we find that the optimal design under ϕ approaching zero might not be the same as that under ϕ estimated by the maximum likelihood estimation. This shows that the global patterns of a network play a role in determining optimal designs. Lastly, we discuss three real-world networks and show that our methods are not only applicable for specific graphs, but also for general networks.

Studying optimal designs under ϕ estimated by the maximum likelihood estimation is a challenging task. In addition, deriving a powerful testing method for the hypothesis $\mathrm{H}_0 : \phi = 0$ is crucial since Theorem 1 is derived under ϕ approaching zero. As pointed out by a reviewer, we realize that the equation in (2) may not be able to mathematically characterize the connection probabilities for a few nodes in very small-scale graphs. We leave the above problems for future research.

Appendix

A.1. $m = 3$ with $\phi \to 0$

In Section 4.1, we have derived numerical results by four types of graphs under $m = 2$. Here, we examine the numerical results for $m = 3$. When $m = 3$ and $\phi \to 0$, $p_{11} = p_{22} = p_{33} = 0.731$ and $p_{12} = p_{13} = p_{23} = 0.5$.

Scenario 1. Complete Bipartite Graph

We illustrate the scenario of the complete bipartite graph via an example with twelve units as in Figure 12. We show the top three designs in Table 14. The red one represents the optimal design. The design with the largest L_{12} is D-optimal.

Scenario 2. Cycle Graph

We illustrate this scenario via an example with eleven units as in Figure 13. We have the top three designs in Table 15. The design with the largest L_{23}, one of L_{ij}, is D-optimal.

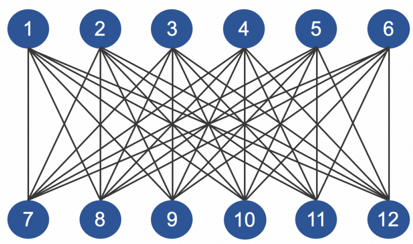


Figure 12: Complete Bipartite Graph with N=12.

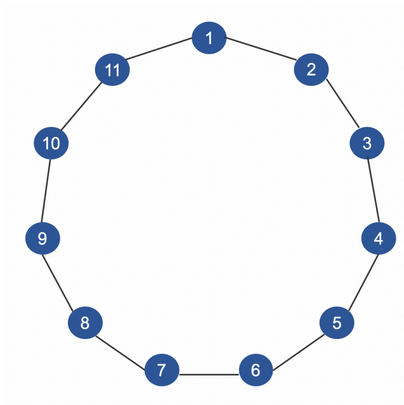


Figure 13: Cycle Graph with N=11.

Table 14: Selected Designs for Scenario 1 as $\phi \to 0$ and $m = 3$.

Treatment assignment	L_{11}	L_{22}	L_{33}	L_{12}	L_{13}	L_{23}	$\mathbf{I}_1$	$\mathbf{I}_2$	$\mathbf{I}_1\mathbf{I}_2$
$\{3,2,2,2,2,2,1,1,1,1,1,1\}$	0	0	0	30	6	0	30	13608	408240
$\{3,3,3,3,3,2,2,1,1,1,1,1\}$	0	1	0	5	25	5	50	8063	403145
$\{3,3,2,2,2,2,1,1,1,1,1,1\}$	0	0	0	24	12	0	48	7776	373248

Note. $\mathbf{I}_1 = \mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})$, $\mathbf{I}_2 = \mathbf{I}_2(\boldsymbol{\theta})$, and $\mathbf{I}_1\mathbf{I}_2 = \mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})\mathbf{I}_2(\boldsymbol{\theta})$.

Table 15: Selected Designs for Scenario 2 as $\phi \to 0$ and $m = 3$.

Treatment assignment	L_{11}	L_{22}	L_{33}	L_{12}	L_{13}	L_{23}	$\mathbf{I}_1$	$\mathbf{I}_2$	$\mathbf{I}_1\mathbf{I}_2$
$\{2,3,2,3,2,3,2,3,2,1,1\}$	1	0	0	2	0	8	40	660	26416
$\{3,2,1,2,1,2,1,2,1,2,1\}$	0	0	0	9	1	1	25	1018	25438
$\{3,1,3,2,1,2,1,2,1,2,1\}$	0	0	0	7	3	1	40	539	21560

Note. $\mathbf{I}_1 = \mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})$, $\mathbf{I}_2 = \mathbf{I}_2(\boldsymbol{\theta})$, and $\mathbf{I}_1\mathbf{I}_2 = \mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})\mathbf{I}_2(\boldsymbol{\theta})$.

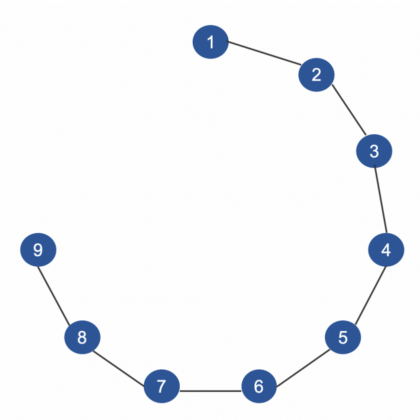


Figure 14: Path Graph with N=9.

Table 16: Selected Designs for Scenario 3 as $\phi \to 0$ and $m = 3$.

Treatment assignment	L_{11}	L_{22}	L_{33}	L_{12}	L_{13}	L_{23}	$\mathbf{I}_1$	$\mathbf{I}_2$	$\mathbf{I}_1\mathbf{I}_2$
$\{\mathbf{3},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{1}\}$	0	0	0	7	1	1	16	396	6336
$\{\mathbf{2},\mathbf{3},\mathbf{2},\mathbf{3},\mathbf{2},\mathbf{3},\mathbf{2},\mathbf{1},\mathbf{1}\}$	1	0	0	2	0	6	24	232	5577
$\{\mathbf{2},\mathbf{3},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{1},\mathbf{2},\mathbf{1},\mathbf{1}\}$	1	0	0	6	0	2	16	298	4774

Note. $\mathbf{I}_1 = \mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})$, $\mathbf{I}_2 = \mathbf{I}_2(\boldsymbol{\theta})$, and $\mathbf{I}_1\mathbf{I}_2 = \mathbf{I}_1(\boldsymbol{\theta};\mathbf{n})\mathbf{I}_2(\boldsymbol{\theta})$.

Scenario 3. Path Graph

We illustrate a path graph with nine units as in Figure 14. We have the top three designs in Table 16. The design with the largest L_{12} is D-optimal.

Scenario 4. Example 2 in Parker, Gilmour, and Schormans (2017)

Similar to Section 4, the unsymmetry in the graph leads to numerous nonisomorphic designs. Hence, we only compare the results with Chang, Phoa, and Huang (2021); see Table 17. With respect to the criterion we propose, the design chosen in this article is better. The D-optimal design has the largest L_{12}.

Table 17: Comparison in Optimal Designs for Scenario 4 as $\phi \to 0$ and $m = 3$.

This article									
Treatment assignment	L_{11}	L_{22}	L_{33}	L_{12}	L_{13}	L_{23}	$\mathbf{I}_1$	$\mathbf{I}_2$	$\mathbf{I}_1\mathbf{I}_2$
$\{\mathbf{3}, \mathbf{1}, \mathbf{1}, \mathbf{2}, \mathbf{3}, \mathbf{1}, \mathbf{2}, \mathbf{2}, \mathbf{2}, \mathbf{1}\}$	2	3	1	13	1	2	32	1403	44898
Chang, Phoa, and Huang (2021)									
Treatment assignment	L_{11}	L_{22}	L_{33}	L_{12}	L_{13}	L_{23}	$\mathbf{I}_1$	$\mathbf{I}_2$	$\mathbf{I}_1\mathbf{I}_2$
$\{\mathbf{1}, \mathbf{2}, \mathbf{3}, \mathbf{3}, \mathbf{2}, \mathbf{3}, \mathbf{1}, \mathbf{1}, \mathbf{2}, \mathbf{1}\}$	4	2	2	5	5	4	36	419	15091
$\{\mathbf{1}, \mathbf{2}, \mathbf{3}, \mathbf{1}, \mathbf{2}, \mathbf{3}, \mathbf{3}, \mathbf{1}, \mathbf{2}, \mathbf{3}\}$	2	2	3	4	6	5	36	469	16872

Note. $\mathbf{I}_1 = \mathbf{I}_1(\boldsymbol{\theta}; \mathbf{n})$, $\mathbf{I}_2 = \mathbf{I}_2(\boldsymbol{\theta})$, and $\mathbf{I}_1\mathbf{I}_2 = \mathbf{I}_1(\boldsymbol{\theta}; \mathbf{n})\mathbf{I}_2(\boldsymbol{\theta})$.

A.2. $m = 3$ with estimated ϕ

In this section, we show the numerical results for the condition that ϕ is estimated by the MLE and $m = 3$. Therefore, it results in different p_{kl} and the determinants given different designs.

Scenario 1. Complete Bipartite Graph

For the scenario of the complete bipartite graph, we show the optimal design in Section A.1 and the top two designs in Table 18. The red one represents the optimal design in Section A.1. The orange one represents the optimal design for ϕ estimated by the MLE. The range of $\hat{\phi}$ is from -0.05 to 2.93. We find that the optimal design when ϕ approaches zero is the worst in this condition; since $\hat{\phi} = 2.93$ causes $p_{12} = p_{13} = 1$, the determinant is zero. This consequence is similar when $m = 2$.

Scenario 2. Cycle Graph

In this case, we show the top three designs in Table 19. The range of $\hat{\phi}$ is from -0.88 to -0.03. The optimal design in Section A.1 is also D-optimal here. This consequence is also similar when $m = 2$.

Scenario 3. Path Graph

In this scenario, we present the top three designs in Table 20. The range of $\hat{\phi}$ is from -0.78 to -0.03. The D-optimal design is the same as that in Section A.1.

Table 18: Selected Designs for Scenario 1 under $\hat{\phi}$ = MLE and $m = 3$.

Treatment assignment	L_{11}	L_{22}	L_{33}	L_{12}	L_{13}	L_{23}	$\hat{\phi}$
{3, 2, 2, 2, 2, 2, 1, 1, 1, 1, 1, 1}	0	0	0	30	6	0	2.93
{3, 2, 2, 2, 2, 1, 2, 1, 1, 1, 1, 1}	5	4	0	21	5	1	0.03
{3, 2, 2, 2, 2, 1, 3, 2, 1, 1, 1, 1}	4	4	1	17	5	5	0.02

Treatment assignment	p_{11}	p_{22}	p_{33}	p_{12}	p_{13}	p_{23}	$\mathbf{I}_1$	$\mathbf{I}_2$	$\mathbf{I}_1\mathbf{I}_2$
{3, 2, 2, 2, 2, 2, 1, 1, 1, 1, 1, 1}	0.73	0.73	0.73	1.00	1.00	0.50	30	0	0
{3, 2, 2, 2, 2, 1, 2, 1, 1, 1, 1, 1}	0.76	0.75	0.73	0.63	0.53	0.51	30	6438	193134
{3, 2, 2, 2, 2, 1, 3, 2, 1, 1, 1, 1}	0.75	0.75	0.74	0.60	0.53	0.53	50	3845	192244

Note. $\mathbf{I}_1 = \mathbf{I}_1(\boldsymbol{\theta}; \mathbf{n})$, $\mathbf{I}_2 = \mathbf{I}_2(\boldsymbol{\theta})$, and $\mathbf{I}_1\mathbf{I}_2 = \mathbf{I}_1(\boldsymbol{\theta}; \mathbf{n})\mathbf{I}_2(\boldsymbol{\theta})$.

Table 19: Selected Designs for Scenario 2 under $\hat{\phi}$ = MLE and $m = 3$.

Treatment assignment	L_{11}	L_{22}	L_{33}	L_{12}	L_{13}	L_{23}	$\hat{\phi}$
{2, 3, 2, 3, 2, 3, 2, 3, 2, 1, 1}	1	0	0	2	0	8	−0.07
{3, 2, 1, 2, 1, 2, 1, 2, 1, 2, 1}	0	0	0	9	1	1	−0.08
{3, 1, 3, 2, 1, 2, 1, 2, 1, 2, 1}	0	0	0	7	3	1	−0.12

Treatment assignment	p_{11}	p_{22}	p_{33}	p_{12}	p_{13}	p_{23}	$\mathbf{I}_1$	$\mathbf{I}_2$	$\mathbf{I}_1\mathbf{I}_2$
{2, 3, 2, 3, 2, 3, 2, 3, 2, 1, 1}	0.72	0.73	0.73	0.47	0.50	0.37	40	616	24641
{3, 2, 1, 2, 1, 2, 1, 2, 1, 2, 1}	0.73	0.73	0.73	0.33	0.48	0.48	25	899	22481
{3, 1, 3, 2, 1, 2, 1, 2, 1, 2, 1}	0.73	0.73	0.73	0.30	0.41	0.47	40	458	18334

Note. $\mathbf{I}_1 = \mathbf{I}_1(\boldsymbol{\theta}; \mathbf{n})$, $\mathbf{I}_2 = \mathbf{I}_2(\boldsymbol{\theta})$, and $\mathbf{I}_1\mathbf{I}_2 = \mathbf{I}_1(\boldsymbol{\theta}; \mathbf{n})\mathbf{I}_2(\boldsymbol{\theta})$.

Table 20: Selected Designs for Scenario 2 under $\hat{\phi}$ = MLE and $m = 3$.

Treatment assignment	L_{11}	L_{22}	L_{33}	L_{12}	L_{13}	L_{23}	$\hat{\phi}$
$\{\mathbf{3}, \mathbf{2}, \mathbf{1}, \mathbf{2}, \mathbf{1}, \mathbf{2}, \mathbf{1}, \mathbf{2}, \mathbf{1}\}$	0	0	0	7	1	1	−0.07
$\{\mathbf{2}, \mathbf{3}, \mathbf{2}, \mathbf{3}, \mathbf{2}, \mathbf{3}, \mathbf{2}, \mathbf{1}, \mathbf{1}\}$	1	0	0	2	0	6	−0.03
$\{\mathbf{3}, \mathbf{1}, \mathbf{3}, \mathbf{2}, \mathbf{1}, \mathbf{2}, \mathbf{1}, \mathbf{2}, \mathbf{1}\}$	0	0	0	5	3	1	−0.12

Treatment assignment	p_{11}	p_{22}	p_{33}	p_{12}	p_{13}	p_{23}	$\mathbf{I}_1$	$\mathbf{I}_2$	$\mathbf{I}_1\mathbf{I}_2$
$\{\mathbf{3}, \mathbf{2}, \mathbf{1}, \mathbf{2}, \mathbf{1}, \mathbf{2}, \mathbf{1}, \mathbf{2}, \mathbf{1}\}$	0.73	0.73	0.73	0.38	0.48	0.48	16	372	5944
$\{\mathbf{2}, \mathbf{3}, \mathbf{2}, \mathbf{3}, \mathbf{2}, \mathbf{3}, \mathbf{2}, \mathbf{1}, \mathbf{1}\}$	0.72	0.73	0.73	0.48	0.50	0.45	24	230	5529
$\{\mathbf{3}, \mathbf{1}, \mathbf{3}, \mathbf{2}, \mathbf{1}, \mathbf{2}, \mathbf{1}, \mathbf{2}, \mathbf{1}\}$	0.73	0.73	0.73	0.36	0.41	0.47	24	176	4225

Note. $\mathbf{I}_1 = \mathbf{I}_1(\boldsymbol{\theta}; \mathbf{n})$, $\mathbf{I}_2 = \mathbf{I}_2(\boldsymbol{\theta})$, and $\mathbf{I}_1\mathbf{I}_2 = \mathbf{I}_1(\boldsymbol{\theta}; \mathbf{n})\mathbf{I}_2(\boldsymbol{\theta})$.

Table 21: Comparison in Optimal Designs for Scenario 4 under $\hat{\phi}$ =MLE and $m = 3$.

This article								
Treatment assignment	L_{11}	L_{22}	L_{33}	L_{12}	L_{13}	L_{23}	$\mathbf{I}_1$	$\mathbf{I}_2$
$\{\mathbf{2}, \mathbf{1}, \mathbf{1}, \mathbf{1}, \mathbf{1}, \mathbf{3}, \mathbf{2}, \mathbf{2}, \mathbf{2}, \mathbf{1}\}$	5	1	0	14	1	1	20	2065
	p_{11}	p_{22}	p_{33}	p_{12}	p_{13}	p_{23}	$\hat{\phi}$	$\mathbf{I}_1\mathbf{I}_2$
	0.73	0.73	0.73	0.50	0.50	0.50	0.00	41306
Chang, Phoa, and Huang (2021)								
Treatment assignment	L_{11}	L_{22}	L_{33}	L_{12}	L_{13}	L_{23}	$\mathbf{I}_1$	$\mathbf{I}_2$
$\{\mathbf{1}, \mathbf{2}, \mathbf{3}, \mathbf{3}, \mathbf{2}, \mathbf{3}, \mathbf{1}, \mathbf{1}, \mathbf{2}, \mathbf{1}\}$	4	2	2	5	5	4	36	414
	p_{11}	p_{22}	p_{33}	p_{12}	p_{13}	p_{23}	$\hat{\phi}$	$\mathbf{I}_1\mathbf{I}_2$
	0.67	0.70	0.70	0.42	0.42	0.43	−0.07	14913
Treatment assignment	L_{11}	L_{22}	L_{33}	L_{12}	L_{13}	L_{23}	$\mathbf{I}_1$	$\mathbf{I}_2$
$\{\mathbf{1}, \mathbf{2}, \mathbf{3}, \mathbf{1}, \mathbf{2}, \mathbf{3}, \mathbf{3}, \mathbf{1}, \mathbf{2}, \mathbf{3}\}$	2	2	3	4	6	5	36	462
	p_{11}	p_{22}	p_{33}	p_{12}	p_{13}	p_{23}	$\hat{\phi}$	$\mathbf{I}_1\mathbf{I}_2$
	0.71	0.71	0.69	0.45	0.42	0.44	−0.05	16646

Note. $\mathbf{I}_1 = \mathbf{I}_1(\boldsymbol{\theta}; \mathbf{n})$, $\mathbf{I}_2 = \mathbf{I}_2(\boldsymbol{\theta})$, and $\mathbf{I}_1\mathbf{I}_2 = \mathbf{I}_1(\boldsymbol{\theta}; \mathbf{n})\mathbf{I}_2(\boldsymbol{\theta})$.

Scenario 4. Example 2 in Parker, Gilmour, and Schormans (2017)

In this example, the optimal design in Section A.1 is not optimal here. See Table 21 for details. Likewise, we compare the results with Chang, Phoa, and Huang (2021) in Table 21. The design chosen in this article is better.

From the four scenarios we discussed, we derive a similar conclusion in Section 4. Only the second scenario and the third scenario have the same optimal designs for two conditions. That is, the results for ϕ approaching zero may be not applicable to ϕ estimated by the MLE.

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網路效應模型在無向網路結構之最佳設計

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摘　要

在生活中，具有網路結構的例子無所不在，例如在農業實驗、生物信息學、醫學實驗、機器學習、物理學、社會科學和許多其他科學領域，再加上社交網路的快速發展，網路相關的議題已經成為一個新興的研究領域。為一個實驗單位指派處理會影響該實驗單位及其鄰居，並同時產生了處理效應和網路效應。在實驗設計的文獻中，Parker, Gilmour, and Schormans (2017) 和 Chang, Phoa, and Huang (2021) 都採用了線性網路效應模型來處理網路實驗。然而，這種模型並未得到廣泛應用。Kolaczyk and Csárdi (2014) 回顧了網路的統計模型，例如指數隨機圖模型和網路區塊模型。Zhang *et al.* (2020) 考慮了一種基於網路的邏輯斯迴歸模型來描述網路效應。本文擴展 Kolaczyk and Csárdi (2014) 以及 Zhang *et al.* (2019) 的想法提出了一種新的網路統計模型，並尋找最佳設計的條件。最後，我們通過模擬和真實例子來說明我們的理論且提供相對應的最佳設計。

關鍵詞: 社交網路、處理效應、網路效應、網路建模、二分圖/循環圖/路徑圖、D 最佳化準則。

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