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Investigations of Binomial Group Testing Models

DOCTORAL DISSERTATION

Natural Sciences,
Mathematics (N 001)

VILNIUS 2025

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LIST OF ABBREVIATIONS

Abbreviation	Explanation
a.s.	Almost surely
A2	Square Array procedure
BTA	Binomial testing assumptions
BGT	Binomial group testing
$Be(p)$	Bernoulli distribution with parameter p
CGT	Combinatorial group testing
CLT	Central limit theorem
COCP	Continuous scale optimal cut-point
DOCP	Discrete scale optimal cut-point
D	Dorman procedure
GT	Group testing
H	Halving procedure
LDP	Large deviation principle
LLN	Law of large numbers
lhs	Left-hand side
MD	Modified Dorman procedure
MGF	Moment generating function
OCP	Optimal cut-point
PGT	Probalistic group testing
PT	Pairwise testing procedure
QC	Quality control
rhs	Right-hand side
ST	Sterrett procedure
s.t.	Such that
UCP	Universal cut-point
w.r.t	With respect to

Notation

Notation	Explanation
G_X	Average testing savings per item (aka gain)
L^X	Loss function
N	Cohort size
N_{opt}^X	Optimal value of the tested cohort size when applying procedure X for the case of a known prevalence p
$N_\star^X$	Optimal value of the tested cohort size when applying procedure X for the case of an unknown prevalence p
$\dot{N}$	Derivative of a latent function N
T_X	Random number of tests required to identify all defectives when applying procedure X
θ_X	Average number of tests required to identify all defectives when applying procedure X
t_X	Average number of tests per single item in a cohort when applying procedure X
$p_{X,c}$	Optimal continuous scale cut-point for procedure X
p_c^X	Optimal (discrete scale) cut-point for procedure X

Chapter 1

Introduction

1.1 Topic and early history of Group Testing

In many real-life settings, the task of testing is frequent. For example, physicians routinely apply tests to screen for diseases, manufacturers test goods to identify defective items, statisticians utilize tests to validate hypotheses, etc. Group Testing (GT), also known as Pool Testing, refers to a set of methods devoted to this task. The distinguishing feature of any GT method is an attempt to save testing efforts by replacing single items' tests with tests of groups of items. Hence the name.

Today, more than 80 years have passed since the recorded historical beginning of GT. It is usually associated with a seminal paper [19] published by Robert Dorfman in 1943. In that paper, Dorfman addressed the following problem. During World War II, the US Army conscripts had to be tested for syphilis. Syphilis required an accurate blood test, known nowadays as the Wassermann test, which was carried out after a sample of each soldier's blood had been taken. Under usual circumstances, syphilis was a rare disease, and the vast majority of the tests carried out came back negative. Therefore, Dorfman pointed out that the total number of tests for syphilis testing could be significantly reduced by pooling samples. This meant that blood samples from a large number of soldiers had to be taken and mixed into a single pooled sample so that the initial syphilis test was not performed on each soldier's blood sample. If the result was negative for the pooled sample, all soldiers whose blood samples were included in the pooled sample were healthy and free of syphilis. If the test was positive, one knew that at least one of the soldiers in the group had syphilis, and the whole cohort needed to be retested one by one. This first GT model demonstrated how to save by testing groups. Unfortunately, as reported in [20], it was not put into practice then, yet it inspired further investigations in this direction. These investigations were not immediate since World War II ended, the need for GT for massive testing disappeared, and the scientific community put it aside for quite a long time. In 1957, Sterret published a paper [73] describing a new testing scheme[1] which has some advantages compared with the original Dorfman's, and it took two years more for the seminal work by Sobel and Groll [72], the two Bell Laboratories Scientists, to make a break-through. This long (74 page) paper published in 1959 spawned a sequence of important GT-related papers to appear in 1960's [24, 25, 70, 71, 79] and to set in motion GT field afresh.

1.2 Examples of applications

Although the concept of group testing was first formulated in the context of medical testing of patients, it soon became apparent that use cases are not limited to this field alone. Below, we provide a sample of various applications illustrating its spread. The list is far from exhaustive yet sufficient to give an impression of breadth.

Medicine and biology It is not surprising that GT counts down a vast number of applications devoted to screening for a particular infectious disease like HIV [58, 61, 65], hepatitis B [15, 23, 28, 60], and most recently COVID-19 [13, 47, 49, 52, 64]. There are, however, many others.

In DNA testing, one looks for true genomic sub-sequences in relatively short fragments of DNA. The possibility of mixing samples taken from patients means that one can apply group testing, significantly reducing the number of tests and, hence, costs. The topic was so important that Du and Hwang (two famous investigators in the GT field) have published a dedicated monograph [41].

Another application in biology is the counting of infected/exposed objects. Not all cases require the identification of every item that is infected. Often, only the proportion of infected matters. For example, when monitoring the spread of diseases while preserving the confidentiality of individuals [68], or inspecting the spread of diseases among a wide variety of insects [21].

[1] it will be explicated in the sequel

Communications and networking Multi-access channels are channels that can be accessed, communicated, and messaged by multiple users. The basic problem here is identifying the users having information to transmit (active users). Hayes [35] was among the first who discovered that the GT approach is applicable in this context and can be successfully applied for the identification of active users. Several subsequent works were discussed by Wolf [82], who related the communications community's efforts to employ GT to the general GT theory developed so far. Among many investigations after that, paper [50] by Goodrich and Hirschberg is worth mentioning. Similar to predecessors, they studied GT algorithms for resolving broadcast conflicts on multi-access channels and for identification of the dead sensors in a mobile and wireless network. Their approach enriched the standard GT model, allowing the result of each test to be non-binary and indicate the number of defective items contained in the tested subset.

Cybersecurity, database systems, data compression An important cybersecurity problem is to efficiently determine which files on a computer/distributed storage have changed. In the general GT context, the changed files correspond to the defective items. M. T. Goodrich, M. J. Atallah, R. Tamassia [31] and T. Madej [51] proposed GT procedures devoted to solving problems of this kind.

Another cybersecurity problem is the detection of various virtual attacks. Khattab et al. [44], Xuan et al. [87] and Gurani et al. [32] described how GT could be used to detect denial-of-service attacks. They divided a server into several virtual servers and monitored which received high traffic. This way, the highest traffic users are identified.

For effective database management, it may be helpful to classify items as having high demand. Cormode and Muthukrishnan [26] suggested how to use GT for achieving such item classification.

Hong and Ladner [36] described an adaptive algorithm for image data compression, whereas Shavit et al. [67] did this for video data compression.

Relation to Theoretical Computer Science There are many works demonstrating a clear relationship between GT and Theoretical Computer Science. For example, Hwang and coauthors in a series of papers [27, 40, 85] employ the fact that GT procedures for finding a single defective can be cast in terms of optimal binary search trees (aka Hu-Tucker trees). Chen et al. [11] propose GT procedures based on the Shannon-entropy criteria, whereas Hsu [37] develops GT procedures based on the Huffman lower bound and Shannon-entropy criteria. Triesch [78] and later Allemann [6] employ hypergraphs to construct very effective GT procedures. Among many others, Aldridge's paper [4] delineates a relationship with coding theory, whereas his recent review with coauthors [5] provides a systematic view of GT from the informational perspective and contains many examples of applications.

Quality control The field of Quality Control (QC) is rich in GT applications, pretty much like that of medicine and biology. We do not list here specific ones yet point out the monograph [42] and review [75]. Inspecting the references therein, the reader can find many various GT procedures related to the field of QC.

1.3 Classification of Group Testing methods

There are several ways to classify GT procedures. The first and most common is to distinguish between combinatorial GT (CGT) and probabilistic GT (PGT). In CGT, one assumes that, given a set of $N \in \mathbb{N}$ objects, there can be at most or exactly $1 \leq d \leq N$ defectives[2]. In order to identify these defective items and reduce the number of tests utilized, combinatorial methods are applied. In CGT, the worst case scenario (i.e., the one requiring the largest possible number of tests) is of primary interest. In PGT, one assumes that each item to be classified has a probability of defectiveness and also specifies dependence between items. This way, the data-generating mechanism is introduced, and because of randomness, the focus usually lies in reducing an average number of tests by taking into account the data-generating mechanism.

The second way to classify GT procedures is to distinguish between adaptive ones and non-adaptive ones. In adaptive procedures, testing is done sequentially, and one can utilize the results of the tests carried out so far in the subsequent tests. In non-adaptive procedures, all tests usually run in parallel, and there is no opportunity to make use of accrued information. Hybrid procedures are also met in the literature.

[2] or else contaminated, infected, etc.; in all the Thesis, we use these adjectives as well as their counterparts (non-defective, pure, non-infected, etc.) interchangeably; in all cases, they mean the same: an object or a group of objects having (respectively, not having) property of interest

There are several other criteria employed in the classification of GT procedures. Some of them apply only to specific sub-classes (e.g., only to adaptive procedures). Below, we list a few.

> *Test kit quality*. In many practical applications, it is unreasonable to assume that the test kit at hand obeys 100 percent sensitivity and/or specificity. Therefore, one can split the GT procedures into those assuming perfect testing and those assuming testing with errors.
>
> *Cohort size*. Often there are natural constraints preventing from testing arbitrarily large groups. E.g., in medical screening, it is common to observe the so-called dilution effect: pooling of too many specimens inflates the test's sensitivity/specificity drastically; thus, only procedures with upper bounded cohort size are applicable. It is, therefore, possible to classify GT procedures into size-constrained/unconstrained.
>
> *Nesting*. One says that an adaptive GT procedure belongs to the class of nested procedures provided the following holds: at each testing stage (except the first one), the cohort to be tested next is a subset of a contaminated items' set, i.e., the set known to contain defectives. The class of nested procedures is very large and common in applications.
>
> *Test output*. The procedures can also be classified by their output. Most common scenario is that of binary procedures: given the set to test, such procedure outputs 1 provided at least one item in the tested set is contaminated and it outputs 0 provided all items are pure; there are no further indications which items (if any) are contaminated and how much items of this kind there are in the tested set. However, some procedures can output the (estimated) number of contaminated items.

In this Thesis, we investigate only size unconstrained binary PGT procedures corresponding to perfect testing and satisfying Binomial Testing Assumptions described in Subsection 2.1. Almost all of them are nested.

1.4 Structure of the Thesis

The remaining part of the thesis contains three chapters. In Chapter 2, we give notation and provide all necessary background. It includes description of:

(a) general Binomial Testing Assumptions under which all subsequent analysis is done;

(b) several GT procedures, which are repeatedly used in the sequel;

(c) general GT results required for understanding of our ones;

(d) typical GT analysis tasks.

Chapter 3 is devoted to the statement of our results, some examples of applications, and a related literature review. Corresponding proofs are given in Chapter 5. Chapter 4 is devoted to discussion. Finally, there is a summary in Lithuanian placed at the very end.

Chapter 2

Background

2.1 Binomial Testing Assumptions

As mentioned in the Introduction 1, we consider only PGT models. However, even here, the most general model is intractable analytically and concrete GT procedures are formulated under additional assumptions. Before proceeding to their statement, we remind that, in the Thesis, we consider only binary tests: when applied to the group at hand, such test outputs one if the group contains at least one contaminated item, and it outputs zero provided the group is pure. Generally, N stands for the size of the initial cohort of the items to be tested. It can be further parameterized by an integer $n \geq 1$, and such parametrization (including a trivial one $N(n) = n$) depends on the algorithm of the procedure under consideration (see Subsection 2.2 for concrete examples).

In what follows, we always assume that:

(BTA1) initially, each item in the cohort to be tested can be contaminated with the same constant probability $p \in (0, 1)$;

(BTA2) items are independent;

(BTA3) test kit under consideration is perfect (i.e., sensitivity = specificity = 100%) and does not depend on the size of the tested group.

Assumptions (BTA1)–(BTA3) are called Binomial Testing Assumptions (BTA). Imposing them, we can formalize our setup by the following probabilistic model:

- Let $Y_1, \dots, Y_N$ be i.i.d. $\sim Be(p)$ random variables (r.vs.) representing the cohort of interest;
- $Y_i = 1 \iff$ item i is contaminated (then $Y_i = 0 \iff$ item i is pure);
- For any testing procedure X and any non-empty $A \subset \{Y_1, \dots, Y_N\}$, $X(A) = \mathbb{1}\{\Sigma_{Y_i \in A} Y_i > 0\}$.

Given cohort $C = \{Y_1, \dots, Y_N\}$ and test procedure X, let T_X denote the random number of tests required to identify all contaminated in C and let $\theta_X(N, p) = \mathrm{E}\, T_X$ be its average. Note that θ_X is a function of two arguments: $N \in \mathbb{N}, p \in (0, 1)$. For convenience, q stands for $1 - p$ in the entire Thesis.

2.2 Several Group Testing procedures

In this subsection, we describe several binomial GT procedures serving as examples and objects of investigation in the sequel. The graphic schemes of the procedures are presented in figures 2.1–2.5.

Dorfman procedure D This procedure was already described in the Introduction 1. It spans two steps:

Step1: test initial pooled sample IP;

Step2: if IP tests negative, finish; otherwise retest each item individually.

One can see that $T_D = 1 + N\mathbb{1}\{Y_1 + \dots + Y_N > 0\}$. Therefore,

$$\theta_D(N, p) = 1 + N\,\mathrm{E}\,\mathbb{1}\{Y_1 + \dots + Y_N > 0\} = 1 + N(1 - q^N). \quad (2.1)$$

Modified Dorfman procedure MD Sobel and Groll [72] observed that the D procedure is inconsistent and suggested a fix: if the initial pool tested positively and having retested $N - 1$ items there were no defectives, there is no need to retest the last one. In what follows, we denote this procedure MD. By description,

$$T_{MD} = 1 + (N-1)\mathbb{1}\{Y_1 + \dots + Y_N > 0\} + \mathbb{1}\{Y_1 + \dots + Y_{N-1} > 0\}.$$

Therefore,

$$\theta_{MD}(N, p) = 1 + (N-1)(1-q^N) + 1 - q^{N-1} = 1 - pq^{N-1} + N(1-q^N). \quad (2.2)$$

Sterrett procedure ST Sterrett [73] proposed another modification of the D procedure. His testing algorithm is as follows:

Step1: test initial pooled sample IP;

Step2: if IP tests negative, finish; otherwise go to Step3;

Step3: retest each item one by one until the first contaminated is identified; if the whole cohort is already tested, finish; otherwise, treating the set of the remaining untested items as a new initial cohort, go to Step1 and start over.

In [72] it was shown that

$$\theta_{ST}(N,p) = 2q - p^{-1}(1 - q^{N+1}) + (2 - q)N. \tag{2.3}$$

Pairwise testing algorithm PT Pairwise testing algorithm was investigated by Yao and Hwang in [85]. Its description is as follows:

Step1: if there is only one item in the cohort C, test it and finish; if there are no items at all, finish; otherwise proceed to Step2;

Step2: having a cohort of $N \geq 2$, choose a pair of items, form a pool, and test it;

Step3:

- if the pool tests negative, classify tested items as pure, set $N = N - 2$, $C = C \setminus \{\text{tested pair}\}$;
- if the pool tests positive, retest one item; in case that item tests negative, classify the remaining item as contaminated, set $N = N - 2$, $C = C \setminus \{\text{tested pair}\}$; if that item tests positive, set $N = N - 1$, $C = C \setminus \{\text{retested item}\}$.

Step4: go to Step1.

Remark 2.2.1. There is no difference which pair of items to choose in Step 2. In what follows, we always choose the last two. □

In [85] it was demonstrated that

$$\theta_{PT}(N,p) = N\frac{2 - q^2}{1 + q} + \frac{q^2 + q - 1}{(1 + q)^2}(1 - (-q)^N). \tag{2.4}$$

Square Array procedure A2 This procedure was introduced by Phatarfod and Sudbury [63] and later generalized by Berger, Mandell and Subrahmanya [9]. To apply it, one has to have $N = n^2, n \in \mathbb{N}$, items in total. Assuming this holds true, the algorithm reads as follows:

Step1: put samples of all items on a square $n \times n$ matrix;

Step2: make n pools corresponding to rows and n pools corresponding to columns; test them;

Step3: if all pools test negatively, finish; otherwise retest items I_{ij} satisfying condition "row i and column j tested positively".

An average number of tests was computed by Phatarfod and Sudbury [63]:

$$\theta_{A2}(N,p) = 2n + n^2\left(1 - 2q^n + q^{2n-1}\right) = 2\sqrt{N} + N\left(1 - 2q^{\sqrt{N}} + q^{2\sqrt{N}-1}\right). \quad (2.5)$$

Halving procedure H It is difficult to trace back who has introduced this procedure first as it has tight relationships to binary search problem. For the purposes of GT in quality control, it was discussed by Johnson et. al. [42]. To apply it, one has to have $N = 2^n, n \geq 1$ items in total. As the name suggests, the corresponding algorithm works by testing halves. Below comes a precise description.

Step1: Test initial pool. If it tests negative, finish; otherwise, go to Step 2.

Step2: Split the initial cohort into two equal subsets. Apply the procedure recursively (i.e., starting from Step 1) to each half.

An average number of tests required by this procedure (see, e.g., [69]) equals

$$\theta_H(N,p) = 1 + 2N \sum_{k=1}^{\log_2 N} \frac{1 - q^{2^k}}{2^k}. \quad (2.6)$$

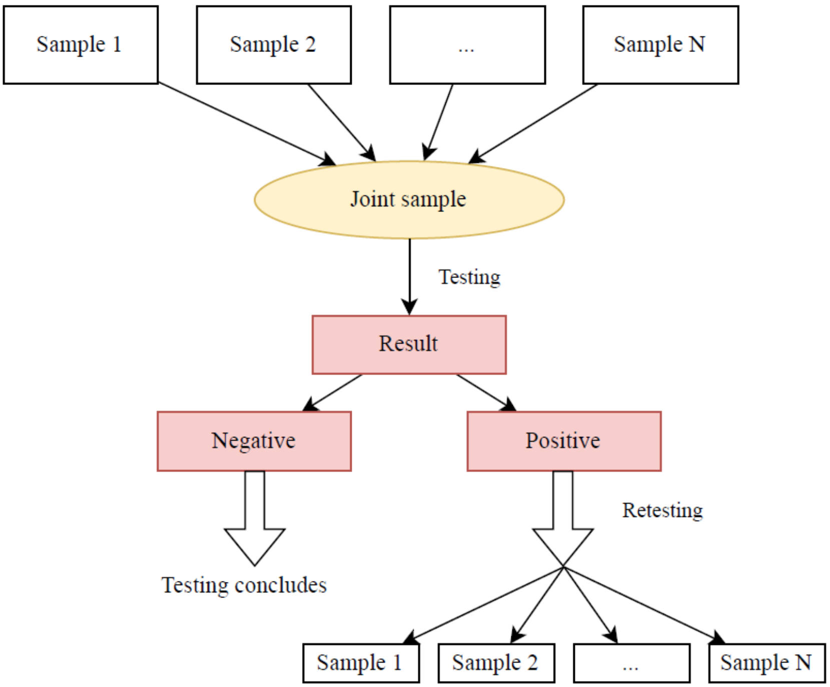

Figure 2.1: Dorfman testing scheme [19].

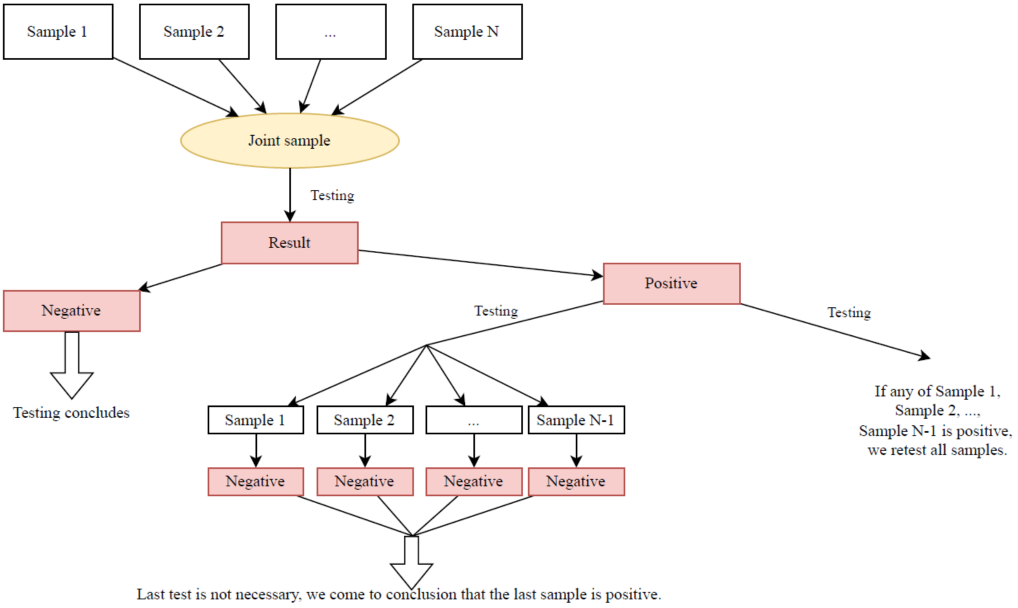

Figure 2.2: Modified Dorfman testing scheme [72].

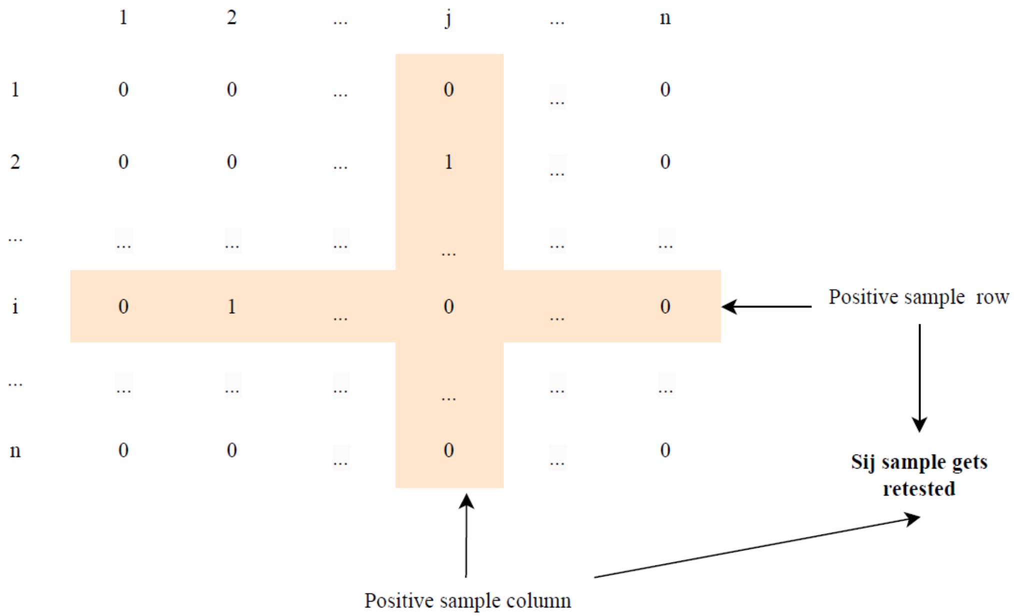

Figure 2.3: Square Array testing scheme [63].

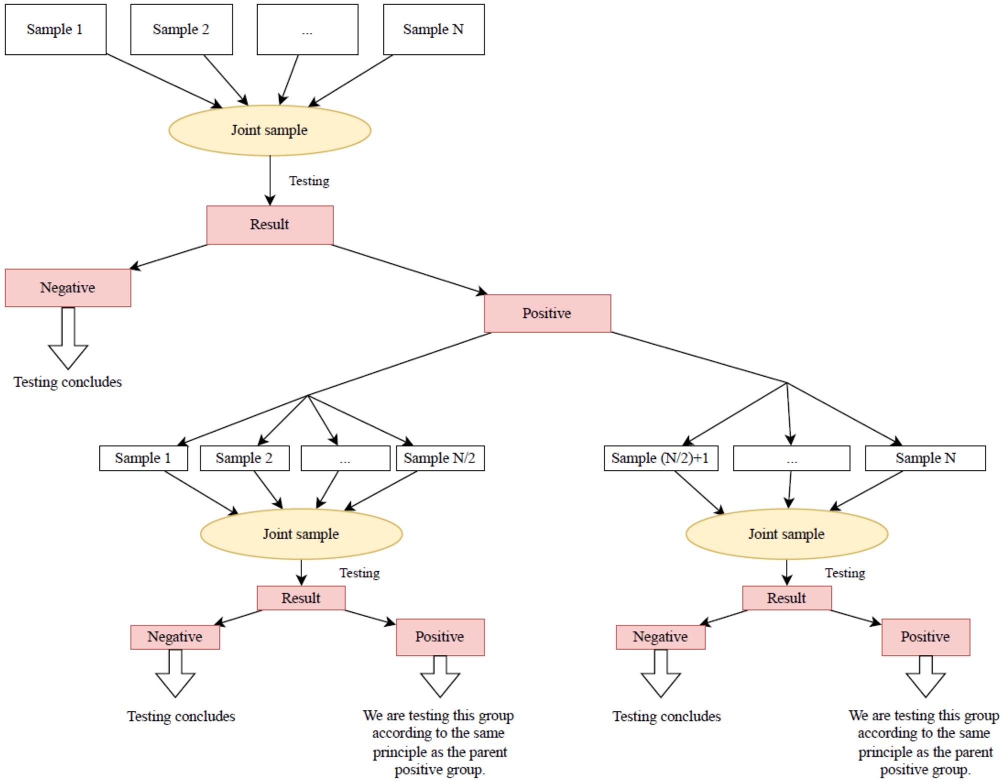

Figure 2.4: Halving testing scheme.

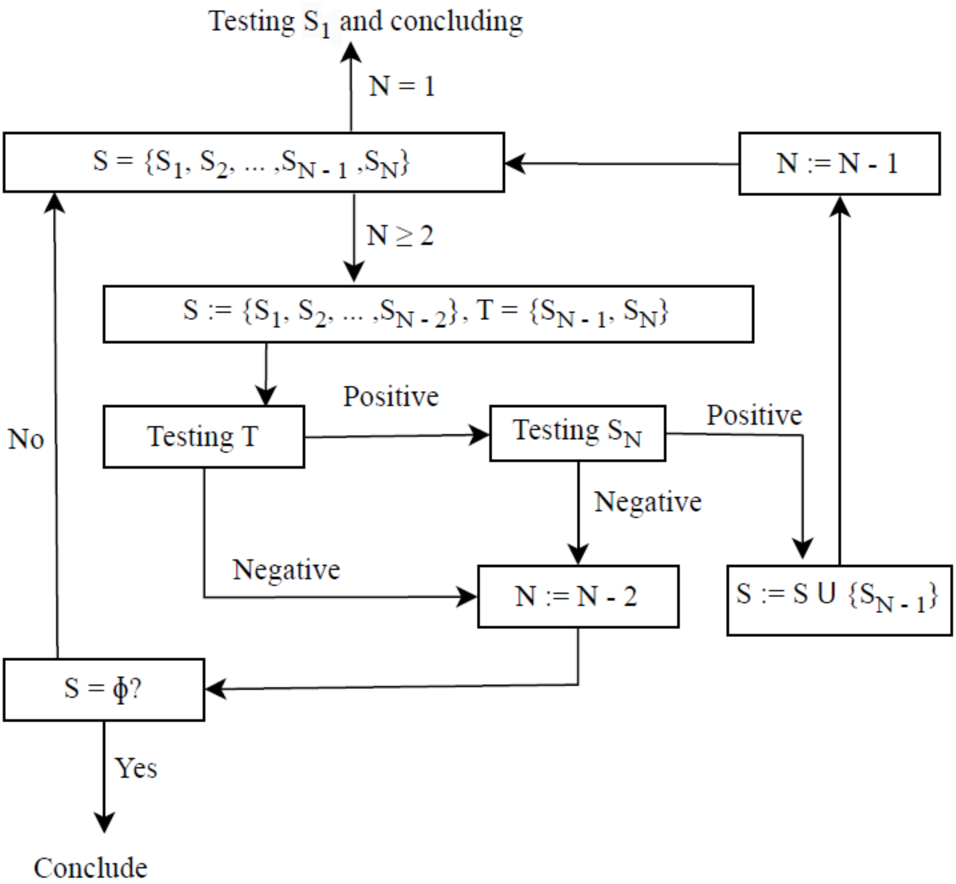

Figure 2.5: Pairwise testing scheme [85].

2.3 Typical Group Testing tasks

Let X be a procedure of interest. It is reasonable to assume that it differs from other procedures not only w.r.t. the testing scheme but also w.r.t. an average number of tests $\theta_X(N,p)$. Since the primary aim of GT is to minimize this quantity and the contamination probability p may be regarded as fixed by nature, one of the typical GT tasks is to find the optimal value of the tested cohort size N_{opt}^X. To state this optimization problem formally, one usually considers the function

$$\mathbb{N} \times (0,1) \ni (N,p) \mapsto t_X(N,p) := \frac{\theta_X(N,p)}{N} \tag{2.7}$$

whose value is an average number of tests per single item in a cohort of size N. Then, any minimizer of this function w.r.t. N is called optimal configuration and denoted by N_{opt}^X. Note that we assume fixed p, i.e. $N_{opt}^X \in \arg\min_{N\in\mathbb{N}} t_X(N,p)$. Therefore, N_{opt}^X depends on p. This has several important consequences discussed below.

The function $(0,1) \ni p \mapsto N_{opt}^X(p)$ shows how large should be the sizes of the tested cohorts to have average testing savings per item (aka gain)

$$G_X(p) := 1 - t_X(N_{opt}^X(p), p) \tag{2.8}$$

maximal (in the long run). It is intuitively clear that, for any reasonable X, $(0,1) \ni p \mapsto N_{opt}^X(p)$ should be non-increasing, and in all the remaining parts of the Thesis, we assume this by default. Then values of $G_X(p)$ close to 1 should be observed for small p's. In practice, testing pools of arbitrarily large sizes may be infeasible because of the dilution effect: large pool sizes change test kit characteristics (usually, sensitivity drops down drastically). Knowing the maximal tolerable pool size $N_{\max}$ of the test kit at hand allows one to find the range R_X of p's for which $N_{opt}^X(p) \leq N_{\max}$. For this, explicit functional form of $(0,1) \ni p \mapsto N_{opt}^X(p)$ is desirable.

An explicit form of the latter function yields an ability to address another typical GT problem: a comparison of several competing procedures. Say, $X_i, i = 1, \ldots, k$, are procedures applicable to the problem at hand. One can investigate both gains $G_{X_i}(p)$ (see Eq. (2.8)) and sizes $N_{opt}^{X_i}(p)$ for different values of p and, taking into account various scenarios, choose preferable procedures.

Finally, there is one more typical GT task tightly related to N_{opt}^X: finding optimal cut-point (OCP) $p_c^X \in (0,1)$. As noted earlier, intuition suggests that group testing should be profitable only for sufficiently small prevalence p. To be more specific, recall Dorfman procedure D: if p is small, then testing will oftentimes end up after a single initial pool test; however, if p is close to 1, almost every group of size $N \geq 2$ will be contaminated, and in addition to single pool test there will be N individual tests; hence, instead of having only N individual tests, one will have $N+1$ tests. The above OCP problem therefore translates to finding value $p_c^X \in (0,1)$ s.t. $\forall p \in (p_c^X, 1)$ $N_{opt}^X(p) = 1$. In the general BTA context, this problem was addressed by Ungar. In [79], he obtained the following fundamental GT result.

Theorem 2.3.1. *Binomial GT makes sense if and only if* $p \in \left(0, \frac{3-\sqrt{5}}{2}\right)$*: for* $p \in \left(\frac{3-\sqrt{5}}{2}, 1\right)$*, there does not exist GT procedure performing better than individual testing; for* $p \in \left(0, \frac{3-\sqrt{5}}{2}\right)$ *there always exists at least one procedure* X *s.t.* $t_X(N_{opt}^X(p), p) < 1$.

In the binomial GT, the value $\frac{3-\sqrt{5}}{2}$ is known under the name of Universal Cut-Point (UCP). For some GT procedures, it is achievable. That is,

$$G_X(p) = 0 \Longleftrightarrow p \geq \frac{3-\sqrt{5}}{2}.$$

However, there are procedures for which

$$G_X(p) = 0 \Longleftrightarrow p \geq p_c^X \text{ with } p_c^X < \frac{3-\sqrt{5}}{2}.$$

Therefore, when investigating characteristics of a particular procedure X, it is first of all important to find p_c^X: if the problem at hand is s.t. $p > p_c^X$, one needs to resort to individual testing or look for another GT procedure if $p_c^X < \frac{3-\sqrt{5}}{2}$. Because of Theorem 2.3.1, in all the Thesis, we restrict the range of p to $\left(0, \frac{3-\sqrt{5}}{2}\right)$.

In the end, we mention that there are other binomial GT problems not discussed here. Some of them are difficult and open for quite a long period of time. In our opinion, those described above are the most typical. Nonetheless, dealing with a particular procedure still poses a challenge and requires extensive analysis.

Chapter 3

Results

3.1 Optimal configurations for Modified Dorfman, Sterrett, and Square Array procedures

3.1.1 Theoretical results

In Chapter 2, we have mentioned that finding N_{opt}^X is one of the typical yet very important GT tasks because knowledge of N_{opt}^X allows to utilize X most efficiently. As we know, there are no a lot of results providing explicit expressions of N_{opt}^X.

For the case of the Dorfman procedure D, the optimal configuration was derived by Samuels [66] quite long ago. He has demonstrated that, for[1] $p \in (0, 1-(1/3)^{1/3}) \approx (0, 0.31)$, $N_{opt}^D(p) \in \{\lfloor\sqrt{p^{-1}}\rfloor+1, \lfloor\sqrt{p^{-1}}\rfloor+2\}$ whereas, for $p \geq 1-(1/3)^{1/3}$, $N_{opt}^D(p) = 1$ (the latter result also means that optimal cut-point $p_c^D = 1-(1/3)^{1/3}$ is strictly less than $UCP = \frac{3-\sqrt{5}}{2}$ discussed in Subsection 2.3). However, at the start of our investigations, we discovered that for the modified Dorfman procedure MD, the Sterrett procedure ST, and the square array procedure A2, the analytical expressions of N_{opt}^X were not completely made explicit. To be more precise, for MD and ST procedures, Malinovsky and Albert [55] numerically derived explicit analytical expressions of optimal configurations for a wide range of p's and conjectured that the same expressions are valid

[1] here and in the sequel, $\lfloor x\rfloor$ denotes an integer part of $x \in \mathbb{R}$; $\lceil x\rceil$ equals x if $x \in \mathbb{Z}$ and it equals $\lfloor x\rfloor + 1$ otherwise

for all $p \in (0, UCP)$. In our paper [88], we justified the correctness of their conjectures and proved the following statements.

Theorem 3.1.1. *Let*

$$g_0(p) := \frac{1}{q}\left(\frac{1-2pq}{q\left(1-\ln q\sqrt{\frac{2}{p}}\right)}\right)^{\sqrt{\frac{p}{2}}} \quad \text{for} \quad p \in \left(0, \frac{3-\sqrt{5}}{2}\right). \tag{3.1}$$

Then equation $g_0(p) = 1$ *admits a unique solution* $p_* \approx 0.1711$ *and the following relations hold:*

$$N^S_{opt}(p) \in \left\{\lfloor\sqrt{2p^{-1}}\rfloor, \lfloor\sqrt{2p^{-1}}\rfloor + 1\right\} \text{ for } p \in \left(p_*, \frac{3-\sqrt{5}}{2}\right);$$

$$N^S_{opt}(p) \in \left\{\lfloor\sqrt{2p^{-1}}\rfloor, \lfloor\sqrt{2p^{-1}}\rfloor + 1, \lfloor\sqrt{2p^{-1}}\rfloor + 2\right\} \text{ for } p \in (0, p_*].$$

Theorem 3.1.2. *For all* $p \in \left(0, \frac{3-\sqrt{5}}{2}\right)$*,*

$$N^{MD}_{opt}(p) \in \left\{\lfloor\sqrt{p^{-1}}\rfloor, \lfloor\sqrt{p^{-1}}\rfloor + 1\right\}. \tag{3.2}$$

The A2 procedure was investigated by Hudgens and Kim [38]. They derived quite tight lower and upper bounds yet did not succeed in providing exact expression of optimal A2 configuration and left explicit formulae undiscovered. They also addressed the problem of finding OCP (see Section 2.3) and actually found optimal value p_c^{A2}. In [89], we obtained expression for $N^{A2}_{opt}(p)$ and along the way produced additional insights about p_c^{A2} (see clarifying Remark 3.1.5 below). Before stating our results, we remind that, in the case of A2, cohort size N is parameterized by $n \in \mathbb{N}$ as follows[2]: $N(n) = n^2$. Also, in the setting of A2, it was more convenient for us to treat t_{A2} as a function $[2, \infty) \times (UCP, 1) \ni (n, q) \mapsto t_{A2}(n, q)$ with $n \in [2, \infty)$ ranging continuously rather than a function of (N, p) with a domain $\{n^2 : n \in \mathbb{N}\} \times (0, UCP)$. Keeping this in view, our results read as follows.

Theorem 3.1.3. *Let* $g(q, n) = \frac{2}{n} - 2q^n + q^{2n-1} = t_{A2}(n, q) - 1$. *The following statements hold true:*

[2] see Section 2.2 for the description of A2

(i) For any $(q, n) \in (1/2, 1) \times (2, \infty)$*, system of equations*

$$\begin{cases} 1 = nq^n \left(1 - \frac{q^{n-1}}{2}\right) \\ n \ln q = -\frac{\left(1 - \frac{q^{n-1}}{2}\right)}{(1-q^{n-1})} \end{cases} \tag{3.3}$$

has a unique solution $(q_*, n_*) \approx (0.748416, 4.453524)$*.*

(ii) For any fixed $q \in (q_*, 1)$ *and with respect to* n*, equation* $g(q, n) = 0$ *admits two solutions* $n_L, n_U : 2 < n_L < n_* < n_U < \infty$*. On* (n_L, n_U)*,* $n \mapsto g(q, n)$ *attains values in* $(-\infty, 0)$ *whereas on* $(2, \infty) \setminus [n_L, n_U]$ *it attains values in* $(0, \infty)$*.*

(iii) For any fixed $q \in (q_*, 1)$*, the region* (n_L, n_U) *is the one where A2 is efficient, i.e.,* $t_{A2}(q, n) < 1$ *for* $n \in (n_L, n_U)$*. In that region, there exists a unique (and, therefore, global) minimizer* n_{min} *of* $(2, \infty) \ni n \mapsto t_{A2}(q, n)$*. For* $q \in [0.755, 1)$*, it is given by*

$$n_{min} = \frac{1}{p^{\frac{2}{3}}} + \frac{1}{2p^{\frac{1}{3}}} + 0.2 + 3p^2 + t_* \tag{3.4}$$

for some $t_* \in [0, 1]$*.*

(iv) $(2, \infty) \ni n \mapsto t_{A2}(n, q)$ *also has a unique (and, therefore, global) maximizer located in the region* (n_U, ∞)*. For any fixed* $q \in (0, q_*)$*, A2 is never optimal, i.e.,* $(2, \infty) \ni n \mapsto t_{A2}(n, q)$ *attains values in* $(1, \infty)$*.*

Corollary 3.1.4. *Let* $g(q, n)$ *be as in Theorem 3.1.3. Then* $g(q, 5) = 0$ *has a unique solution* $q_5 \approx 0.750209961$*. For all* $q \in (q_5, 1)$*,* $n_{opt}(q)$ *belongs to the set*

$$\left\{ \left\lfloor \frac{1}{p^{\frac{2}{3}}} + \frac{1}{2p^{\frac{1}{3}}} + 3p^2 + 0.2 \right\rfloor + i : i = 0, 1, 2 \right\}. \tag{3.5}$$

Remark 3.1.5. Inspecting the statements above, it might be tempting to conclude that our results are not exhaustive: it is unclear what happens in the region (q_*, q_5) and what is an expression for $n_{opt}(q)$ there. Applying Theorem 3.1.3 for a fixed $q \in (q_*, q_5)$, we have that $t_{A2}(n_{min}, q) < 1$ with $n_{min} = n_{min}(q)$ of (iii). However, this $n_{min}(q) \in (4, 5)$ and $\min(t_{A2}(4, q), t_{A2}(5, q)) > 1$ when $q \in (q_*, q_5)$. We do not provide separate proof of this fact and only mention that technical details can be filled in after inspection of the proofs presented in Chapter 5. Hudgens and Kim [38] operated on the discrete scale and deduced that region $(q_5, 1)$

is the one where $\{5, 6, \ldots\} \ni n \mapsto t_{A2}(n, q)$ is efficient. Having proved that $n = 2, 3, 4$ are never optimal, they actually verified that $(q_5, 1)$ is the region where practical application of A2 makes sense. Therefore, in this direction, our input adds the missing part to the theoretical characterization of A2. However, it is an honest deal to say that theoretical findings about OCP, though interesting, have ho additional practical value. $\square$

3.1.2 Examples

In this subsection, we provide two examples illustrating the usefulness of our results. The first of our examples is most interesting in the asymptotic regime as $p \to 0+$. Since in this case Dorfman procedure D and modified Dorfman procedure MD are equivalent, we exclude MD. Also, in both examples, we switch back to our usual convention and treat t_X as a function of (N, p).

The figures and calculations were produced by making use of an open-source computer algebra system SymPy [59] and the Python packages lying in the core kit for scientific numerical programming with Python: NumPy [34], SciPy [80], Matplotlib [39] and Pandas [81], [77]. The same software was employed in the proofs provided in Chapter 5.

Example 1: Comparison of procedures To illustrate performance of different procedures, we compare A2, D, S and H in terms of magnitude of optimal configuration N^X_{opt} and gain (defined by Eq. (2.8)) across the range $p \in (0, 0.249790)$ where application of all of them seems reasonable[3]. In what follows, N^X_* stands for the unrounded optimal configuration, i.e. the minimizer of the continuous argument function $[1, \infty) \ni N \mapsto t_X(N, p)$. We have chosen to operate on the continuous scale and use $t_X(N^X_*(p), p)$ instead of $t_X(N^X_{opt}(p), p)$ since it is much easier to interpret information visually in comparison to the discrete case. Recall that, in the case of A2, $N = n^2$, where n is the number of rows (columns) in the square array used in the definition of A2. In this example (as well as in the second one), this reparametrization remains in force: writing $t_{A2}(N, p)$, we actually mean $t_{A2}(n_{min}(q), q)$ of Theorem 3.1.3 with n_{min} given by (3.4). From results of [66], [69] and those above

[3] the restriction of the range is due to A2 which does not make sense for larger p's

it follows that

$$N_*^{A2}(p) = n_{min}^2(p) = p^{-\frac{4}{3}}(1 + o(1)), \quad N_*^D(p) = \sqrt{p^{-1}}(1 + o(1)),$$
$$N_*^S(p) = \sqrt{2p^{-1}}(1 + o(1)), \quad N_*^H(p) = -\frac{1}{2\log_2 q}(1 + o(1))$$

and that

$$t_{A2}(N_*^{A2}(p), p) = 3p^{\frac{2}{3}}(1 + o(1)), \quad t_D(N_*^D(p), p) = 2\sqrt{p}(1 + o(1)),$$
$$t_{ST}(N_*^S(p), p) = \sqrt{2p}(1 + o(1)),$$
$$t_H(N_*^H(p), p) = -(2p\log_2 p)(1 + o(1))$$

as $p \to 0+$.

Figure 3.1 shows the behavior of N_*^X and gain G_X of the four procedures considered. Due to the raise to the square of n_{min}, N_*^{A2} grows to infinity much faster than the counterparts of the remaining schemes, and, because of this, in the top left sub-figure, the range of p starts quite far from the origin and the accompanying bottom left sub-figure on the log scale is given. The latter clearly depicts the relationships

$$\ln\left(N_*^D(p)\right), \ \ln\left(N_*^S(p)\right) \sim -\frac{1}{2}\ln(p),$$
$$\ln\left(N_*^H(p)\right) \sim -\ln(p), \quad \ln\left(N_*^{A2}(p)\right) \sim -\frac{4}{3}\ln(p), \quad (3.6)$$

following from the formulae given above and clearly showing that the asymptotic slope of $\ln\left(N_*^{A2}(p)\right)$ on the $-\ln p$ scale is the largest one.

Talking about gains depicted in the right top sub-figure, one can see that the D procedure always performs worse than other competitors. However, each of A2, S and H have their own regions where they perform best. The bottom right sub-figure illustrates that, for p tending to zero, the H procedure's gain growth rate is the biggest one.

Example 2: Optimal configuration when the prevalence is unknown
In reference [54], the authors looked for the pool size leading to optimal testing by making use of procedure D when the prevalence is unknown. They employed two approaches. Both (approaches) were based on the following loss function. Given procedure X, define

$$L^X(N, p) = t_X(N, p) - t_X(N_{opt}^X(p), p), \quad (3.7)$$

where $N_{opt}^X = N_{opt}^X(p) \in \arg\min_{N\in\{1,2,\dots\}} t_X(N, p)$ is the optimal configuration when the prevalence p is known. It is clear that $L^X(N, p) \geq$

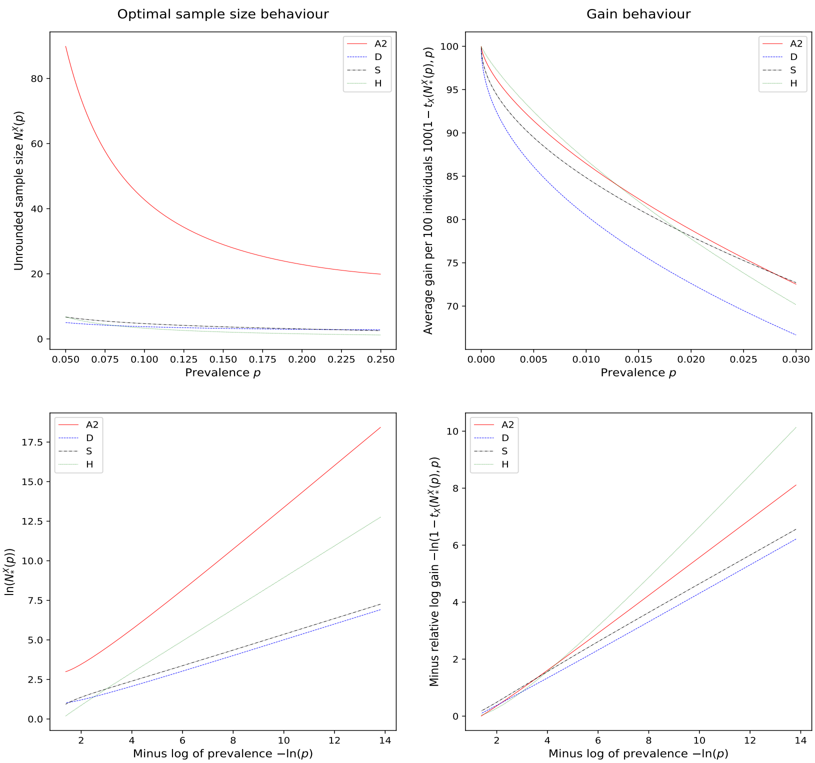

Figure 3.1: Graph showing the behavior of optimal pool sizes and gains on original and log–log scales.

$0\ \forall (N,p) \in \mathbb{N} \times (0,1)$ and, for a given p, $L^X(N,p) = 0$ precisely when $N \in \arg\min_{N\in\{1,2,\ldots\}} t_X(N,p)$. In what follows, to distinguish between $N^X_{opt}(p)$ and optimal configuration suitable for unknown p's, the latter configuration is denoted by $N^X_\star$.

The first approach in [54] was to make use of mini–max strategy and take $N^X_\star$ as a minimizer of

$$\{1,2,\ldots\} \ni N \mapsto \sup_p L^X(N,p). \tag{3.8}$$

The second approach was to make use of the Bayesian paradigm and, after putting the prior π on p, to take $N_\star^X$ as a minimizer of

$$\{1,2,\ldots\} \ni N \mapsto \mathrm{E}_\pi(L^X(N,p)) = \mathrm{E}_\pi(t_X(N,p)) - c(\pi), \\ c(\pi) = \mathrm{E}_\pi(t_X(N_{opt}^X(p),p)). \quad (3.9)$$

In this example, we have adopted both approaches to the case of A2. When using the Bayesian one, π was taken uniform over $(0, 0.249790)$. Thereby, we have modeled a situation when the only prior information is that the application of A2 makes sense (see Corollary 3.1.4). Also, we have modified (3.9) and used

$$\{1,2,\ldots\} \ni N \mapsto \mathrm{E}_\pi(L^X(N,p))^2 = \mathrm{E}_\pi\left(t_X(N,p) - t_X(N_{opt}^X(p),p)\right)^2 \quad (3.10)$$

instead. To justify our choice, note that, in (3.9), $c(\pi)$ does not depend on N. Therefore, minimization of the target function amounts to minimization of $\{1,2,\ldots\} \ni N \mapsto \mathrm{E}_\pi(t_X(N,p))$ and the corresponding minimizer depends only on the prior π. This way important information carrying function $p \mapsto t_X(N_{opt}^X(p),p)$ remains unutilized. It seems, however, more reasonable to look for an estimate minimizing the distance to optimal value function and depending on this function.

Figures 3.2–3.3 show graphs of (3.8) and (3.10) for the case of $X = A2$ and the previously mentioned prior π. Numerical estimation yielded the following values:

- $N_\star^{A2}(p) = 12^2$ for the case of mini–max approach;
- $N_\star^{A2}(p) = 7^2$ for the case of Bayesian approach.

We did not make any attempt to rigorously prove that these values are the only global minimizers of the target loss.

Finishing the example, it is important to note that, though the strategy discussed above leads to sub-optimal testing in a stable environment when the prevalence is close to constant and its reliable estimation is possible, it appears to be a reasonable strategy when the prevalence is varying rapidly and is difficult to capture by data at hand. Therefore, at least in the initial stage, it can be considered as a good alternative for optimal testing during pandemics like COVID-19. Of course, under such circumstances, one can (and should) use various priors motivated by expert knowledge and/or domain-specific factors.

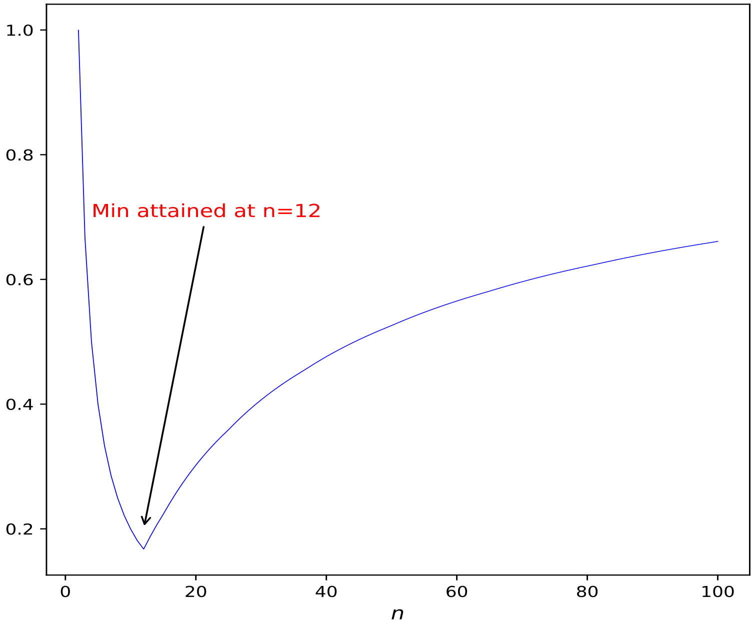

Figure 3.2: Graph of $\{2,3,\ldots\} \ni n \mapsto \sup_q(t_{A2}(n,q) - t_{A2}(n_{opt}(q),q)$

3.2 Algorithm for finding optimal cut-point

3.2.1 Theoretical results

In Subsection 2.3, we have discussed the importance of finding OCP for a given procedure X. However, to our best knowledge, Ungar's Theorem 2.3.1 is the only result of the general nature addressing this problem. All other works were tied to investigations of particular procedures. In our work [90], we proposed an algorithm suitable for finding an approximate value of OCP for a class of BTA satisfying procedures and allowing to recover exact OCP in many cases. Along the way, we have discovered an interesting connection of independent interest between GT and Bifurcation Theory. Our method applies to the class of binomial GT procedures satisfying the following constraints.

(M0) $\exists c \geq 2$ s.t. X is a-priori known to be useless for $N \in [1, c)$.

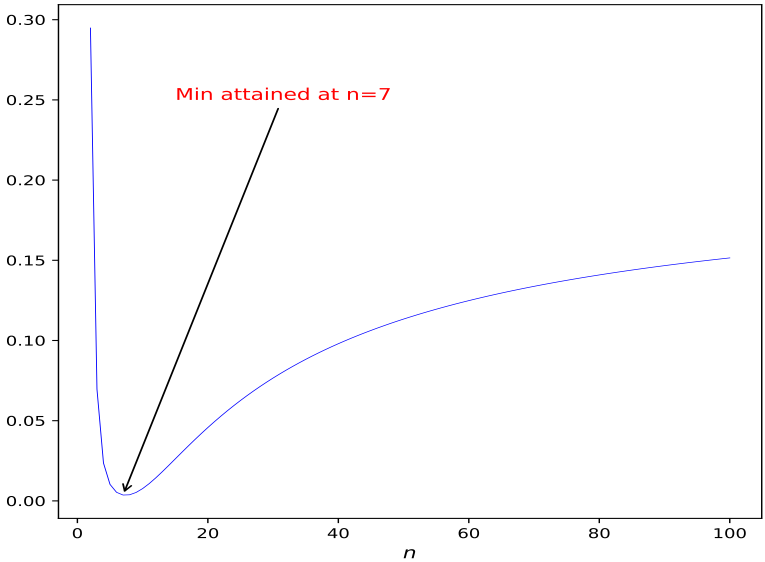

Figure 3.3: Graph of $\{2, 3, \ldots\} \ni n \mapsto \mathrm{E}_\pi(t_{A2}(n, q) - t_{A2}(n_{opt}^{A2}(q), q))^2$

(M1) Function $\mathbb{N} \times (0, UCP] \ni (N, p) \mapsto \theta_X(N, p)$ can be treated as a continuous function on $[c, \infty) \times (0, UCP]$ differentiable in the whole interior of its domain.

(M2) $\forall N \in (c, \infty)$ function $(0, UCP] \ni p \mapsto \theta_X(N, p)$ is strictly increasing.

(M3) $\forall N \in (c, \infty)\; t_X(N, UCP) > 1$.

(M4) $\forall N \in (c, \infty)\; \exists p \in (0, UCP) : t_X(N, p) < 1$.

Our results are given in two propositions stated below. The first one characterizes the properties of the OCP.

Proposition 3.2.1. *Assume (M0)–(M4). Let* $p_{X,c} = \sup\{p \in (0, UCP) \mid \exists N \in (c, \infty) : t_X(N, p) < 1\}$. *Then* $\forall p \in (0, p_{X,c})$ *procedure* X *makes sense on the continuous scale;* $\forall p \in (p_{X,c}, UCP]$ *it makes no sense at all, that is,*

$$(N, p) \in (c, \infty) \times (p_{X,c}, UCP] \Rightarrow t_X(N, p) > 1. \tag{3.11}$$

The second proposition demonstrates that under (M0)–(M4), there exists a generic procedure for finding $p_{X,c}$, and it can be naturally cast in terms of the Bifurcation Theory as follows. Treating $p \in (0, UCP]$ as a control parameter and $N \in (c, \infty)$ as a function of some latent continuous argument, consider an autonomous dynamical system

$$\dot{N} = t_X(N, p) - 1. \tag{3.12}$$

Proposition 3.2.2. *Assume (M0)–(M4). $p_{X,c}$ is a bifurcation point of the system (3.12) and one can distinguish between three types of possible bifurcations.*

> *(b0) $p_{X,c}$ is the only value of the control parameter for which (3.12) admits fixed points in (c, ∞). In this case $p_{X,c} < UCP$ and all $N \in (c, \infty)$ solve $t_X(N, p_{X,c}) = 1$.*

If there exists $p_l \in (0, p_{X,c})$ for which (3.12) admits a fixed point $N \in (c, \infty)$, there are two possibilities:

> *(b1) (3.12) has fixed points in (c, ∞) for all $p \in [p_l, p_{X,c})$ yet there are no fixed points corresponding to $p_{X,c}$;*
>
> *(b2) (3.12) has fixed points in (c, ∞) for all $p \in [p_l, p_{X,c}]$ including $p_{X,c}$ which then is necessary smaller than UCP.*

In all cases, bifurcation curve induces a differentiable map $(c, \infty) \ni N \mapsto p_N \in (0, p_{X,c}]$. Therefore, $p_{X,c}$ can be determined by finding its maximum. For bifurcations of types (b0) and (b2), this amounts to solving a system

$$\begin{cases} t_X(N, p) = 1, \\ \frac{\partial}{\partial N} t_X(N, p) = 0 \end{cases} \tag{3.13}$$

(with respect to both N and p) and then picking up a largest p value from the set $S = \{(N, p) \in (c, \infty) \times (0, UCP] \mid (N, p) \text{ solves } (3.12)\}$. For the bifurcation of type (b1), $p_{X,c} = \max(\lim_{N \to c+} p_N, \lim_{N \to \infty} p_N)$. In particular, this holds true when (3.13) has no solution lying in $(c, \infty) \times (0, UCP]$.

In this subsection, we do not comment on the restrictiveness of conditions (M0–M4) and postpone this to the dedicated Section of Chapter 4. However, before proceeding to examples, we provide several clarifying remarks.

Remark 3.2.3. Prop. 3.2.2 establishes the procedure for finding OCP on the continuous scale (COCP). In practice, one operates on the discrete one since the number of tested items N is integer. As a rule, discrete scale OCP (DOCP), so far in the Thesis denoted as p_c^X, is lower than $COCP = p_{X,c}$ of Prop. 3.2.1. However, the difference is usually small (see examples in Section 3.2.2) whereas the determination of DOCP is often times quite involved. Moreover, in the case of (b2), DOCP$= p_c^X$ can often be recovered as follows:

- take N_c s.t. $(N_c, p_{X,c})$ solves (3.13);
- set $DOCP = \max(p_{\lfloor N_c \rfloor}, p_{\lceil N_c \rceil})$.

In the case of (b1), DOCP is very likely to coincide with COCP. □

Remark 3.2.4. We have seen that, in some cases (like that of A2), cohort size $N = N(n)$ is a function of $n \in \mathbb{N}$ and it is more convenient to treat θ_X, t_X and other related functions as functions of (n, p) rather than functions of (N, p). Replacing N by n in (M0)–(M4) and then in all functions in Propositions 3.2.1–3.2.2 does not change conclusions of these Propositions provided $(c, \infty) \ni n \mapsto N(n)$ is differentiable and strictly increasing. □

Remark 3.2.5. We are inclined to think that bifurcations (b1)–(b2) are the prevalent ones since we are unaware of practical examples of (b0) satisfying our assumptions. Yet Subsection 3.2.2.5 contains an example showing that a counterpart of (b0) may occur on the discrete scale. We were unable to exclude this type theoretically. Thus, appealing to the mentioned example, we are inclined to think that (b0) is not a redundant case but an exceptional one, corresponding to optimal procedures (see the discussion in Chapter 4). □

3.2.2 Examples

In this section, we provide several examples demonstrating applications of Prop. 3.2.2. We also provide two examples of the procedures violating our conditions. Figures appearing in this subsection were produced by making use of Desmos Graphing Calculator [17].

3.2.2.1 Dorfman procedure D

Recall that

$$\theta_D(N,p) = 1 \cdot q^N + (N+1)(1-q^N) = N+1-Nq^N, \tag{3.14}$$
$$t_D(N,p) = \frac{\theta_D(N,p)}{N} = 1 + \frac{1}{N} - q^N.$$

We put $c = 2$ in (M0) and have it (testing one item does not require D procedure). (M1) obviously holds. Since $\frac{\partial}{\partial p} t_D(N,p) = Nq^{N-1} > 0$ for all $N \in (2,\infty)$, (M2) holds as well. As for (M3), note that

$$\frac{\mathrm{d}}{\mathrm{d}N} t_D(N, UCP) = \frac{\mathrm{d}}{\mathrm{d}N}\left(1 + \frac{1}{N} - \left(\frac{\sqrt{5}-1}{2}\right)^N\right) =$$
$$-\frac{1}{N^2} - \left(\frac{\sqrt{5}-1}{2}\right)^N \ln\left(\frac{\sqrt{5}-1}{2}\right).$$

Equating this to zero (and solving numerically) one finds out that this function has a unique minimum at $N_{\min} \approx 2.888$ and $\min\limits_{N>2} t_D(N, UCP) \approx t_D(2.888, UCP) = 1.097$. Moreover, it has a maximum at $N_{\max} \approx 5.75$ and then decreases to $\lim\limits_{N\to\infty} t_D(N, UCP) = 1$. Since $t_D(2, UCP) = \frac{\sqrt{5}}{2} > 1$, (M3) holds. Finally, from (3.14) it follows that

$$\forall N \in (2,\infty) \ \lim_{p\to 0+} t_D(N,p) = \frac{1}{N}.$$

Therefore, (M4) holds as well.

Figure 3.4 shows a plot of the inverted bifurcation map $N \mapsto p_N$ described in Prop. 3.2.2. In this case, it admits analytical expression: $p_N = 1 - \left(\frac{1}{N}\right)^{\frac{1}{N}}$. System (3.13) is given by

$$\begin{cases} \frac{1}{N} = q^N, \\ -\frac{1}{N^2} = q^N \ln q, \end{cases} \tag{3.15}$$

and can be solved analytically too. Its solution is $(N_*, p_{D,c}) = (\mathrm{e}, 1 - \mathrm{e}^{-\mathrm{e}^{-1}})$. Recall that Samuels' [66] analysis led to $DOCP = 1 - 3^{-3^{-1}}$. Our COCP is quite close. Moreover, we can recover DOCP by applying the method described in the Remark 3.2.3. In this particular case the method works and affirms Samuels' result.

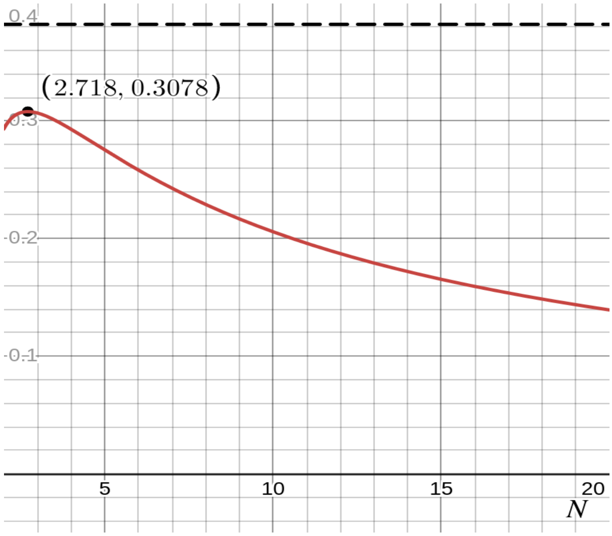

Figure 3.4: plot of $N \mapsto p_N$ (solid line) for the procedure D; dashed line shows constant line $p = UCP = \frac{3-\sqrt{5}}{2}$; maximal value yields $COCP = 1 - \mathrm{e}^{-\mathrm{e}^{-1}} \approx 0.3078$; value $p_{\lceil \mathrm{e} \rceil} = 1 - 3^{-3^{-1}}$ is equal to DOCP.

3.2.2.2 Square Array procedure A2

As we know, in the case of A2,

$$\theta_{A2}(N, p) = 2\sqrt{N} + N\left(1 - 2q^{\sqrt{N}} + q^{2\sqrt{N}-1}\right) \tag{3.16}$$

for $N(n) = n^2, n \in \mathbb{N}$. Therefore, for the sake of convenience and in view of Remark 3.2.4, we make a change of variables and treat both t_{A2} and θ_{A2} as functions of (n, p). We carry this convention to all related functions as well. This yields

$$t_{A2}(n, p) = \frac{2}{n} + 1 - 2q^n + q^{2n-1} = \frac{2}{n} + (1 - q^n)^2 + pq^{2n-1}. \tag{3.17}$$

From the latter expression, it follows that A2 makes sense only for $n > 2$. Bearing in mind the practical aspect (i.e., the fact that cohort sizes are integers) we therefore set $c = 3$ in[4] (M0). Note that, due to the design of the procedure, this truncation actually restricts sizes of the tested cohorts to start from $9 = 3 \times 3$ (not 3). It is obvious that (M1) holds.

[4] relying on results of Subsection 3.1.1, we could even set $c = 5$

Since $\forall p \in (0, UCP]$

$$\frac{\partial}{\partial p}\theta_{A2}(n,p) = n^2\left(2nq^{n-1} - (2n-1)q^{2n-2}\right) = \\ n^2\left(q^{2n-2} + 2nq^{n-1}(1-q^{n-1})\right) > 0,$$

(M2) holds as well.

Justification of (M3) can be done by accomplishing the following steps:

- check that $\frac{\partial}{\partial n}t_{A2}(n,p) = -\frac{2}{n^2} - 2q^n \ln q(1-q^{n-1})$ and $\frac{\partial^2}{\partial n^2}t_{A2}(n,p) = \frac{4}{n^3} - 2q^n \ln^2 q(1-2q^{n-1})$;
- numerically solve $\left.\frac{\partial^2}{\partial n^2}t_{A2}(n,p)\right|_{p=UCP} = 0$ and obtain two roots: $n_1 \approx 5.278, n_2 \approx 9.448$;
- verify that n_1 corresponds to the maximum whereas n_2 corresponds to the minimum of $n \mapsto \frac{\partial}{\partial n}t_{A2}(n, UCP)$ and that

  $$\frac{\partial}{\partial n}t_{A2}(n_1, UCP) < -0.0055 < 0;$$

- conclude that $n \mapsto t_{A2}(n, UCP)$ is decreasing and (M3) holds since

  $$\lim_{n\to\infty} t_{A2}(n, UCP) = 1.$$

Finally, from the last expression given in (3.17), it follows that

$$t_{A2}(n,p) \xrightarrow[p\to 0+]{} \frac{2}{n} \leq \frac{2}{3}.$$

Hence (M4).

Figure 3.5 shows the inverted bifurcation curve $(3,\infty) \ni n \mapsto p_n$ of Prop. 3.2.2. System (3.13) is given by

$$\begin{cases} \frac{2}{n} - 2q^n + q^{2n-1} = 0, \\ -\frac{1}{n^2} - q^n(1-q^{n-1})\ln q = 0. \end{cases}$$

As can be seen from the curve, it has a unique solution $(n_*, p_{A2,c}) \approx (4.454, 0.252)$. Recall that Kim and Hudgens [38] analysis on the discrete scale yielded $DOCP = 0.2498$. This point precisely coincides with $p_{\lceil n_* \rceil}$. Thus, the method described in 3.2.3 again led to the recovery of the DOCP.

Figure 3.5: plot of $n \mapsto p_n$ (solid line) for the procedure A2; dashed line shows constant line $p = UCP = \frac{3-\sqrt{5}}{2}$; maximal value yields $COCP \approx 0.2516$; $p_5 \approx 0.2498$ is equal to DOCP.

3.2.2.3 Modified Dorfman procedure MD

For MD,

$$t_{MD}(N,p) = 1 - q^N + \frac{1 - pq^{N-1}}{N}. \tag{3.18}$$

We set $c = 2$ and (M0) is satisfied (again, as in the case of procedure D, testing one item does not require procedure MD). As usually, (M1) is obvious. Since

$$\frac{\partial}{\partial p} t_{MD}(N,p) = Nq^{N-1} - \frac{1}{N}\left(q^{N-1} - (N-1)pq^{N-2}\right) = q^{N-1}\left(N - \frac{1}{N}\right) + \frac{N-1}{N}pq^{N-2} > 0$$

for any fixed $N \in (2,\infty)$, (M2) holds. $\forall N \in (2,\infty)$ $\lim\limits_{p \to 0+} t_{MD}(N,p) = \frac{1}{N} < 1$. Hence (M4). Finally, verification of (M3) can be done in the same way as in the case of procedure A2. Since an exercise is quite lengthy and tedious, we omit the details as well as check that system (3.13) does not admit solution lying in $(2,\infty) \times (0, UCP]$. The latter means that we have a bifurcation of type (b1). Since $t_{MD}(2, UCP) = 1$, we conclude that

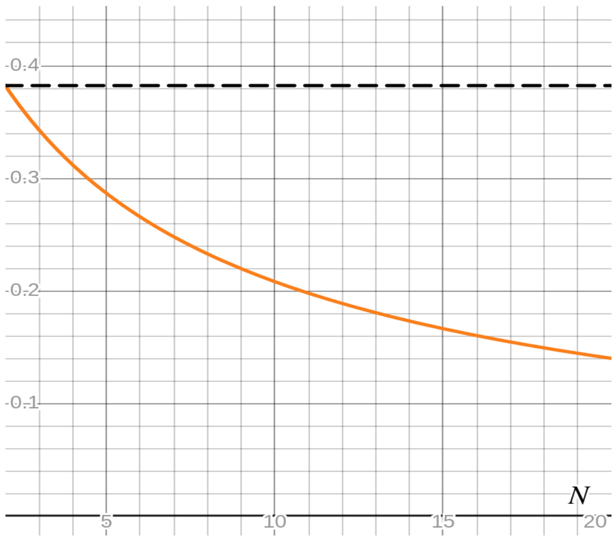

Figure 3.6: plot of $N \mapsto p_N$ (solid line) for the procedure MD; dashed line shows constant line $p = UCP = \frac{3-\sqrt{5}}{2}$.

$p_{MD,c} = \lim\limits_{N \to 2+} p_N = UCP$. Figure 3.6 provides graphical illustration of the said.

As noted in the Remark 3.2.5, this time $COCP = DOCP = UCP$.

3.2.2.4 Sterrett procedure ST

As we know, for procedure ST,

$$t_{ST}(N,p) = 2 - q + \frac{2q - (1-q)^{-1}(1-q^{N+1})}{N}. \tag{3.19}$$

Setting $c = 2$ in (M0), one has that (M0)–(M1) readily hold. A way to verify (M2) lies in showing that $(1-UCP, 1) \ni q \mapsto t_{ST}(N,p)$ is decreasing. Since

$$\frac{\partial}{\partial q} t_{ST}(N,p) = \left(\frac{2}{N} - 1\right) - \frac{1}{N}\left(\frac{1-q^{N+1}}{1-q}\right)'_q,$$

one sees that the term $2/N - 1 < 0$ for any $N > 2$ and it suffices to note that

$$\left(\frac{1-q^{N+1}}{1-q}\right)'_q = \left(1 + q + \cdots + q^N\right)'_q > 0.$$

(M4) follows by noting that, for any fixed $N > 2$,

$$\lim_{p\to 0+} t_{ST}(N,p) = \lim_{q\to 1-} t_{ST}(N,p) = 1 + \frac{2 - \lim_{q\to 1-} \frac{\left(1-q^{N+1}\right)'_q}{(1-q)'_q}}{N} = 1 + \frac{2 - \frac{N+1}{1}}{N} = \frac{1}{N} < 1.$$

As in the previous example, we omit verification of (M3). It amounts to a careful analysis of the derivative of $(2,\infty) \ni N \mapsto t_{ST}(N, UCP)$. One can also show that the system (3.13) does not admit solutions (N,p) lying in $(2,\infty) \times (0, UCP]$. Since UCP solves $t_{ST}(2,p) = 1$ (w.r.t. p), we again have that $p_{ST,c} = \lim_{N\to 2+} p_N = UCP$ as in the previous example. Figure 3.7 demonstrates that the bifurcation curve qualitatively exhibits the same behavior too. Again, note that $COCP = DOCP = UCP$.

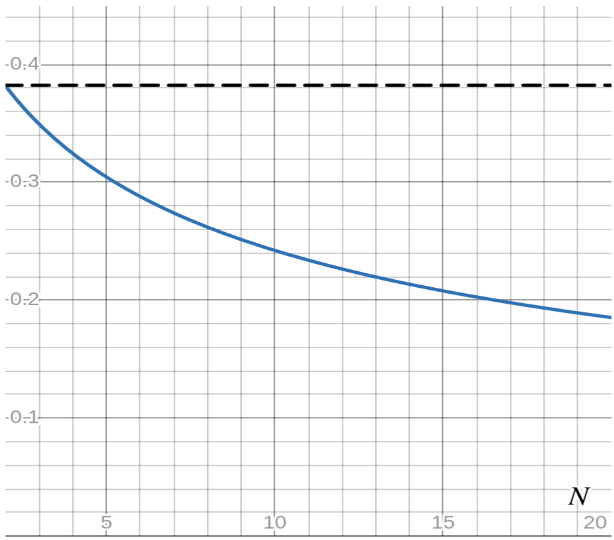

Figure 3.7: plot of $N \mapsto p_N$ (solid line) for the procedure ST; dashed line shows constant line $p = UCP = \frac{3-\sqrt{5}}{2}$.

3.2.2.5 Examples violating our assumptions

The first example is the PT procedure. Since

$$\theta_{PT}(N,p) = N\frac{2-q^2}{1+q} + \frac{q^2+q-1}{(1+q)^2}(1-(-q)^N),$$

it is clear that one can not extend θ_{PT} to the continuously differentiable function w.r.t. N. Hence, (M1) does not hold. (M3) does not hold as well. Indeed, UCP solves $q^2 + q - 1 = 0$; also $\frac{2-q^2}{1+q}\Big|_{p=UCP} = 1$ and

$$\frac{2-q^2}{1+q} < 1 \iff 0 < q^2 + q - 1 \iff p \in (0, UCP). \tag{3.20}$$

Another example of this kind is the procedure H. Recall that here the cohort size $N(n) = 2^n, n \in \mathbb{N}$, and

$$\theta_H(N,p) = 1 + 2^{n+1} \sum_{k=1}^{n} \frac{1-q^{2^k}}{2^k}.$$

Thus, it again violates (M1).

3.3 Probabilistic analysis of the Pairwise testing procedure

In [85], it was proved that, for $p \in \left[1 - \frac{1}{\sqrt{2}}, UCP\right]$, the PT procedure is optimal in the class of nested procedures. That is, for any nested procedure X and for any $N \in \mathbb{N}$, $\theta_{PT}(N,p) \le \theta_X(N,p)$ uniformly over $p \in \left[1 - \frac{1}{\sqrt{2}}, UCP\right]$. Despite this fundamental property, the PT procedure did not receive considerable attention in the literature. After getting familiar with the PT and retrieving citing literature, we have discovered that out of fifteen citing references [1–3, 12, 22, 29, 30, 43, 48, 53, 55, 56, 76, 83, 84] retrieved by us[5] from Google Scholar, Malinovsky [53] was the only who investigated a problem having a direct relationship to the PT procedure. All other researchers touched the paper of Yao and Hwang [85] merely as a reference having a connection to GT with a mild relation to their own problem. These circumstances motivated us to give a broader probabilistic characterization of the PT procedure [91]. We succeeded in deriving an exact analytical expression of the moment-generating function (MGF) for the number of tests performed by the PT procedure. With the help of the MGF, it was possible to obtain common limiting theorems: strong law of large numbers (SLLN), central limit theorem (CLT), and large deviations principle (LDP). To state formal results, we need several notions.

For short, let $\Theta_N \equiv T_{PT}$ denote the number of conducted tests required for an identification of all defectives in a given binomial set

[5] the list was generated on 28th of June, 2022; non-English references were excluded

having N items, and let $Y_i, i = 1, \dots, N$, be an indicator of an ith item status (1 stands for the defective one). Then $Y_i \sim Be(p)$. Also, let $\bar{Y}_i := 1 - Y_i$ and

$$M_0 = \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}, \quad M_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{3.21}$$

Our first result gives an explicit expression for Θ_N in terms of the above quantities.

Proposition 3.3.1. *Let* $A = \left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix} \right\}$ *and* $B_k = \begin{pmatrix} Y_k & \bar{Y}_k \\ 1 & 0 \end{pmatrix}$ *for* $k = 1, \dots, N$*. Then* $\Theta_2 = 3Y_2 + \bar{Y}_2(1 + Y_1), \quad \Theta_3 = 2 + \bar{Y}_3 Y_2 + Y_3 \Theta_2$*, and*

$$\begin{aligned} \Theta_N &= 1 + Y_N(\bar{Y}_{N-1} Y_{N-2} + 2) + Y_{N-1} + \\ &\sum_{j=3}^{N-1} (\bar{Y}_{j-1} Y_{j-2} + Y_{j-1} + 1) \left(Y_j + \bar{Y}_{j-1} \mathbb{1}\left\{B_N B_{N-1} \cdots B_{j+1} \in A\right\}\right) + \\ &\qquad Y_2 + \bar{Y}_2 \mathbb{1}\left\{B_N B_{N-1} \cdots B_3 \in A\right\} \text{ for } N \geqslant 4. \end{aligned} \tag{3.22}$$

The expression above provides insight into the structure of Θ_N. Our next result provides the announced explicit formula of the MGF.

Theorem 3.3.2. *Let* $M_{\Theta_N}(\lambda)$ *denote the moment generating function of* Θ_N *at* $\lambda \in \mathbb{R}$*. Set*

$$\alpha_i = \alpha_i(\lambda) = \frac{1}{2}\left(p\mathrm{e}^{2\lambda} + (-1)^i \sqrt{p^2 \mathrm{e}^{4\lambda} + 4q\mathrm{e}^{\lambda}(q + p\mathrm{e}^{\lambda})}\right), \; i = 0, 1; \tag{3.23}$$

$$\kappa_N = \kappa_N(\lambda) = \frac{\alpha_0^N - \alpha_1^N}{\alpha_0 - \alpha_1} \text{ for } N \geqslant 0. \tag{3.24}$$

Then $M_{\Theta_N}(\lambda) =$

$$\begin{aligned} \mathrm{e}^{2\lambda}\Big[&\left((1-q)^2 \mathrm{e}^{3\lambda} + q(1-q)^2 \mathrm{e}^{2\lambda} + q(1-q^2)\mathrm{e}^{\lambda} + q^2\right) \kappa_{N-2} + \\ q &\left((1-q)^2 \mathrm{e}^{3\lambda} + q(1-q)(2-q)\mathrm{e}^{2\lambda} + 2q^2(1-q)\mathrm{e}^{\lambda} + q^3\right) \kappa_{N-3}\Big] \end{aligned} \tag{3.25}$$

for $N \geqslant 3$.

The remaining results are the consequences of the previous one.

Corollary 3.3.3. $\mathrm{E}\,\Theta_N = N\frac{2-q^2}{1+q} + \frac{q^2+q-1}{(1+q)^2}(1-(-q)^N)$,

$$\operatorname{Var}\Theta_N = N\frac{(1-q)}{(q+1)^3}\Big(q\left(q^3+3q^2+5q+4\right)+ (-q)^N(2q+4)\left(q^2+q-1\right)\Big)+ \frac{\left(1-(-q)^N\right)}{(q+1)^4}\left(q\left(5q^2+3q-7\right)+(-q)^N\left(q^2+q-1\right)^2\right), N \geqslant 3. \tag{3.26}$$

Corollary 3.3.4. *The following asymptotic results apply to Θ_N as $N\to\infty$.*

LLN: $\frac{\Theta_N}{N} \xrightarrow{L_2} \frac{2-q^2}{1+q}$ *and* $\frac{\Theta_N}{N} \xrightarrow{a.s.} \frac{2-q^2}{1+q}$.

CLT: $\sqrt{N}\left(\frac{\Theta_N}{N}-\frac{2-q^2}{1+q}\right) \xrightarrow{d} N(0,\sigma^2)$, $\sigma^2 = \frac{q(1-q)\left(q^3+3q^2+5q+4\right)}{(q+1)^3}$.

LDP: $\frac{\Theta_N}{N}$ *satisfies the Large Deviation Principle with a good rate function I equal to the Legendre transform of $\mathbb{R}\ni\lambda\mapsto\ln\alpha_0(\lambda)$ with $\alpha_0(\lambda)$ given by (3.23). That is, for any closed $C\subset\mathbb{R}$ and any open $O\subset\mathbb{R}$,*

$$\limsup_{N\to\infty}\frac{1}{N}\ln\mathrm{P}\left(\frac{\Theta_N}{N}\in C\right)\le-\inf_{x\in C}I(x)$$

and

$$-\inf_{x\in O}I(x)\le\liminf_{N\to\infty}\frac{1}{N}\ln\mathrm{P}\left(\frac{\Theta_N}{N}\in O\right),$$

where $I(x)=\sup_{\lambda\in\mathbb{R}}\left(x\lambda-\ln\alpha_0(\lambda)\right)$.

Chapter 4

Discussion and conclusions

In this chapter, we have collected several remarks about the results stated in Chapter 3. In our opinion, these remarks fall out of the scope of the related literature review yet are worth mentioning. For each section of Chapter 3, we devote a separate section. The last section is devoted to several concluding observations of a general nature.

4.1 About results of Section 3.1

It is always possible to obtain numerical solutions of optimal configurations. However, examples given in Subsection 3.1.2 clearly demonstrate that analytic expressions are very useful. Moreover, in an asymptotic regime, numerical solutions are of minimal applicability because of computational errors, and the absence of analytic expressions prevents the asymptotic analysis.

To get a quick example, consider the asymptotic regime when $p \to 0+$. From results of Section 3.1

$$t_{MD}(N^{MD}_{opt}(p), p) = \frac{2 + o(1)}{N^{MD}_{opt}(p)} \text{ and } t_{ST}(N^{ST}_{opt}(p), p) = \frac{2 + o(1)}{N^{ST}_{opt}(p)}.$$

Therefore, taking into account Theorems 3.1.1–3.1.2,

$$\lim_{p \to 0+} \frac{t_{MD}(N^{MD}_{opt}(p), p)}{t_{ST}(N^{ST}_{opt}(p), p)} = \lim_{p \to 0+} \frac{N^{ST}_{opt}(p)}{N^{MD}_{opt}(p)} = \sqrt{2}. \tag{4.1}$$

Hence, for small p's, testing optimally by using the procedure MD results in an average number of tests per object, which is approximately 1.4

times larger than the average number of tests per object obtained by applying procedure ST at its optimal configuration. Analyses of a similar kind appear in the literature. E.g., in [57], the limit (4.1) appears with MD replaced by D and is the same. This means that asymptotically the original and the modified Dorfman procedures are identical. However, their behavior differs for p's far from the origin (see [55]).

4.2 About results of Section 3.2

In this Section, we discuss conditions (M0)–(M4) of Section 3.2 with a focus on their meaning and restrictiveness.

(M0) may be viewed as a condition required to confine the range of the dynamical system we make use of when looking for the $COCP = p_{X,c}$. Together with (M3), it also defines the boundary value for the determination of $p_{X,c}$ for the case $p_{X,c} = UCP$. In a usual case, one can set $c = 2$ and have it since, in this context, $c = 2$ means that taking one item, we do not need any GT procedure: to identify the defectiveness of a single item, one always needs one test[1].

Constraint (M1) is the most restrictive since not all binomial GT procedures can be naturally extended to have a differentiable mean with respect to both arguments (though in the case of p this always holds true). Nonetheless, this particular assumption is the one we heavily rely on. It also enables us to draw the connection with the bifurcation theory.

Other constraints can be justified naturally and attributed to many binomial GT procedures in general.

(M2) states that an average number of tests per batch spanning N items should increase together with the rate of defectiveness. For justification, we mention another fundamental result due to Yao and Hwang [86] who have demonstrated that $\forall N \in \mathbb{N}$, function $(0, UCP] \ni p \mapsto \inf_X \theta_X(N,p)$, with an infimum being taken over all possible BGT procedures, is strictly increasing.

At first glance, it may seem that (M3) rules out procedures having $p_{X,c} = UCP$. As demonstrated by example, this is not the case. In fact, it restricts the subset of GT procedures to those having $p_{X,c}$ on the boundary of the domain of the bifurcation curve. We are inclined to

[1] see examples in Subsection 3.2.2

think that this way, we rule out optimal procedures, i.e., those which are best performing in certain classes. However, we do not treat this as a drawback since, for optimal procedures, one generally expects $p_{X,c} = UCP$.

Finally, (M4) in technical terms states that we focus on the procedures applicable to any number of tested items, at least for some p's in the range of their sensibility. This is very often the case since many procedures are suitable for large-scale testing when the rate of defectiveness is small.

In case (M0)–(M4) hold, our algorithm appears to be efficient. There is a word of caution: one has to choose c in (M0) carefully. The point is that the dynamical system defined by (3.12), when viewed on a wider domain, may exhibit more complicated bifurcations. Figure 4.1 provides a convincing graphical illustration.

Turning to the types of bifurcations, one sees that, in terms suggested by Strogatz [74], (b1) is usually the saddle point bifurcation, whereas for (b2) the system admits fixed points for all but boundary value of the control parameter $p \in (0, UCP]$. We are inclined to think that the dynamical system approach we took could be extended to GT procedures violating (M1) and successfully used to investigate other general properties of GT procedures, yet one needs to work on the discrete scale.

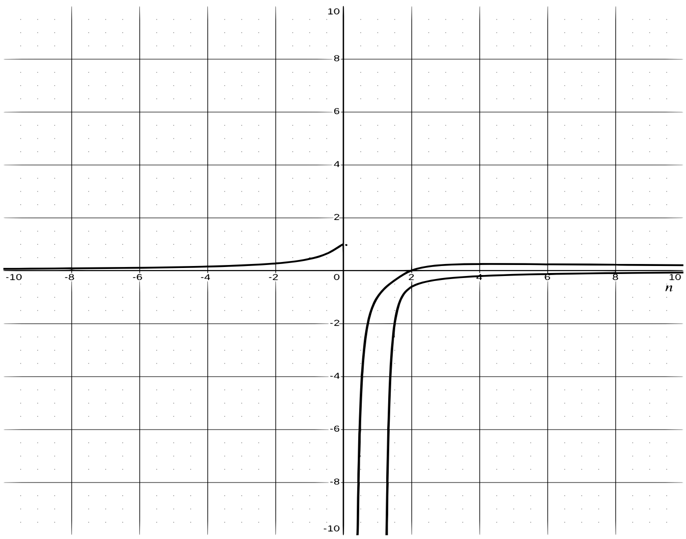

Figure 4.1: plot of bifurcation curve for procedure A2 when the domain of the dynamical system (3.12) is extended to the whole real line.

We end by noting that relationships (3.20) uncover an interesting fact:

$$\forall N \in (2, \infty)\, t_{PT}(N, UCP) = 1,$$

which means that the PT procedure is "almost" of type (b0). Yao and Hwang [85] proved that the PT is an optimal nested testing procedure if and only if $p \in \left[1 - \frac{\sqrt{2}}{2}, \frac{3-\sqrt{5}}{2}\right]$. This suggests that procedures of type (b0) are likely to be those which are optimal in some region.

4.3 About results of Section 3.3

We did not provide any specific examples of applications of results stated in Section 3.3 beyond moment calculations presented in Corollary 3.3.3. Despite that, one can list several reasons supporting the relevance of our analysis.

- Though the definition of an optimal procedure is usually tied to an average number of tests, when choosing between several procedures, it is desirable to evaluate their performance by taking into account multiple aspects. For example, procedure *Pr1* may perform slightly better than *Pr2* regarding an average number of tests. However, *Pr1* may have a considerably larger variance than *Pr2* and, therefore, the previously mentioned slight gain of *Pr1* could be gladly traded by the practitioner in favor of *Pr2*.
- We have already mentioned that the importance of the PT remained unrecognized in the literature, and there is more to say on that.
  - Many GT procedures described in the literature have limited applicability in certain areas due to the *dilution effect* described in 1.3. Recall that basically this means the following. Given procedure X and fixed p, $N^X_{opt}(p)$ may be too large and inflate the operating characteristics (sensitivity and/or specificity) of the test kit at hand making them unacceptably low (aka diluting) for that particular application[2]. With respect to this property, the PT procedure is a very favorable option: it requires only pools of size $N = 2$, and this holds true for all p's in the region of its optimality $\left[\frac{2-\sqrt{2}}{2}, \frac{3-\sqrt{5}}{2}\right]$.

[2]in theory, (BTA3) stated in Section 2.1 prevents from this; however, in practice, it may be a serious obstacle

– The region $\left[\frac{2-\sqrt{2}}{2}, \frac{3-\sqrt{5}}{2}\right]$ where the PT procedure performs optimally is bounded away from zero in contrast to many other GT procedures which do better for p's close to zero. In certain applications, this property may be of significant importance. For example, when screening for a quite widespread infectious disease.

- In [85] it was conjectured that there exists such $p_0 \in \left[\frac{2-\sqrt{2}}{2}, \frac{3-\sqrt{5}}{2}\right]$ that for $p \in \left[p_0, \frac{3-\sqrt{5}}{2}\right]$ the PT procedure is optimal over all (not necessarily nested) procedures satisfying the BTA.

- Our Proposition 3.3.1 demonstrates that, despite apparently simple recurrence governing the evolution of Θ_N (see Eq. (5.22)), the resulting dependence structure is not so simple. At least we were not able to analyze its behavior neither by making use of Markov chains theory, nor by making use of martingale theory. A well-developed apparatus of weakly dependent sequences also did not promise easy deduction of Corollary 3.3.4. More than that, even direct moment calculation exercise, though accomplishable for $\mathrm{E}\,\Theta_N$ at a reasonable price (see Lemma in Section 4 of [85]), becomes much more involved when it comes to $\mathrm{Var}\,\Theta_N$ and higher order moments. This way, $(\Theta_N)_{N\geqslant 2}$ yields an example of a sequence of positive integer-valued random variables having an interesting probabilistic structure encountered in practical application and not designed artificially for learning or other purposes.

Finally, we believe that our results may be useful for the solution of several unresolved conjectures. Namely, the one stated in [85] and mentioned above, and the generalized PT optimality conjecture stated in [53].

4.4 Several concluding remarks

In the Thesis, we have focused on the PGT procedures satisfying the BTA. Such a framework may seem too simplified for the real setting. However, this is not generally true. For some applications (say, in quality control or computer science), these assumptions are justifiable. Moreover, though developed quite long ago, simple procedures like D, MD, and ST are not outdated and still in use even in large scale projects. E.g., the American Red Cross makes use of Dorfman procedure for the screening of blood donations for HIV and hepatitis [18] whereas, in Lithuania, Dorfman procedure was not long ago applied to test for COVID-19 employees of larger firms and pupils attending public schools [7]. There are several reasons explaining why the BTA-based procedures are still in use.

Convenience. Even though since the original work of Dorfman many procedures tied to particular needs of applications considered were developed, the organizational flow of the whole project may not afford to apply more elaborated procedures. In such cases, simple procedures appear to be a good alternative, resulting in cost savings.

Specifics of application. It appears that one of the reasons for the emergence of A2 in genetic applications was testing equipment: it was such that A2 was very handy option.

Tolerable errors. Though there exist a lot of generalizations allowing imperfectness of the test (e.g., [46], [45], [33], [8], [10]), as noted by several authors [9], [38], [55], procedures assuming perfect tests can be quite accurate since modern tests exhibit very small errors.

Investigations of the BTA-based PGT procedures remain essential due to other reasons as well.

For example, binomial testing procedures may serve as a basement for more elaborated ones: procedures MD and ST were built on the top of D; in [46] and [33], A2 serves as a basis for extensions incorporating imperfectness of the test and dilution effect; in [8] extensions addressing subject-specific risk characteristics and imperfect tests are proposed for the D procedure whereas in [10] the authors do the same focusing only on the heterogeneity of the population.

For another example of the usefulness of the BTA-based procedures, consider benchmarking. The BTA-based procedures, being more simple to treat analytically, provide theoretically justified benchmark thresholds for more elaborated procedures that assume the imperfectness of the test and/or other specific conditions.

In view of the said, our findings seem to be useful input to the existing GT knowledge base.

Chapter 5

Proofs

5.1 Proofs of results stated in Section 3.1

Before proceeding to the proofs, we give several remarks. In [55] it was demonstrated that, for a fixed $p \in (0, \frac{3-\sqrt{5}}{2})$, function $[1, \infty) \ni N \mapsto t_{ST}(N,p)$ admits a unique absolute minimum which is attained at the unique zero of $[1, \infty) \ni N \mapsto \frac{\partial}{\partial N} t_{ST}(N,p)$, say $N_*^{ST}(p)$. Therefore, $N_{opt}^{ST}(p) \in \{\lfloor N_*^{ST}(p) \rfloor, \lfloor N_*^{ST}(p) \rfloor + 1\}$, and the choice between two possible values is made by evaluating whether $t_{ST}(\lfloor N_*^{ST}(p) \rfloor, p) > t_{ST}(\lfloor N_*^{ST}(p) \rfloor + 1, p)$ or $t_{ST}(\lfloor N_*^{ST}(p) \rfloor, p) \leq t_{ST}(\lfloor N_*^{ST}(p) \rfloor + 1, p)$ holds true. For the case of the procedure MD, Pfeifer and Enis [62] have obtained a quite similar result stated below.

Theorem 5.1.1. *[Pfeifer and Enis [62], Lemma 2] For a fixed $p \in \left(0, \frac{3-\sqrt{5}}{2}\right)$, function $[1, \infty) \ni N \mapsto t_{MD}(N,p)$ admits a unique absolute minimum attained at the smallest zero of $[1, \infty) \ni N \mapsto \frac{\partial}{\partial N} t_{MD}(N,p)$, say $N_*^{MD}(p)$. In the set*

$$A^{MD} = \left\{ (p, N) \in \left(0, \frac{3-\sqrt{5}}{2}\right) \times [1, \infty) : t_{MD}(N,p) < 1 \right\},$$

$N_*^{MD}(p)$ is the only zero of $N \mapsto \frac{\partial}{\partial N} t_{MD}(N,p)$.

From (2.1) and (2.2) it follows that

$$t_D(N,p) = 1 - q^N + \frac{1}{N} \text{ and } t_{MD}(N,p) = t_D(N,p) - \frac{pq^{N-1}}{N}.$$

Therefore, $t_D(N,p) - t_{MD}(N,p) = \frac{pq^{N-1}}{N} > 0$. Hence, appealing to the result of Samuels [66] mentioned in Section 3.1, we thus conclude that looking for $N_{opt}^{MD}(p)$ corresponding to $p \in (0, 1-(1/3)^{1/3})$, one can apply the same algorithm as for $N_{opt}^{ST}(p)$ above: it is enough to find the unique $N_*^{MD}(p)$ and then select $N_{opt}^{MD}(p) \in \{\lfloor N_*^{MD}(p) \rfloor, \lfloor N_*^{MD}(p) \rfloor + 1\}$. In the region $\left[1-(1/3)^{1/3}, \frac{3-\sqrt{5}}{2}\right)$ additional care is needed.

Proof of Theorem 3.1.1. Consider equation $\frac{\partial}{\partial N} t_{ST}(N,p) = 0$. Simple rearrangement shows that it is equivalent to equality

$$\frac{1}{\ln q} - \frac{1-2pq}{\ln q}\left(\frac{1}{q}\right)^{N+1} = N. \tag{5.1}$$

Denote the lhs by $h(N)$. Then (5.1) means that $N_*^{ST}(p)$ is a fixed point of $h : [0, \infty) \to \mathbb{R}$. Since h is translated and scaled increasing exponential function with $h(0) < 0$, that fixed point is unique in agreement with the results discussed above. Moreover, in view of these results, it suffices to demonstrate that $N_*^{ST}(p) \in \left[\sqrt{2p^{-1}} - 1, \sqrt{2p^{-1}} + 1\right]$ in order to deduce that $N_{opt}^{ST}(p) \in \left\{\lfloor \sqrt{2p^{-1}} \rfloor + i : i \in \{-1, 0, 1, 2\}\right\}$. Taking into account the exponential form of h, the latter will follow provided we show that

$$h\left(\sqrt{\frac{2}{p}} + 1\right) > \sqrt{\frac{2}{p}} + 1 \quad \text{and} \quad h\left(\sqrt{\frac{2}{p}} - 1\right) < \sqrt{\frac{2}{p}} - 1. \tag{5.2}$$

For each $m \in \{-1, 0, 1\}$, define a function $\left(0, \frac{3-\sqrt{5}}{2}\right) \ni p \mapsto g_m(p)$ by

$$g_m(p) = \frac{1}{q}\left(\frac{1-2pq}{q^{1+m}\left(1 - \ln q \sqrt{\frac{2}{p}}\left(1 + m\sqrt{\frac{p}{2}}\right)\right)}\right)^{\sqrt{\frac{p}{2}}}. \tag{5.3}$$

By simple rearrangement, it follows that (5.2) is equivalent to

$$g_1(p) > 1 \quad \text{and} \quad g_{-1}(p) < 1. \tag{5.4}$$

Figure 5.1 shows the graphs of g_1, g_0, and g_{-1}. These suggest that relationships (5.4) do hold outside the zero neighborhood though, due to resolution issues, the true behavior close to the origin may be masked.

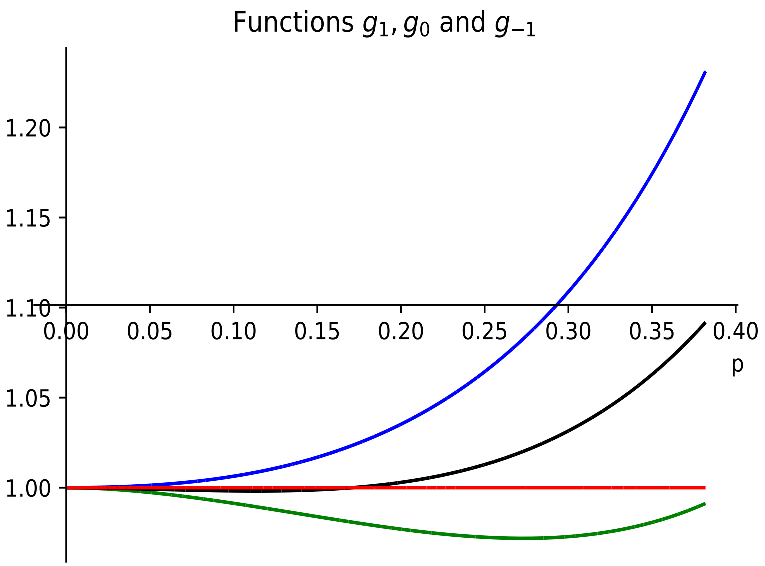

Figure 5.1: Functions g_m on $\left(0, \frac{3-\sqrt{5}}{2}\right)$: g_1 plotted in blue, g_0 plotted in black, and g_{-1} plotted in green.

To see that here $g_1(p) > 1$ and $g_{-1}(p) < 1$, consider expansion

$$\ln g_m(p) =$$
$$\sqrt{\frac{p}{2}}\left(\ln(1-2pq) - (1+m)\ln q - \ln\left(1 - \ln q\left(m + \sqrt{\frac{2}{p}}\right)\right)\right)$$
$$- \ln q = \sqrt{\frac{p}{2}}\left(p(1+m-2q) + p^2\left(\frac{1+m}{2} - 2q^2\right) + O(p^3)\right) +$$
$$m\sqrt{\frac{p}{2}}\ln q + \sqrt{\frac{1}{2p}}(\ln q)^2\left(1 + m\sqrt{\frac{p}{2}}\right)^2 + \frac{2}{3}\frac{(\ln q)^3}{p}\left(1 + m\sqrt{\frac{p}{2}}\right)^3 +$$
$$\frac{1}{\sqrt{2}}\frac{(\ln q)^4}{p^{3/2}}\left(1 + m\sqrt{\frac{p}{2}}\right)^4 + O\left(p^3\right). \quad (5.5)$$

Plugging in $m = \pm 1$ yields

$$\ln g_{-1}(p) = \sqrt{\frac{p}{2}}\left(-2pq(1+pq+O(p^2)\right) - \sqrt{\frac{p}{2}}\ln q\left(1-\frac{\ln q}{p}\right) - (\ln q)^2 + \frac{\sqrt{p}(\ln q)^2}{2\sqrt{2}} + \frac{2}{3}\frac{(\ln q)^3}{p}\left(1-\sqrt{\frac{p}{2}}\right)^3 + \frac{(\ln q)^4}{\sqrt{2}p^{\frac{3}{2}}}\left(1-\sqrt{\frac{p}{2}}\right)^4 + O\left(p^3\right) = -\sqrt{\frac{p}{2}}\left(2p+\ln q\left(2+O(p)\right)\right) - (\ln q)^2\left(1-\frac{2}{3}\frac{\ln q}{p}\left(1-\sqrt{\frac{p}{2}}\right)^3\right) + O\left(p^{\frac{5}{2}}\right) = -\frac{5}{3}p^2 + O\left(p^{\frac{5}{2}}\right).$$

and

$$\ln g_{1}(p) = \sqrt{\frac{p}{2}}\left(3p^2-2(pq)^2+O(p^3)\right) + \sqrt{\frac{p}{2}}\ln q\left(1+\frac{\ln q}{p}\right) + (\ln q)^2 + \frac{\sqrt{p}(\ln q)^2}{2\sqrt{2}} + \frac{2}{3}\frac{(\ln q)^3}{p}\left(1+\sqrt{\frac{p}{2}}\right)^3 + \frac{(\ln q)^4}{\sqrt{2}p^{\frac{3}{2}}}\left(1+\sqrt{\frac{p}{2}}\right)^4 + O\left(p^3\right) = (\ln q)^2\left(1+\frac{2}{3}\frac{\ln q}{p}\left(1+\sqrt{\frac{p}{2}}\right)^3\right) = \frac{1}{3}p^2 + O\left(p^{\frac{5}{2}}\right).$$

Hence, $g_1(0+0) = g_{-1}(0+0) = 1$ and $g_1(p) > 1, g_{-1}(p) < 1$ for all $p \in (0,\delta)$ provided $\delta > 0$ is small enough. One can further show that g_1' is positive on $(0, \frac{3-\sqrt{5}}{2})$, whereas, in case of g_{-1}', the following hold true: it has a unique zero $x_0 \in (0, \frac{3-\sqrt{5}}{2})$; it is negative on $(0, x_0)$ and positive on $(x_0, \frac{3-\sqrt{5}}{2})$; finally, $\lim_{x\to\frac{3-\sqrt{5}}{2}-} g_{-1}(x) \approx 0.9912$. Calculations being lengthy and tedious nonetheless require only standard calculus and we, therefore, omit the details. Putting all together, relationships (5.4) do hold. Taking into account all the said and then by the similar argument as above, it follows that

$$N_*^{ST}(p) \in \left[\sqrt{2p^{-1}}-1, \sqrt{2p^{-1}}\right] \iff g_0(p) \geq 1$$

and

$$N_*^{ST}(p) \in \left[\sqrt{2p^{-1}}, \sqrt{2p^{-1}}+1\right] \iff g_0(p) \leq 1.$$

Also, since $\left(0, \frac{3-\sqrt{5}}{2}\right) \ni p \mapsto N_*^{ST}(p)$ is continuous and strictly decreasing[1], $g_0 - 1$ has a unique zero $p_* \in (0, \frac{3-\sqrt{5}}{2})$ (see figure 5.2) and sets $g_0^{-1}((-\infty, 1]), g_0^{-1}([1,\infty))$ are connected, i.e., intervals $(0, g_0^{-1}(\{1\})]$,

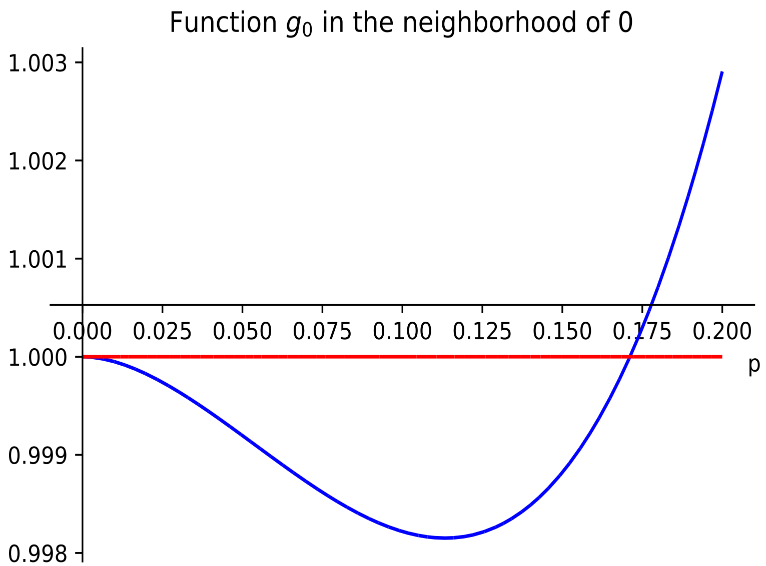

Figure 5.2: The behavior of g_0 near the origin: the point of intersection with 1 is the cut-off point p_*. For p's on the left from it, $N_{opt}^{ST}(p) \in \{\lfloor\sqrt{2p^{-1}}\rfloor, \lfloor\sqrt{2p^{-1}}\rfloor + 1, \lfloor\sqrt{2p^{-1}}\rfloor + 2\}$, whereas for p's on the right, $N_{opt}^{ST}(p) \in \{\lfloor\sqrt{2p^{-1}}\rfloor, \lfloor\sqrt{2p^{-1}}\rfloor + 1\}$

$\left[g_0^{-1}(\{1\}), \frac{3-\sqrt{5}}{2}\right)$ respectively. To finish the proof, it remains to demonstrate that $\left\lfloor\sqrt{\frac{2}{p}}\right\rfloor - 1$ is never optimal on $\left(p_*, \frac{3-\sqrt{5}}{2}\right)$. For this, consider a function

$$f(p) = t_{ST}\left(\left\lfloor\sqrt{\frac{2}{p}}\right\rfloor - 1, p\right) - t_{ST}\left(\left\lfloor\sqrt{\frac{2}{p}}\right\rfloor, p\right) =$$
$$\mathbb{1}\left\{p \in \left(p_*, \frac{2}{9}\right]\right\}\left(t_{ST}(1,p) - t_{ST}(2,p)\right) +$$
$$\mathbb{1}\left\{p \in \left(\frac{2}{9}, \frac{3-\sqrt{5}}{2}\right)\right\}\left(t_{ST}(2,p) - t_{ST}(3,p)\right)$$

on $\left(p_*, \frac{3-\sqrt{5}}{2}\right)$. It is left continuous and has a single point of discontinuity equal to $\frac{2}{9}$. Since f' is negative on $\left(p_*, \frac{2}{9}\right) \cup \left(\frac{2}{9}, \frac{3-\sqrt{5}}{2}\right)$, invoking left

[1]this needs some reasoning yet we omit the details

continuity, we infer that its minimal values are $f(2/9)$ on $(p_*, 2/9]$ and $f\left(\frac{3-\sqrt{5}}{2}-\right)$ on $\left(\frac{2}{9}, \frac{3-\sqrt{5}}{2}\right)$ respectively. By direct substitution and because of left continuity, $f\left(\frac{3-\sqrt{5}}{2}-\right) = 0$, whereas numerical estimation yields $f(2/9) \approx 0.018976$. The verification of the enumerated properties of f requires only lengthy standard calculus and we omit it. The graph of f illustrating its behavior is given in figure 5.3. □

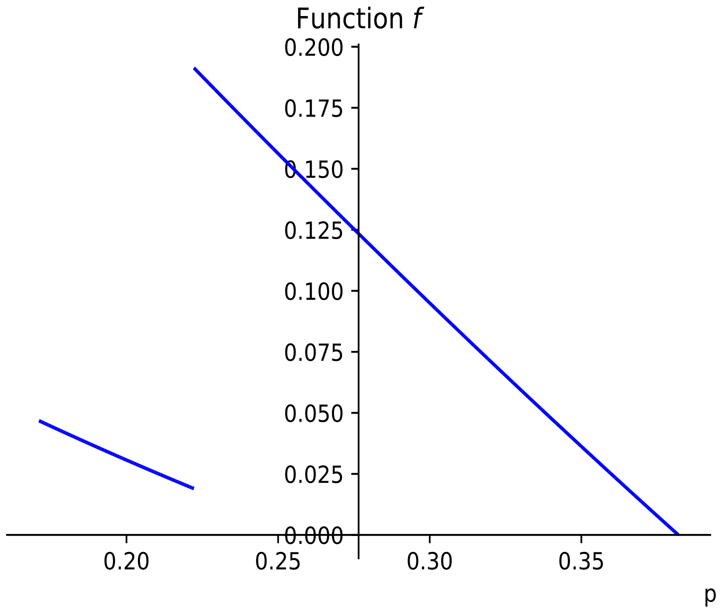

Figure 5.3: The behavior of function $f(p) = t_{ST}\left(\left\lfloor\sqrt{\frac{2}{p}}\right\rfloor - 1, p\right) - t_{ST}\left(\left\lfloor\sqrt{\frac{2}{p}}\right\rfloor, p\right)$ on $\left(p_*, \frac{3-\sqrt{5}}{2}\right)$.

Proof of Theorem 3.1.2. For the sake of clarity, we split the proof into three steps. As in the proof of Theorem 3.1.1, some tedious details are omitted and only the sketch is given.

Step 1: slicing A^{MD}. In this step, we show that

$$\left\{\left(p, \frac{1}{\sqrt{p}} + 1 - \frac{5}{2}p\right) : p \in \left(0, \frac{3-\sqrt{5}}{2}\right)\right\} \subseteq A^{MD}, \tag{5.6}$$

where A^{MD} is the same as in the statement of Theorem 5.1.1. To this end, note that, by elementary rearrangement,

$$t_{MD}(N,p) < 1 \iff 1 < q^{N-1}(Nq+p) = q^{N-1}((N-1)q+1) = \\ [\text{denoting } N-1 = x] = q^x(1+qx) \iff 0 < x\ln q + \ln(1+qx).$$

Plugging in $N = \sqrt{p^{-1}} + 1 - (5/2)p$, we then obtain the condition we need to check:

$$\left(\frac{1}{\sqrt{p}} - \frac{5p}{2}\right)\ln q + \ln\left(1 + q\left(\frac{1}{\sqrt{p}} - \frac{5p}{2}\right)\right) > 0.$$

Putting $y = \sqrt{p}$ this translates to checking that

$$f(y) = \left(\frac{1}{y} - \frac{5y^2}{2}\right)\ln(1-y^2) + \ln\left(1 + (1-y^2)\left(\frac{1}{y} - \frac{5y^2}{2}\right)\right)$$

is positive on its domain $\left(0, \sqrt{\frac{3-\sqrt{5}}{2}}\right)$. One can show that f is strictly convex on $\left(0, \sqrt{\frac{3-\sqrt{5}}{2}}\right)$. Consequently, f' is non-decreasing and upper bounded by $\lim_{x \to \sqrt{\frac{3-\sqrt{5}}{2}}-} f'(x) \approx -1.66$. This, in turn, yields that f is decreasing and lower bounded by $\lim_{x \to \sqrt{\frac{3-\sqrt{5}}{2}}-} f(x) \approx 0.024$.

Step 2: bracing the optimal points. Rewrite equation $\frac{\partial}{\partial N} t_{MD}(N,p) = 0$ as follows:

$$-\frac{q}{p}\left(N^2 + \frac{1}{\ln q}\left(\frac{1}{q}\right)^N\right) + \frac{1}{\ln q} = N,$$

and denote the function on the rhs by $f(N,p)$. Then each fixed point of $N \mapsto f(N,p)$ is the zero of $\frac{\partial}{\partial N} t_{MD}(N,p)$. In particular, the statement applies to $N_*^{MD}(p)$. In this step, by making use of this observation, we show that $N_*^{MD}(p)$ (the detailed explanation of the latter fact is given in *Step* 3) does not deviate a lot from $\sqrt{p^{-1}}$. To achieve the goal, we consider points

$$N = N(\theta) = \left(\frac{1}{\sqrt{p}} + 1 - \frac{5}{2}p\right)\theta + \left(\frac{1}{\sqrt{p}} - p\right)(1-\theta) = \\ \frac{1}{\sqrt{p}} - p + \theta\left(1 - \frac{3}{2}p\right), \theta \in [0,1], \quad (5.7)$$

and demonstrate that

$$\forall p \in \left(0, \frac{3-\sqrt{5}}{2}\right) \exists! \theta \in [0,1] : f(N(\theta), p) = N(\theta) \iff$$
$$\forall p \in \left(0, \frac{3-\sqrt{5}}{2}\right) \exists! \theta \in [0,1] : p^{\frac{3}{2}}(f(N(\theta), p) - N(\theta)) = 0. \quad (5.8)$$

For convenience, put $h(\theta, p) = p^{\frac{3}{2}}(f(N(\theta), p) - N(\theta))$. Calculating derivative yields

$$\frac{\partial}{\partial \theta} h(\theta, p) = p^{\frac{3}{2}} \left(\frac{\partial}{\partial N} f(N, p) - 1 \right) \frac{\partial}{\partial \theta} N(\theta) =$$
$$p^{\frac{3}{2}} \left(-\frac{q}{p} \left(2N(\theta) - \left(\frac{1}{q}\right)^{N(\theta)} \right) - 1 \right) \left(1 - \frac{3}{2}p\right) \quad (5.9)$$

and then, since $\frac{\partial}{\partial \theta} N(\theta)$ does not depend on θ,

$$\frac{\partial^2}{\partial \theta^2} h(\theta, p) = p^{\frac{3}{2}} \left(\frac{\partial^2}{\partial N^2} f(N, p) \right) \left(\frac{\partial}{\partial \theta} N(\theta) \right)^2 =$$
$$-q\sqrt{p} \left(2 + \left(\frac{1}{q}\right)^{N(\theta)} \ln q \right) \left(1 - \frac{3}{2}p\right)^2. \quad (5.10)$$

For a fixed p, consider the term $\left(2 + \left(\frac{1}{q}\right)^{N(\theta)} \ln q\right)$. Since $N(\theta) \uparrow$, it is upper bounded by $\left(2 + \left(\frac{1}{q}\right)^{N(1)} \ln q\right)$. By making use of the second derivative test, one can show that $p \mapsto \left(2 + \left(\frac{1}{q}\right)^{N(1)} \ln q\right)$ is strictly concave and has negative derivative on $\left(0, \frac{3-\sqrt{5}}{2}\right)$. Therefore, it is lower bounded by its left limit at $\frac{3-\sqrt{5}}{2}$. The value of the latter is approximately equal to 0.93. It follows then from (5.10) that, for any fixed $p \in \left(0, \frac{3-\sqrt{5}}{2}\right)$, $\theta \mapsto \frac{\partial^2}{\partial \theta^2} h(\theta, p)$ is negative on $[0, 1]$. Hence, for any fixed $p \in \left(0, \frac{3-\sqrt{5}}{2}\right)$, $\theta \mapsto h(\theta, p)$ is concave and has therefore a decreasing derivative. Inspection of $p \mapsto \frac{\partial}{\partial \theta} h(0, p)$ reveals that $\theta \mapsto \frac{\partial}{\partial \theta} h(\theta, p)$ is negative for any fixed p meaning that the range of $\theta \mapsto h(\theta, p)$ is equal to $[h(1, p), h(0, p)]$. Finally, omitting the details of a tedious exercise of verification that the range of $p \mapsto h(1, p)h(0, p)$ lies in $(-\infty, 0)$, we finish proof of this step and conclude that (5.8) indeed holds.

Step 3: the end of the proof. By *Step 2*, for each $p \in \left(0, \frac{3-\sqrt{5}}{2}\right)$, there exists $N(p) \in \left(\frac{1}{\sqrt{p}} - p, \frac{1}{\sqrt{p}} + 1 - \frac{5}{2}p\right)$ which solves $\frac{\partial}{\partial N} t_{MD}(N, p) = 0$. By *Step 1*, $N(p) \in A^{MD}$. Therefore, by Theorem 5.1.1, $N(p)$ is the unique global minimizer of $[1, \infty) \ni N \mapsto t_{MD}(N, p)$, i.e., $N(p) = N_*^{MD}(p)$. This implies that $N_{opt}^{MD}(p) \in \{\lfloor\sqrt{p^{-1}}\rfloor - 1, \lfloor\sqrt{p^{-1}}\rfloor, \lfloor\sqrt{p^{-1}}\rfloor + 1\}$, and it remains to exclude the point $\lfloor\sqrt{p^{-1}}\rfloor - 1$. The route is as follows. First, by making exactly the same technique as in *Step 2*, show that $N(p) \in \left(\frac{1}{\sqrt{p}}, \frac{1}{\sqrt{p}} + 1 - \frac{5}{2}p\right)$ for $p \in (0, 0.3)$. Second, note that integer parts of $\frac{1}{\sqrt{p}} - p$ and $\frac{1}{\sqrt{p}}$ coincide for $p \in \left[0.3, \frac{3-\sqrt{5}}{2}\right)$. Figure 5.4 provides a good visual summary of the whole proof and explains the need of this workaround in particular. □

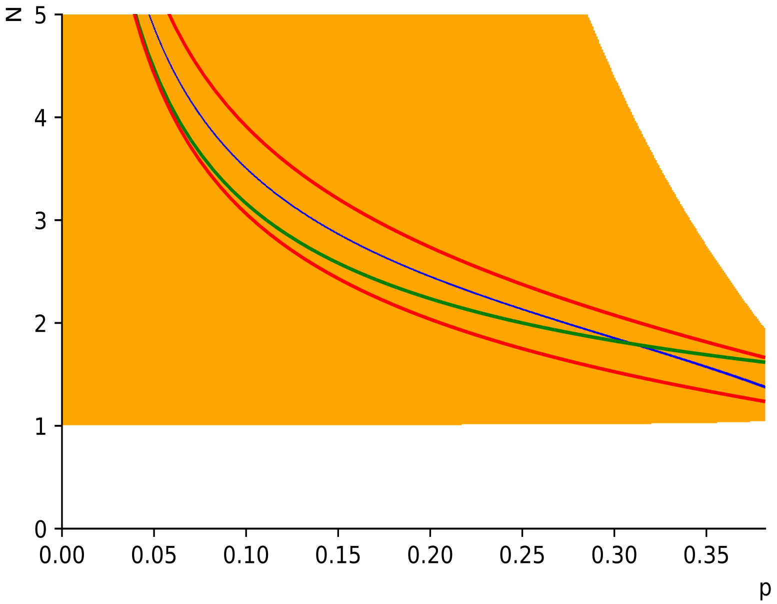

Figure 5.4: orange area corresponds to $\{(N, p) : t_{MD}(N, p) < 1\}$; upper and lower red lines show bracing functions $p \mapsto \sqrt{p^{-1}} + (1 - (5/2)p)$ and $p \mapsto \sqrt{p^{-1}} - p$ respectively; green line shows function $p \mapsto \sqrt{p^{-1}}$; blue line shows $p \mapsto N_*^{MD}(p)$

We note that in the proof of Theorem 3.1.3 below, *Step 1* is a repetition of Lemma 1 in [38]. Nonetheless, we have decided to rewrite it here because it is very short and, along the way, some notions used in the sequel appear.

Proof of Theorem 3.1.3. Step 1. We first show that, for any fixed $n \in (2,\infty)$, there exists a unique $q_n \in (0,1)$ such that

$$g(q_n,n)=0, \quad g(q,n)<0\,\forall q\in(q_n,1) \quad \text{and} \quad g(q,n)>0\,\forall q\in(0,q_n).$$

To this end, note that

$$\frac{\partial}{\partial q}g(q,n) = -2nq^{n-1}+(2n-1)q^{2n-2} = \\ -2nq^{n-1}\left(1-\frac{2n-1}{2n}q^{n-1}\right)<0\,\forall n\in(2,\infty).$$

Thus, given $n \in (2,\infty)$, $q \mapsto g(q,n)$ is decreasing on $(0,1)$. Since $g(0+,n)=\frac{2}{n}>0$ and $g(1-,n)=\frac{2}{n}-1<0$, the claim holds true.

Step 2. From *Step 1* it follows that, for any fixed $q\in(0,1)$, we have a well defined function $n\mapsto q_n$ which is given implicitly by equation $g(q_n,n)=0$. Since this function is continuous, its range $I\subset(0,1)$ is an interval. Next, for $\varepsilon\in(0,1)$ and $n=2+\varepsilon$,

$$g(1-\varepsilon,n)=\frac{2}{n}-2(1-n\varepsilon+O(\varepsilon^2))+(1-(2n-1)\varepsilon+O(\varepsilon^2)) = \\ \frac{-\varepsilon}{2+\varepsilon}+\varepsilon+O(\varepsilon^2)>0,$$

provided ε is small enough. Hence, analysis accomplished in *Step 1* implies that $q_{2+\varepsilon}\in(1-\varepsilon,1)$. Therefore, $I=(q_*,1)$ for some $q_*\in(1/2,1)$. To justify the lower bound $1/2$, note that

$$g(1/2,n)>0 \Longleftrightarrow 2^n > n\left(1-\frac{1}{2^n}\right).$$

Since the rhs holds true for all $n>2$, it follows that $\forall n>2\; g(1/2,n)>0$. Also note that $\forall\,(q,n)\in(0,q_*)\times(2,\infty)\; g(q,n)>0$ since an opposite contradicts the definition of q_*.

Step 3. Fix $q\in(q_*,1)$. By *Step 1–Step 2*, $g(q,n)=0$ has at least one solution $n=n(q)$ (suffices it to take n such that $q_n=q$). To show that there are two solutions, put $c=\frac{1}{2q}$, make a change of variable $q^n=x$, and rewrite $g(q,n)=0$ in a form

$$-\ln q = -\ln x(x-cx^2). \tag{5.11}$$

Consider function $h(x) = -(x - cx^2)\ln x$ for $x \in (0,1)$. Note that

$$\frac{\mathrm{d}}{\mathrm{d}x}h(x) = -\left((1-cx) + (1-2cx)\ln x\right) = 0 \iff -\ln x = \frac{1-cx}{1-2cx}. \tag{5.12}$$

Since $1 - cx > 1 - c > 0$ and $-\ln x > 0$ for all $x \in (0,1)$, it follows that $1 - 2cx > 0$ as well, provided x solves (5.12). Therefore, the range of possible solutions of (5.12) shrinks to $(0, q)$. Moreover, relationships $\lim_{x\to 0+} \frac{\mathrm{d}}{\mathrm{d}x}h(x) = \infty$, $\lim_{x\to 1-} \frac{\mathrm{d}}{\mathrm{d}x}h(x) = c - 1 < 0$ imply that (5.12) has at least one solution. Since $\frac{1-cx}{1-2cx} + \ln x = 1 + \frac{cx}{1-2cx} + \ln x$ increases on $(0,q)$, the solution is unique. Denote it x_0. Based on the sign of the derivative, we have that $h \uparrow$ on $(0, x_0)$ and $h \downarrow$ on $(x_0, 1)$. Hence, at x_0, h attains its maximum and (5.11) admits exactly two solutions if $h(x_0) > -\ln q$, one solution if $h(x_0) = -\ln q$, and has no solutions if $h(x_0) < -\ln q$. By the choice of q (recall that $q > q_*$), the last case can not hold. To exclude the second one, note that the function $\left(\frac{1}{2}, \frac{1}{2q_*}\right) \ni c \mapsto x_0(c)$ is well defined and decreasing since

$$\begin{aligned} -\ln x_0 &= \frac{1-cx_0}{1-2cx_0} \Rightarrow \\ -\frac{\mathrm{d}}{\mathrm{d}c}\ln x_0(c) &= -\frac{\frac{\mathrm{d}}{\mathrm{d}c}x_0(c)}{x_0(c)} = \frac{\mathrm{d}}{\mathrm{d}c}\frac{1-cx_0}{1-2cx_0} = \frac{x_0 + c\frac{\mathrm{d}}{\mathrm{d}c}x_0(c)}{(1-2cx_0)^2} \Rightarrow \\ &\qquad\qquad \frac{\mathrm{d}}{\mathrm{d}c}x_0(c) = \frac{-x_0^2}{(1-2cx_0)^2 + cx_0} < 0. \end{aligned}$$

Therefore, $(q_*, 1) \ni q \mapsto x_0(q)$ is increasing. Taking into account that $q \mapsto -\ln q$ is decreasing, we finally deduce that $h(x_0) > -\ln q$ for all $q \in (q_*, 1)$. The monotonicity of $q \mapsto x_0(q)$ and $q \mapsto -\ln q$ also leads to the conclusion that q_* can be solved from equation

$$-\ln q_* = h(x_0(q_*))$$

along with a unique $n_* \in (2, \infty)$. Hence (i).

Step 4. Assume the setting of *Step 3*. Let $0 < x_L = q^{n_U} < x_U = q^{n_L} < q$ denote two solutions of (5.11). By above, $h(x) > -\ln q \iff x \in (x_L, x_U)$. Reverting to $(0, \infty) \ni n \mapsto g(q, n)$, this reads as $g(q,n) < 0 \iff n \in (n_L, n_U)$. Note that $n \mapsto g(q,n) > 0$ in the neighborhood of ∞. Also, from *Step 1*–*Step 2*, we have that $n \mapsto g(q,n) > 0$ in the right neighborhood of 2 and that $n_U \in (2, \infty)$. Therefore, continuity of $n \mapsto g(q,n) > 0$ yields that $n_L \in (2, \infty)$ as well. Finally, it is clear that $n_L < n_* < n_U$ (see figure 5.5 for a graphical illustration). Hence (ii).

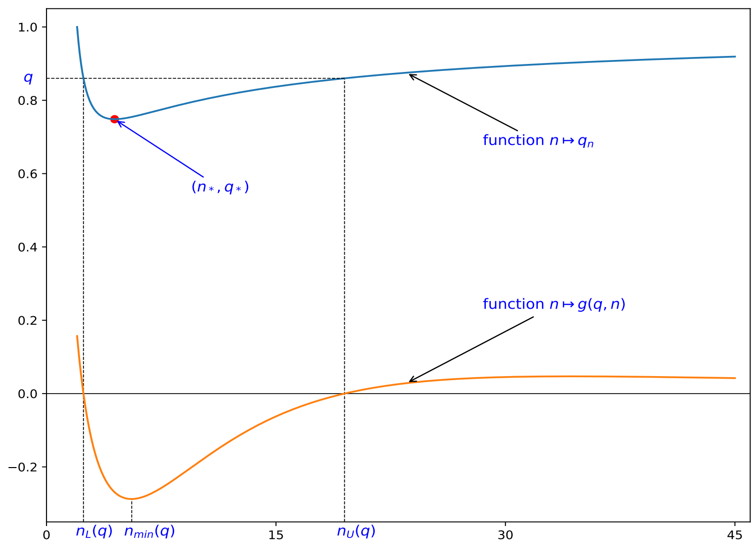

Figure 5.5: Graph illustrating relationships of $n \mapsto q_n$ and related quantities. The lower curve corresponds to $q = 0.86$.

Step 5. In this step, we identify the number and location of zeroes of the derivative of $(2, \infty) \ni n \mapsto g(q, n)$ having fixed $q \in (q_*, 1)$. From analysis given in *Step 4*, it follows that $(2, \infty) \ni n \mapsto g(q, n)$ has at least two extremes: there must be a minimum in (n_L, n_U) (since function is negative here), and maximum in (n_U, ∞) (since the function is positive here and $\lim_{n\to\infty} g(q, n) = 0+$. To see that there are no other extremes, consider an equation

$$\frac{\partial}{\partial n} g(q, n) = -\frac{2}{n^2} - 2q^n \ln q + 2q^{2n-1} \ln q = 0, \tag{5.13}$$

and rewrite it by making use of notions introduced in *Step 3* as follows:

$$-x \ln x = \sqrt{-\ln q}\sqrt{\frac{x}{1-2cx}}, x \in \left(0, \frac{1}{2c}\right) = (0, q). \tag{5.14}$$

Next, note that:

- $h_1(x) = -x \ln x$ is strictly convex–up and positive on $(0, 1)$ with $\lim_{x\to 0+} h_1(x) = \lim_{x\to 1-} h_1(x) = 0+$;

- $h_2(x) = \sqrt{\frac{x}{1-2cx}}$ is strictly positive and increasing on $(0, \frac{1}{2c}) = (0, q)$, it has one inflection point and $\lim_{x \to 0+} h_2(x) = 0$, $\lim_{x \to q-} h_2(x) = \infty$.

Taking this information into account, we conclude that (5.14) can have at most two solutions and confirm thereby the assertion stated above.

Step 6. It remains to justify expression (3.4). Let

$$n(q,t) = \frac{1}{p^{\frac{2}{3}}} + \frac{1}{2p^{\frac{1}{3}}} + 0.2 + 3p^2 + t, \quad t \in [0,1]. \tag{5.15}$$

It suffices to prove that, for all $q \in [0.755, 1)$, the following statements hold true:

(a) $\max(g(q, n(q,0)), g(q, n(q,1)) < 0$; and

(b) $\exists t \in [0,1] : \frac{\partial}{\partial n} g(q,n)\Big|_{n=n(q,t)} = 0$.

Analytical calculations behind (a) and (b) are standard yet very lengthy and tedious. Therefore, we omit the details and end up with a graphical proof and a sketch of the analytical one.

Figures 5.6–5.7 show graph of $q \mapsto \max(g(q, n(q,0)), g(q, n(q,1)))$ from which it is evident that (a) holds. Analytical proof consists of the following steps.

(s1) Calculate $\frac{\partial}{\partial q} g(q, n(q,i)), i = 0,1$.

(s2) Check that $\frac{\partial}{\partial q} g(q, n(q,i)) < 0, i = 0,1$ on $[0.755, 1)$ and deduce that $g(q, n(q,i))$ decrease on [0.755,1).

(s3) Conclude that (a) indeed holds since

$$g(0.755, n(0.755, 0)) \approx -0.002258, \quad g(0.755, n(0.755, 1)) \approx -0.013690.$$

Turning to (b), first rewrite (5.13) as follows:

$$-n^2 q^n \ln q(1 - q^{n-1}) = 1.$$

Next, consider function $h(t,q) = -n^2(q,t) q^{n(q,t)} \ln q(1 - q^{n(q,t)-1}) - 1$ with $n(q,t)$ given by (5.15) and $q \in [0.755, 1)$. Since $t \mapsto h(t,q)$ is continuous, it suffices to show that, for any $q \in [0.755, 1)$, $h(0,q) < 0$ and $h(1,q) > 0$. Figure 5.8 shows graphs of $q \mapsto h(0,q), q \mapsto h(1,q)$. These confirm (b). Considering analytical part, the following is the suggested route.

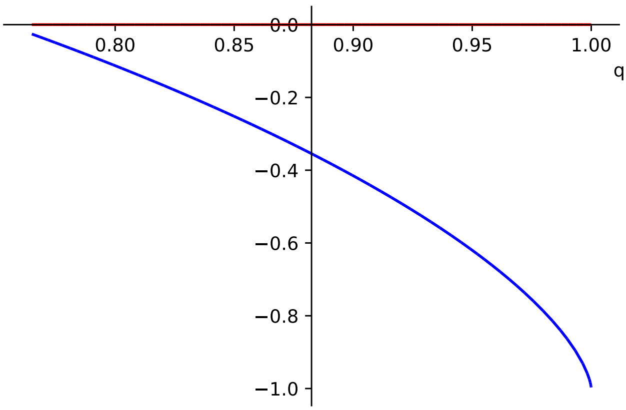

Figure 5.6: Graph of $q \mapsto \max(g(q,n(q,0)), g(q,n(q,1)))$ for $q \in [0.765, 1)$. For reference, a function identically equal to 0 is plotted in red.

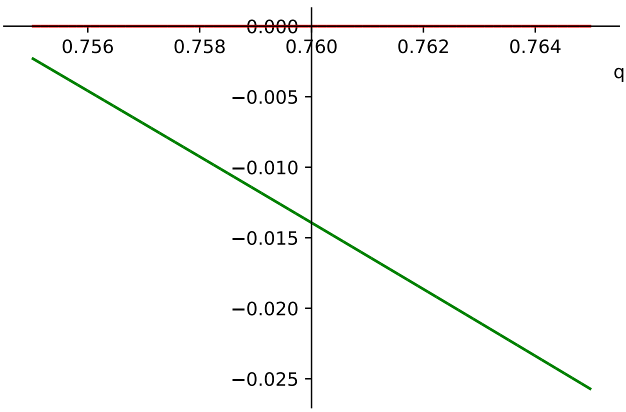

Figure 5.7: Graph of $q \mapsto \max(g(q,n(q,0)), g(q,n(q,1))$ for $q \in [0.755, 0.765]$. For reference, a function identically equal to 0 is plotted in red.

(s1) Calculate $\frac{\partial^2}{\partial q^2} h(i,q), i = 0, 1$.

(s2) Check that $\frac{\partial^2}{\partial q^2} h(0,q) > 0$ whereas $\frac{\partial^2}{\partial q^2} h(1,q) < 0$ on $[0.755, 1)$ and deduce that $h(0,q)$ is convex downwards whereas $h(1,q)$ is convex upwards on [0.755,1).

(s3) By making use of Taylor's expansion, check that $\lim_{q\to 1-} h(0,q) = 0-$ and $\lim_{q\to 1-} h(1,q) = 0+$.

(s4) Conclude that (b) indeed holds since

$$h(0, 0.755) \approx -0.2645889 \quad \text{and} \quad h(1, 0.755) \approx 0.081749. \qquad \square$$

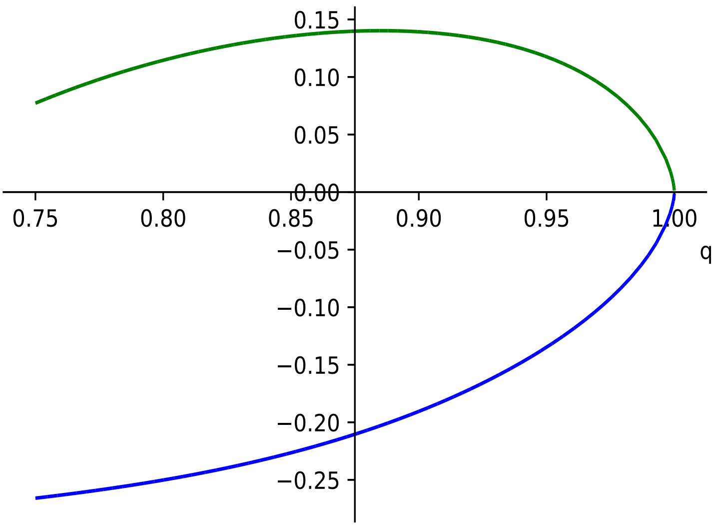

Figure 5.8: Graphs of $q \mapsto h(0,q), q \in [0.755, 1)$ (plotted in blue) and $q \mapsto h(1,q), q \in [0.755, 1)$ (plotted in green).

Proof of Corollary 3.1.4. Uniqueness of q_5 was established in *Step 1* of the proof of Theorem 3.1.3. Hudgens and Kim [38] (Lemmas 2, 7, and 14) have demonstrated that $n_{opt}(q) \notin \{2,3,4\}$ $\forall q \in (0,1)$. From their results we also have that $\forall q \in (q_*, 0.755]$ $n_{opt}(q) = 5$. It is straightforward to verify that

$$\forall\, q \in (q_5, 0.755] \left\lfloor \frac{1}{p^{\frac{2}{3}}} + \frac{1}{2p^{\frac{1}{3}}} + 3p^2 + 1.2 \right\rfloor = 5.$$

Hence the claim in the region $(q_5, 0.755]$. For $q \in [0.755, 1)$, it follows from Theorem 3.1.3 by noting that at least one of numbers in the set (3.5) belongs to $\{n \in (2,\infty) : t_{A2}(n,q) < 1\}$ because of (a) in Step 6 of proof of Theorem 3.1.3. $\square$

5.2 Proofs of results stated in Section 3.2

Proof of Proposition 3.2.1. Take $p \in (0, p_{X,c})$. By the definition of $p_{X,c}$, there exists $N \in (c,\infty) : t_X(N,p) < 1$. Hence, Xmakes sense for that p. Since $p \in (0, p_{X,c})$ was arbitrary, it holds true for all $p \in (0, p_{X,c})$.

Next, assume that $p_{X,c} < \mathrm{UCP}$ (otherwise implication (3.11) is obvious) and take $p \in (p_{X,c}, \mathrm{UCP}]$. Case "$\exists N \in (c,\infty) : t_X(N,p) < 1$" contradicts the definition of $p_{X,c}$. Hence, $\forall N \in (c,\infty)\ t_X(N,p) \geq 1$. Assuming that $t_X(N,p) = 1$ for some $N \in (c,\infty)$ again leads to contradiction. Indeed, take $p' \in (p_{X,c}, p)$ and employ (M2) to deduce that

$$t_X(N,p') < t_X(N,p) = 1 \Rightarrow p_{X,c} = \sup\{p \in (0,\mathrm{UCP}) \mid \exists N \in (c,\infty) : t_X(N,p) < 1\} \geq p' > p_{X,c}. \quad \square \tag{5.16}$$

Proof of Proposition 3.2.2. First, note that $t_X(N, p_{X,c}) \geq 1$ for all $N \in (c,\infty)$ provided $p_{X,c} < \mathrm{UCP}$. Assuming an opposite leads to the same contradiction as in (5.16). With this in view, we proceed to the analysis of the distinct types of possible bifurcations.

Case (b0). Since $p_{X,c}$ solves $t_X(N, p_{X,c}) = 1$ for some $N \in (c,\infty)$, (M3) implies that $p_{X,c} < \mathrm{UCP}$. Further, note that

$$\forall (N,p) \in (c,\infty) \times (0, p_{X,c})\ t_X(N,p) < 1. \tag{5.17}$$

must hold since the existence of $(N,p) \in (c,\infty) \times (0, p_{X,c})$ s.t. $t_X(N,p) \geq 1$ contradicts the premise[2] "$p_{X,c}$ is the only value of the control parameter for which dynamical system (3.13) admits fixed points in (c,∞)".

Fix arbitrary $(N_1, p_1) \in (c,\infty) \times (0, p_{X,c})$ and take $p_2 \in (p_{X,c}, \mathrm{UCP})$. By Prop. 3.2.1, $t_X(N_1, p_2) > 1$. By (M2), $[p_1, p_2] \ni p \mapsto t_X(N_1, p)$ is strictly increasing. Therefore, there exists unique $p_0 \in (p_1, p_2)$ s.t.

[2] $t_X(N,p) = 1$ is clearly impossible; assuming strict inequality $t_X(N,p) > 1$, to reach a contradiction, employ (M2) and (M4)

$t_X(N_1, p_0) = 1$. By the premise, $p_0 = p_{X,c}$. Since N_1 was arbitrary, it follows that

$$\forall\, N \in (c, \infty)\, t_X(N, p_{X,c}) = 1 \tag{5.18}$$

and $p_{X,c}$ is the unique value of the control parameter $p \in (0, \mathrm{UCP})$ obeying this property. Differentiating both sides of (5.18) with respect to N one finds out that (3.13) holds as well.

Case (b1)–(b2). Assume that there exists $(N_l, p_l) \in (c, \infty) \times (0, p_{X,c})$ s.t. $t_X(N_l, p_l) = 1$. Take arbitrary $p \in (p_l, p_{X,c})$. Since $p > p_l$, it follows that $t_X(N_l, p) > 1$ because of (M2). On the other hand, by the definition of $p_{X,c}$, there exists $N_p \in (c, \infty)$ s.t. $t_X(N_p, p) < 1$. Therefore, by the Intermediate Value Theorem and continuity of $N \mapsto t_X(N, p)$, there exists $N_1 \in (\min(n_p, N_l), \max(n_p, N_l))$ s.t. $t_X(N_1, p) = 1$. Since this holds for any $p \in [p_l, p_{X,c})$, we have (b1) provided $\forall N \in (c, \infty)\, t_X(N, p_{X,c}) > 1$. Otherwise, we have (b2) and $p_{X,c}$ then can't be equal to UCP because of (M3).

Inversion of the bifurcation curve. When dealing with (b0), we have already shown that the bifurcation curve defines a constant map $(c, \infty) \ni N \mapsto p_N \equiv p_{X,c}$. As for (b1)–(b2), note that, for any fixed $N \in (c, \infty)$, the following applies:

- by the said in the very beginning of the proof and (M3),

$$\forall N\, t_X(N, p_{X,c}) \geq 1; \tag{5.19}$$

- by (M4),

$$\forall N\, \exists p \in (0, p_{X,c}) : t_X(N, p) < 1; \tag{5.20}$$

- (5.19)–(5.20) and (M2) imply existence of a unique $p_N \in (0, p_{X,c}]$ s.t. $t_X(N, p_N) = 1$.

Therefore, we have a well defined map $(c, \infty) \ni N \mapsto p_N \in (0, p_{X,c}]$. By (M1)–(M2), $p \mapsto t_X(N, p)$ is differentiable and increasing for any $N \in (c, \infty)$. Therefore, $\forall N \in (c, \infty)\, \frac{\partial}{\partial p} t_X(N, p) > 0$ and one can apply the Implicit Function Theorem to $\varphi(N, p) = t_X(N, p) - 1$ to deduce that $N \mapsto p_N$ is differentiable as well. Moreover, differentiating both sides of $t_X(N, p_N) = 1$ and applying the chain rule, we have that

$$\frac{\partial}{\partial N} t_X(N, p_N) + \frac{\partial}{\partial p} t_X(N, p_N) \frac{\partial}{\partial N} p_N = 0 \Rightarrow \frac{\partial}{\partial N} p_N = -\frac{\frac{\partial}{\partial N} t_X(N, p_N)}{\frac{\partial}{\partial p} t_X(N, p_N)}.$$

$$(5.21)$$

Therefore, looking for extremes of $N \mapsto p_N$ one has to solve

$$\frac{\partial}{\partial N} t_X(N, p_N) = 0 \Longleftrightarrow \frac{\partial}{\partial N} p_N = 0$$

with respect to N. Since p_N also solves $t_X(N, p) = 1$, extremes and corresponding values can be obtained by solving (3.13). For bifurcations of type (b0) and (b2), maximal value $p_{X,c}$ is attained at some inner point(s) $N_c \in (c, \infty)$; for the bifurcation of type (b1), the maximal value lies on the boundary of its domain. □

5.3 Proofs of results stated in Section 3.3

Proof of Proposition 3.3.1. By the description of the testing procedure,

$$\begin{aligned}\Theta_N =&(1 + \Theta_{N-2})\mathbb{1}\{Y_N + Y_{N-1} = 0\} + \\ &(2 + \Theta_{N-1})\mathbb{1}\{Y_N + Y_{N-1} > 0\} Y_N + \\ &(2 + \Theta_{N-2})\mathbb{1}\{Y_N + Y_{N-1} > 0\} \bar{Y}_N = \\ &\bar{Y}_N(1 + Y_{N-1}) + 2Y_N + \Theta_{N-1}Y_N + \Theta_{N-2}\bar{Y}_N \end{aligned} \tag{5.22}$$

since

$$\mathbb{1}\{Y_N + Y_{N-1} = 0\} = \bar{Y}_N\bar{Y}_{N-1}, \quad \mathbb{1}\{Y_N + Y_{N-1} > 0\} Y_N = Y_N, \\ \text{and} \quad \mathbb{1}\{Y_N + Y_{N-1} > 0\} \bar{Y}_N = \bar{Y}_N Y_{N-1}.$$

Let

$$\tau_1 = \begin{pmatrix}1\\0\end{pmatrix}, \quad A_1 = \tau_1, \quad \tau_k \overset{k\geqq 2}{=} \begin{pmatrix}\Theta_k\\ \Theta_{k-1}\end{pmatrix}, \quad A_k \overset{k\geqq 2}{=} \begin{pmatrix}\bar{Y}_k(1 + Y_{k-1}) + 2Y_k\\ 0\end{pmatrix},$$

and let $B_k, k \geqslant 1$, be as in the statement of the Proposition. From (5.22) it follows that

$$\begin{aligned}&\tau_N = A_N + B_N\tau_{N-1} = \ldots = \\ &A_N + \sum_{k=1}^{N-2} B_N B_{N-1} \ldots B_{N-k+1} A_{N-k} + B_N \ldots B_2\tau_1 = \\ &A_N + \sum_{j=3}^{N} B_N \ldots B_j A_{j-1} + B_N \ldots B_2\tau_1 = A_N + \sum_{j=2}^{N} B_N \ldots B_j A_{j-1}.\end{aligned}$$

Define

$$
\begin{aligned}
&M_0 = \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}, \; M_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \; M_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \; M_3 = \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix}, \\
&S = \{M_0, M_1, M_2, M_3\}, \qquad (5.23)
\end{aligned}
$$

Then S forms a semi-group with respect to ordinary matrix multiplication since

$$
\begin{aligned}
&M_0^2 = M_0,\; M_0M_1 = M_3,\; M_0M_3 = M_3,\; M_1M_0 = M_0,\; M_1^2 = M_2, \\
&M_1M_3 = M_3,\; M_3M_0 = M_0,\; M_3M_1 = M_0,\; M_3^2 = M_3. \qquad (5.24)
\end{aligned}
$$

Let $J_i = \{j \in \{2,, \ldots, n\} \mid Y_j = i\}, i = 0, 1$. Note that $\forall i \; B_i = Y_iM_0 + \bar{Y}_iM_1 \in S$ and that M_0 is an absorbing element of S. Therefore, by (5.24)

$$
\sum_{j \in J_1} B_N \ldots B_j A_{j-1} = \sum_{j \in J_1} M_0 A_{j-1} = \sum_{j=2}^{N} Y_j M_0 A_{j-1}
$$

and

$$
\begin{aligned}
\sum_{j \in J_0} B_N \ldots B_j A_{j-1} = \sum_{j=2}^{N} \bar{Y}_j \Big(&\mathbb{1}\{B_N \ldots B_j M_1 = M_0\} M_0 + \\
\mathbb{1}\{B_N \ldots B_j M_1 = M_1\} M_1 + &\mathbb{1}\{B_N \ldots B_j M_1 = M_2\} M_2 + \\
&\mathbb{1}\{B_N \ldots B_j M_1 = M_3\} M_3 \Big) A_{j-1}.
\end{aligned}
$$

To extract Θ_N from τ_N, it suffices to multiply τ_N by $(1\;0)$ from the left. Since

$$
(1\;0)M_iA_{j-1} = \begin{cases} 0, \text{ for } i = 1, 3 \text{ and all } j; \\ \bar{Y}_{j-1}(1 + Y_{j-2}) + 2Y_{j-1}, \text{ for } i = 0, 2 \text{ and } j \geqslant 3; \\ 1, \text{ for } i = 0, 2 \text{ and } j = 2, \end{cases}
$$

after the collection of terms, we finally end up with an expression (3.22). □

Proof of Theorem 3.3.2. Step 1: auxiliary recurrence. For $\lambda_1, \lambda_2 \in \mathbb{R}$, let

$$
M_{i,N}(\lambda_1, \lambda_2) = \mathrm{E}\left(\mathrm{e}^{\lambda_1 \Theta_N + \lambda_2 \Theta_{N-1}} \mid X_N = i\right), \quad i = 0, 1. \qquad (5.25)
$$

By equation (5.22),

$$
\begin{aligned}
M_{0,N}(\lambda_1,\lambda_2) = \mathrm{E}\left(\mathrm{e}^{\lambda_1(1+X_{N-1}+\Theta_{N-2})+\lambda_2\Theta_{N-1}}\right) = \\
p\,\mathrm{E}\left(\mathrm{e}^{\lambda_1(2+\Theta_{N-2})+\lambda_2\Theta_{N-1}} \mid X_{N-1}=1\right) + \\
q\,\mathrm{E}\left(\mathrm{e}^{\lambda_1(1+\Theta_{N-2})+\lambda_2\Theta_{N-1}} \mid X_{N-1}=0\right) = \\
p\mathrm{e}^{2\lambda_1} M_{1,N-1}(\lambda_2,\lambda_1) + q\mathrm{e}^{\lambda_1} M_{0,N-1}(\lambda_2,\lambda_1); \\
M_{1,N}(\lambda_1,\lambda_2) = \mathrm{E}\left(\mathrm{e}^{\lambda_1(2+\Theta_{N-1})+\lambda_2\Theta_{N-1}}\right) = \\
\mathrm{e}^{2\lambda_1}\left(pM_{1,N-1}(\lambda_1+\lambda_2,0) + qM_{0,N-1}(\lambda_1+\lambda_2,0)\right).
\end{aligned}
\tag{5.26}
$$

For $\lambda \in \mathbb{R}$, let

$$
\begin{aligned}
m_{1,N} = m_{1,N}(\lambda) = M_{1,N}(\lambda,0), \quad m_{2,N} = m_{2,N}(\lambda) = M_{0,N}(\lambda,0), \\
m_{3,N} = m_{3,N}(\lambda) = M_{1,N}(0,\lambda), \quad m_{4,N} = m_{4,N}(\lambda) = M_{0,N}(0,\lambda); \\
A = A(\lambda) = \mathrm{e}^{2\lambda}\begin{pmatrix} p & q \\ 0 & 0 \end{pmatrix}, \quad B = B(\lambda) = \begin{pmatrix} 0 & 0 \\ \mathrm{e}^{2\lambda}p & \mathrm{e}^{\lambda}q \end{pmatrix}, \\
C = \begin{pmatrix} p & q \\ p & q \end{pmatrix}, \quad O = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}.
\end{aligned}
\tag{5.27}
$$

From (5.26) it then follows that $m_N = m_N(\lambda) = (m_{1,N}, m_{2,N}, m_{3,N}, m_{4,N})^\top$ satisfies recurrent equation

$$
m_N = \begin{pmatrix} A & B \\ C & O \end{pmatrix} m_{N-1} = \cdots = \begin{pmatrix} A & B \\ C & O \end{pmatrix}^{N-1} m_1. \tag{5.28}
$$

Writing

$$
\begin{pmatrix} A & B \\ C & O \end{pmatrix}^{N} = \begin{pmatrix} A_N & B_N \\ C_N & D_N \end{pmatrix}
$$

and applying inductive argument, one finds out that the 2×2 blocks A_N, B_N, C_N, D_N satisfy

$$
\begin{cases} A_N = AA_{N-1} + BC_{N-1}, \\ C_N = CA_{N-1}; \end{cases} \tag{5.29}
$$

$$
\begin{cases} B_N = AB_{N-1} + BD_{N-1}, \\ D_N = CB_{N-1}; \end{cases} \tag{5.30}
$$

with $A_0 = D_0 = Id$ and $C_0 = B_0 = O$. Consider system (5.29). Since $A = \begin{pmatrix} e^{2\lambda} & 0 \\ 0 & 0 \end{pmatrix} C$, we have that

$$A_N = \begin{pmatrix} e^{2\lambda} & 0 \\ 0 & 0 \end{pmatrix} C A_{N-1} + BC_{N-1} = \begin{pmatrix} e^{2\lambda} & 0 \\ 0 & 0 \end{pmatrix} C_N + BC_{N-1}. \quad (5.31)$$

Therefore,

$$C_N = C \left(\begin{pmatrix} e^{2\lambda} & 0 \\ 0 & 0 \end{pmatrix} C_{N-1} + BC_{N-2} \right). \quad (5.32)$$

Let κ_N be defined by (3.24). We claim that $C_N = \kappa_N C$ solves (5.32). For $N = 2$ (as well as $N = 0, 1$) the claim holds by the direct check. Assume it holds for $k \leqslant N$ with $N \geqslant 2$. Noting that

$$C \begin{pmatrix} e^{2\lambda} & 0 \\ 0 & 0 \end{pmatrix} C = pe^{2\lambda} C, \; CBC = qe^{\lambda}(q + pe^{\lambda})C$$

and then applying inductive assumption and multiplication yields

$$C_{N+1} = C \left(\kappa_N \begin{pmatrix} e^{2\lambda} & 0 \\ 0 & 0 \end{pmatrix} C + \kappa_{N-1} BC \right) = \\ (pe^{2\lambda}\kappa_N + qe^{\lambda}(q + pe^{\lambda})\kappa_{N-1})C = \kappa_{N+1} C$$

since an expression for κ_N given in (3.24) is precisely the solution of the second order linear difference equation

$$\kappa_{N+1} = pe^{2\lambda}\kappa_N + qe^{\lambda}(q + pe^{\lambda})\kappa_{N-1}, \quad \kappa_1 = 1, \quad \kappa_0 = 0.$$

Substituting $C_N = \kappa_N C$ to (5.31), we obtain an expression for A_N.

System (5.30) is handled in the same way by noting that it is identical to (5.29) and only the initial conditions differ leading thereby to the following solution:

$$D_N = \kappa_{N-1} D_2, \quad B_N = \begin{pmatrix} e^{2\lambda} & 0 \\ 0 & 0 \end{pmatrix} D_N + BD_{N-1} \text{ for } N \geqslant 1. \quad (5.33)$$

Step 2: final expression. From the results of *Step 1*, we obtain an expression for m_n given by (5.28) since m_1 is readily available and equal to[3] $(e^{\lambda}, e^{\lambda}, 1, 1)^{\top}$:

$$m_n = \begin{pmatrix} (e^{\lambda} A_{N-1} + B_{N-1}) \begin{pmatrix} 1 \\ 1 \end{pmatrix} \\ (e^{\lambda} C_{N-1} + D_{N-1}) \begin{pmatrix} 1 \\ 1 \end{pmatrix} \end{pmatrix}.$$

[3] note that $\Theta_1 \equiv 1, \Theta_0 \equiv 0$

Noting that

$$\mathrm{E}\,\mathrm{e}^{\lambda\Theta_N} = p\,\mathrm{E}\left(\mathrm{e}^{\lambda\Theta_N} \mid X_N = 1\right) + q\,\mathrm{E}\left(\mathrm{e}^{\lambda\Theta_N} \mid X_N = 0\right) = pm_{1,N} + qm_{2,N},$$

we finally arrive to expression (3.25). □

Proof of Corollary 3.3.3. Recall that the k-th derivative of the moment generating function evaluated at zero yields the k-th moment. Therefore, to obtain the announced formulae, one simply needs to differentiate expression (3.25). Though conceptually an exercise is trivial, the calculations require tedious work. Therefore, we provide key steps and some intermediate quantities, yet omit the detailed listing in order not to overwhelm the Thesis with trivial content. For the sake of convenience, we make a change of variables $x = \mathrm{e}^{\lambda}$ and work with the probability generating function $G(x) = \mathrm{E}\,x^{\Theta_N} = M_{\Theta_N}(\ln x)$. By (3.24)–(3.25) and a slight abuse of notation,

$$\begin{aligned}
&G(x) = g_1(x)\kappa_{N-2}(x) + g_2(x)\kappa_{N-3}(x) \text{ with}\\
&g_1(x) = \left((1-q)^2x^3 + q(1-q)^2x^2 + q(1-q^2)x + q^2\right)x^2,\\
&g_2(x) = q\left((1-q)^2x^3 + q(1-q)(2-q)x^2 + 2q^2(1-q)x + q^3\right)x^2,\\
&\alpha_i = \alpha_i(x) = \frac{1}{2}\left(px^2 + (-1)^i\sqrt{p^2x^4 + 4qx(q+px)}\right), \text{ for } i = 0, 1,\\
&\text{and} \quad \kappa_N = \kappa_N(x) = \frac{\alpha_0^N(x) - \alpha_1^N(x)}{\alpha_0(x) - \alpha_1(x)} \text{ for } N \geqslant 0.
\end{aligned} \tag{5.34}$$

Then

$$\begin{aligned}
\mathrm{E}\,\Theta_N = G'(1) = g_1'(1)\kappa_{N-2}(1) + g_1(1)\kappa_{N-2}'(1) +&\\
g_2'(1)\kappa_{N-3}(1) + g_2(1)\kappa_{N-3}'(1)&
\end{aligned} \tag{5.35}$$

and

$$\begin{aligned}
&\mathrm{E}\,\Theta_N(\Theta_N - 1) = G''(1) = g_1''(1)\kappa_{N-2}(1) + 2g_1'(1)\kappa_{N-2}'(1) +\\
&g_1(1)\kappa_{N-2}''(1) + g_2''(1)\kappa_{N-3}(1) + 2g_2'(1)\kappa_{N-3}'(1) + g_2(1)\kappa_{N-3}''(1).
\end{aligned} \tag{5.36}$$

Therefore, $\operatorname{Var}\Theta_N = G''(1) + G'(1) - (G'(1))^2$ and to verify the announced formulae, one needs to check the validity of the equalities

$$\alpha_0(1) = 1, \quad \alpha_1(1) = -q, \quad \alpha_0'(1) = \frac{2-q^2}{1+q}, \quad \alpha_1'(1) = -\frac{q^2}{1+q},$$
$$\alpha_0''(1) = 4\frac{1-q}{q+1} - \frac{2}{(q+1)^3}, \quad \alpha_1''(1) = -\frac{2\,(1-q)^2}{q+1} + \frac{2}{(q+1)^3},$$
$$g_1(1) = 1, \quad g_2(1) = q,$$
$$g_1'(1) = q^3 - q^2 - 3q + 5, \quad g_2'(1) = -q\left(q^2 + 2q - 5\right),$$
$$g_1''(1) = 6q^3 - 2q^2 - 22q + 20, \quad g_2''(1) = 2q\left(q^3 - 2q^2 - 8q + 10\right),$$
$$\kappa_N(1) = \frac{1-(-q)^N}{1+q},$$
$$\kappa_N'(1) = N\frac{2-q^2}{(1+q)^2} + \frac{(-q)^N(2-q(1+q)N)-2}{(1+q)^3},$$
$$\kappa_N''(1) = \frac{2N\,(1-q)\left(2+(1-q)\,(-q)^{N-1}\right)}{(q+1)^2} +$$
$$\frac{N\,(N-1)\left(\left(2-q^2\right)^2 - (-q)^{N+2}\right) - 2\,(1-q)\,(3-q)\left(1-(-q)^N\right)}{(q+1)^3} -$$
$$\frac{2N\left(-2q^2+5+(-q)^{N-1}\left(2q^2+1\right)\right)}{(q+1)^4} + 12\frac{1-(-q)^N}{(q+1)^5},$$

substitute them into (5.35)–(5.36), and carefully compute the terms. □

Proof of corollary 3.3.4. *Step 1: expansions.* Applying Taylor's formula, we obtain the following equalities (for $\lambda \to 0$):

$$p^2\mathrm{e}^{4\lambda} + 4q\mathrm{e}^{\lambda}\left(q + p\mathrm{e}^{\lambda}\right) =$$
$$(1+q)^2\left[1 + \frac{4\lambda}{(1+q)^2} + 2\lambda^2\left(\frac{2-q}{1+q}\right)^2 + O(\lambda^3)\right];$$
$$\sqrt{p^2\mathrm{e}^{4\lambda} + 4q\mathrm{e}^{\lambda}(q + p\mathrm{e}^{\lambda})} =$$
$$(1+q)\left(1 + \frac{2\lambda}{(1+q)^2} + \lambda^2\left(\left(\frac{2-q}{1+q}\right)^2 - \frac{2}{(1+q)^4}\right) + O(\lambda^3)\right);$$
$$\alpha_0 = 1 + \lambda\frac{2-q^2}{1+q} + \frac{\lambda^2}{2}\left(2(1-q) + \frac{(2-q)^2}{(1+q)} - \frac{2}{(1+q)^3}\right) + O(\lambda^3);$$
$$\alpha_1 = -q - \lambda\frac{q^2}{1+q} + \frac{\lambda^2}{2}\left(2(1-q) - \frac{(2-q)^2}{(1+q)} + \frac{2}{(1+q)^3}\right) + O(\lambda^3). \tag{5.37}$$

Let c_{ij} denote a coefficient near λ^j in the expansion of $\frac{\alpha_i}{(-q)^i}$ for $j = 0, 1, 2$ and $i = 0, 1$. Then

$$\ln\left(\frac{\alpha_i}{(-q)^i}\right)^N = N\left(c_{i1}\lambda + \left(c_{i2} - \frac{c_{i1}^2}{2}\right)\lambda^2\right) + O(N\lambda^3). \tag{5.38}$$

Consequently,

$$\begin{aligned}(\alpha_0 - \alpha_1)\kappa_N(\lambda) = \alpha_0^N - \alpha_1^N = \mathrm{e}^{N\ln\alpha_0} - (-1)^N \mathrm{e}^{N\ln\left(q\frac{\alpha_1}{-q}\right)} = \\ \exp\left\{N\left(c_{01}\lambda + \left(c_{02} - \frac{c_{01}^2}{2}\right)\lambda^2\right) + O(N\lambda^3)\right\} - \\ (-1)^N \exp\left\{N\left(c_{11}\lambda + \left(c_{12} - \frac{c_{11}^2}{2}\right)\lambda^2\right) + N\ln q + O(N\lambda^3)\right\}.\end{aligned} \tag{5.39}$$

Finally, let $g_i(x)$ denote the same polynomials as given in (5.34). Taylor expanding yields

$$g_1(\mathrm{e}^\lambda) = 1 + O(\lambda), \quad g_2(\mathrm{e}^\lambda) = q + O(\lambda).$$

Combining all above, we then obtain the following asymptotic expansion for the moment-generating function:

$$M_{\Theta_N}(\lambda) = \frac{1 + O(\lambda)}{1 + q + O(\lambda)}\left((1 + O(\lambda))\kappa_{N-2}(\lambda) + (q + O(\lambda))\kappa_{N-3}(\lambda)\right) \tag{5.40}$$

with asymptotic expressions for $\kappa_{N-2}, \kappa_{N-3}$ stemming from (5.39).

Step 2: LLN. To prove relationship $\frac{\Theta_N}{N} \xrightarrow{L_2} \frac{2-q^2}{1+q}$, note that, by Corollary 3.3.3,

$$\begin{aligned}\mathrm{E}\left(\frac{\Theta_N}{N} - \frac{2-q^2}{1+q}\right)^2 = \mathrm{E}\left(\frac{\Theta_N}{N} - \mathrm{E}\,\frac{\Theta_N}{N}\right)^2 + \left(\mathrm{E}\,\frac{\Theta_N}{N} - \frac{2-q^2}{1+q}\right)^2 = \\ \frac{1}{N^2}\left(\mathrm{Var}\,\Theta_N + \left(\frac{q^2+q-1}{(1+q)^2}\left(1 - (-q)^N\right)\right)^2\right) = O\left(\frac{1}{N}\right).\end{aligned}$$

To prove a.s. convergence, we bound the probability

$$\begin{aligned}\mathrm{P}\left(\left|\frac{\Theta_N}{N} - \frac{2-q^2}{1+q}\right| > \gamma\frac{\ln N}{\sqrt{N}}\right) = \\ \mathrm{P}\left(\frac{\Theta_N}{\sqrt{N}} - \sqrt{N}\frac{2-q^2}{1+q} > \gamma\ln N\right) + \\ \mathrm{P}\left(\frac{\Theta_N}{\sqrt{N}} - \sqrt{N}\frac{2-q^2}{1+q} < -\gamma\ln N\right),\end{aligned}$$

where $\gamma > 0$ is arbitrary yet fixed constant. By Markov's inequality,

$$\mathrm{P}\left(\frac{\Theta_N}{\sqrt{N}} - \sqrt{N}\frac{2-q^2}{1+q} > \gamma \ln N\right) \le \\ \mathrm{e}^{-\sqrt{N}\frac{2-q^2}{1+q}-\gamma\ln N}\,\mathrm{E}\,\mathrm{e}^{\frac{\Theta_N}{\sqrt{N}}} = \mathrm{e}^{-\sqrt{N}\frac{2-q^2}{1+q}-\gamma\ln N} M_{\Theta_N}\left(\frac{1}{\sqrt{N}}\right).$$

From results obtained in *Step 1* and after some rearrangement, it follows that

$$M_{\Theta_N}\left(\frac{1}{\sqrt{N}}\right) = \left(1 + O\left(\frac{1}{\sqrt{N}}\right)\right)\left(\mathrm{e}^{c_{01}\sqrt{N}+c_{02}-\frac{c_{01}^2}{2}+O(\frac{1}{\sqrt{N}})} - \\ (-1)^N \mathrm{e}^{c_{11}\sqrt{N}+c_{12}-\frac{c_{11}^2}{2}+N\ln q+O(\frac{1}{\sqrt{N}})}\right).$$

Since $c_{01} = \frac{2-q^2}{1+q}$ and

$$c_{11}\sqrt{N} - \frac{2-q^2}{1+q}\sqrt{N} + c_{12} - \frac{c_{11}^2}{2} + N\ln q = N\ln q\left(1 + O\left(\frac{1}{\sqrt{N}}\right)\right),$$

we obtain that

$$\mathrm{e}^{-\sqrt{N}\frac{2-q^2}{1+q}-\gamma\ln N} M_{\Theta_N}\left(\frac{1}{\sqrt{N}}\right) = \mathrm{e}^{-\gamma\ln N} O(1) \le \frac{C_q}{N^\gamma}$$

for some constant $C_q \in (0,\infty)$ independent of γ. In the same way,

$$\mathrm{P}\left(\frac{\Theta_N}{N} - \frac{2-q^2}{1+q} < -\gamma\frac{\ln N}{\sqrt{N}}\right) \le \mathrm{e}^{\sqrt{N}\frac{2-q^2}{1+q}-\gamma\ln N} M_{\Theta_N}\left(-\frac{1}{\sqrt{N}}\right) \le \frac{C_q}{N^\gamma},$$

provided C_q in the previous inequality was chosen large enough. Taking $\gamma > 1$, we then have that

$$\sum_{N=2}^{\infty} \mathrm{P}\left(\left|\frac{\Theta_N}{N} - \frac{2-q^2}{1+q}\right| > \gamma\frac{\ln N}{\sqrt{N}}\right) \le 2C_q \sum_{N=1}^{\infty} \frac{1}{N^\gamma} < \infty.$$

Hence the claim.

Step 3: CLT. It suffices to show that

$$M_{\sqrt{N}\left(\frac{\Theta_N}{N} - \frac{2-q^2}{1+q}\right)}(t) \xrightarrow[N\to\infty]{} M_\xi(t), \quad \xi \sim N(0,\sigma^2)$$

for some fixed $\varepsilon > 0$ and any fixed $t \in (-\varepsilon, \varepsilon)$. Applying expansions obtained in the *Step 1* and the reasoning similar to that of *Step 2*, we have

$$M_{\sqrt{N}\left(\frac{\Theta_N}{N}-\frac{2-q^2}{1+q}\right)}(t) = \mathrm{e}^{-t\sqrt{N}\frac{2-q^2}{1+q}} M_{\Theta_N}\left(\frac{t}{\sqrt{N}}\right) =$$
$$\mathrm{e}^{-tc_{01}\sqrt{N}}\left(1+O\left(\frac{1}{\sqrt{N}}\right)\right)\left[\mathrm{e}^{tc_{01}\sqrt{N}+t^2\left(c_{02}-\frac{c_{01}^2}{2}\right)+O(\frac{1}{\sqrt{N}})}-\right.$$
$$\left.(-1)^N \mathrm{e}^{tc_{11}\sqrt{N}+t^2\left(c_{12}-\frac{c_{11}^2}{2}\right)+N\ln q+O(\frac{1}{\sqrt{N}})}\right] =$$
$$\left(1+O\left(\frac{1}{\sqrt{N}}\right)\right)\mathrm{e}^{t^2\left(c_{02}-\frac{c_{01}^2}{2}\right)+O(\frac{1}{\sqrt{N}})}+O\left(q^N\right) \xrightarrow[N\to\infty]{} \mathrm{e}^{t^2\left(c_{02}-\frac{c_{01}^2}{2}\right)}.$$

Direct calculations show that $c_{02} - \frac{c_{01}^2}{2} = \frac{\sigma^2}{2}$.

Step 4: LDP. To prove the final claim, we apply Gärtner-Ellis (GE) Theorem (see [16], Section 2.3) to $Z_N = \frac{\Theta_N}{N}$. First, note that, for any fixed $\lambda \in \mathbb{R}$,

$$\alpha_0(\lambda) > |\alpha_1(\lambda)| \Rightarrow \lim_{N\to\infty}\frac{\kappa_{N-3}(\lambda)}{\kappa_{N-2}(\lambda)} = \frac{1}{\alpha_0(\lambda)} \Rightarrow$$
$$\Lambda(\lambda) := \lim_{N\to\infty}\frac{1}{N}\ln M_{Z_N}(N\lambda) = \lim_{N\to\infty}\frac{1}{N}\ln M_{\Theta_N}(\lambda) =$$
$$\lim_{N\to\infty}\frac{1}{N}\ln\alpha_0^N(\lambda) = \ln\alpha_0(\lambda) \in \mathbb{R}.$$

Since $\mathbb{R} \ni \lambda \mapsto \Lambda(\lambda)$ is differentiable at every $\lambda \in \mathbb{R}$, it follows that all GE assumptions hold and Θ_N satisfies LDP with a good rate function I equal to the Legendre transform of Λ. □

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Santrauka (Summary in Lithuanian)

Tyrimų sritis

Grupinio testavimo[4] (GT) modeliai taikomi tais atvejais, kai reikia klasifikuoti objektus pagal tyrėją dominantį požymį į dvi grupes — turinčius požymį ir neturinčius požymio. Nuo įprasto ištisinio testavimo, kai testuojami visi objektai, GT modeliai skiriasi tuo, kad individualių objektų testavimas atskirose viso testavimo proceso fazėse keičiamas jų grupių (iš čia pavadinimas) testavimu taip bandant sutaupyti bendrą testų skaičių ir sumažinti su jais susijusias išlaidas. Tradiciškai literatūroje metodologijos pradininku laikomas R. Dorfman, straipsnyje [19] aprašęs pirmą grupinio testavimo procedūrą (toliau ją vadinsime D procedūra), skirtą tirti JAV karių, dalyvavusių antrame pasauliniame kare, kraujo mėginius sifilio užkratui rasti. Jo idėja buvo tokia. Turint N kraujo mėginių, reikia juos sumaišyti ir ištirti gautą grupės mėginį. Jei testas užkrato nerodo, visi N tiriamųjų sveiki; jei rodo — reikia ištestuoti kiekvieną tiriamąjį individualiai. Reguliariomis sąlygomis sifilis nėra dažna liga, todėl tokia metodika leidžia sutaupyti nemažai testų, nes testuojant masiškai N dydžio grupėmis dominuos sveikų tiriamųjų grupės, kurioms vietoje N testų pakaks vieno testo, ir tik retais atvejais pasitaikys grupės su infekuotais asmenimis (tada grupei bus sunaudotas $N + 1$ testas).

Per 80 metų, praėjusių nuo [19] straipsnio publikavimo, GT idėja išplito į įvairias žmonijos veiklos sritis, kuriose reikia testuoti ir identifikuoti požymį turinčius objektus. Šiandien šie modeliai sutinkami medicinoje (identifikuojant pacientus, sergančius infekcinėmis (ir kitomis) ligomis kaip ŽIV [58, 61, 65], hepatitas B [15, 23, 28, 60] ar COVID-

[4]kitaip — kaupinių testavimo

19 [13, 47, 49, 52, 64]), informacinių technologijų sektoriuje (aktyvių vartotojų [35, 82] ar neveikiančių jutiklių [50] komunikaciniuose tinkluose paieška; taikymai kibernetinio saugumo [31, 32, 44, 51, 87], duomenų bazių valdymo [26], kodavimo teorijos ir duomenų spūdos [36, 67] srityse), kokybės kontrolėje [42] ir kitur. Tai dinamiška, aktyviai tebevystoma ir tiriama sritis.

Tyrimų objektas ir uždaviniai

Sąvokos, žymenys ir prielaidos

Tyrėją dominantis požymis priklauso nuo taikymo srities, todėl jį turintys objektai skirtingose srityse vadinami skirtingai. Gamyboje — tai defektiniai gaminiai, medicinoje — infekuoti pacientai, komunikaciniame tinkle — pasyvūs mazgai ir t.t. Apibrėžtumo dėlei visoje tolimesnėje santraukos dalyje požymį turinčius objektus vadinsime defektiniais, o jo neturinčius — gerais, nedefektiniais arba be defekto.

N raide žymėsime testuojamos grupės dydį. Kai kuriuose GT modeliuose jis gali būti parametrizuojamas natūraliu parametru n (konkretus pavyzdys pateikiamas tolimesniame poskyryje); tada N bus n funkcija: $\mathbb{N} \ni n \mapsto N(n) \in \mathbb{N}$.

Nagrinėsime binarinius testavimo modelius. Juose tariama, kad grupės testo rezultatas gali būti tik dvireikšmis: jei grupėje yra bent vienas defektinis objektas, testo rezultatas lygus 1; jei visi objektai be defekto — rezultatas lygus 0. Jei grupei, kurioje yra daugiau nei vienas objektas (vieno objekto grupės irgi galimos), pritaikytas testas teigiamas, tai jis nenusako kurie objektai turi defektą.

Pagrindinės prielaidos, kuriomis remiasi disertacijoje nagrinėti modeliai, vadinamos *binominio testavimo prielaidomis* (BTP) ir formuluojamos taip:

(BTP1) testavimo pradžioje kiekvienas objektas gali būti defektinis su ta pačia eigoje nekintančia tikimybe $p \in (0, 1)$;

(BTP2) objektai yra nepriklausomi;

(BTP3) naudojamas (fizinis) testas yra tobulas (jautrumas ir specifiškumas yra lygūs 100%) ir nepriklauso nuo testuojamos grupės dydžio.

Remdamiesi BTP galime griežtai apibrėžti disertacijoje nagrinėtą bendrą modelį.

- Tegu $Y_1, \ldots, Y_N$ yra nepriklausomi vienodai pasiskirstę Bernulio atsitiktiniai dydžiai (toliau a.d.);
- $Y_i = 1 \iff i$-asis objektas defektinis (toki atveju $Y_i = 0 \iff i$-asis objektas yra be defekto);
- Bet kuriai testavimo procedūrai X ir bet kokiai netuščiai $A \subset \{Y_1, \ldots, Y_N\}$ teisinga lygybė $X(A) = \mathbb{1}\{\Sigma_{Y_i \in A} Y_i > 0\}$.

Turint grupę $C = \{Y_1, \ldots, Y_N\}$ ir testavimo procedūrą X, T_X žymės (atsitiktinį) testų skaičių, reikalingą tam, kad identifikuoti visus defektinius aibės C elementus; $\theta_X(N, p) = \mathrm{E}\, T_X$ žymės a.d. T_X vidurkį. Atkreipsime dėmesį, kad θ_X yra dviejų argumentų ($N \in \mathbb{N}$ ir $p \in (0, 1)$) funkcija. Visoje santraukoje q žymės dydį $1 - p$.

Nagrinėti modeliai

Šiame poskyryje pateikiami konkrečių disertacijoje tirtų GT procedūrų, tenkinančių BTP, algoritmai.

Dorfman procedūra D Šią procedūrą jau aprašėme įvade. Ją sudaro du žingsniai.

> Žingsnis nr. 1: testuojame visos grupės jungtinį mėginį JM;
>
> Žingsnis nr. 2: jei JM testas neigiamas, baigiame; priešingu atveju pakartotinai testuojame kiekvieną objektą individualiai.

Iš procedūros aprašymo išplaukia lygybė

$$T_D = 1 + N\mathbb{1}\{Y_1 + \cdots + Y_N > 0\};$$

todėl,

$$\theta_D(N, p) = 1 + N\,\mathrm{E}\,\mathbb{1}\{Y_1 + \cdots + Y_N > 0\} = 1 + N(1 - q^N). \quad \text{(S.1)}$$

Modifikuota Dorfman procedūra MD Sobel ir Groll darbe [72] pastebėjo, kad D procedūroje galimas perteklinis testas ir pasiūlė tokią pataisą: jeigu pradinis jungtinio mėginio testas buvo teigiamas ir pakartotinai ištestavus $N-1$ objektų defektinis vis dar nebuvo aptiktas, tai paskutinio objekto testuoti nebereikia (ir taip aišku, kad jis defektinis). Remiantis procedūros aprašymu

$$T_{MD} = 1 + (N-1)\mathbb{1}\{Y_1 + \cdots + Y_N > 0\} + \mathbb{1}\{Y_1 + \cdots + Y_{N-1} > 0\}.$$

Taigi,

$$\theta_{MD}(N,p) = 1+(N-1)(1-q^N)+1-q^{N-1} = 1-pq^{N-1}+N(1-q^N). \quad \text{(S.2)}$$

Sterrett procedūra ST Sterrett [73] pasiūlė kitą D procedūros modifikaciją, nusakomą tokiu algoritmu.

Žingsnis nr. 1: testuojame visos grupės jungtinį mėginį JM;

Žingsnis nr. 2: jei JM testas neigiamas, baigiame; priešingu atveju vykdome žingsnį nr. 3;

Žingsnis nr. 3: pakartotinai testuojame po vieną objektą tol, kol aptinkame pirmą defektinį; jei ištestuota visa grupė, baigiame; priešingu atveju likusią netestuotą grupės dalį laikome nauja pradine grupe ir jai taikome algoritmą pradėdami nuo žingsnio nr. 1.

Darbe [72] buvo parodyta, kad

$$\theta_{ST}(N,p) = 2q - p^{-1}(1-q^{N+1}) + (2-q)N. \quad \text{(S.3)}$$

Porinė testavimo procedūra PT Ši procedūra nagrinėta Yao ir Hwang darbe [85]. Ji nusakoma žemiau pateikiamu algoritmu, kurio kiekviename žingsnyje aibė C žymi testuojamų objektų aibę.

Žingsnis nr. 1: jei aibėje C yra vienintelis elementas, atliekame jo testavimą ir baigiame; jei elelementų išvis nėra, baigiame; priešingu atveju vykdome žingsnį nr. 2;

Žingsnis nr. 2: iš aibės C, turinčios $N \geq 2$ objektų, parenkame du; suformuojame jungtinį mėginį ir ištestavę jį vykdome žingsnį nr. 3;

Žingsnis nr. 3:

- jei jungtinio mėginio testas neigiamas, priskiriame abu objektus grupei be defekto, $N = N - 2$, $C = C \setminus \{\text{testuota pora}\}$;
- jei jungtinio mėginio testas teigiamas, parenkame bet kurį iš dviejų objektų ir pakartotinai ištestuojame; jei jo testas neigiamas, priskiriame netestuotą objektą grupei su defektu, $N = N - 2$, $C = C \setminus \{\text{testuota pora}\}$; jei jo testas teigiamas, $N = N - 1$, $C = C \setminus \{\text{pakartotinai testuotas objektas}\}$.

Žingsnis nr. 4: pradėti viską iš naujo nuo žingsnio nr. 1.

Darbe [85] išvesta ši a.d. T_{PT} vidurkio formulė:

$$\theta_{PT}(N,p) = N\frac{2-q^2}{1+q} + \frac{q^2+q-1}{(1+q)^2}(1-(-q)^N). \tag{S.4}$$

Kvadratinės matricos procedūra A2 Procedūra[5] pasiūlyta Phatarfod and Sudbury [63]; vėliau apibendrinta Berger, Mandell ir Subrahmanya [9]. Norint taikyti procedūrą, reikia, kad bendras mėginių skaičius N būtų pavidalo $N = n^2, n \in \mathbb{N}$. Galiojant šiai sąlygai, procedūra nusakoma žemiau pateikiamu algoritmu.

Žingsnis nr. 1: išdėstome turimus mėginius ant $n \times n$ kvadratinės matricos;

Žingsnis nr. 2: suformuojame n jungtinių mėginių, atitinkančių eilutes, ir n jungtinių mėginių, atitinkančių stulpelius; ištestuojame šiuos $2n$ mėginius;

Žingsnis nr. 3: jei visi testai neigiami, baigiame; priešingu atveju pakartotinai testuojame objektus I_{ij}, tenkinančius sąlygą „eilutės i stulpelio j testai teigiami“.

Phatarfod ir Sudbury [63] apskaičiavo vidutinį A2 testų skaičių:

$$\theta_{A2}(N,p) = 2n + n^2\left(1-2q^n+q^{2n-1}\right) = 2\sqrt{N} + N\left(1-2q^{\sqrt{N}}+q^{2\sqrt{N}-1}\right). \tag{S.5}$$

[5] žymuo A2 nuo angl. square array

Disertacijoje spręsti Grupinio testavimo uždaviniai

Prieš įvardindami disertacijoje spręstus uždavinius, aptarsime tipinius GT uždavinius.

Tipniai Grupinio testavimo uždaviniai

Tegu X — fiksuota GT procedūra. Kadangi pagrindinis GT tikslas yra minimizuoti $\theta_X(N,p)$ ir paprastai tikimybę p galima (bent jau trumpuoju laikotarpiu) laikyti nekintančia, vienas tipinių GT teorijos uždavinių — rasti optimalų testuojamos grupės dydį N, kai tikimybė p laikoma nekintančia. Formaliai problema nusakoma pasitelkiant funkciją

$$\mathbb{N} \times (0,1) \ni (N,p) \mapsto t_X(N,p) := \frac{\theta_X(N,p)}{N}, \tag{S.6}$$

žyminčią vidutinį testų skaičių, tenkantį vienam objektui tuo atveju, kai testuojamos grupės dydis yra N. Bet kuris globalus šios funkcijos minimumo taškas $N \in \arg\min_{N\in\mathbb{N}} t_X(N,p)$ vadinamas optimalia konfigūracija ir žymimas N_{opt}^X. Kadangi p yra fiksuota, $N_{opt}^X = N_{opt}^X(p)$ priklauso nuo p. Iš to išplaukia keli svarbūs pastebėjimai.

Funkcija $(0,1) \ni p \mapsto N_{opt}^X(p)$ rodo kaip kinta optimalios grupės dydis, kai testuojame maksimizuodami vidutinį išlošį

$$G_X(p) := 1 - t_X(N_{opt}^X(p), p) \tag{S.7}$$

ilgoje testavimo (grupėmis) serijoje. Intuityviai aišku, kad bet kuriai tipinei testavimo procedūrai X funkcija $(0,1) \ni p \mapsto N_{opt}^X(p)$ bus nedidėjanti, $G_X(p) \xrightarrow[p\to 0+]{} 1-$, o $N_{opt}^X(p) \xrightarrow[p\to 0+]{} \infty$. Kai kuriuose praktiniuose taikymuose egzistuoja natūralūs apribojimai testuojamų grupių dydžiams, kuriuos peržengus testo charakteristikos tampa nebepriimtinos — drastiškai sumažėja jautrumas ir/arba specifiškumas. Žinant maksimalią slenkstinę vertę $N_{\max}$, kurią peržengus stebimas minėtas efektas, galima rasti sritį $R_X = \{p \in (0,1) : N_{opt}^X(p) \le N_{\max}\}$; tam reikia išreikštinio funkcijos $(0,1) \ni p \mapsto N_{opt}^X(p)$ pavidalo. Išreikštinis šios funkcijos pavidalas leidžia palyginti kelias procedūras ir pasirinkti labiausiai tinkančią turimai problemai: jei $X_i, i = 1,\ldots,k$, yra problemai tinkančios procedūros, galima apskaičiuoti išlošius $G_{X_i}(p)$ ir grupių dydžius $N_{opt}^{X_i}(p)$ skirtingoms p reikšmėms bei kiekvienai p reikšmei atsirinkti labiausiai tinkančią procedūrą.

Su funkcija N_{opt}^X tampriai susijęs dar vienas tipinis GT uždavinys — optimalaus tikimybinio slenksčio (OTS) $p_c^X \in (0,1)$ radimas. Šio uždavinio apibrėžimą iš pradžių paaiškinsime neformaliai. Kaip minėta įvade D procedūros atveju ir kaip sufleruoja intuicija, GT metodika turėtų pasiteisinti tik tada, kai defekto tikimybė p pakankamai maža. Pvz., prisiminus Dorfman procedūrą aišku, kad didelėms p reikšmėms grupėje iš N objektų dažnai pasitaikys bent vienas defektinis ir tokiais atvejais, užuot naudoję N testų testuodami individualiai, taikydami D procedūrą naudosime $N+1$ testą; todėl OTS radimo uždavinys formuluojamas taip: fiksavus procedūrą X reikia rasti tokią $p_c^X \in (0,1)$ reikšmę, kad $\forall p \in (p_c^X, 1)$ $N_{opt}^X(p) = 1$. Bendrame BTP kontekste šią problemą sprendė Ungar. Darbe [79] jis gavo šį fundamentalų GT rezultatą.

Teorema S.0.1. *Binominių GT procedūrų taikymas turi prasmę tada ir tik tada, kai $p \in \left(0, \frac{3-\sqrt{5}}{2}\right)$: jei $p \notin \left(\frac{3-\sqrt{5}}{2}, 1\right)$, tai neegzistuoja GT procedūros, kuri vidutiniškai naudotų mažiau nei vieną testą objektui (t.y., $t_X(N_{opt}^X(p), p) \geq 1$ su bet kokia procedūra X); jei $p \in \left(0, \frac{3-\sqrt{5}}{2}\right)$, tai atsiras bent viena tokia procedūra X, kad $t_X(N_{opt}^X(p), p) < 1$.*

Binominio GT literatūroje skaičius $\frac{3-\sqrt{5}}{2}$ dažnai vadinamas universaliu tikimybiniu slenksčiu (toliau UCP nuo angl Universal Cut-Point). Kai kurioms GT procedūroms jis sutampa su p_c^X, t.y.

$$G_X(p) = 0 \iff p \geq \frac{3-\sqrt{5}}{2}.$$

Kita vertus, egzistuoja tokios procedūros, kurioms

$$G_X(p) = 0 \iff p \geq p_c^X \text{ su } p_c^X < \frac{3-\sqrt{5}}{2}.$$

Taigi, tiriant konkrečią procedūrą X, visų pirma svarbu surasti p_c^X. Atsižvelgiant į teoremą S.0.1, visoje disertacijoje (ir santraukoje), funkcijos, priklausančios nuo p, nagrinėjamos tik intervale $\left(0, \frac{3-\sqrt{5}}{2}\right)$.

Disertacijoje spręsti uždaviniai

- Trims GT procedūroms — MD, ST ir A2 — spręstas išreikštinio N_{opt}^X pavidalo radimo uždavinys.

- Specifiniam procedūrų poklasiui, tenkinančiam BTP, konstruotas p_c^X radimo algoritmas.
- Ieškotas būdas, leidžiantis charakterizuoti a.d. T_{PT} skirstinį taip įvertinant PT procedūros tikimybines savybes.

Disertacijos struktūra

Disertaciją sudaro penki skyriai. Pirmasis skirtas įvadui. Jame aptariama GT idėja, apžvelgiama raidos istorija, pateikiami taikymų pavyzdžiai iš įvairių veiklos sričių. Antrame skyriuje apibrėžiamos disertacijoje vartojamos sąvokos ir žymėjimai, detaliai aprašomas disertacijos tyrimo objektas. Trečiajame skyriuje suformuluoti teoriniai tyrimų rezultatai, pateikiami taikymų pavyzdžiai. Ketvirtasis skyrius skirtas rezultatų aptarimui ir baigiamosioms pastaboms. Paskutiniame skyriuje surinkti teorinių rezultatų įrodymai.

Rezultatų apžvalga

Kiekvienam disertacijoje spręstam uždaviniui skiriamas atskiras poskyris, kuriame suformuluoti gauti teoriniai rezultatai ir aptariama susijusi literatūra.

Optimalios Modifikuotos Dorfman, Sterrett ir Kvadratinės matricos procedūrų konfigūracijos

Mūsų žiniomis, darbų, kuriuose ieškota analizinė N_{opt}^X išraiška, nėra daug. D procedūra nagrinėta Samuels straipsnyje [66]. Jame parodyta, kad[6] $N_{opt}^D(p) \in \{\lfloor\sqrt{p^{-1}}\rfloor + 1, \lfloor\sqrt{p^{-1}}\rfloor + 2\}$, kai $p \in (0, 1 - (1/3)^{1/3}) \approx (0, 0.31)$ ir $N_{opt}^D(p) = 1$, kai[7] $p \geq 1 - (1/3)^{1/3}$. Modifikuotos Dorfman procedūros MD, Sterrett procedūros ST ir kvadratinės matricos procedūros A2 atvejais tikslios analizinės išraiškos N_{opt}^X nebuvo žinomos ilgą laiką. Tiksliau tariant, MD ir ST atveju, Malinovsky ir Albert [55]

[6]čia ir toliau $\lfloor x \rfloor$ žymi sveikąją skaičiaus $x \in \mathbb{R}$ dalį; $\lceil x \rceil = x$, kai $x \in \mathbb{Z}$ ir $\lceil x \rceil = \lfloor x \rfloor + 1$, kai $x \in \mathbb{R} \setminus \mathbb{Z}$

[7]pastarasis rezultatas taip pat rodo, kad procedūros D atveju $p_c^D = 1 - (1/3)^{1/3}$ yra griežtai mažesnis už universalų slenkstį $UCP = \frac{3-\sqrt{5}}{2}$

skaitiškai nuspėjo šias išraiškas gana plačiame p reikšmių intervale ir iškėlė hipotezę, kad jos turėtų būti tokios pat visoms $p \in (0, UCP)$ reikšmėms. Mūsų darbe [88] mes patvirtinome jų hipotezes įrodydami žemiau pateikiamas teoremas.

Teorema S.0.2. *Tegu*

$$g_0(p) := \frac{1}{q}\left(\frac{1-2pq}{q\left(1-\ln q\sqrt{\frac{2}{p}}\right)}\right)^{\sqrt{\frac{p}{2}}} \quad su \quad p \in \left(0, \frac{3-\sqrt{5}}{2}\right). \tag{S.8}$$

Aibė $g_0^{-1}(\{1\})$ *sudaryta iš vieno taško* $p_* \approx 0.1711$.

$$N_{opt}^{ST}(p) \in \left\{\lfloor\sqrt{2p^{-1}}\rfloor, \lfloor\sqrt{2p^{-1}}\rfloor + 1\right\}, \textit{kai } p \in \left(p_*, \frac{3-\sqrt{5}}{2}\right);$$

$$N_{opt}^{ST}(p) \in \left\{\lfloor\sqrt{2p^{-1}}\rfloor, \lfloor\sqrt{2p^{-1}}\rfloor + 1, \lfloor\sqrt{2p^{-1}}\rfloor + 2\right\}, \textit{kai } p \in (0, p_*].$$

Teorema S.0.3. *Su visomis* $p \in \left(0, \frac{3-\sqrt{5}}{2}\right)$ *reikšmėmis*

$$N_{opt}^{MD}(p) \in \left\{\lfloor\sqrt{p^{-1}}\rfloor, \lfloor\sqrt{p^{-1}}\rfloor + 1\right\}. \tag{S.9}$$

A2 procedūra tirta Hudgens ir Kim darbe [38]. Autoriams pavyko gauti gana tikslius apatinius ir viršutinius $N_{opt}^{A2}(p)$ rėžius, tačiau analizinė šios funkcijos išraiška liko nežinoma. Jie taip pat nagrinėjo OTS problemą ir surado p_c^{A2} reikšmę. Darbe [89] mums pavyko išvesti analizinę $N_{opt}^{A2}(p)$ išraišką ir pateikti papildomų įžvalgų apie p_c^{A2} (žr. pastabą S.0.6 apačioje). Prieš formuluodami gautus rezultatus, priminsime, kad A2 atveju testuojamos grupės dydis N parametrizuojamas natūraliu parametru n: $N(n) = n^2$. Be to, A2 atveju mums buvo patogiau traktuoti t_{A2} kaip funkciją $[2,\infty) \times (UCP, 1) \ni (n, q) \mapsto t_{A2}(n, q)$ su tolydžiu argumentu $n \in [2, \infty)$ užuot laikius ją argumentų (N, p), kintančių aibėje $\{n^2 : n \in \mathbb{N}\} \times (0, UCP)$, funkcija. Žemiau pateikiamuose teiginiuose šis susitarimas galioja.

Teorema S.0.4. *Tegu* $g(q, n) = \frac{2}{n} - 2q^n + q^{2n-1} = t_{A2}(n, q) - 1$.

(i) *Srityje* $(q, n) \in (1/2, 1) \times (2, \infty)$ *egzistuoja vienintelis sistemos*

$$\begin{cases} 1 = nq^n\left(1 - \frac{q^{n-1}}{2}\right) \\ n \ln q = -\frac{\left(1-\frac{q^{n-1}}{2}\right)}{(1-q^{n-1})} \end{cases}$$

sprendinys $(q_*, n_*) \approx (0.748416, 4.453524)$.

(ii) n *atžvilgiu bet kokiai fiksuotai* $q \in (q_*, 1)$ *reikšmei lygtis* $g(q, n) = 0$ *turi du sprendinius* $n_L, n_U : 2 < n_L < n_* < n_U < \infty$. *Intervale* (n_L, n_U) *funkcija* $n \mapsto g(q, n)$ *įgyja neigiamas reikšmes, o aibėje* $(2, \infty) \setminus [n_L, n_U]$ *— teigiamas.*

(iii) Fiksuotai $q \in (q_*, 1)$ *reikšmei A2 procedūra efektyvi intervale* (n_L, n_U), *t.y.* $t_{A2}(q, n) < 1$ *su visais* $n \in (n_L, n_U)$. *Šiame intervale egzistuoja vienintelis (ir todėl globalus) funkcijos* $(2, \infty) \ni n \mapsto t_{A2}(q, n)$ *minimumo taškas* n_{min}. *Jei* $q \in [0.755, 1)$, *tai*

$$n_{min} = \frac{1}{p^{\frac{2}{3}}} + \frac{1}{2p^{\frac{1}{3}}} + 0.2 + 3p^2 + t_*$$

su $t_* \in [0, 1]$.

(iv) Fiksuotai $q \in (q_*, 1)$ *reikšmei intervale* (n_U, ∞) *funkcija* $(2, \infty) \ni n \mapsto t_{A2}(n, q)$ *taip pat turi vienintelį (ir todėl globalų) maksimumo tašką. Bet kokiai* $q \in (0, q_*)$ *reikšmei A2 nėra optimali: funkcija* $(2, \infty) \ni n \mapsto t_{A2}(n, q)$ *įgyja reikšmes intervale* $(1, \infty)$.

Išvada S.0.5. *Tegu* $g(q, n)$ *tokia pati kaip teoremoje S.0.4. Lygtis* $g(q, 5) = 0$ *turi vienintelį sprendinį* $q_5 \approx 0.750209961$. *Visoms* $q \in (q_5, 1)$ *reikšmėms* $n_{opt}(q)$ *priklauso aibei*

$$\left\{ \left\lfloor \frac{1}{p^{\frac{2}{3}}} + \frac{1}{2p^{\frac{1}{3}}} + 3p^2 + 0.2 \right\rfloor + i : i = 0, 1, 2 \right\}.$$

Pastaba S.0.6. Gali susidaryti įspūdis, kad pateikti rezultatai nėra išsamūs (neaišku kokia yra $n_{opt}(q)$ reikšmė, kai $q \in (q_*, q_5)$). Taip nėra: remiantis teorema S.0.4, bet kokiai $q \in (q_*, q_5)$ reikšmei $t_{A2}(n_{min}, q) < 1$ su $n_{min} = n_{min}(q)$ iš (iii) dalies; iš disertacijoje pateikiamo įrodymo išplaukia, kad $n_{min}(q) \in (4, 5)$ ir $\min(t_{A2}(4, q), t_{A2}(5, q)) > 1$, kai $q \in (q_*, q_5)$. Hudgens ir Kim [38] analizavo A2 diskrečioje skalėje, t.y. tardami, kad $n \in \mathbb{N}$. Jie įrodė, kad:

- imant $n = 2, 3, 4$ ir bet kokią q reikšmę procedūra A2 nėra optimali;
- $\forall q \in (q_5, 1)$ funkcija $\{5, 6, \ldots\} \ni n \mapsto t_{A2}(n, q)$ įgyja reikšmes mažesnes už 1.

Faktiškai jų rezultatai reiškia, kad $(q_5, 1)$ — tai tas intervalas, kuriame A2 efektyvi arba kitaip — kad $p_c^{A2} = 1 - q_5$. Kaip matome, mūsų analizė pateikia papildomų įžvalgų apie p_c^{A2} ir procedūros A2 elgesį tolydžioje skalėje. Įžvalgos įdomios iš teorinės pusės, tačiau pridėtinės praktinės vertės nesuteikia. $\square$

Optimalaus tikimybinio slenksčio paieškos algoritmas

OTS paieška p_c^X — svarbi problema: konkrečioje situacijoje žinodami, kad $p > p_c^X$, iškart žinome, kad procedūros X taikymas prasmės neturi. Vis dėlto, mūsų žiniomis, teorema S.0.1 yra vienintelis bendro pobūdžio rezultatas, skirtas šiai problemai. Kitų autorių darbuose p_c^X radimas siejamas su konkrečios procedūros analize. Darbe [90] mes pasiūlėme algoritmą, leidžiantį surasti apytikrę OTS reikšmę ir dažnais atvejais rekonstruoti tikslią reikšmę p_c^X gana plačiai BTP tenkinančių procedūrų klasei. Analizės metu mes taip pat atskleidėme įdomų ryšį tarp GT ir dinaminių sistemų bifurkacijų teorijos. Pasiūlytas algoritmas tinka binominio testavimo procedūroms, tenkinančioms šiuos apribojimus.

(M0) $\exists c \geq 2$ toks, kad a-priori žinoma, jog procedūra X neefektyvi, kai $N \in [1, c)$.

(M1) Funkcija $\mathbb{N} \times (0, UCP] \ni (N, p) \mapsto \theta_X(N, p)$ gali būti traktuojama kaip tolydžiai kintančių argumentų funkcija aibėje $[c, \infty) \times (0, UCP]$ ir yra diferencijuojama šios aibės viduje.

(M2) $\forall N \in (c, \infty)$ funkcija $(0, UCP] \ni p \mapsto \theta_X(N, p)$ yra griežtai didėjanti.

(M3) $\forall N \in (c, \infty)\, t_X(N, UCP) > 1$.

(M4) $\forall N \in (c, \infty)\, \exists p \in (0, UCP) : t_X(N, p) < 1$.

Mūsų rezultatai pateikiami dviejuose žemiau suformuluotuose teiginiuose. Pirmasis charakterizuoja OTS savybes.

Teiginys S.0.1. *Tarkime, kad tenkinamos prielaidos (M0)–(M4). Tegu* $p_{X,c} = \sup\{p \in (0, UCP) \mid \exists N \in (c, \infty) : t_X(N, p) < 1\}$. *Tada* $\forall p \in (0, p_{X,c})$ *procedūra* X *efektyvi tolydžioje skalėje;* $\forall p \in (p_{X,c}, UCP]$ *ji neefektyvi jokia prasme, t.y.*

$$(N, p) \in (c, \infty) \times (p_{X,c}, UCP] \Rightarrow t_X(N, p) > 1.$$

Antrasis teiginys rodo, kad galiojant (M0)–(M4) egzistuoja $p_{X,c}$ radimo algoritmas, kuris gali būti aprašomas bifurkacijų teorijos terminais. Iš tikrųjų, traktuodami $p \in (0, UCP]$ kaip kontroliuojamą parametrą, o $N \in (c, \infty)$ — kaip latentinio tolydaus kintamojo funkciją, įveskime dinaminę sistemą, apibrėžiamą lygtimi

$$\dot{N} = t_X(N, p) - 1. \tag{S.10}$$

Teiginys S.0.2. *Tarkime, kad tenkinamos prielaidos (M0)–(M4); tada $p_{X,c}$ yra sistemos (S.10) bifurkacijos taškas ir galima išskirti tris žemiau aprašytus bifurkacijų tipus.*

(b0) $p_{X,c}$ yra vienintelė kontroliuojamo parametro reikšmė su kuria (S.10) turi fiksuotų taškų intervale (c, ∞). Šiuo atveju $p_{X,c} < UCP$ ir bet kuris $N \in (c, \infty)$ yra lygties $t_X(N, p_{X,c}) = 1$ sprendinys.

Jei egzistuoja tokia reikšmė $p_l \in (0, p_{X,c})$, kad (S.10) turi fiksuotą tašką $N \in (c, \infty)$, tai galimi du atvejai:

(b1) (S.10) turi fiksuotų taškų intervale (c, ∞) su visomis $p \in [p_l, p_{X,c})$ reikšmėmis, tačiau nėra fiksuotų taškų, atitinkančių reikšmę $p_{X,c}$;

(b2) (S.10) turi fiksuotų taškų intervale (c, ∞) su visomis $p \in [p_l, p_{X,c}]$ reikšmėmis įskaitant $p_{X,c}$ reikšmę, kuri šiuo atveju yra griežtai mažesnė už UCP.

Visais atvejais bifurkacijos kreivė indukuoja diferencijuojamą atvaizdį $(c, \infty) \ni N \mapsto p_N \in (0, p_{X,c}]$ ir $p_{X,c}$ lygus jo maksimumui. Turint (b0) ir (b2) tipų bifurkacijas, šis taškas gali būti surastas sprendžiant dviejų kintamųjų sistemą

$$\begin{cases} t_X(N, p) = 1, \\ \frac{\partial}{\partial N} t_X(N, p) = 0 \end{cases} \tag{S.11}$$

(t.y. N ir p atžvilgiu) ir parenkant maksimalią p reikšmę iš aibės $S = \{(N, p) \in (c, \infty) \times (0, UCP] \mid (N, p)$ yra sistemos (S.10) sprendinys$\}$. Turint (b1) tipo bifurkaciją $p_{X,c} = \max(\lim_{N \to c+} p_N, \lim_{N \to \infty} p_N)$; pastaroji lygybė galioja ir tuo atveju, kai sistema (S.11) neturi sprendinių aibėje $(c, \infty) \times (0, UCP]$.

Pateiksime kelias aiškinamąsias pastabas.

Pastaba S.0.7. Remiantis teiginiu S.0.2 galima rasti OTS tolydžioje skalėje (TOTS). Praktikoje testuojamos grupės dydis N yra sveikaskaitinis; todėl dirbama diskrečioje skalėje. Paprastai diskretus OTS (toliau DOTS), iki šiol žymėtas ir toliau žymimas tuo pačiu simboliu p_c^X, yra mažesnis už $TOTS = p_{X,c}$ iš teiginio S.0.1, tačiau skirtumai dažniausiai nežymūs (pavyzdžiai pateikiami disertacijoje). Kadangi p_c^X radimas dažnai sudėtingas, $p_{X,c}$ yra nebloga aproksimacija. Be to, kaip iliustruoja disertacijoje pateikiami pavyzdžiai, (b2) atveju DOTS neretai galima surasti naudojantis tokiu algoritmu:

- parenkame tokį N_c, kad pora $(N_c, p_{X,c})$ yra (S.11) sistemos sprendinys;
- imame $DOTS = \max(p_{\lfloor N_c \rfloor}, p_{\lceil N_c \rceil})$.

(b1) atveju DOTS dažnai sutaps su TOTS. □

Pastaba S.0.8. Procedūros A2 pavyzdys rodo, kad kai kuriais atvejais grupės dydis $N = N(n)$ yra argumento $n \in \mathbb{N}$ funkcija ir patogiau traktuoti θ_X, t_X bei kitas susijusias funkcijas kaip argumento (n, p) (o ne (N, p)) funkcijas. Keičiant N į n sąlygose (M0)–(M4) ir visose susijusiose funkcijose, nekeičia tvirtinimų S.0.2–S.0.1 išvadų jei $(c, \infty) \ni n \mapsto N(n)$ yra diferencijuojama ir griežtai didėjanti. □

Pastaba S.0.9. Mūsų manymu, bifurkacijos (b1)–(b2) yra dominuojančios — mes nesugebėjome rasti pavyzdžio, atitinkančio tipą (b0). Kita vertus, mes nesugebėjome eliminuoti šio atvejo teoriškai. □

Baigdami trumpai aptarsime sąlygų (M0)–(M1) prasmę ir stiprumą.

(M0) galima traktuoti kaip sąlygą, reikalingą apriboti dinaminės sistemos (S.10) kitimo sritį. Jos neapribojus, bifurkacijos kreivės forma galėtų smarkiai pasikeisti (atitinkamas pavyzdys pateikiamas disertacijoje). Kartu su sąlyga (M3), ji apibrėžia kraštinę reikšmę $p_{X,c}$ radimui tais atvejais, kai $p_{X,c} = UCP$. Tipinėje situacijoje galima imti $c = 2$; tada (M0) bus tenkinama, o lygybė $c = 2$ jokio esminio apribojimo nededa, nes nagrinėjamame kontekste ji tereiškia, kad testuojant aibę iš vieno elemento jokia GT nereikalinga — vienam elementui visada reikia vieno testo.

Sąlyga (M1) yra stipriausia. Ją tenkina toli gražu ne visos procedūros. Pvz., procedūrai PT ji negalioja — iš lygties (S.4) matome, kad $\theta_{PT}(N, p)$

neišeina pratęsti iki funkcijos aibėje $[c, \infty) \times (0, UCP)$, įgyjančios reikšmes intervale $[0, \infty)$. Iš esmės ši sąlyga ir apibrėžia klasę, kuriai mūsų pasiūlytas metodas tinka, nes kitas sąlygas galima traktuoti kaip „natūralias“ ir tinkančias daugeliui GT procedūrų, tenkinančių BTP.

(M2) reiškia, kad didėjant defekto tikimybei vidutinis testų skaičius, tenkantis N dydžio grupei, irgi turėtų augti. Sąlygos pagrįstumui galima paminėti fundamentalų Yao ir Hwang darbą [86], kuriame parodyta, kad $\forall N \in \mathbb{N}$ funkcija $(0, UCP] \ni p \mapsto \inf_X \theta_X(N, p)$, kurioje infimumas imamas pagal visas galimas BTP tenkinančias procedūras, yra griežtai didėjanti.

Gali pasirodyti, kad (M3) eliminuoja visas procedūras, kurioms $p_{X,c} = UCP$. Disertacijoje pateikiami pavyzdžiai rodo, kad taip nėra. Mūsų manymu, (M3) eliminuoja optimalias procedūras[8]. Tai nėra trūkumas, nes optimalioms procedūroms lygybė $p_{X,c} = UCP$ labai tikėtina.

Galiausiai (M4) techniškai išreiškia faktą, kad mes nagrinėjame tik tas procedūras, kurios savo efektyvioje srityje turi prasmę bet kokiam testuojamų objektų skaičiui bent jau atskiroms defektyvumo tikimybių reikšmėms. Ši sąlyga galioja daugeliui procedūrų, nes, kaip minėta anksčiau, dažniausiai $N^X_{opt}(p) \xrightarrow[p \to 0+]{} \infty$.

Porinės testavimo procedūros analizė

Tarp disertacijoje tirtų procedūrų PT užima išskirtinę vietą: darbe [85] buvo parodyta, kad intervale $p \in \left[1 - \frac{1}{\sqrt{2}}, UCP\right]$ PT procedūra yra globaliai optimali įdėtųjų procedūrų (angl. nested procedures) klasėje[9]. Kitaip tariant, imant bet kokią įdėtąją procedūrą X ir bet kokį $N \in \mathbb{N}$, $\theta_{PT}(N, p) \leq \theta_X(N, p)$ tolygiai $p \in \left[1 - \frac{1}{\sqrt{2}}, UCP\right]$ atžvilgiu. Nepaisant to, PT procedūra nebuvo plačiai nagrinėjama GT literatūroje. Nusprendę ją tirti ir peržiūrėję [85] citavusius straipsnius[10] e-platformoje Google Scholar, aptikome, kad iš penkiolikos surastų straipsnių [1–3, 12, 22, 29,

[8] t.y. tokias, kurioms vidurkis $\theta_X(N, p)$ minimalus kažkuriame $(a, b) \subset (0, UCP)$

[9] Procedūra vadinama įdėta, jei testai atliekami nuosekliai vienas po kito ir ji tenkina šiuos reikalavimus: 1) kiekviename testavimo žingsnyje galima naudotis visa ankstesne testavimo metu sukaupta informacija; 2) žinant, kad aibė, turinti daugiau nei vieną elementą, yra defektinė, kitame žingsnyje testuojamas tikrinis jos poaibis. Ši klasė labai plati. MD, ST ir PT procedūros jai priklauso.

[10] sąrašas generuotas 2022 metų birželio 28 d.; straipsniai parašyti ne anglų kalba nenagrinėti

30, 43, 48, 53, 55, 56, 76, 83, 84] vienintelis Malinovsky [53] nagrinėjo problemą, turinčią tiesioginį ryšį su PT procedūra. Visi likę tyrėjai citavo Yao ir Hwang darbą [85] tik kaip turintį ryšį su jų sprendžiamais uždaviniais. Peržiūrėta literatūra lėmė pasirinkimą pateikti detalesnę tikimybinę PT procedūros charakterizaciją. Darbe [91] mums pavyko išvesti a.d. T_{PT} momentų generuojančios funkcijos (MGF) išraišką ir jos pagalba įrodyti kelias ribines teoremas — centrinę ribinę (CRT), didžiųjų skaičių dėsnį (DSD) ir didelių nuokrypių principą (DNP). Prieš pateikdami rezultatų formuluotes, įvesime kelis pažymėjimus.

Tegu $\Theta_N \equiv T_{PT}$ žymi bendrą testų skaičių, kurio reikia norint identifikuoti visus defektinius objektus dydžio N aibėje. Tegu $Y_i \sim Be(p), i = 1, \ldots, N$ žymi i-ojo objekto būsenos indikatorių (1 atitinka defektinį). Galiausiai, tegu $\bar{Y}_i := 1 - Y_i$ ir

$$M_0 = \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}, \quad M_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{S.12}$$

Pirmasis rezultatas nusako Θ_N struktūrą įvestų dydžių terminais.

Teiginys S.0.3. *Tegu* $A = \left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix} \right\}$ *ir* $B_k = \begin{pmatrix} Y_k & \bar{Y}_k \\ 1 & 0 \end{pmatrix}$, $k = 1, \ldots, N$. *Tada* $\Theta_2 = 3Y_2 + \bar{Y}_2(1 + Y_1)$, $\quad \Theta_3 = 2 + \bar{Y}_3 Y_2 + Y_3 \Theta_2$,

$$\Theta_N = 1 + Y_N(\bar{Y}_{N-1}Y_{N-2} + 2) + Y_{N-1} + \sum_{j=3}^{N-1} (\bar{Y}_{j-1}Y_{j-2} + Y_{j-1} + 1) \left(Y_j + \bar{Y}_{j-1}\mathbb{1}\{B_N B_{N-1} \cdots B_{j+1} \in A\}\right) + Y_2 + \bar{Y}_2 \mathbb{1}\{B_N B_{N-1} \cdots B_3 \in A\}, \text{ kai } N \geqslant 4.$$

Kitas rezultatas aprašo minėtą išreikštinį MGF pavidalą.

Teorema S.0.10. *Tegu* $M_{\Theta_N}(\lambda)$ *žymi a.d.* Θ_N *MGF taške* $\lambda \in \mathbb{R}$. *Apibrėžkime*

$$\alpha_i = \alpha_i(\lambda) = \frac{1}{2}\left(pe^{2\lambda} + (-1)^i \sqrt{p^2 e^{4\lambda} + 4qe^{\lambda}(q + pe^{\lambda})}\right), \ i = 0, 1; \tag{S.13}$$

$$\kappa_N = \kappa_N(\lambda) = \frac{\alpha_0^N - \alpha_1^N}{\alpha_0 - \alpha_1} \text{ su } N \geqslant 0. \tag{S.14}$$

$\forall N \geqslant 3$ *teisinga lygybė* $M_{\Theta_N}(\lambda) =$

$$\mathrm{e}^{2\lambda}\Big[\Big((1-q)^2\mathrm{e}^{3\lambda}+q(1-q)^2\mathrm{e}^{2\lambda}+q(1-q^2)\mathrm{e}^{\lambda}+q^2\Big)\,\kappa_{N-2}+$$
$$q\left((1-q)^2\mathrm{e}^{3\lambda}+q(1-q)(2-q)\mathrm{e}^{2\lambda}+2q^2(1-q)\mathrm{e}^{\lambda}+q^3\right)\kappa_{N-3}\Big].$$

Likę rezultatai išplaukia iš teoremos S.0.10.

Išvada S.0.11. $\mathrm{E}\,\Theta_N = N\frac{2-q^2}{1+q}+\frac{q^2+q-1}{(1+q)^2}(1-(-q)^N)$,

$$\mathrm{Var}\,\Theta_N = N\frac{(1-q)}{(q+1)^3}\Big(q\left(q^3+3q^2+5q+4\right)+$$
$$(-q)^N\left(2q+4\right)\left(q^2+q-1\right)\Big)+$$
$$\frac{\left(1-(-q)^N\right)}{(q+1)^4}\left(q\left(5q^2+3q-7\right)+(-q)^N\left(q^2+q-1\right)^2\right),N\geqslant 3.$$

Išvada S.0.12. *Jei* $N\to\infty$*, tai a.d.* Θ_N *tenkina žemiau nurodytus sąryšius.*

DSD: $\frac{\Theta_N}{N}\xrightarrow{L_2}\frac{2-q^2}{1+q}$ *ir* $\frac{\Theta_N}{N}\xrightarrow{b.v.}\frac{2-q^2}{1+q}$.

CRT: $\sqrt{N}\left(\frac{\Theta_N}{N}-\frac{2-q^2}{1+q}\right)\xrightarrow{d}N(0,\sigma^2)$, $\sigma^2=\frac{q(1-q)\left(q^3+3q^2+5q+4\right)}{(q+1)^3}$.

DNP: $\frac{\Theta_N}{N}$ *tenkina didelių nuokrypių principą (DNP) su nuokrypių funkcija* I*, lygia* $\mathbb{R}\ni\lambda\mapsto\ln\alpha_0(\lambda)$ *Ležandro transformacijai* ($\alpha_0(\lambda)$ *apibrėžiama* (S.13)). *Kitaip tariant, bet kokiai uždarai* $C\subset\mathbb{R}$ *ir bet kokiai atvirai* $O\subset\mathbb{R}$,

$$\limsup_{N\to\infty}\frac{1}{N}\ln\mathrm{P}\left(\frac{\Theta_N}{N}\in C\right)\leq-\inf_{x\in C}I(x)$$
ir
$$-\inf_{x\in O}I(x)\leq\liminf_{N\to\infty}\frac{1}{N}\ln\mathrm{P}\left(\frac{\Theta_N}{N}\in O\right),$$

su $I(x)=\sup_{\lambda\in\mathbb{R}}\left(x\lambda-\ln\alpha_0(\lambda)\right)$.

Išvados

Apie disertacijos turinį Šiame disertaciniame darbe ištirtos keturios grupinio testavimo procedūros — modifikuota Dorfman (MD), Sterrett (ST), kvadratinės matricos (A2) ir porinio testavimo (PT). MD ir ST procedūroms matematiškai pagrįstos iki tol literatūroje hipotetinėmis laikytos analizinės optimalių konfigūracijų išraiškos. A2 procedūros optimalios konfigūracijos analizinės išraiškos pavidalas buvo nežinomas. Disertacijoje jis surastas ir matematiškai pagrįstas.

PT procedūrai surasta testų skaičiaus skirstinio momentų generuojanti funkcija. Pasinaudojant ja (tinkamai transformuotam testų skaičiui) įrodytos trys ribinės teoremos — centrinė ribinė teorema, didžiųjų skaičių dėsnis ir didelių nuokrypių principas.

Be jau aprašytų uždavinių išspręstas dar vienas — pasiūlytas procedūros apytikrio optimalaus tikimybinio slenksčio radimo algoritmas, tinkantis gana plačiai binominio testavimo procedūrų klasei.

Visais atvejais gauti rezultatai iliustruoti taikymų pavyzdžiais.

Apie rezultatų reikšmę Disertacijoje nagrinėtos tikimybinio testavimo procedūros, tenkinančios binominio testavimo prielaidas. Vienuose taikymuose šios prielaidos yra pateisinamos (pvz., gamyba, kompiuterių mokslas), kituose per daug ribojančios (pvz., kai kurie medicininiai ar socialiniai taikymai), todėl disertacijos rezultatai tinka būtent pirmųjų atvejų analizei. Nepaisant to, kad grupinio testavimo procedūros, tinkančios specifiniams atvejams, aktyviai tebevystomos, disertacijoje nagrinėtosios nėra pasenusios ir dažnai naudojamos masiniame testavime. Geras pavyzdys — neseniai praėjusi COVID-19 pandemija, kurios metu Dorfman procedūra buvo naudojama ir Lietuvoje testuojant moksleivius mokyklose [7] bei kitose šalyse [14]. Atsižvelgiant į išsakytas pastabas, binominio testavimo procedūrų tyrimai išlieka aktualūs ir disertacijoje gautus rezultatus galima laikyti naudingu indėliu į binominio testavimo teoriją.

Rezultatų naujumas

Autorės žiniomis, visi disertacijoje gauti rezultatai yra nauji ir iki šiol literatūroje jokia forma nepublikuoti.

Aprobacija

Disertacijos rezultatai pristatyti keturiose tarptautinėse mokslinėse konferencijose.

1. Čižikovienė, Ugnė; Skorniakov, Viktor. *On the optimal configuration of a square array group testing algorithm* // NBBC21: 8th Nordic-Baltic biometrics virtual conference, 7-10 June 2021, Helsinki, Finland.
2. Čižikovienė, Ugnė; Skorniakov, Viktor. *On the optimal configuration of the modified Dorfman and Sterrett group testing schemes* // IBC2022: 31st International Biometric Conference, 10 - 15 July 2022, Riga, Latvia.
3. Čižikovienė, Ugnė; Skorniakov, Viktor. *On the optimal Pairwise Group Testing Algorithm* // ECMI 2023: 22nd ECMI conference on industrial and applied mathematics, June 26 – 30, 2023, Wrocław, Poland.
4. Čižikovienė, Ugnė; Skorniakov, Viktor. *On the Generic Cut-Point Detection Procedure in the Binomial Group Testing* // The international scientific conference dedicated to the 160th anniversary of Prof. Dr. Hermann Minkowski, June 20 – 22, 2024, Kaunas, Lithuania.

Publikacijos

Disertacija parašyta keturių žemiau išvardintų straipsnių pagrindu. Trys pirmieji publikuoti Web of Science indeksuojamuose žurnaluose. Ketvirtasis priimtas spaudai į Web of Science indeksuojamą žurnalą *TWMS Journal of Applied and Engineering Mathematics*.

1. Čižikovienė, Ugnė, and Viktor Skorniakov. “On a Couple of Unresolved Group Testing Conjectures”. *Communications in Statistics - Theory and Methods*, vol. 52, no. 8, Apr. 2023, pp. 2448–60. DOI.org (Crossref), https://doi.org/10.1080/03610926.2021.1953531.
2. Čižikovienė, Ugnė, and Viktor Skorniakov. “On the Optimal Configuration of a Square Array Group Testing Algorithm”. *Statistics and Its Interface*, vol. 16, no. 4, 2023, pp. 579–91. DOI.org (Crossref), https://doi.org/10.4310/22-SII746.

3. Čižikovienė, Ugnė, and Viktor Skorniakov. “On the Optimal Pairwise Group Testing Algorithm”. *Brazilian Journal of Probability and Statistics*, vol. 38, no. 2, June 2024. DOI.org (Crossref), https://doi.org/10.1214/24-BJPS603.

4. Čižikovienė, Ugnė, and Viktor Skorniakov. "On the Generic Cut–Point Detection Procedure in the Binomial Group Testing". *arXiv: 2304.07263*, *arXiv*, 14 Apr. 2023. arXiv.org, https://doi.org/10.48550/arXiv.2304.07263.

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Užsienio kalbos	Anglų, rusų, italų

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Publications by the Author

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1. Čižikovienė, Ugnė, and Viktor Skorniakov. "On a Couple of Unresolved Group Testing Conjectures". *Communications in Statistics - Theory and Methods*, vol. 52, no. 8, Apr. 2023, pp. 2448–60. DOI.org (Crossref), https://doi.org/10.1080/03610926.2021.1953531.

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