Existence theorems for some group testing strategies

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Abstract. Group testing problems are considered as examples of discrete search problems. Existence theorems for optimal nonsequential designs developed for the general discrete search problems in [1] are applied for construction of upper bounds for the length of optimal group testing strategies in the case of additive model. The key point in the study is derivation of analytic expressions for the so-called Renyi coefficients. In addition, some asymptotic results are obtained and an asymptotic design problem is considered. The results particularly imply that if the number of significant factors is relatively small comparing with the total number of factors then the choice of the test collections all containing a half of the total number of factors is asymptotically optimal in a proper sense.

Key words: Group testing, factor screening, existence theorems, experimental design, significant factors.

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1 Introduction

Group testing, known also as factor screening and search for significant factors, is a vast area with many papers developing both theoretical and applied aspects. A general statement of the group testing problem that covers many particular statements is as follows. Assume that n factors (elements, items, variables, etc.) $x_1, \ldots, x_n$ are given and some of them are *defective* (significant, important, etc.). The problem is to determine which factors are defective by testing several factor groups, that is subsets of the set $\underline{X} = \{x_1, \ldots, x_n\}$. The problems differ in

(i) prior information concerning the number of defective factors,

(ii) constraints on the test groups, and

(iii) information we are getting by inspecting the groups.

This work is concerned with the problems determined by

(i) the number of defective factors is either equal to or not greater than t where t is a given number, $1 \leq t \leq n$,

(ii) there is either no constraints on the test groups or the groups contain exactly s elements or the groups contain s elements or less, $1 \leq s \leq n$, and

(iii) by inspecting a group $Z, Z \subset \underline{X}$ we receive a number of defective factors in Z (additive, or quantitative model).

Also, we only consider the *nonsequential* strategies (called also static, nonadaptive, passive, etc.) when all tests have to be specified without knowing the outcomes of other tests.

The paper by R.Dorfman [2], devoted to sequential procedures of blood testing for detection of syphilitic men, is usually considered as the first work on the theory of group testing. The blood testing and many other practical problems are described by the binary model where by inspecting a group Z one receives 1 if there is at least one defective in Z and 0 otherwise. This model is perhaps the most important and well studied. During more than 50 years of the history of the group testing many other mathematical models have been also developed and advanced results have been achieved. Among many classical papers in the field of group testing we mention only several dealing with statistical and probabilistic aspects: [3, 4, 5, 6]. A recent monograph [7] covers the major part of the main achievements in the group testing theory. The readers mainly interested in applications may also find very useful the collection of papers [8].

In the present work we apply the probabilistic method of [1] to prove the existence of nonsequential designs that detect all defective factors by performing N tests where N is called the length of the design and small values of N are preferable. The probabilistic method for proving existence theorems for nonsequential search designs was proposed by A.Renyi in a classical paper [6] and since then it was applied to different search problems, examples can be found in [7] and the forthcoming monograph [9].

Section 2 formulates the problem of group testing as an example of a general search problem and provides general existence theorems. In Section 3 upper bound for the length of optimal strategies are established in some particular cases. Section 3 can be regarded as an introduction to Section 4 where the general case is solved. In Section 5 a problem of an asymptotically optimal experimental design is considered where a design set rather than design points is to be chosen in an optimal way.

We do not consider the important problem of finding strategies with small length N. We refer to [10] for construction of sequential algorithms in the case when the number of defective factors is either known or bounded and to [11, 12] for design construction in particular cases. In this respect we also mention a well–known paper [5] which not only considers some schemes of design construction but also demonstrates a lot of interesting properties of design matrices for a group testing problem being more general than the problem considered in the present work.

In asymptotic considerations we only consider the case when the number of defective factors is small compared to the total number of factors n. This is the main point which makes the difference between the asymptotic results of the present paper and the results obtained in a series of papers [13, 14, 15] where the nonsequential group testing problem for the additive model is considered with no constraints on both the test groups and the number of defective factors. The above papers yield the result $N_{\min} \sim \frac{2n}{\log_2 n}$, $n \to \infty$, for the minimal length of a nonsequential strategy which guarantees detection of all defectives. We show that if the number of defective factors is small compared to n then typically $N_{\min} \leq c \log n$ for some constant c which does not depend on n but may depend on information concerning the number of defectives, constraints on the test groups and required probability of correct decision.

2 Group testing as a search problem, general existence theorems

2.1 General discrete search problems

Our approach is to consider group testing problems from a general view of discrete search. To do this let us start with a rather general formulation of discrete search problems which is borrowed from [1].

Definition 2.1. A *discrete search problem* is a triple $(\mathcal{T}, \mathcal{X}, f)$ where $\mathcal{T} = \{T\}$ is a target field, that is a collection of all possible target combinations T, $\mathcal{X} = \{X\}$ is a *test field,* that is a collection of all possible test combinations, and $f : \mathcal{X} \times \mathcal{T} \to \mathcal{Y}$ is a *search function* mapping $\mathcal{X} \times \mathcal{T}$ to some space $\mathcal{Y}$.

A value $f(X, T)$ for fixed $X \in \mathcal{X}$ and $T \in \mathcal{T}$ is called a *test* result at a test combination X when the unknown target combination is T.

Definition 2.2. A target $T \in \mathcal{T}$ is *achievable* if for any other $T' \in \mathcal{T}$ there exist $X \in \mathcal{X}$ such that $f(X, T) \neq f(X, T')$. A search problem $\{\mathcal{T}, \mathcal{X}, f\}$ is *solvable* if every $T \in \mathcal{T}$ is achievable.

If a search problem is not solvable then there exist targets which are impossible to find. We shall only consider the search problems that are solvable.

For the group testing problems both $\mathcal{X}$ and $\mathcal{T}$ are certain collections of factor groups. We mainly consider the problems when $\mathcal{T}$ is either $\mathcal{G}_t$ or $\mathcal{G}_{\leq t}$ and analogously $\mathcal{X}$ is either $\mathcal{G}_s$ or $\mathcal{G}_{\leq s}$. Here $1 \leq t < n$, $1 \leq s \leq n$, n is the total number of factors,

$$\mathcal{G}_k = \{\{x_{i_1}, \ldots, x_{i_k}\},\ \ 1 \leq i_1 < \ldots i_k \leq n\} \tag{1}$$

is the collection of all factor groups containing exactly k factors,

$$\mathcal{G}_{\leq k} = \bigcup_{j=0}^{k} \mathcal{G}_j \tag{2}$$

is the collection of the groups containing k factors or less. As for the test function, we only consider the function $f(X, T) = |X \cap T|$ where $|A|$ denotes the number of elements in a set A. This corresponds to the so-called "additive group testing" model.

2.2 Strongly separating designs

Definition 2.3. A nonsequential design $\mathcal{X}_N$ of a length N is a collection of test combinations $\mathcal{X}_N = \{X_1, \dots, X_N\}$ which are chosen before the observations start.

If we apply a nonsequential design then for any $i > 0$ the test results $f(X_1, T), \dots, f(X_{i-1}, T)$ can not be used to select X_i. We shall not consider other types of designs and will usually omit the word "nonsequential" while referring to a nonsequential design.

To ensure that a design $\mathcal{X}_N$ finds an unknown target T whatever the target $T \in \mathcal{T}$ is, the design should separate all $T \in \mathcal{T}$, that is to say to be *strongly separating.*

Definition 2.4. A design $\mathcal{X}_N = \{X_1, \dots, X_N\}$ *separates* T in $\mathcal{T}$ if for any $T' \in \mathcal{T}$, $T' \neq T$ there exist a test group $X \in \mathcal{X}_N$ which separates the pair (T, T') that is $f(X, T) \neq f(X, T')$. A design $\mathcal{X}_N$ is *strongly separating* if it separates all T in $\mathcal{T}$.

The following basic result of [1] will be used to establish the existence of the group testing strategies.

Theorem 2.1. *Let $(\mathcal{T}, \mathcal{X}, f)$ be a solvable search problem, $|\mathcal{T}| = M \geq 4$, $|\mathcal{X}| = R$, and for a fixed $T_i, T_j \in \mathcal{T}$ $(1 \leq j < i \leq M)$ let $k_{ij} = k(T_i, T_j)$ be the number of $X \in \mathcal{X}$ such that $f(X, T_i) = f(X, T_j)$, that is*

$$k_{ij} = |X \in \mathcal{X} : \ f(X, T_i) = f(X, T_j)| \quad \text{for } T_i, T_j \in \mathcal{T}\,. \tag{3}$$

Then there exists a nonsequential strongly separating search design with the sample size

$$N \ \leq \ N^* = \min\left\{ k = 1, 2, \dots \text{ such that } \sum_{i=1}^{M} \sum_{j=1}^{i-1} \left(\frac{k_{ij}}{R} \right)^k \leq 1 \right\}. \tag{4}$$

The proof can be found in [1, 9]. However, for the sake of completeness we outline the proof of the theorem.

Proof. Let us consider the test groups $X_i \in \mathcal{X}_N$ $(i = 1, \dots, N)$ as uniformly distributed on $\mathcal{X}$ mutually independent random elements and estimate the probability q_N that at least one N-collection of these random elements constitutes a strongly separating design $\mathcal{X}_N$. Let A_{ij} be the event that T_i and T_j are not separated by all $X_i \in \mathcal{X}_N$. By independence, $\text{Prob}(A_{ij}) = \left(\frac{k_{ij}}{R}\right)^N$. Then $1 - q_N = \text{Prob}(\cup_{i<j} A_{ij})$ is the probability of that the random design $\mathcal{X}_N$ is not strongly separating. But

$$\text{Prob}(\cup_{i<j} A_{ij}) < \sum_{i<j} \text{Prob}(A_{ij}) = \sum_{i<j} \left(\frac{k_{ij}}{R} \right)^N$$

where the fact that the inequality is strict follows from dependence of random events A_{ij} for $M \geq 4$. The first value of N, such that the right hand side of this inequality is smaller than or equal to 1, gives (4). $\square$

The sampling procedure above for $X_i \in \mathcal{X}$ corresponds to the random sampling from $\mathcal{X}$ with replacement. If to use the random sampling from $\mathcal{X}$ without replacement then the same arguments lead to the upper bound for the length of the optimal design

$$N \ \leq \ N^+ = \min\left\{ k = 1, 2, \dots : \ \sum_{i=1}^{M} \sum_{j=1}^{i-1} \frac{k_{ij}(k_{ij} - 1) \dots (k_{ij} - k + 1)}{R(R - 1) \dots (R - k + 1)} < 1 \right\} \tag{5}$$

where we use the assumption $\frac{0}{0} = 0$. This upper bound is always smaller than or equal to (4) but it is a little more complex to compute. For large enough values of $R = |\mathcal{X}|$ we do not know cases when the estimates (4) and (5) are different. Therefore, we shall always compute (4) and use (4) in asymptotic considerations. Computation of (5) is analogous and all asymptotic conclusions are the same for (4) and (5).

Computation of (4) and (5) for a particular search problem corresponds to an existence proof of a strongly separating design $\mathcal{X}_N$ of the length $N \leq N^*$ or $N \leq N^+$. Derivation of formulas for the coefficients (3) implies the derivation of the upper bounds (4), (5) and constitutes the main objective of the present work. A general case will be considered in Section 4.

2.3 Weakly separating designs

Strongly separating can be weakened to say that the problem is solved for most targets in $\mathcal{T}$.

Definition 2.5. Let a search problem $(\mathcal{T}, \mathcal{X}, f)$ be solvable and γ be a fixed number, $0 \leq \gamma \leq 1$. A design $\mathcal{X}_N$ is called γ*-separating design* if

$$\frac{|\, \{T \in \mathcal{T}: \text{ design } \mathcal{X}_N \text{ separates } T \text{ in } \mathcal{T}\} \,|}{|\, \mathcal{T} \,|} \geq 1 - \gamma\,. \tag{6}$$

Note that the definition of γ-separating designs can be generalized to the case when there is a nonuniform prior measure on $\mathcal{T}$ and that in the present notation 0-separating designs are exactly the same as strongly separating designs.

The difference between the concepts of strongly separating and γ-separating designs is as follows. If one has to construct a design which separates all the targets then he should use a strongly separating design. However if one has got a search problem and he would be satisfied with a design that solves his problem in a majority of cases then it is worthwhile to use a γ-separating design. As we shall see later one can typically guarantee the existence of γ-separating designs with a much smaller length than for the strongly separating designs.

The following theorem is a generalization of Theorem 2.1 for the case of γ-separating designs.

Theorem 2.2. *Let $(\mathcal{T}, \mathcal{X}, f)$ be a solvable search problem, $|\mathcal{T}| = M \geq 2$ and $|\mathcal{X}| = R$, $0 < \gamma < 1$ be a fixed number and k_{ij} be defined by* (3). *Then there exists a non-sequential γ-separating design with sample size*

$$N \;\leq\; N_\gamma = \min\left\{ k = 1, 2, \ldots : \sum_{i=1}^{M} \sum_{j \neq i} \left(\frac{k_{ij}}{R} \right)^k < M\gamma, \right\}, \tag{7}$$

Proof. The proof is analogous to the proof of Theorem 2.1, the difference is that we do not need to separate all pairs of different $T_i, T_j \in \mathcal{T}$: for fixed $T_i \in \mathcal{T}$ the probability of that T_i is not separated from at least one $T_j \in \mathcal{T}$ after N random tests is less than or equal to $\sum_{j \neq i} \left(\frac{k_{ij}}{R} \right)^N$ and we have $1 - \sum_{j \neq i} \left(\frac{k_{ij}}{R} \right)^N$ as a lower bound for the probability of that T_i is separated from all others $T_j \in \mathcal{T}$. Summation over i and the use of (6) implies (7). $\square$

Note that the values of $\gamma < \frac{2}{M}$ are meaningless and the asymptotic formula (4) for the case of strongly separating designs almost coincides with (7) for $\gamma = \frac{2}{M}$. (The only difference is that we have strict inequality inside the curly brackets in (7).) Note also that analogously to derivation of (5) one can use random sampling without replacement in $\mathcal{X}$ as a randomization scheme and get formulas analogous to (5).

Another interpretation can be given to the value N_γ determined via (7). Indeed, assume that the target T is uniformly distributed in $\mathcal{T}$ and we are interested in the probability of separation of T by independent randomly selected test groups $X_i,\ i = 1, \dots, N$, in $\mathcal{X}$. Then the proof of Theorem 2.2 shows that for $N \geq N_\gamma$ the probability that a random design $\{X_1, \dots, X_N\}$ separates an unknown target $T \in \mathcal{T}$ is $\geq 1 - \gamma$.

3 Examples

This section provides some simple examples where straightforward computation provides the desired result and gives an insight into the general case. All results of this section can be obtained as consequences of general results of Section 4.

3.1 One defective element

The assumption of this subsection is that the number of defective elements $t = 1$. This means that $\mathcal{T} = \mathcal{G}_1$, i.e. the target set $\mathcal{T} = \{T_1, \dots, T_n\}$ consists of n one-element sets $T_i = \{x_i\},\ i = 1, \dots, n$. In the case $t = 1$ the test function $f(X, T) = |X \cap T|$ assumes values on the two-point set $\{0, 1\}$. This problem was considered in a number of papers [6, 16, 17]

The main reason to the simplicity of this case is that the coefficients k_{ij} defined by (3) do not depend on i, j for all sets $\mathcal{X}$ we are considering. According to [6] the case when k_{ij} do not depend on i, j is known as homogeneous of order 2 and the existence theorems of the group testing designs have been established mostly for this case. The method used to prove the existence is a particular case of the method of the present paper and is known as the method of random design. Essentially all results of this section can be found in [6]. Better upper bounds for the case $\mathcal{T} = \mathcal{G}_1$, $\mathcal{X} = \mathcal{G}_{\leq s}$ have been obtained in [16] and [17].

Different situations arise depending on the assumption on the collection of test sets $\mathcal{X}$. Consider first the case when there are no restrictions on the test sets, that is $\mathcal{X} = \mathcal{G}_{\leq n}$.

Theorem 3.1. *Let $n \geq 4$, $\mathcal{T} = \mathcal{G}_1$ and $\mathcal{X} = \mathcal{G}_{\leq n}$. Then $k_{ij} = 2^{n-1}$ for any $T_i, T_j \in \mathcal{T}$ ($T_i \neq T_j$), and*

$$N^* = \min\left\{k : \binom{n}{2}\left(\frac{1}{2}\right)^k \leq 1\right\} = \lceil \log_2 n(n-1) - 1 \rceil, \quad N_\gamma = \lceil \log_2 (n-1) - \log_2 \gamma \rceil \quad (8)$$

where $\lceil a \rceil$ denotes the smallest integer larger than or equal to a.

Proof. Note first that $R = |\mathcal{X}| = 2^n$. To compute k_{ij} let us fix two different sets $T_i, T_j \in \mathcal{T}$, note the form $T_i = \{x_i\}$ for them and represent $k_{ij} = |\mathcal{X}_0| + |\mathcal{X}_1|$ where

$$\mathcal{X}_k = \{X \in \mathcal{X} : f(X, T_i) = f(X, T_j) = k\}. \quad (9)$$

The set $\mathcal{X}_0$ consists of all non-empty subsets of the $(n-2)$-element set $X \setminus \{x_i, x_j\}$ and therefore the number of elements in it equals

$$|\mathcal{X}_0| = \sum_{k=0}^{n-2} \binom{n-2}{k} = 2^{n-2}.$$

The number of elements in $\mathcal{X}_1$ also equals $|\mathcal{X}_1| = 2^{n-2}$ since $\mathcal{X}_1$ contains the factor groups consisting of either x_i or x_j and any other factors, i.e. any elements from the set $X \setminus \{x_i, x_j\}$. Formulas (8) follow now from (4) and (7) . $\square$

Corollary 3.1 *Under the assumptions of* Theorem 3.1 *there exists a strongly separating design of the length*

$$N \leq \lceil 2 \log_2 n - 1 \rceil. \tag{10}$$

The formula (10) in its asymptotic form $N \sim 2 \log_2 n,$ as $n \to \infty$, is well known [6] in the theory of group testing as an upper bound for the length of the optimal strongly separating design obtained by the method of random design. Note also that the optimal design, which uses orthogonal arrays to construct optimal designs, is also well known and achieves a better order $N \sim \log_2 n,\ n \to \infty$.

Theorem 3.2. *Assume that* $n \geq 4,\ \mathcal{T} = \mathcal{G}_1,\ \mathcal{X} = \mathcal{G}_s,\ 2 \leq s \leq n-2.$ *Then*

$$k_{ij} = \binom{n-2}{s} + \binom{n-2}{s-2} = \left(1 - 2\frac{s(n-s)}{n(n-1)}\right) \binom{n}{s}.$$

for any $T_i, T_j \in \mathcal{T}$ $(T_i \neq T_j)$ *and*

$$N^* = \lceil C_{n,s}(\log_2 n(n-1) - 1) \rceil\,, \quad N_\gamma = \lceil C_{n,s}(\log_2 (n-1) - \log_2 \gamma) \rceil \tag{11}$$

where $C_{n,s} = -1/\log_2(1 - \frac{2s(n-s)}{n(n-1)})$.

Proof. The proof is similar to the proof of Theorem 3.1. The difference is in that $R = |\mathcal{X}| = \binom{n}{s}$ and for $|\mathcal{X}_0|$ and $|\mathcal{X}_1|$:

$$|\mathcal{X}_0| = \binom{n-2}{s}, \quad |\mathcal{X}_1| = \binom{n-2}{s-2}.$$

These formulas follow from that $\mathcal{X}_0$ contains all groups of s factors taken from the factor collection $X \setminus \{x_i, x_j\}$ and $\mathcal{X}_1$ consists of the factor groups which include either x_i or x_j and any $s-2$ factors from the set $X \setminus \{x_i, x_j\}$. $\square$

When $n \to \infty$ one can easily get the asymptotic form of N^* in (11):

$$N^* \sim \frac{2 \log_2 n}{-\log_2(1 - \frac{2s(n-s)}{n(n-1)})}, \quad n \to \infty, \tag{12}$$

and, if there is a freedom in selection of s, one can consider the problem of an asymptotically optimal choice of s minimizing the right-hand side of (12). This is a kind of experimental design problem since a choice of s determines the choice of the set $\mathcal{X}$ where we perform observations.

Assume that $n \to \infty, \quad s = s(n) \to \infty, \quad \frac{s}{n} \to \lambda$ where $\lambda, 0 < \lambda < 1$, is a number to be chosen. Under this assumption, (12) can be rewritten as

$$N^* \sim \frac{2\log_2 n}{-\log_2(\lambda^2 + (1-\lambda)^2)}, \quad n \to \infty, \tag{13}$$

Obviously, the minimal value of the right-hand side of (13) is achieved for $\lambda = \frac{1}{2}$ and equals $2\log_2 n$ (which coincides with the asymptotic formula for N^* in the case above when $\mathcal{X} = \mathcal{G}_{\leq n}$). It is also easy to see that if $\lambda = 0$ or 1 then we do not get the logarithmic order of the rate of $N^* = N^*(n), \ n \to \infty$.

In Section 4 we will show that the asymptotic considerations in the general case lead to basically the same conclusions concerning the choice of s.

3.2 Two defectives

Assume first that there are exactly two defectives, i.e. $\mathcal{T} = \mathcal{G}_2$, and there are no restrictions on the test sets X.

Theorem 3.3. *Let* $\mathcal{T} = \mathcal{G}_2, \ \mathcal{X} = \mathcal{G}_{\leq n}, \ n \geq 4$. *Then*

$$N^* = \min\left\{ k = 1, 2, \ldots : \ 3\binom{n}{4}\left(\frac{3}{8}\right)^k + 3\binom{n}{3}\left(\frac{1}{2}\right)^k \leq 1 \right\}. \tag{14}$$

Proof. Fix a pair of different sets $T_i, T_j \in \mathcal{T}$, and note that they both contain two elements with at least one element different. Consider first the case (i) when $|T_i \cap T_j| = 0$, i.e. when the sets T_i, T_j consist of different elements. Note that there are $3\binom{n}{4}$ different pairs $\{T_i, T_j\}$ consisting of different elements.

Since the test function $f(X,T) = |X \cap T|$ can get one of three values $0, 1, 2$ we can represent

$$k_{ij} = \sum_{j=0}^{2} |\mathcal{X}_j| \tag{15}$$

where $\mathcal{X}_j$ are defined by (9).

The set $\mathcal{X}_0$ contains all factor groups containing factors from the set $X \setminus (T_i \cup T_j)$ which contains $n-4$ factors. Therefore

$$|\mathcal{X}_0| = \sum_{k=0}^{n-4} \binom{n-4}{k} = 2^{n-4}$$

The set $\mathcal{X}_1$ consists of the factor groups which contain one factor from T_i, another factor from T_j, there are 4 different ways to select these two factors, and any combination of the factors from the set $X \setminus (T_i \cup T_j)$. This gives

$$|\mathcal{X}_1| = 4\sum_{k=0}^{n-4} \binom{n-4}{k} = 2^{n-2}$$

The set $\mathcal{X}_2$ includes the factor groups with all four factors from T_i and T_j and any combination of factors from the set $X \setminus (T_i \cup T_j)$. This gives

$$|\mathcal{X}_2| = \sum_{k=0}^{n-4} \left(\begin{array}{c} n-4 \\ k \end{array} \right) = 2^{n-4}$$

Altogether the above formulas give $k_{ij} = 3\,2^{n-3}$ for the case (i).

Consider now the case (ii) when the two-element factor groups T_i and T_j have one common element. There are $3 \left(\begin{array}{c} n \\ 3 \end{array} \right)$ different combinations of these factor groups.

In case (ii) we again have three possible values for f and the representation (15). The set $X \setminus (T_i \cup T_j)$ contains now $n-3$ elements rather than $n-4$. This analogously with (i) gives $|\mathcal{X}_0| = 2^{n-3}$ and $|\mathcal{X}_2| = 2^{n-3}$. The set $\mathcal{X}_1$ contains the groups of two kinds: they either contain the factor which is common for the pair (T_i, T_j), and there are 2^{n-3} of such groups, or they do not contain the common factor but contain the two other from the set $T_i \cup T_j$, and again there are 2^{n-3} of such groups. In total this gives $k_{ij} = 2^{n-1}$ for the case (ii). Bearing in mind $R = 2^n$ we now apply (4) and get (14). $\square$

Consider now the case when the number of defective factors is either 1 or 2, that is $\mathcal{T} = \mathcal{G}_1 \cup \mathcal{G}_2$ and there are no restrictions on the test sets.

Theorem 3.4. *Let $\mathcal{T} = \mathcal{G}_1 \cup \mathcal{G}_2$, $\mathcal{X} = \mathcal{G}_{\leq n}, n \geq 4$. Then*

$$N^* = \min \left\{ k = 1, 2, \ldots : 3 \left(\begin{array}{c} n+1 \\ 4 \end{array} \right) \left(\frac{3}{8} \right)^k + 3 \left(\begin{array}{c} n+1 \\ 3 \end{array} \right) \left(\frac{1}{2} \right)^k \leq 1 \right\}.$$

Proof. We use the arguments to the proof to Theorem 3.3 and add three more cases to what has been considered there.

Case (iii). Both T_i and T_j consist of one factor. This case was considered in the proof of Theorem 3.1. There are $\left(\begin{array}{c} n \\ 2 \end{array} \right)$ different pairs (T_i, T_j) of that kind and $k_{ij} = 2^{n-1}$.

Case (iv). T_i and T_j consist of different number of factors and do not intersect. There are $3 \left(\begin{array}{c} n \\ 3 \end{array} \right)$ different ways to choose such combination. Since only 0 and 1 are possible values of f we have the representation (0) where $|\mathcal{X}_0|$ and $|\mathcal{X}_1|$ can be computed analogously to the above: $|\mathcal{X}_0| = 2^{n-3}$, $|\mathcal{X}_1| = 2^{n-2}$. This gives $k_{ij} = 3\,2^{n-3}$ for the case (iv).

Case (v). T_i and T_j consist of different number of factors and intersect. There are $2 \left(\begin{array}{c} n \\ 2 \end{array} \right)$ different pairs of this type. Again, 0 and 1 are the values that the test function f can get. As before $\mathcal{X}_0$ contains all nonempty factor groups with the factors from the set $X \setminus (T_i \cup T_j)$ which gives in the present case $|\mathcal{X}_0| = 2^{n-2}$. The set $\mathcal{X}_1$ contains the factor groups that include the factor common for T_i and T_j and any combination of factors from $X \setminus (T_i \cup T_j)$. This gives $|\mathcal{X}_1| = 2^{n-2}$. Combining we get $k_{ij} = 2^{n-1}$ for the case (v). Application of (4) gives the required. $\square$

We omit here the asymptotic considerations referring to Section 5 for a general case.

4 General Case

4.1 Branching of the target field

The result of this section allows one to compute the number of elements in the subsets of the target field of the form (1) and (2) where, as will be shown below, the coefficients k_{ij} are equal.

Let $0 \le p \le m \le l \le n,\ p < l$. Denote

$$\mathcal{T}(n,l,m,p) = \{(T_i,T_j) \in \mathcal{G}_{\le n} \times \mathcal{G}_{\le n} :\ T_i \ne T_j,\ |T_i| = l,\ |T_j| = m,\ |T_i \cap T_j| = p\} \qquad (16)$$

Theorem 4.1. *The number of different non-ordered pairs in $\mathcal{T}(n,l,m,p)$ equals*

$$Q(n,l,m,p) = \begin{cases} \begin{pmatrix} & & n & \\ p & m{-}p & l{-}p & n{-}l{-}m{+}p \end{pmatrix} & \text{if } m < l \\ \frac{1}{2}\begin{pmatrix} & & n & \\ p & m{-}p & m{-}p & n{-}2m{+}p \end{pmatrix} & \text{if } m = l \end{cases} \qquad (17)$$

where

$$\begin{pmatrix} & n & \\ n_1 & n_2 \ \ldots & n_k \end{pmatrix} = \frac{n!}{n_1!\, n_2! \ldots n_k!} \quad (n_r \ge 0,\ \sum_{r=1}^{k} n_r = n\ )$$

is the multinomial coefficient.

Proof. Consider first the case $m < l$. There are $\begin{pmatrix} n \\ l+m-p \end{pmatrix}$ possibilities to select $l+m-p$ elements that belong to at least one of two groups $T_i,\ T_j$, the number of possibilities to select l elements belonging to T_i from $l+m-p$ is $\begin{pmatrix} l+m-p \\ l \end{pmatrix}$, and one can select p elements that belong to $T_i \cap T_j$ from these l elements by $\begin{pmatrix} l \\ p \end{pmatrix}$ variants. Multiplying we have

$$Q(n,l,m,p) = \begin{pmatrix} n \\ l{+}m{-}p \end{pmatrix} \begin{pmatrix} l{+}m{-}p \\ l \end{pmatrix} \begin{pmatrix} l \\ p \end{pmatrix} = \begin{pmatrix} & & n & \\ p & m{-}p & l{-}p & n{-}l{-}m{+}p \end{pmatrix}$$

The case $m = l$ differs from the case $m < l$ in that the symmetry in selection of T_i and T_j reduces by half the number of possibilities. $\square$

4.2 Existence theorems for balanced test fields

This section introduces a concept of a a-balanced test field, where a stands for "additive", and provides a formula for an upper bound of optimal group testing designs in the cases when the target field is of the form (1) or (2) and the test field is a-balanced. Examples of the a-balanced test fields $\mathcal{X}$ will be given in the next subsection.

Let $(T, T') \in \mathcal{T}(n, l, m, p)$, where the set $\mathcal{T}(n, l, m, p)$ is defined through (16) and $X \in \mathcal{X}_{qr}(T, T')$ where

$$\mathcal{X}_{qr}(T, T') = \{X \in \mathcal{X} : \ |X \cap T| = |X \cap T'| = q \geq 0, \ \ |X \cap (T \cap T')| = r \geq 0\} \tag{18}$$

where q and r are some integers.

Definition 4.1. Let

$$0 \leq p \leq m \leq l \leq n, \ \ p < l; \ \ 0 \leq r \leq q \leq m.$$

We shall call the test field $\mathcal{X}$ *a-balanced* if the number $|\mathcal{X}_{qr}(T, T')|$ does not depend on a choice of the pair $(T, T') \in \mathcal{T}(n, l, m, p)$. For a-balanced test fields $\mathcal{X}$ the number $|\mathcal{X}_{qr}(T, T')|$ for $(T, T') \in \mathcal{T}(n, l, m, p)$ will be denoted $R(n, l, m, p, q, r)$.

Theorem 4.2. *Let* $0 \leq p \leq m \leq l \leq n$, $p < l$, $\mathcal{X}$ *be a a-balanced test field, in the sense of* Definition 4.1, *and* $T_i, T_j \in \mathcal{T}(n, l, m, p)$ *be a fixed pair of target groups. Then*

$$k_{ij} = \sum_{r=0}^{p} \sum_{q=r}^{m-p+r} R(n, l, m, p, q, r) \tag{19}$$

and the value of k_{ij} *is the same for all pairs* $(T_i, T_j) \in \mathcal{T}(n, l, m, p)$.

Proof. Suppose $T_i, T_j \in \mathcal{T}(n, l, m, p)$ and $X \in \mathcal{X}_{qr}(T_i, T_j)$. One can easily see that the sets $X_{qr}(T_i, T_j)$ defined by (18) may be non-empty only if

$$0 \leq r \leq p, \ \ 0 \leq q - r \leq m - p\,. \tag{20}$$

Recall that $k_{ij} = |\{X \in \mathcal{X} : \ |X \cap T_i| = |X \cap T_j|\}|$. Using the notation (9) and (18) we can write

$$k_{ij} = \sum_{q} |\mathcal{X}_q| = \sum_{q} \sum_{r} |\mathcal{X}_{qr}| = \sum_{q} \sum_{r} R(n, l, m, p, q, r) \tag{21}$$

where we have used the fact that $(T_i, T_j) \in \mathcal{T}(n, l, m, p)$.

Now we use (20) to establish bounds for q and r in (21) such that the sets $\mathcal{X}_{qr}$ are non-empty:

$$k_{ij} = \sum_{r=0}^{p} \sum_{u=0}^{m-p} R(n, l, m, p, u + r, r) = \sum_{r=0}^{p} \sum_{q=r}^{m-p+r} R(n, l, m, p, q, r)$$

where we have used the variable $u = q - r$. $\square$

If the test field $\mathcal{X}$ is a-balanced in the sense of Definition 4.1 and one has analytic expressions for the coefficients $R(n, l, m, p, q, r)$ then the upper bound N^* can be expressed in a closed form by separating the set of all pairs $\{(T_i, T_j), \ i < j\}$ into a union of disjoint sets $\mathcal{T}(n, l, m, p)$ and computing the coefficients k_{ij} for the pairs in these sets. Theorem 4.1 gives formulas for computing the number of different pairs in the sets $\mathcal{T}(n, l, m, p)$ and

Theorem 4.2 guarantees that k_{ij} are the same for all pairs in $\mathcal{T}(n,l,m,p)$ and provides explicit formulas for the values of k_{ij}. This gives the following formula for N^*:

$$N^* = \min\left\{k : \sum_{l,m}\sum_{p:p\le m,p<l} Q(n,l,m,p)\left(\frac{1}{R}\sum_{r=0}^{p}\sum_{q=r}^{m-p+r} R(n,l,m,p,q,r)\right)^k \le 1\right\} \tag{22}$$

where $R = |\mathcal{X}|$, and the first summation is over $0 \le m \le l \le t$ for the case $\mathcal{T} = \mathcal{G}_{\le t}$ and $l = m = t$, that is the first summation disappears in (22), for the case $\mathcal{T} = \mathcal{G}_t$. Analogous formula for γ-separating designs is

$$N_\gamma = \min\left\{k : \sum_{l,m}\sum_{p:p\le m,p<l} Q(n,l,m,p)\left(\frac{1}{R}\sum_{r=0}^{p}\sum_{q=r}^{m-p+r} R(n,l,m,p,q,r)\right)^k < \frac{\gamma|\mathcal{T}|}{2}\right\} \tag{23}$$

4.3 Examples of balanced test fields

Let us consider some examples of a-balanced test fields and derive explicit formulas for $R(n,l,m,p,q,r)$. The following statement is basic in this respect.

Theorem 4.3. *Let $\underline{X} = \{x_1,\dots,x_n\}$ be a collection of $n \ge 2$ factors and integers n,m,l,p,q,r be such that*

$$0 \le p \le m \le l \le n,\ p < l,\ \ 0 \le r \le p,\ \ 0 \le q - r \le m - p.$$

Then the test field

$$\mathcal{X} = \mathcal{G}_s = \{X = \{x_{i_1},\dots,x_{i_s}\},\ \ 1 \le i_1 < \dots i_s \le n\}, \tag{24}$$

$1 \le s \le n$, *is a-balanced and*

$$R(n,l,m,p,q,r) = \binom{p}{r}\binom{l-p}{q-r}\binom{m-p}{q-r}\binom{n-l-m+p}{s+r-2q} \tag{25}$$

where we assume

$$\binom{b}{a} = 0 \quad \text{for } a < 0 \quad \text{and } a > b. \tag{26}$$

Proof. Assume that (T_i, T_j) be any pair in $\mathcal{T}(n,l,m,p)$ and integers n,m,l,p,q,r be as in the statement of the theorem. By definition $R(n,l,m,p,q,r)$ is the number of the test groups $X \in \mathcal{X}_{qr}$. In the case (24) this number can be computed as follows. To construct a factor group $X \in \mathcal{X}_{qr}$ select first r factors from the set $T_i \cap T_j$ (there are $\binom{p}{r}$ possibilities to do this); then, for fixed $r \le p$, for two sets $T_i \setminus T_j$ and $T_j \setminus T_i$, we select $u = q - r$ ($0 \le u \le m - r$) factors from both, we can do this by

$$\binom{m-p}{u}\binom{l-p}{u} = \binom{m-p}{q-r}\binom{l-p}{q-r}$$

choices; finally we include $s-r-2u = s+r-2q$ factors into X from the set $\underline{X} \setminus (T_i \cup T_j)$ containing $n-l-m+p$ factors (obviously, we have $\begin{pmatrix} n-l-m+p \\ s+r-2q \end{pmatrix}$ possibilities to do this).

Note that if s is either rather small, i.e. $s < 2m-p$, or large, $s > n-l-m+p$, then some variants among those considered above are impossible but the corresponding summands are excluded from the sum due to the convention (26).

To finish the proof we only mention that the above calculation of $R(n,l,m,p,q,r)$ does not depend on the choice of a pair $(T_i,T_j) \in \mathcal{T}(n,l,m,p)$. $\square$

Let us show how to compute values $R(n,l,m,p,q,r)$ in the cases when the test field $\mathcal{X}$ can be represented as

$$\mathcal{X} = \mathcal{X}_J = \cup_{j\in J} \mathcal{G}_j \tag{27}$$

where $J \subset \{0,1,\ldots,n\}$ and $\mathcal{G}_j$ is defined in (1). Note that in particular cases $J=\{s\}$ and $J=\{0,1,\ldots,s\}$ one has $\mathcal{X}_J = \mathcal{G}_s$ and $\mathcal{X}_J = \mathcal{G}_{\le s}$, respectively.

Lemma 4.1. *Let the test field $\mathcal{T}$ be fixed, $\mathcal{X} = \mathcal{X}' \cup \mathcal{X}''$ where $\mathcal{X}' \cap \mathcal{X}'' = \emptyset$, $R' = |\mathcal{X}'|$, $R'' = |\mathcal{X}''|$, and $\{k'_{ij};\ T_i,T_j \in \mathcal{T}\}$, $\{k''_{ij};\ T_i,T_j \in \mathcal{T}\}$ be two sets of the coefficients* (3) *for the test fields $\mathcal{X}'$ and $\mathcal{X}''$, respectively. Then $R = |\mathcal{X}| = R' + R''$ and*

$$k_{ij} = |\{X \in \mathcal{X} \text{ such that } |X \cap T_i| = |X \cap T_j|\}| = k'_{ij} + k''_{ij} \tag{28}$$

for any pair $T_i,T_j \in \mathcal{T}$.

Lemma 4.1 implies that if $\mathcal{X}' \cap \mathcal{X}'' = \emptyset$ and both $\mathcal{X}'$ and $\mathcal{X}''$ are a-balanced in the sense of Definition 4.1 with families of R-values $\{R'(n,l,m,p,q,r)\}_{l,m,p,q,r}$ and $\{R''(n,l,m,p,q,r)\}_{l,m,p,q,r}$ then the set $\mathcal{X} = \mathcal{X}' \cup \mathcal{X}''$ is also a-balanced and

$$R(n,l,m,p,q,r) = R'(n,l,m,p,q,r) + R''(n,l,m,p,q,r) \tag{29}$$

for any l,m,p,q,r. Application of (22) and (23) give expressions for N^* and N_γ in the case when the test field is $\mathcal{X} = \mathcal{X}' \cup \mathcal{X}''$.

4.4 Existence theorems

We provide in this section several existence theorems for the group testing designs. These theorems are corollaries of previous results of Section 4.

Combining (22), (25) and the results of Theorems 4.1 and 4.2 we get the following two statements.

Corollary 4.1. *Let $\mathcal{T} = \mathcal{G}_t$ and $\mathcal{X} = \mathcal{G}_s$ where $n \ge 4,\ 1 \le t < n,\ 1 \le s < n$. Then there exists a nonsequential group testing design with the sample size $N \le N^* = N^*(n,t,s)$ where*

$$N^*(n,t,s) = \min\left\{ k = 1,2,\ldots :\ \frac{1}{2}\sum_{p=0}^{t-1} \begin{pmatrix} n \\ p\ \ t{-}p\ \ t{-}p\ \ n{-}2t{+}p \end{pmatrix} \right.$$

$$\left. \times \left(\sum_{r=0}^{p} \sum_{q=r}^{t-p+r} \begin{pmatrix} p \\ r \end{pmatrix} \begin{pmatrix} t-p \\ q-r \end{pmatrix}^2 \begin{pmatrix} n-2t+p \\ s+r-2q \end{pmatrix} \right)^k \le \begin{pmatrix} n \\ s \end{pmatrix}^k \right\} \tag{30}$$

and there exists a nonsequential γ-separating design with the sample size $N \le N^* = N_\gamma(n,t,s)$ *where*

$$N_\gamma(n,t,s) = \min\Bigg\{ k = 1,2,\dots : \sum_{p=0}^{t-1} \binom{n}{p\ \ t{-}p\ \ t{-}p\ \ n{-}2t{+}p}$$

$$\times \left(\sum_{r=0}^{p} \sum_{q=r}^{t-p+r} \binom{p}{r} \binom{t-p}{q-r}^2 \binom{n-2t+p}{s+r-2q} \right)^k < \gamma \binom{n}{t} \binom{n}{s}^k \Bigg\} \tag{31}$$

Corollary 4.2. *Let $\mathcal{T} = \mathcal{G}_{\le t}$ and $\mathcal{X} = \mathcal{G}_s$ where $n \ge 4,\ 1 \le t < n,\ 1 \le s < n$. Then there exists a nonsequential group testing design with the sample size* $N \le N^* = N^*(n, \le t, s)$ *where*

$$N^*(n,\le t,s) = \min\Bigg\{ k = 1,2,\dots : \frac{1}{2} \sum_{m=0}^{t} \sum_{p=0}^{m-1} \binom{n}{p\ \ m{-}p\ \ m{-}p\ \ n{-}2m{+}p}$$

$$\times \left(\sum_{r=0}^{p} \sum_{q=r}^{m-p+r} \binom{p}{r} \binom{m{-}p}{q{-}r}^2 \binom{n{-}2m{+}p}{s{+}r{-}2q} \right)^k + \sum_{l=1}^{t} \sum_{m=1}^{l-1} \sum_{p=0}^{m} \binom{n}{p\ \ l{-}p\ \ m{-}p\ \ n{-}l{-}m{+}p}$$

$$\times \left(\sum_{r=0}^{p} \sum_{q=r}^{m-p+r} \binom{p}{r} \binom{l{-}p}{q{-}r} \binom{m{-}p}{q{-}r} \binom{n{-}l{-}m{+}p}{s{+}r{-}2q} \right)^k \le \binom{n}{s}^k \Bigg\}$$

The additivity property (29) implies the following statements.

Corollary 4.3. *Let $\mathcal{T} = \mathcal{G}_t$ and $\mathcal{X} = \mathcal{G}_{\le s}$ where $n \ge 4,\ 1 \le t < n,\ 1 \le s \le n$. Then there exists a nonsequential group testing design with the sample size* $N \le N^* = N^*(n, t, \le s)$ *where*

$$N^*(n,t,\le s) = \min\Bigg\{ k = 1,2,\dots \text{ such that } \frac{1}{2} \sum_{p=0}^{t-1} \binom{n}{p\ \ t{-}p\ \ t{-}p\ \ n{-}2t{+}p}$$

$$\times \left(\sum_{v=0}^{s} \sum_{r=0}^{p} \sum_{q=r}^{t-p+r} \binom{p}{r} \binom{t-p}{q-r}^2 \binom{n-2t+p}{v+r-2q} \Big/ \sum_{v=0}^{s} \binom{n}{v} \right)^k \le 1 \Bigg\}$$

Corollary 4.4. *Let $n \ge 4,\ 1 \le t < n$, $\mathcal{T} = \mathcal{G}_t$ and $\mathcal{X} = \mathcal{G}_{\le n}$ be the collection of 2^n subsets of $\underline{X}$. Then there exists a nonsequential group testing design with the sample size* $N \le N^* = N^*(n, t, \le n)$ *where*

$$N^*(n,t,\le n) = \min\Bigg\{ k : \frac{1}{2} \sum_{p=0}^{t-1} \binom{n}{p\ \ t{-}p\ \ t{-}p\ \ n{-}2t{+}p} \left(2^{2p-2t} \sum_{u=0}^{t-p} \binom{t-p}{u}^2 \right)^k \le 1 \Bigg\}$$

and there exists a nonsequential γ-separating design with the sample size $N \le N^* = N_\gamma(n,t,\le n)$ where

$$N_\gamma(n,t,\le n) = \min\left\{k : \sum_{p=0}^{t-1} \binom{n}{p\ \ t{-}p\ \ t{-}p\ \ n{-}2t{+}p} \left(2^{2p-2t} \sum_{u=0}^{t-p} \binom{t-p}{u}^2\right)^k < \gamma \binom{n}{t}\right\}$$

Corollary 4.5. *Let $n \ge 4$, $1 \le t < n$, $\mathcal{T} = \mathcal{G}_{\le t}$ and $\mathcal{X} = \mathcal{G}_{\le n}$ be the collection of 2^n subsets of $\underline{X}$. Then there exists a nonsequential group testing design with the sample size $N \le N^* = N^*(n,\le t,\le n)$ where*

$$N^*(n,\le t,\le n) = \min\left\{ k = 1,2,\ldots : \frac{1}{2}\sum_{m=0}^{t}\sum_{p=0}^{m-1} \binom{n}{p\ \ m{-}p\ \ m{-}p\ \ n{-}2m{+}p}\right.$$

$$\times \left(2^{-2m+2p} \sum_{u=0}^{m-p} \binom{m-p}{u}^2\right)^k + \sum_{l=1}^{t}\sum_{m=0}^{l-1}\sum_{p=0}^{m} \binom{n}{p\ \ l{-}p\ \ m{-}p\ \ n{-}l{-}m{+}p}$$

$$\left. \times \left(2^{-l-m+2p} \sum_{u=0}^{m-p} \binom{l-p}{u}\binom{m-p}{u}\right)^k \le 1\right\}$$

Corollaries 4.4 and 4.5 give expressions for N^* in the case when $\mathcal{X}$ is the collection of all non-empty subsets of $\underline{X}$ which is certainly one of the most important cases. We shall not provide formulas for N^* and N_γ in other particular cases, they can be derived in the same manner.

5 Asymptotic bounds

In this section we consider the asymptotic behavior of N^* and N_γ computed above when the number of factors n is large. Using the fact that whatever the target set $\mathcal{T} \subseteq \mathcal{G}_{\le n}$ is the test made with the test group $X = \underline{X}$ reduces the problem to the case $\mathcal{T} = \mathcal{G}_t$ for some t, we only consider this assumption for $\mathcal{T}$.

The principal cases are the cases (30) and (31) when $\mathcal{X} = \mathcal{G}_s$ and $\mathcal{T} = \mathcal{G}_t$ and

$$n \to \infty,\ \ t = t(n) \ge 2,\ \ \frac{t(n)}{\log n} \to 0,\ \ s = s(n) \to \infty,\ \ \frac{s(n)}{n} \to \lambda, \tag{32}$$

where $t = t(n)$ may be fixed or $t(n) \to \infty$ as $n \to \infty$, $\lambda,\ 0 < \lambda < 1,$ is some number. (It is easy to demonstrate that if $\lambda = 0$ or 1 then we could not get the logarithmic order of the rate of $N^* = N^*(n),\ n \to \infty$, and therefore these cases are not interesting from the asymptotic point of view.) The case considered in Corollary 4.4, when $\mathcal{X} = \mathcal{G}_{\le n}$, is also important. As we show below, see Corollary 5.1, the asymptotic upper bounds in this case coincide with the bounds for $\mathcal{X} = \mathcal{G}_{\lceil n/2 \rceil}$.

Straightforward application of the Stirling formula

$$k! \sim \sqrt{2\pi k} k^k e^{-k}, \quad k \to \infty,$$

to the coefficients (17) implies that if (32) is valid then

$$\lim_{n\to\infty} N^*(n,t,\le s)/N^*(n,t,\max\{s\}) = 1 \ \text{ for } \ s \le n/2 \tag{33}$$

$$\lim_{n\to\infty} N^*(n,t,\le s)/N^*(n,t,n/2) = 1 \ \text{ for } \ s \ge n/2 \tag{34}$$

and particularly

$$\lim_{n\to\infty} N^*(n,t,\le n)/N^*(n,t,n/2) = 1 \tag{35}$$

where $N^*(n,t,\lambda n) = N^*(n,t,\lceil \lambda n \rceil)$ for any λ.

The asymptotic formulas (33)–(35) show that an asymptotic expression for $N^*(n,t,s)$ would immediately yield analogous expressions in many other cases including the case when $\mathcal{X}$ contain all 2^n subsets of $\underline{X}$. Analogous relations hold in the case of γ-separability.

Assume that $\mathcal{X} = \mathcal{G}_s$ and (32) holds. Using the Stirling formula we get for $(T_i,T_j) \in \mathcal{T}(n,l,m,p)$

$$\frac{k_{ij}}{R} = \sum_{r=0}^{p} \sum_{q=r}^{m-p+r} \binom{p}{r} \binom{l-p}{q-r} \binom{m-p}{q-r} \binom{n-l-m+p}{s+r-2q} \Big/ \binom{n}{s}$$

$$\sim k_{ij}^{\mathrm{as}} = (1-\lambda)^{l+m-2p} \sum_{u=0}^{m-p} \left(\frac{\lambda}{1-\lambda}\right)^{2u} \binom{l-p}{u} \binom{m-p}{u}, \quad n \to \infty,$$

where we have used the variable $u = q - r$. For the case $m = l = t$ which should only be considered if $\mathcal{T} = \mathcal{G}_t$ we have

$$\frac{k_{ij}}{R} \sim k_{ij}^{\mathrm{as}} = (1-\lambda)^{2t-2p} \sum_{u=0}^{t-p} \left(\frac{\lambda}{1-\lambda}\right)^{2u} \binom{m-p}{u}^2, \ \text{ if } n \to \infty.$$

This implies

$$k_{ij}^{\mathrm{as}} = (1-\lambda)^2 + \lambda^2 \ge \frac{1}{2} \ \text{ for } \ m = l = t, \ p = t-1 \tag{36}$$

where the strict inequality holds if and only if $\lambda \ne \frac{1}{2}$.

On the other hand, if $\lambda = \frac{1}{2}$ then for any m, l, p

$$k_{ij}^{\mathrm{as}} = \left(\frac{1}{2}\right)^{l+m-2p} \sum_{u=0}^{m-p} \binom{l-p}{u} \binom{m-p}{u} \tag{37}$$

This implies that $k_{ij}^{\mathrm{as}} \le \frac{1}{2}$ where the strict inequality holds only if $m = l = p - 1$:

$$k_{ij}^{\mathrm{as}} = \frac{1}{2} \ \text{ if } m = l = p + 1.$$

The above consideration leads to a suggestion that $\lambda = \frac{1}{2}$ is the optimal value of λ. The following theorem proves this suggestion for the case $\mathcal{T} = \mathcal{G}_t$ and establishes an asymptotic formulas for $N^*(n,t,\lambda n)$ and $N_\gamma(n,t,n/2)$.

Theorem 5.1. *Assume that $\mathcal{X} = \mathcal{G}_s$, $\mathcal{T} = \mathcal{G}_t$ (32) holds and let γ and λ be fixed numbers, $0 < \gamma < 1$, $0 < \lambda < 1$. Then*

$$N^*(n, t, \lambda n) \sim g_\lambda (t+1) \log_2 n, \quad n \to \infty, \tag{38}$$

$$N_\gamma(n, t, n/2) \sim \frac{t \log_2 n}{2t - \log_2 (2t)! + 2 \log_2 t!}, \quad n \to \infty, \tag{39}$$

where

$$g_\lambda = \frac{1}{-\log_2(\lambda^2 + (1-\lambda)^2)} \tag{40}$$

and the minimal value of the constant g_λ equals 1 and is achieved for $\lambda = \frac{1}{2}$.

Proof. Note that $m = l = t$ in the case $\mathcal{X} = \mathcal{G}_s$, $\mathcal{T} = \mathcal{G}_t$.

Consider the case of strongly separating designs. Establish first an asymptotic lower bound $L = L(n, t, \lambda n)$ for $N(n, t, \lambda n)$ such that

$$\liminf_{n \to \infty} \frac{N(n, t, \lambda n)}{L(n, t, \lambda n)} \geq 1\,. \tag{41}$$

To do this, take only the term with $p = t - 1$ in the sum over p in (30) and apply (36). This gives the equation

$$\frac{1}{2} \binom{n}{t-1 \;\; 1 \;\; 1 \;\; n{-}t{-}1} \left((1-\lambda)^2 + \lambda^2 \right)^L = 1$$

for $L = L(n, t, \lambda n)$. Using the Stirling formula and solving the asymptotic equation with respect to L we get

$$\frac{1}{2} \frac{n^{t+1}}{(t-1)!} \left((1-\lambda)^2 + \lambda^2 \right)^L = 1, \tag{42}$$

$$L(n, t, \lambda n) \sim g_\lambda (t+1) \log_2 n, \quad n \to \infty. \tag{43}$$

To prove that $g_\lambda(t+1)\log_2 n$ is indeed asymptotically equivalent to $N(n, t, \lambda n)$ we need to show that the terms corresponding to $p = 0, 1, \ldots, t-2$ are asymptotically negligible in the sum (30) relative to the term with $p = t - 1$. The proof is similar for all p and we consider only the term corresponding to $p = 0$. This term is the biggest comparing with $p = 1, \ldots, t-2$ which follows from

$$\binom{n}{0 \;\; t \;\; t \;\; n{-}2t} \Big/ \sum_{p=0}^{t-1} \binom{n}{p \;\; t{-}p \;\; t{-}p \;\; n{-}2t{+}p} \to 1 \quad \text{if} \quad n \to \infty$$

Denote by $A(n, t, k, 0)$ and $A(n, t, k, t{-}1)$ the terms in the sum (30) over p corresponding to $p = 0$ and $p = t - 1$, respectively. To prove that the term corresponding to $p = 0$ is asymptotically negligible means to prove that

$$\frac{A(n, t, N(n, t, \lambda n), 0)}{A(n, t, N(n, t, \lambda n), t-1)} \to 0 \;\; \text{for} \;\; n \to \infty. \tag{44}$$

Due to (43) and (41) this would follow from the asymptotic relation

$$\frac{A(n,t,g_\lambda(t+1)\log_2 n,0)}{A(n,t,g_\lambda(t+1)\log_2 n,t-1)} \to 0 \text{ for } n\to\infty. \tag{45}$$

which we are going to prove.

For simplicity consider only the principal case $\lambda=\frac{1}{2}$ and first establish the asymptotic behavior of $A(n,t,(t+1)\log_2 n,t-1)$:

$$A(n,t,(t+1)\log_2 n,t-1)\sim C_t,\ n\to\infty$$

where C_t is a constant not depending on n, it is actually $C_t=1/(2(t-1)!)$.

Consider now $A(n,t,(t+1)\log_2 n,0)$. Using (37) in the case $m=t,\ p=0$ we have

$$k_{ij}^{\mathrm{as}}(0)=\left(\frac{1}{2}\right)^{2t}\sum_{u=0}^{t}\binom{t}{u}^2=\left(\frac{1}{2}\right)^{2t}\frac{(2t)!}{(t!)^2}$$

This gives for $n\to\infty$

$$A(n,t,(t+1)\log_2 n,0)=\frac{1}{2}\binom{n}{0\ t\ t\ n{-}2t}\left(\left(\frac{1}{2}\right)^{2t}\frac{(2t)!}{(t!)^2}\right)^{(t+1)\log_2 n}$$

$$\sim\frac{n^{2t}}{2((t)!)^2}\left(\left(\frac{1}{2}\right)^{2t}\frac{(2t)!}{(t!)^2}\right)^{(t+1)\log_2 n}=\frac{1}{2((t)!)^2}\left(\left(\frac{1}{2}\right)^{2t^2/(t+1)}\frac{(2t)!}{(t!)^2}\right)^{(t+1)\log_2 n}$$

The case $t=1$ has been considered in Section 3. For $t\geq 2$ the function of t

$$\left(\frac{1}{2}\right)^{2t^2/(t+1)}\frac{(2t)!}{(t!)^2}$$

is smaller than 1 and monotonically decreases to 0 if $t\to\infty$. This completes the proof of (45) and (38). Proof of (39) is similar and is based on the asymptotically equivalent form for $N_\gamma(n,t,\frac{1}{2}n)$:

$$N_\gamma(n,t,n/2)\sim\min\{k=1,2,\ldots:\frac{n^{2t}}{((t)!)^2}\left(k_{ij}^{\mathrm{as}}(0)\right)^k<\frac{\gamma n^t}{t!}\},\quad n\to\infty\,. \tag{46}$$

□

Two important remarks on Theorem 5.1 are: (i) the value $\lambda=\frac{1}{2}$ is asymptotically optimal, including the case of γ-separability, and (ii) for $\lambda=\frac{1}{2}$ and any fixed $0<\gamma<1$

$$\lim_{n\to\infty}\frac{N^*(n,t,n/2)}{N_\gamma(n,t,n/2)}=\alpha(t)=\frac{1}{t}(t+1)(2t-\log_2(2t)!+2\log_2(t)!)$$

with $\alpha(t)\sim\frac{1}{2}(\log_2 t-\log_2\pi)$ when $t\to\infty,\ t/\log n\to 0$ when $n\to\infty$. This shows that γ-separability is a weaker restriction on a design than the strong separability.

The technique applied to prove Theorem 5.1 allows to obtain more precise asymptotic approximations for $N^*(n,t,\lambda n)$ and $N_\gamma(n,t,n/2)$ than those given in (38) and (39).

Corollary 5.1. *Let the assumptions of* Theorem 5.1 *hold. Then*

$$N^*(n,t,\lambda n) \sim N_0^{(\mathrm{as})}(n,t,\lambda) = \left\lceil \frac{(t+1)\log_2 n - \log_2(t-1)! - 1}{-\log_2(\lambda^2 + (1-\lambda)^2)} \right\rceil, \quad n \to \infty, \tag{47}$$

$$N_\gamma(n,t,n/2) \sim N_\gamma^{(\mathrm{as})}(n,t,n/2) = \left\lceil \frac{t\log_2 n - \log_2(t!\gamma)}{2t - \log_2(2t)! + 2\log_2 t!} \right\rceil, \quad n \to \infty, \tag{48}$$

where g_λ is defined in (40).

To derive the approximation (47) we need to solve asymptotic equation (42) not neglecting the terms small comparing with the leading term (43). Analogously, to derive (48) we have to rewrite (46) as an equation for N_γ and solve it neglecting neither of the terms.

6 Numerical results

In this section we present some numerical results relating to optimal choice of $s = s(n)$ and computation of the values $N^* = N^*(\mathcal{X})$ by (4), (47) and N_γ by (7), (48).

Numerical results show that there is only a small range of values of s where minimum of $N^*(\mathcal{G}_s)$ over s is achieved. Table 1 provides typical results. Interestingly, in the cases $\mathcal{T} = \mathcal{G}_t$ and $\mathcal{T} = \mathcal{G}_{\le t}$ when t is small compared to n, the optimal values of s depend on n but do not depend on t. An empirical formula for optimal s is $s^* = \lceil \frac{n+1}{2} \rceil$, which is in agreement with Theorem 5.1. Unlike in the asymptotic case where

$$\lim_{n\to\infty} N^*(\mathcal{G}_{s^*})/N^*(\mathcal{G}_{\le n}) = 1,$$

for small n the difference between $N^*(\mathcal{X}_{s^*})$ and $N^*(\mathcal{G}_{\le n})$ is sometimes significant which can be seen from Table 1. Analogous results hold for the case when N_γ is considered as the characteristic of interest.

Table 1 contains values of N^* for $\mathcal{T} = G_{\le 3},\ \mathcal{X} = G_s,\ s = \lambda n$ for different values of n and λ. In brackets values of N^+ are given, if they are different from the values of N^*.

λ	$n=10$	$n=20$	$n=50$	$n=100$	$n=150$
0.1	∞(10)	79 (64)	105	125	137
0.2	28 (21)	37	50	59	65
0.3	18 (16)	29	34	37	41
0.4	13 (12)	17	23	28	30
0.5	11 (10)	15	21	25	27
0.6	11 (10)	15	21	27	29
0.7	12	17	25	32	35
0.8	17 (14)	26	36	45	49
0.9	∞(10)	50 (44)	70	86	94
$\mathcal{X} = \mathcal{G}_{\le n}$	12	16	21	25	27

Table 1. Values of N^* and N^+ for $\mathcal{T} = G_{\le 3},\ \mathcal{X} = \mathcal{G}_{\lambda n}$ and different values of n and λ.

Table 2 contains values of $N^{(\mathrm{as})} = N^{(\mathrm{as})}(n, t, n/2)$ and $N_\gamma^{(\mathrm{as})} = N_\gamma^{(\mathrm{as})}(n, t, n/2)$ computed via (47) and (48), respectively, for $\gamma = 0.05$ and $\gamma = 0.0001$. Comparison of the asymptotic values presented in Table 2 with the exact formulas (4) and (7) for N^* and N_γ has shown that the approximations (47) and (48) are very precise for large values of n: for values of t and n given in Table 2 the minimal difference between asymptotic expressions and exact values was detected only for the case $t = 2,\ n = 100$, in the other cases the results coincide.

n	$\mathcal{T}_2$			$\mathcal{T}_3$			$\mathcal{T}_5$		
	$N^{(\mathrm{as})}$	$N^{(\mathrm{as})}_{0.05}$	$N^{(\mathrm{as})}_{0.0001}$	$N^{(\mathrm{as})}$	$N^{(\mathrm{as})}_{0.05}$	$N^{(\mathrm{as})}_{0.0001}$	$N^{(\mathrm{as})}$	$N^{(\mathrm{as})}_{0.05}$	$N^{(\mathrm{as})}_{0.0001}$
100	19	12	19	25	13	19	35	15	20
500	26	16	22	34	18	23	49	21	26
1000	29	17	23	38	19	25	55	24	28
2000	32	18	25	42	21	26	61	26	31
5000	36	20	27	48	24	29	69	30	34
10000	39	22	28	52	25	31	75	32	37
20000	42	23	29	56	27	32	81	35	39
30000	44	24	30	58	28	33	84	36	40

Table 2. Values of $N^{(\mathrm{as})}$ and $N_\gamma^{(\mathrm{as})}$ for $\mathcal{X} = G_{n/2}$, $\mathcal{T} = \mathcal{G}_t$, $t = 2, 3, 5$, $\gamma = 0.05, 0.0001$ and different values of n.

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