Conjectures on Optimal Nested Generalized Group Testing Algorithm

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Abstract

Consider a finite population of \( N \) items, where item \( i \) has a probability \( p_i \) to be defective. The goal is to identify all items by means of group testing. This is the generalized group testing problem (hereafter GGTP). In the case of \( p_1 = \cdots = p_N = p \), Yao and Hwang (1990) proved that the pairwise testing algorithm is the optimal nested algorithm, with respect to the expected number of tests, for all \( N \) if and only if \( p \in \left[1 - \frac{1}{\sqrt{2}}, \frac{3 - \sqrt{5}}{2}\right] \) (R-range hereafter) (an optimal at the boundary values).

In this note, we present a result that helps to define the generalized pairwise testing algorithm (hereafter GPTA) for the GGTP. We present two conjectures: (1) when all \( p_i, i = 1, \ldots, N \) belong to the R-range, GPTA is the optimal procedure among nested procedures applied to \( p_i \) of nondecreasing order; (2) if all \( p_i, i = 1, \ldots, N \) belong to the R-range, GPTA the optimal nested procedure, i.e., minimises the expected total number of tests with respect to all possible testing orders in the class of nested procedures. Although these conjectures are logically reasonable, we were only able to empirically verify the first one up to a particular level of \( N \). We also provide a short survey of GGTP.

Keywords: Individual testing; pairwise testing

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1 Introduction

1.1 Common $p$ case

Robert Dorfman introduced the concept of group testing in 1943 as a need to administer syphilis tests to millions of individuals drafted into the U.S. Army during World War II. Interesting historical details related to the problem formulation can be found in Du and Hwang (1999). The nice description of the Dorfman (1943) procedure is given by Feller (1950): “A large number, $N$, of people are subject to a blood test. This can be administered in two ways. (i) Each person is tested separately. In this case $N$ tests are required. (ii) The blood samples of $k$ people can be pooled and analyzed together. If the test is negative, this one test suffices for the $k$ people. If the test is positive, each of the $k$ persons must be tested separately, and all $k + 1$ tests are required for the $k$ people. Assume the probability $p$ that the test is positive is the same for all and that people are stochastically independent.”

Procedure (ii) is commonly referred to as the Dorfman group testing procedure.

Since then, the group testing has widespread applications. Partial list included quality control in product testing (Sobel and Groll, 1959), communication networks (Wolf, 1985), American Red Cross screening of blood donations for HIV (Dood et al., 2002), identification of rare alleles (Shental et al., 2010), among others.

Consider a set $S$ of $N$ items, where each item has the probability $p$ to be defective, and the probability $q = 1 - p$ to be good independent from the other items. Following the accepted notation in the group testing literature, we call this set a binomial set (Sobel and Groll, 1959). A group test applied to the subset $x$ is a binary test with two possible outcomes, positive or negative. The outcome is negative if all $x$ items are good, whereas the outcome is positive if at least one item among $x$ items is defective. We call such a set defective or contaminated. The goal is complete identification of all $N$ items with the minimum expected number of tests.

Every reasonable group testing algorithm should satisfy the following properties (Sobel and Groll, 1959; Ungar, 1960): (P1) items that are classified as positive or negative will never be tested again, and (P2) the test is not performed if its outcome can be inferred from previous test results. In addition, if a subset of good items $I'$ is removed from the defective set $I$, then
the remaining items $I - I'$ form a defective set, and it follows from (P2) that this defective set should not be tested as a whole group.

A nested class of group testing algorithms was introduced by Sobel and Groll (1959) [see also Hwang (1976) and Yao and Hwang (1990)], and can be described as follows:

(a) At each stage $t$ ($t = 0, 1, \ldots, T$) of the execution of a nested algorithm, the set $S$ is partitioned into disjoint sets $B_t, C_t,$ and $D_t,$ where set $C_t$ is a set of classified units, set $B_t$ is a binomial set, and set $D_t$ is a defective set. At the beginning of the process at stage (stage 0), $B_0 = S,$ and both $C_0$ and $D_0$ are empty. At the termination of the process (stage $T$), $C_T = S,$ and both $B_T$ and $D_T$ are empty. If at any stage during the process $|D_t| = 1,$ then, according to (P1) above, this sole defective item should be moved from set $D_t$ into set $C_t.$

(b) At each stage $t$ of the algorithm execution, if $D_{t-1}$ is not empty, then a proper subset $D'_{t-1}$ of $D_{t-1}$ is tested. If the outcome of testing $D'_{t-1}$ is positive, then $C_t = C_{t-1},$ $D_t = D'_{t-1}$ and $B_t = N - C_t - D_t$ (follows from Result 1 below); if the outcome of testing $D'_{t-1}$ is negative, then $C_t = C_{t-1} + D'_{t-1},$ $D_t = D_{t-1} - D'_{t-1},$ and $B_t = B_{t-1}.$ Otherwise, if $D_{t-1}$ is empty and $B_{t-1}$ is not empty, then a subset $B'_{t-1}$ of $B_{t-1}$ is tested. If the outcome of testing $B'_{t-1}$ is positive, then $C_t = C_{t-1},$ $D_t = B'_{t-1},$ and $B_t = B_{t-1} - B'_{t-1};$ if the outcome of testing $B'_{t-1}$ is negative, then $C_t = C_{t-1} + B'_{t-1},$ $D_t = D_{t-1},$ and $B_t = B_{t-1} - B'_{t-1}.$

An optimal nested procedure in the form of a dynamic programming algorithm was found by Sobel and Groll (1959). Subsequently, Sobel (1960) and Hwang (1976) improved its computational efficiency. Recently, Zaman and Pippenger (2016) provided an asymptotic analysis of the optimal nested procedure. Finally, different aspects concerning the nested class of group testing procedures were summarized and investigated in Malinovsky and Albert (2019). For $N = 2,$ the optimal algorithm coincides with Huffman’s (Huffman, 1952) encoding algorithm (Sobel, 1967). However, the optimal nested algorithm is not optimal for $N \geq 3$ (Sobel, 1960, 1967). An explicit construction, an example showing that the optimal nested procedure is not in fact optimal, can be found in Section 13 of Sobel (1960).
Until today, an optimal group testing procedure for complete identification under a binomial model is unknown for \( p < (3 - \sqrt{5})/2 \) and general \( N \). For \( p \geq (3 - \sqrt{5})/2 \) (or \( 3 - q - q^2 \geq 2, q = 1 - p \)) Ungar (1960) proved that the optimal group testing procedure is individual, one-by-one testing (at the boundary point it is an optimal).

The pairwise nested algorithm belongs to the nested class and was defined by Yao and Hwang (1990). A verbatim definition of it is as follows:

*We define the pairwise testing algorithm by the following two rules:*

(i) If no contaminated set exists, then always test a pair from the binomial set unless only one item is left, in which case we test that item.

(ii) If a contaminated pair is found, test one item of that pair. If that item is good, we deduce the other is defective. Thus we classify both items and only a binomial set remains to be classified. If the tested item is defective, then by a result of Sobel and Groll (1959), the other item together with the remaining binomial set forms a new binomial set. So, both cases reduce to a binomial set. It is easily verified that at all times the unclassified items belong to either a binomial set or, a contaminated pair. Thus the pairwise testing algorithm is well defined and is nested.

The following result offers a closed-form design for the optimal nested procedure, which can be resolved without computational effort, provided that all \( p_i, i = 1, \ldots, N \) belong to the R-range.

**Theorem 1.** Yao and Hwang (1990)  
The pairwise testing algorithm is the unique (up to the substitution of equivalent items) optimal nested algorithm for all \( N \) if and only if \( 1 - 1/\sqrt{2} \leq p \leq (3 - \sqrt{5})/2 \) (at the boundary values the pairwise testing algorithm is an optimal nested algorithm).

### 1.2 The generalized group testing problem

The generalized group testing problem (GGTP): \( N \) stochastically independent units \( u_1, u_2, \ldots, u_N \), where unit \( u_i \) has the probability \( p_i \) (\( 0 < p_i < 1 \)) to be defective and the probability \( q_i = 1 - p_i \) to be good. We assume that the probabilities \( p_1, p_2, \ldots, p_N \) are known
and we can decide the order in which the units will be tested. All units have to be classified as good or defective by group testing. The generalized group testing problem was first introduced by Sobel (1960) on page 144. In this work, two (or more) different kinds of units are presented and can be put into the same test group. In the case of two kinds of units with known probabilities \( q_1 \geq q_2 \), the individual testing is optimal if

\[ 3 - q_1 - q_1q_2 > 2. \]

This result follows the Huffman (1952) encoding algorithm construction when \( N = 2 \) (Sobel, 1960). Since its introduction, GGTP has been investigated (Lee and Sobel (1972); Nebenzahl and Sobel (1973); Katona (1973); Nebenzahl (1975); Hwang (1976); Yao and Hwang (1988a,b); Kurtz and Sidi (1988); Yao and Hwang (1990); Kealy et al. (2014); Malinovsky (2019)). Even for a particular nested group testing algorithm the optimal regime (or, order in which groups/units will be tested) is known only for the Dorfman procedure (Dorfman, 1943) because of Hwang (1976).

For the GGTP, Hwang (1976) proved that under Dorfman’s procedure an optimal partition is an ordered partition (i.e., each pair of subsets has the property such that the numbers in one subset are all greater or equal to every number in the other subset). Then Dorfman’s procedure is performed on each subset. It allowed Hwang to find the optimal solution using a dynamic programming algorithm with the computational effort \( O(N^2) \). But, even using a slightly modified Dorfman procedure or Sterrett (1957) procedure, the ordered partition is not optimal (Malinovsky, 2019). As the total number of possible partitions is the Bell number, it is impossible to use brutal search to obtain an optimal solution, which is unknown (Hwang, 1981; Malinovsky, 2019). Kurtz and Sidi (1988) provided a dynamic programming (DP) algorithm having computational effort \( O(N^3) \) to find an optimal nested procedure for a given order of units \( u_1, \ldots, u_N \) (which order should be preserved at all stages of the testing process). In addition, Kurtz and Sidi (1988) used the Ungar (1960) method and extended Sobel (1960) result from \( N = 2 \) to general \( N \). Namely, they proved that if \( 3 - q_1 - q_1q_2 > 2 \), where \( q_1 \geq \cdots \geq q_N \), then individual testing is optimal. Closely related results were obtained by Yao and Hwang (1988b), and can be summarized as follows:

**Theorem 2.** Yao and Hwang (1988b)

*Assume without loss of generality that \( 0 < p_1 \leq p_2 \leq \cdots \leq p_N < 1 \). Then,
1. If \(3 - q_1 - q_1 q_i > 2\), then there exists an optimal algorithm which tests \(u_i\) individually.

2. Denote by \(k = \sup \{ \sup \{ i = 1, \ldots, N : 3 - q_1 - q_1 q_i > 2 \} , 0 \} \), with \(\sup \{ \phi \} = -\infty\).

   Then there exists an optimal algorithm which tests \(u_{k+1}, \ldots, u_N\) individually.

3. If there exists an optimal algorithm in which \(u_i\) is tested individually, there exists an optimal algorithm in which \(u_j\) is tested individually for all \(j\) with \(p_j > p_i\).

It is important to note that in contrast to Ungar (1960), the results by Kurtz and Sidi (1988) and Yao and Hwang (1988b) provide a sufficient, but not necessary, condition. Yao and Hwang (1988b) constructed an example with \(N = 3, p_1 = 0.1, p_2 = 0.2, p_3 = 0.8\) such that \(3 - q_1 - q_1 q_3 < 2\), where the optimal algorithm tests \(u_3\) individually. In contrast, if \(p_i < (3 - \sqrt{5})/2\) for every \(i = 1, \ldots, N\), then \(3 - q_j - q_j q_i < 2\) for every \(i, j = 1, \ldots, N\) and therefore no item should be tested individually unless there are no items left to combine. In addition, it was shown in Yao and Hwang (1988b) that \(E^* (p_1, \ldots, p_N)\) is nondecreasing in each \(p_i < 1\) for every \(N\), where \(E^* (p_1, \ldots, p_N)\) denotes the expected number of tests for an optimal algorithm in GGTP. In combination with Ungar (1960), this result implies that if \(p_i > (3 - \sqrt{5})/2\) for every \(i = 1, \ldots, N\), then the optimal group testing procedure is to perform individual, one-by-one testing.

2 Description of the Problem, Results and Examples

We want to define the generalized pairwise testing algorithm (GPTA) for the GGTP. Two results below will help to proceed. The first result is a simple generalization of Sobel and Groll (1959) result for the common \(p\) case into GGTP (see also Kurtz and Sidi (1988)).

Result 1 (Sobel and Groll (1959)). In the GGTP, given a defective set \(I\) and given that a proper subset \(I_1, I_1 \subset I\) contains at least one defective unit, then the posteriori distribution of the units in the subset \(I - I_1\) is the same as it was before any testing.

The second result describes an optimal rule for nested testing in the case that at some stage, we have to test two particular units \(a\) and \(b\).
**Result 2.** Suppose that a nested procedure is applied. Also suppose that the $n$ units that remain to be tested, $a, b, u_3, \ldots, u_n$, all have unknown status, and the corresponding probabilities of those units being good are $q_a, q_b, q_3, \ldots, q_n$. We start by testing two units together, as a group, with the corresponding probabilities $q_a$ and $q_b$, where $q_a \geq q_b$. Then, under this setting, when the first group test of units $a$ and $b$ is positive, we then have to test the unit for which the corresponding probability of being good is largest, i.e. unit $a$ (call it algorithm $A$). If the outcome of testing unit $a$ is negative, then the second unit is positive by deduction. Otherwise, if the outcome of testing unit $a$ is positive, then by Result 1 the conditional distribution of the status of the second unit is a Bernoulli distribution with parameter $p_b = 1 - q_b$, and units $b, u_3, \ldots, u_n$ remain to be tested.

**Proof.** The proof is based on direct comparison of two possible algorithms, namely, algorithms $A$ and $B$, where, in algorithm $B$, we first test unit $b$ individually. Denote $T$ as the total number of tests and denote $E(p_{i_1}, \ldots, p_{i_k})$ as the total expected number of tests of units $i_1, \ldots, i_k$ with the corresponding probabilities $p_{i_1}, \ldots, p_{i_k}$ under a nested procedure. The left branch of the tree below represents a negative test result, and the right branch represents a positive test result.

![Algorithm A Tree Diagram](image)

Let $E_A(T)$ and $E_B(T)$ be the expected total number of tests under algorithms $A$ and
We have,

\[ E_A(T) = q_a E(p_3, \ldots, p_N) + (1 - q_a) E(p_a, p_3, \ldots, p_N) + 2 - q_a q_b. \]

\[ E_B(T) = q_b E(p_3, \ldots, p_N) + (1 - q_b) E(p_b, p_3, \ldots, p_N) + 2 - q_a q_b. \]

Since \( E(p_1, p_3, \ldots, p_k) \) is non-decreasing in each \( p_i \) for \( 0 \leq p_i \leq 1 \) (Yao and Hwang, 1988a) and we assume w.l.g. that \( p_a \leq p_b \), we have \( E(p_a, p_3, \ldots, p_N) \leq E(p_b, p_3, \ldots, p_N) \). Therefore, we obtain

\[ E_A(T) - E_B(T) \leq (q_b - q_a) (E(p_b, p_3, \ldots, p_N) - E(p_3, \ldots, p_N)) \leq 0. \]

The last inequality follows from the obvious fact that \( E(p_3, \ldots, p_N) \leq E(p_b, p_3, \ldots, p_N) \).

**Remark 1.** The intuition behind Result 2 is as follows: Suppose that the pair \( \{a, b\} \) test is positive. Then, if a subsequent individual test of one unit from the set \( \{a, b\} \) is negative, we can conclude by deduction (without actual testing) that the second unit is positive (possibility 1). Alternately, if the subsequent individual test is positive, then the status of the remaining unit is unknown, and this unit will at some stage be tested in the group or individually (possibility 2). Since \( q_a \geq q_b \) and we prefer possibility 1 over possibility 2, we should select unit \( a \) to be tested first.
Definition 1. Let \( u_1, u_2, \ldots, u_N \) be the fixed initial order of units to test, for which the corresponding probabilities of being good are \( q_1, \ldots, q_N \). We define the generalized pairwise testing algorithm (GPTA) by the following rules:

(a) Test the pair \( \{u_1, u_2\} \). If the outcome is negative, then continue by testing the next pair unless only one unit is left, in which case we test that unit.

(b) If the outcome is positive, then test the unit with the greater probability of being good, i.e. unit \( u_{j_1} \) where \( j_1 = \arg \max(q_1, q_2) \). If unit \( u_{j_1} \) is found to be good, then the other unit \( u_{j_2} \), where \( j_2 = \arg \min(q_1, q_2) \), is defective by deduction. Otherwise, if the tested unit \( u_{j_1} \) is defective, then by Result 1 the conditional distribution of the status of \( u_{j_2} \) is a Bernoulli distribution with parameter \( p_{j_2} = 1 - q_{j_2} \), and units \( u_{j_2}, u_3, \ldots, u_n \) remain to be tested. Continue with testing the next pair of units.

Note that GPTA does not necessarily preserve the initial predetermined testing order; i.e. even if a defective unit \( u_i \) is tested no later than unit \( u_j \), \( u_i \) may remain in the testing process even after unit \( u_j \) is identified. However, if the initial predetermined testing order follows a nondecreasing order of \( p_i \)'s (\( p_1 \leq p_2 \leq \cdots \leq p_N \)), then GPTA preserves the initial testing order.

It is natural to expect that the result of Yao and Hwang (1990) will hold for GGTP in the case of \( 1 - 1/\sqrt{2} \leq p_i \leq (3 - \sqrt{5})/2, \ i = 1, \ldots, N \). The following example helps us to understand this situation. Here, we compare GGTP with an optimal nested procedure from Kurtz and Sidi (1988) for all possible testing orders. Their procedure requires the initial testing order to be preserved throughout the testing process; otherwise its computational complexity will be exponential as a function of \( N \). Therefore, the procedure of Kurtz and Sidi (1988) does not necessarily satisfy the optimal rule obtained in Result 2 in the case where testing two units, unless the \( p_i \)'s are arranged in nondecreasing order.

Example 1. Suppose \( \{q_1, q_2, q_3, q_4\} = \{0.62, \ 0.62, \ 0.65, \ 0.68\} \).
Table 1: The expected total number of tests $E_P(T)$ for all possible initial testing orders under the GPTA and the expected total number of tests $E_{Ne}(T)$ under an optimal nested ordered procedure following the algorithm by Kurtz and Sidi (1988).

| Permutation | Initial Testing Order | $E_P(T)$ | $E_{Ne}(T)$ |
|-------------|-----------------------|----------|-------------|
| 1           | 0.68 0.65 0.62 0.62   | 3.8576   | 3.8576      |
| 2           | 0.68 0.62 0.65 0.62   | $\mathbf{3.8449}$ | 3.8454      |
| 3           | 0.68 0.62 0.62 0.65   | 3.8545   | 3.8754      |
| 4           | 0.65 0.68 0.62 0.62   | 3.8576   | 3.8691      |
| 5           | 0.65 0.62 0.68 0.62   | $\mathbf{3.8449}$ | 3.8454      |
| 6           | 0.65 0.62 0.62 0.68   | 3.8659   | 3.9054      |
| 7           | 0.62 0.65 0.68 0.62   | $\mathbf{3.8449}$ | 3.8655      |
| 8           | 0.62 0.65 0.62 0.68   | 3.8659   | 3.9255      |
| 9           | 0.62 0.68 0.65 0.62   | $\mathbf{3.8449}$ | 3.8610      |
| 10          | 0.62 0.68 0.62 0.65   | 3.8545   | 3.8910      |
| 11          | 0.62 0.62 0.68 0.65   | 3.8749   | 3.8736      |
| 12          | 0.62 0.62 0.65 0.68   | 3.8863   | 3.9036      |

Comment 1. (Example 1) The following observations were made:

(a) For the initial ordered testing $q_1 \geq q_2 \geq q_3 \geq q_4$ (permutation 1) both algorithms are identical. This permutation is not optimal.

(b) In all cases, instead of permutation 1, the procedure by Kurtz and Sidi (1988) for the given order differs from GPTA, but in all cases the testing group size under their procedure does not exceed 2 and can be 1. For example, under permutation 2 this procedure is presented below with the corresponding $E_{Ne} = 3.8454$. 

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(c) For the permutation 11 the GPTA is not optimal.

(d) The expected length of an optimal prefix Huffman code, which serves as a theoretical and generally non-attainable lower bound (Nebenzahl and Sobel, 1973), is 3.7977344.

(e) Initial testing orders 2, 5, 7, and 9 are optimal with the corresponding expected number of tests equals $E_p(T) = 3.8454$. GPTA corresponding to an initial testing order 2 is presented below.

We conjecture that the result of Yao and Hwang (1990) (Theorem [II]) holds for GGTP. That is, for a given testing order concerning the values $p_1, \ldots, p_N$, an optimal design in the...
closed form can be determined without any computational effort. The precise formulation of this conjecture is presented in the next section.

3 Conjectures

Conjecture 1. Given that \( u_1, u_2, \ldots, u_N \) are labeled according to a non-decreasing order of \( p_1 \leq p_2 \leq \cdots \leq p_N \), such that \( 1 - 1/\sqrt{2} \leq p_i \leq (3 - \sqrt{5})/2 \) for \( i = 1, \ldots, N \), GPTA is the optimal nested ordered algorithm (at the boundary values, the pairwise testing algorithm is an optimal nested algorithm).

Conjecture 1 was empirically verified for \( N \leq 1000 \) in the following manner: We generated \( N \) values from a continuous uniform \([1 - 1/\sqrt{2}, (3 - \sqrt{5})/2]\) distribution and ordered them such that \( p_1 \leq p_2 \leq \cdots \leq p_N \). Then, we applied the optimal ordered (with respect to \( u_1, \ldots, u_N \)) nested procedure by Kurtz and Sidi (1988) along with the optimal pairwise testing procedure. For this particular order, the optimal rule presented in Result 2 automatically holds for the algorithm of Kurtz and Sidi (1988). In both procedures, the expected total number of tests was calculated to verify that the difference between those expectations equals zero. We repeated this process a number of times. However, since the computational effort of the Kurtz and Sidi (1988) algorithm is proportional to \( N^3 \), it is not computationally feasible to make many repetitions when \( N \) is large. Therefore, the number of repetitions was chosen as a decreasing function of \( N \). For the first 100 smallest values of \( N \), we repeated the process 500 times; and for each successive 100 values of \( N \), we decreased the number of repetitions by half, ultimately performing only a single repeat for the 100 largest values of \( N \).

Conjecture 2. For all integer positive values of \( N \) and all \( p_i, i = 1, \ldots, N \) in the interval \([1 - 1/\sqrt{2}, (3 - \sqrt{5})/2]\), the generalized pairwise testing algorithm is the optimal nested procedure (at the boundary values, GPTA is an optimal nested algorithm); that is, within the class of nested procedures, this approach minimizes the expected total number of tests with respect to all possible testing orders.

Remark 2. For \( N = 2 \) and \( 1 - 1/\sqrt{2} \leq p_i \leq (3 - \sqrt{5})/2 \), \( i = 1, 2 \), the optimal nested algorithm is GPTA and it is also the optimal group testing procedure because it coincides
with Huffman’s (Huffman, 1952) encoding algorithm.

If Conjecture 2 is true, it is not clear whether the problem of finding the optimal GPTA with respect to all possible testing orders is a computational tractable problem (Garey and Johnson, 1979). But, it still may be possible to provide proof of existence.

It was suggested by an anonymous reviewer that for even values of \( N \), a guess for an optimal ordering of items may be as follows: Split the units \( u_1, u_2, \ldots, u_N \) with corresponding probabilities \( p_1 \leq p_2 \leq \cdots \leq p_N \) into subsets \( U = \{u_1, \ldots, u_M\} \) and \( \overline{U} = \{u_{M+1}, \ldots, u_N\} \). Then apply GPTA to the testing order \( u_1, u_{M+1}, u_2, u_{M+2}, \ldots, u_M, u_N \). This order appears to be optimal for GPTA in the case of \( N = 4 \), as that was empirically verified. However, this ordering is not optimal for the next even value of \( N \), i.e. \( N = 6 \). At this stage, we do not have a good guess for a best ordering.

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