On the Optimal Pairwise Group Testing Algorithm

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Abstract

Originally suggested for the blood testing problem by Dorfman in 1943, an idea of Group Testing (GT) has found many applications in other fields as well. Among many (binomial) GT procedures introduced since then, in 1990, Yao and Hwang proposed the Pairwise Testing Algorithm (PTA) and demonstrated that PTA is the unique optimal nested GT procedure provided the probability of contamination lies in \( \left[ 1 - \frac{\sqrt{2}}{2}, \frac{3 - \sqrt{5}}{2} \right] \).

Despite the fundamental nature of the result, PTA did not receive considerable attention in the literature. In particular, even its basic probabilistic properties remained unexplored. In this paper, we fill the gap by providing an exhaustive characterization of probabilistic PTA properties.

1 Introduction

Group Testing (GT) refers to a special kind of technique used to identify defective items in a given set. It is widely applied in very diverse areas. The list includes (but is not limited to) quality control, communication and security networking, genetics, experimental physics, an estimation of parameters from probability models, screening for the infectious diseases like HIV, hepatitis and, very recently, COVID-19 (for domain specific references see e.g. [14]). The main idea underlying the method is as follows. Given a set of items to test, one should replace testing of single items by testing of groups of items. Some of these groups, however, can contain single items as well. For example, to identify defective lights in a given set of strings of lights, one can adopt the following scheme for each string: first test the whole string of lights and then retest each single bulb only in case the whole string does not function properly. This idea was first announced in 1943 by Dorfman [6] who suggested to test
pools containing $n$ blood samples and then repeatedly retest only the samples of patients belonging to infected pools. The rationale behind is quite obvious. If the prevalence of the disease is small, then quite often the pooled sample is clean. Hence, instead of testing each sample out of $n$ and consuming this way $n$ test kits, one ends up with a single test. In the literature, the described GT procedure is usually termed as Dorfman scheme, or Dorfman algorithm. Since the appearance of the seminal paper [6], myriads of other GT algorithms originated. The defining feature of each such algorithm is an average number of tests $E_n$ required to identify all defectives in a set spanning $n$ items. Given $n$, an algorithm achieving minimal possible value of $E_n$ is called an optimal algorithm. Characterization of the optimal algorithm without any further assumptions seems to be unfeasible. Therefore, one often operates under the following Binomial Testing Assumptions (BTA).

**BTA1**: all tested items are independent.

**BTA2**: each item is contaminated with the same constant probability $p \in (0, 1)$.

**BTA3**: pooling does not change operating characteristics (namely, sensitivity and specificity) of the test kit$^1$.

**BTA4**: the test kit is perfect, i.e. its sensitivity and specificity are both equal to 1.

From now, and till the end of the paper, we assume that BTA hold. In such case, the tested set of items is called the binomial set and $E_n$ depends on $p$ as well. Though it might be tempting to conclude that BTA simplify the matter substantially, the forthcoming short account (highlighting fundamental results) demonstrates that the truth is different.

In 1960, Ungar [19] proved that, for $p > \frac{3 - \sqrt{5}}{2}$, irrespectively of value of $n \in \mathbb{N}$, an optimal algorithm is to test one-by-one and the minimal value of $E_n = E_n(p)$ is therefore $n$. In 1987, Du and Ko [7] proved that finding an optimal BTA based algorithm is an NP–complete problem (no polynomial time solution is known [20]). In 1988, Yao and Hwang [23] proved that $(0, \frac{3 - \sqrt{5}}{2}) \times \{2, 3, \ldots\} \ni (p, n) \mapsto E_n(p)$ is monotonically increasing in each argument. Finally, in 1990, the same authors [24] proposed the Pairwise Testing Algorithm (PTA) and demonstrated that it is a unique optimal nested BTA based algorithm if and only if $p \in \left[1 - \frac{\sqrt{2}}{2}, \frac{3 - \sqrt{5}}{2}\right]$. Nested algorithms are defined by the following property: if the contaminated subset $C$ is identified, then the next subset to be tested is the proper subset of $C$. Though the optimal nested algorithm is not optimal in the class of all possible GT algorithms, it was demonstrated by Sobel [16], [17] that it is nearly optimal over all algorithms. Hence importance of the above mentioned result [24] on PTA.

Surprisingly, yet it turns out that an exploration of the properties of PTA did not receive a considerable attention in the literature. Even more, out of 15 citing

$^1$when talking about this assumption, one often says that there is no dilution effect
references [3, 21, 22, 18, 2, 4, 9, 12, 1, 10, 13, 15, 11, 8, 14] retrieved by us from Google Scholar, Malinovsky [13] was the only who investigated a problem having a direct relationship to PTA. All others touched the work of Yao and Hwang [24] merely as a reference having a connection to GT with a mild relation to their own problem. These circumstances motivated the current work aiming to give a broader probabilistic characterization of the PTA. Our analysis resulted in the following results for the (properly scaled and/or centered) number of tests performed by PTA: exact analytical expression of the moment generating function (MGF), strong law of large numbers (SLLN), central limit theorem (CLT) and large deviations principle (LDP).

The rest part of the paper is organized as follows. In Section 2, we introduce notions and state the previously announced results in detail. Section 3 contains a short accompanying discussion. Finally, there is an appendix devoted to the proofs.

2 Results

We first introduce the PTA by quoting the definition given in [24], Section 2:

(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 that the other is defective. Thus, we classify both items and only a binomial set remains to be classified. If the tested item is defective, the other item together with the remaining binomial set forms a new binomial set.

Intending to present a full picture, we also restate the main result of Yao and Hwang [24].

Theorem. 2.1 ([24], Theorem 1). The pairwise testing algorithm is the unique (up to the substitution of equivalent items) optimal nested algorithm for all \( n \) if and only if

\[
\frac{2\sqrt{2}}{3} \leq p \leq \frac{6 - \sqrt{5}}{2}.
\]

Let \( T_n \) denote the number of conducted tests required for an identification of all defectives in a given binomial set having \( n \) items, and let \( X_i, i = 1, \ldots, n, \) be an indicator of an \( i \)th item status. In view of introductory discussion, \( X_i \sim B(p) \) are independent random variables with \( p \in (0, 1) \) having a meaning of probability of being defective. Also, let \( \bar{X}_i := 1 - X_i, q := 1 - p, \) and

\[
M_0 = \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}, \quad M_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.
\]

(2.1)

Our first result gives an explicit expression for \( T_n \) in terms of the above quantities.

\(^2\)the list was generated on 28th of June, 2022; non English references were excluded
Proposition. 2.1. Let \( A = \{M_1, M_0, M_3\} \) and \( B_k = \begin{pmatrix} X_k & \bar X_k \\ 1 & 0 \end{pmatrix} \) for \( k = 1, \ldots, n \). Then \( T_2 = 3X_2 + \bar X_2(1 + X_1), T_3 = 2 + \bar X_3X_2 + X_3T_2, \) and

\[
T_n = 1 + X_n(\bar X_n-1X_{n-2} + 2) + X_{n-1} + \\
\sum_{j=3}^{n-1}(\bar X_{j-1}X_{j-2} + X_{j-1} + 1) \{X_j + \bar X_{j-1} \mathbb{1} \{B_nB_{n-1} \cdots B_{j+1} \in A\}\} + \\
X_2 + \bar X_2 \mathbb{1} \{B_nB_{n-1} \cdots B_3 \in A\} \text{ for } n \geq 4.
\] (2.2)

The expression above provides insight into the structure of \( T_n \) whereas the next one completely characterizes its distribution.

Proposition. 2.2. Let \( M_{T_n}(\lambda) \) denote the moment generating function of \( T_n \) at \( \lambda \in \mathbb{R} \). Put

\[
\alpha_i = \alpha_i(\lambda) = \frac{1}{2} \left( pe^{2\lambda} + (-1)^i \sqrt{p^2e^{4\lambda} + 4qe^{\lambda}(q + pe^{\lambda})} \right), \ i = 0, 1; \quad (2.3)
\]

\[
\kappa_n = \kappa_n(\lambda) = \frac{\alpha_n - \alpha_n}{\alpha_n - \alpha_1} \text{ for } n \geq 0.
\] (2.4)

Then

\[
M_{T_n}(\lambda) = e^{2\lambda} \left[ ((1 - q)^2e^{3\lambda} + q(1 - q)^2e^{3\lambda} + q(1 - q^2)e^{\lambda} + q^2)\kappa_{n-2} + \\
q((1 - q)^2e^{3\lambda} + q(1 - q)(2 - q)e^{2\lambda} + 2q^2(1 - q)e^{\lambda} + q^3)\kappa_{n-3} \right].
\] (2.5)

for \( n \geq 3 \).

The remaining results are the consequences of the previous one.

Corollary. 2.1. \( \mathbb{E} T_n = n^2 - \frac{q^2}{1+q} + \frac{2+q}{(1+q)^2}(1 - (-q)^n), \)

\[
\text{Var} T_n = \\
n\frac{(1 - q)}{(q + 1)^3} \left( q(q^3 + 3q^2 + 5q + 4) + (-q)^n (2q + 4) (q^2 + q - 1) \right) + \\
\frac{(1 - (-q)^n)}{(q + 1)^4} \left( q(5q^2 + 3q - 7) + (-q)^n (q^2 + q - 1)^2 \right), \ n \geq 3.
\] (2.6)

Corollary. 2.2. The following asymptotic results apply to \( T_n \) as \( n \to \infty \).

\text{LLN}: \( \frac{T_n}{n} \xrightarrow{L_2} \frac{2-q^2}{1+q} \) and \( \frac{T_n}{n} \xrightarrow{a.s.} \frac{2-q^2}{1+q} \).

\text{CLT}: \( \sqrt{n} \left( \frac{T_n}{n} - \frac{2-q^2}{1+q} \right) \xrightarrow{d} N(0, \sigma^2), \quad \sigma^2 = \frac{\sigma(1-q)(q^3+3q^2+5q+4)}{(q+1)^2}. \)
LDP: \( \frac{T_n}{n} \) satisfies Large Deviation Principle (LDP) 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 (2.3). That is, for any closed \( C \subset \mathbb{R} \) and any open \( O \subset \mathbb{R} \),

\[
\limsup_{n \to \infty} \frac{1}{n} \ln P \left( \frac{T_n}{n} \in C \right) \leq - \inf_{x \in C} I(x)
\]

and

\[
- \inf_{x \in O} I(x) \leq \liminf_{n \to \infty} \frac{1}{n} \ln P \left( \frac{T_n}{n} \in O \right),
\]

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

3 Discussion

There are several reasons supporting relevance of our analysis.

- Though the definition of an optimal algorithm is usually tailored to an average number of tests, when choosing between several algorithms, it is desirable to evaluate their performance taking into account multiple aspects. For example, an algorithm \( A_1 \) may perform slightly better than \( A_2 \) in terms of an average number of tests. However, \( A_1 \) may have considerably larger variance than \( A_2 \) and, therefore, the previously mentioned slight gain of \( A_1 \) could be gladly traded by the practitioner in favour of \( A_2 \).

- We have already mentioned that the importance of PTA remained unrecognized in the literature and there is more to say on that.

  - Many GT algorithms described in the literature (including pioneering Dorfman’s algorithm of [6]) have limited applicability due to the dilution effect. To be more precise, for a typical algorithm of this kind to perform optimally for a given \( p \), one has to test items by grouping them into pools of size \( n = n(p) \). If this \( n \) is large (say 64 items or even more), the operating characteristics (sensitivity and specificity) of the test kit at hand may become unacceptably low (aka dilute) making this way the algorithm unsuitable for that particular application\(^3\). With respect to this property, PTA is a very favourable option: it requires only pools of size \( n = 2 \), and this holds true for all \( p \)'s in the region of its optimality \( \left[ \frac{2 - \sqrt{2}}{2}, \frac{3 - \sqrt{5}}{2} \right] \).

  - The region \( \left[ \frac{2 - \sqrt{2}}{2}, \frac{3 - \sqrt{5}}{2} \right] \) where PTA performs optimally is bounded away from 0 in contrast to many other GT algorithms which do better for \( p \)'s close to 0. In certain applications this property may

\(^3\)In theory, BTA3 stated in the Introduction prevents from this; however, in practice, it may be a serious obstacle
be of significant importance. For example, consider a screening for a quite widespread infectious disease.

• Yao and Hwang [24] conjectured that there exists such $p_0 \in \left[\frac{2-\sqrt{2}}{2}, \frac{3-\sqrt{2}}{2}\right]$ that for $p \in \left[p_0, \frac{3-\sqrt{2}}{2}\right]$ PTA is optimal over all (not necessarily nested) algorithms satisfying BTA.

• Our Prop. 2.1 demonstrates that, despite apparently simple recurrence governing evolution of $T_n$ (see Eq. (A.1)), the resulting dependence structure is not so simple. At least we were not able to analyze its behaviour 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 2.2. More than that, even direct moment calculation exercise, though accomplishable for $E T_n$ at a reasonable price (see Lemma in Section 4 of [24]), becomes much more involved when it comes to $\text{Var} T_n$ and higher order moments. This way, $(T_n)_{n \geq 2}$ 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.

In view of the said above, our input seems to be plausible. Moreover, we are inclined to think that it may be useful for the solution of a couple of unresolved conjectures. Namely, the one stated by Yao and Hwang in [24] and mentioned above, and the generalized PTA optimality conjecture stated in [13].

A Proofs

Proof of Proposition 2.1. By the description of the testing procedure,

$$T_n = (1 + T_{n-2}) \mathbb{I}\{X_n + X_{n-1} = 0\} + (2 + T_{n-1}) \mathbb{I}\{X_n + X_{n-1} > 0\}X_n + (2 + T_{n-2}) \mathbb{I}\{X_n + X_{n-1} > 0\} \tilde{X}_n = \left[\text{since } \mathbb{I}\{X_n + X_{n-1} = 0\} = \bar{X}_n \tilde{X}_{n-1}, \mathbb{I}\{X_n + X_{n-1} > 0\} \tilde{X}_n = \bar{X}_n X_{n-1}\right] = \tilde{X}_n (1 + X_{n-1}) + 2X_n + T_{n-1}X_n + T_{n-2} \tilde{X}_n. \quad (A.1)$$

Put

$$t_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad A_1 = t_1, \quad t_k \overset{k \geq 2}{=} \begin{pmatrix} T_k \\ T_{k-1} \end{pmatrix}, \quad A_k \overset{k \geq 2}{=} \begin{pmatrix} \tilde{X}_k (1 + X_{k-1}) + 2X_k \\ 0 \end{pmatrix},$$

6
and let $B_k, k \geq 1$, be as in the statement of the Proposition. From (A.1) it follows that

$$
t_n = A_n + B_n t_{n-1} = \ldots = A_n + \sum_{k=1}^{n-2} B_n B_{n-1} \ldots B_{n-k+1} A_{n-k} + B_n \ldots B_2 t_1 =
$$

$$A_n + \sum_{j=3}^{n} B_n \ldots B_j A_{j-1} + B_n \ldots B_2 t_1 = A_n + \sum_{j=2}^{n} B_n \ldots B_j A_{j-1}.
$$

Let $M_0, M_1$ be given by (2.1). Denoting

$$M_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad M_3 = \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix}, \quad S = \{M_0, M_1, M_2, M_3\}, \quad (A.2)$$

we have that $S$ forms a semi-group with respect to ordinary matrix multiplication since

$$M_2^2 = M_0, \quad M_0 M_1 = M_3, \quad M_0 M_3 = M_3, \quad M_1 M_0 = M_0, \quad M_1^2 = M_2, \quad (A.3)
$$

$$M_1 M_3 = M_3, \quad M_3 M_0 = M_0, \quad M_3 M_1 = M_0, \quad M_3^2 = M_3,
$$

Let $J_i = \{j \in \{2, \ldots, n\} \mid X_j = i\}, i = 0, 1$. Note that $\forall \, i \, B_i = X_i M_0 + \bar{X}_i M_1 \in S$ and that $M_0$ is an absorbing element of $S$. Therefore, by (A.3)

$$\sum_{j \in J_i} B_n \ldots B_j A_{j-1} = \sum_{j \in J_i} M_0 A_{j-1} = \sum_{j=2}^{n} X_j M_0 A_{j-1}
$$

and

$$\sum_{j \in J_0} B_n \ldots B_j A_{j-1} = \sum_{j=2}^{n} \bar{X}_j \left( \mathbb{1} \{B_n \ldots B_j M_1 = M_0\} M_0 + \mathbb{1} \{B_n \ldots B_j M_1 = M_1\} M_1 + \mathbb{1} \{B_n \ldots B_j M_1 = M_2\} M_2 + \mathbb{1} \{B_n \ldots B_j M_1 = M_3\} M_3 \right) A_{j-1}.
$$

To extract $T_n$ from $t_n$, it suffices to multiply $t_n$ by $(1 \ 0)$ from the left. Since

$$(1 \ 0) M_i A_{j-1} = \begin{cases} 0, \text{ for } i = 1, 3 \text{ and all } j; \\ \bar{X}_{j-1} (1 + X_{j-2}) + 2X_{j-1}, \text{ for } i = 0, 2 \text{ and } j \geq 3; \\ 1, \text{ for } i = 0, 2 \text{ and } j = 2, \end{cases}
$$

after the collection of terms, we finally end up with an expression (2.2). □

**Proof of Proposition 2.2. Step 1: auxiliary recurrence.** For $\lambda_1, \lambda_2 \in \mathbb{R}$, let

$$M_{i,n}(\lambda_1, \lambda_2) = \mathbb{E} \left( e^{\lambda_1 T_n + \lambda_2 T_{n-1}} \mid X_n = i \right), \quad i = 0, 1. \quad (A.4)$$

7
By equation (A.1),
\[
M_{0,n}(\lambda_1, \lambda_2) = E \left(e^{\lambda_1 (1 + X_{n-1} + T_{n-2}) + \lambda_2 T_{n-1}}\right) =
\]
\[
p E \left(e^{\lambda_1 (2 + T_{n-2}) + \lambda_2 T_{n-1}} \mid X_{n-1} = 1\right) +
q E \left(e^{\lambda_1 (1 + T_{n-2}) + \lambda_2 T_{n-1}} \mid X_{n-1} = 0\right) =
\]
\[
pe^{2\lambda_1} M_{0,n-1}(\lambda_2, \lambda_1) + qe^{\lambda_1} M_{0,n-1}(\lambda_2, \lambda_1);
\]

\[
M_{1,n}(\lambda_1, \lambda_2) = E \left(e^{\lambda_1 (2 + T_{n-1} + \lambda_2 T_{n-1})}\right) =
\]
\[
e^{2\lambda_1} (pM_{1,n-1}(\lambda_1 + \lambda_2, 0) + qM_{0,n-1}(\lambda_1 + \lambda_2, 0)).
\]

For \( \lambda \in \mathbb{R} \), put
\[
m_{1,n} = m_{1,n}(\lambda) = M_{1,n}(\lambda, 0), \quad m_{2,n} = m_{2,n}(\lambda) = M_{0,n}(\lambda, 0),
\]
\[
m_{3,n} = m_{3,n}(\lambda) = M_{1,n}(0, \lambda), \quad m_{4,n} = m_{4,n}(\lambda) = M_{0,n}(0, \lambda);
\]
\[
A = A(\lambda) = e^{2\lambda} \begin{pmatrix} p & q \\ 0 & 0 \end{pmatrix}, \quad B = B(\lambda) = \begin{pmatrix} 0 & 0 \\ e^{2\lambda}p & e^{\lambda}q \end{pmatrix},
\]
\[
C = \begin{pmatrix} p & q \\ p & q \end{pmatrix}, \quad O = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}.
\]

From (A.5) it then follows that \( m_n = m_n(\lambda) = (m_{1,n}, m_{2,n}, m_{3,n}, m_{4,n})^T \) satisfies recurrent equation
\[
m_n = \begin{pmatrix} A & B \\ C & O \end{pmatrix} m_{n-1} = \cdots = \begin{pmatrix} A & B \\ C & O \end{pmatrix}^{n-1} m_1
\]

(A.7)

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
\[
\begin{cases}
A_n = AA_{n-1} + BC_{n-1}, \\
C_n = CA_{n-1};
\end{cases}
\]

(A.8)

\[
\begin{cases}
B_n = AB_{n-1} + BD_{n-1}, \\
D_n = CB_{n-1};
\end{cases}
\]

(A.9)

with \( A_0 = D_0 = Id \) and \( C_0 = B_0 = O \). Consider system (A.8). Since \( A = \begin{pmatrix} e^{2\lambda} & 0 \\ 0 & 0 \end{pmatrix} \), we have that
\[
A_n = \begin{pmatrix} e^{2\lambda} & 0 \\ 0 & 0 \end{pmatrix} CA_{n-1} + BC_{n-1} = \begin{pmatrix} e^{2\lambda} & 0 \\ 0 & 0 \end{pmatrix} C_n + BC_{n-1}.
\]

(A.10)
Therefore,

\[ C_n = C \left( \begin{pmatrix} e^{2\lambda} & 0 \\ 0 & 0 \end{pmatrix} C_{n-1} + BC_{n-2} \right). \]  

(A.11)

Let \( \kappa_n \) be defined by (2.4). We claim that \( C_n = \kappa_n C \) solves (A.11). For \( n = 2 \) (as well as \( n = 0, 1 \)) the claim holds by direct check. Assume it holds for \( k \leq n \) with \( n \geq 2 \). Applying inductive assumption and multiplying,

\[ C_{n+1} = C \left( \kappa_n \begin{pmatrix} e^{2\lambda} & 0 \\ 0 & 0 \end{pmatrix} C + \kappa_{n-1} BC \right) = 
\left[ C \begin{pmatrix} e^{2\lambda} & 0 \\ 0 & 0 \end{pmatrix} C = pe^{2\lambda}C, \quad CBC = qe^\lambda(q + pe^\lambda)C \right] = 
(pe^{2\lambda}\kappa_n + qe^\lambda(q + pe^\lambda)\kappa_{n-1})C = \kappa_{n+1}C \]

since an expression for \( \kappa_n \) given in (2.4) 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 (A.10), we obtain an expression for \( A_n \).

System (A.9) is handled in the same way by noting that it is identical to (A.8) and only the initial conditions differ leading thereby to the following solution:

\[ D_n = \kappa_{n-1} D_2, \quad B_n = \begin{pmatrix} e^{2\lambda} & 0 \\ 0 & 0 \end{pmatrix} D_n + BD_{n-1} \text{ for } n \geq 1. \]  

(A.12)

Step 2: final expression. From the results of Step 1, we obtain an expression for \( m_n \) given by (A.7) since \( m_3 \) is readily available and equal to\(^4\) \( (e^\lambda, e^\lambda, 1, 1)^T \):

\[ m_n = \begin{pmatrix} (e^\lambda A_{n-1} + B_{n-1}) \frac{1}{1} \\ (e^\lambda C_{n-1} + D_{n-1}) \frac{1}{1} \end{pmatrix}. \]

Noting that

\[ E e^{\lambda T_n} = p E \left( e^{\lambda T_n} \mid X_n = 1 \right) + q E \left( e^{\lambda T_n} \mid X_n = 0 \right) = pm_{1,n} + qm_{2,n}, \]

we finally arrive to expression (2.5).

Proof of Corollary 2.1. Recall that the \( k \)-th derivative of the moment generating function evaluated at 0 yields the \( k \)-th moment. Therefore, to obtain the announced formulae, one simply needs to differentiate expression (2.5). 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 paper with the trivial content. For the sake

\( ^4 \)note that \( T_1 \equiv 1, T_0 \equiv 0 \)

9
of convenience, we make change of variables \( x = e^{\lambda} \) and work with probability generating function \( G(x) = E x^{T_n} = M_{T_n}(\ln \lambda) \). By (2.4)–(2.5) and slight abuse of notation,

\[
G(x) = g_1(x) \kappa_{n-2}(x) + g_2(x) \kappa_{n-3}(x) \quad \text{with}
\]

\[
g_1(x) = ((1 - q)^2 x^3 + q(1 - q)^2 x^2 + q(1 - q^2) x + q^2) x^2,
\]

\[
g_2(x) = q ((1 - q)^2 x^3 + q(1 - q)(2 - q)x^2 + 2q^2(1 - q)x + q^3) x^2,
\]

\[
\alpha_i = \alpha_i(x) = \frac{1}{2} \left( px^2 + (-1)^i \sqrt{p^2 x^4 + 4qx(q + px)} \right), \quad \text{for } i = 0, 1, \text{ and}
\]

\[
\kappa_n = \kappa_n(x) = \frac{\alpha_0^n(x) - \alpha_1^n(x)}{\alpha_0(x) - \alpha_1(x)} \text{ for } n \geq 0. \tag{A.13}
\]

Then

\[
E T_n = G'(1) = g_1'(1) \kappa_{n-2}(1) + g_1(1) \kappa_{n-3}'(1) + g_2(1) \kappa_{n-3}'(1) \tag{A.14}
\]

and

\[
E T_n(T_n - 1) = G''(1) = g_1''(1) \kappa_{n-2}(1) + 2g_1'(1) \kappa_{n-3}(1) + g_1(1) \kappa_{n-3}'(1) + g_2(1) \kappa_{n-3}'(1) \tag{A.15}
\]

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

\[
\alpha_0(1) = 1, \quad \alpha_1(1) = -q, \quad \alpha_0'(1) = \frac{2 - q^2}{1 + q}, \quad \alpha_1'(1) = -\frac{q^2}{1 + q},
\]

\[
\alpha_0''(1) = \frac{4}{q + 1} - \frac{2}{(q + 1)^3}, \quad \alpha_1''(1) = -\frac{2(1 - q)^2}{q + 1} + \frac{2}{(q + 1)^3},
\]

\[
g_1(1) = 1, \quad g_2(1) = q,
\]

\[
g_1'(1) = q^3 - q^2 - 3q + 5, \quad g_2'(1) = -q (q^2 + 2q - 5),
\]

\[
g_1''(1) = 6q^3 - 2q^2 - 22q + 20, \quad g_2''(1) = 2q (q^3 - 2q^2 - 8q + 10),
\]

10
Applying Taylor’s formula, we obtain the following equalities (for $\lambda \to 0$):

$$p^2 e^{4\lambda} + 4q e^{\lambda} (q + pe^{\lambda}) = (1 + q)^2 \left[ 1 + \frac{4\lambda}{(1 + q)^2} + \frac{(2 - q)^2}{1 + q} + O(\lambda^3) \right];$$

$$\sqrt{p^2 e^{4\lambda} + 4q e^{\lambda} (q + pe^{\lambda})} = 1 + \frac{2\lambda}{(1 + q)^2} +$$

$$\lambda^2 \left( \frac{2 - q}{1 + q} + \frac{2}{(1 + q)^2} + O(\lambda^3); \right)$$

$$\alpha_0 = 1 + \frac{2 - q^2}{1 + q} + \frac{\lambda^2}{2} \left( 2(1 - q) + \frac{(2 - q)^2}{1 + q} - \frac{2}{(1 + q)^3} \right) + O(\lambda^3);$$

$$\alpha_1 = -q - \lambda \frac{q^2}{1 + q} + \frac{\lambda^2}{2} \left( 2(1 - q) - \frac{(2 - q)^2}{1 + q} + \frac{2}{(1 + q)^3} \right) + O(\lambda^3).$$

(A.16)

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

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

(A.17)

Consequently,

$$(\alpha_0 - \alpha_1) \kappa_n(\lambda) = \frac{\alpha_0^n - \alpha_1^n}{(-q)^n} = e^{n \ln \alpha_0} - (-1)^n e^{n \ln \left( \frac{\alpha_1}{\alpha_0} \right)} =$$

$$\exp \left\{ n \left( c_{i1} \lambda + \left( c_{i2} - \frac{c_{i1}^2}{2} \right) \lambda^2 \right) + O(n \lambda^3) \right\} -$$

$$(-1)^n \exp \left\{ n \left( c_{i1} \lambda + \left( c_{i2} - \frac{c_{i1}^2}{2} \right) \lambda^2 \right) + n \ln q + O(n \lambda^3) \right\}. \quad (A.18)$$

Finally, let $g_i(x)$ denote the same polynomials as given in (A.13). Taylor expanding yields

$$g_1(e^\lambda) = 1 + O(\lambda), \quad g_2(e^\lambda) = q + O(\lambda).$$
Combining all above, we then obtain the following asymptotic expansion for the moment generating function:

$$M_{T_n}(\lambda) = \frac{1}{1 + q + O(\lambda)} \left((1 + O(\lambda))\kappa_{n-2}(\lambda) + (q + O(\lambda))\kappa_{n-3}(\lambda)\right), \quad \lambda \to 0,$$

(A.19)

with asymptotic expressions for $\kappa_{n-2}, \kappa_{n-3}$ stemming from (A.18).

**Step 2: LLN.** To prove relationship $\frac{T_n}{n} \xrightarrow{L^2} \frac{2-q^2}{1+q}$, note that, by Corollary 2.1,

$$E \left(\frac{T_n}{n} - \frac{2-q^2}{1+q}\right)^2 = E \left(\frac{T_n}{n} - E \frac{T_n}{n}\right)^2 + E \left(E \frac{T_n}{n} - \frac{2-q^2}{1+q}\right)^2 = \frac{1}{n^2} \left(\text{Var} T_n + \left(\frac{q^2 + q - 1}{(1+q)^2} (1 - (-q)^n)\right)^2\right) = O\left(\frac{1}{n}\right).$$

To prove a.s. convergence, we show that the following sufficient condition holds:

$$\forall \varepsilon > 0 \sum_{n=2}^{\infty} P\left(\left|\frac{T_n}{n} - \frac{2-q^2}{1+q}\right| > \varepsilon\right) < \infty. \quad (A.20)$$

To this end, we bound the probability

$$P\left(\left|\frac{T_n}{n} - \frac{2-q^2}{1+q}\right| > \frac{\ln n}{\sqrt{n}}\right) = P\left(\frac{T_n}{\sqrt{n}} - \sqrt{n} \frac{2-q^2}{1+q} > \gamma \ln n\right) + P\left(\frac{T_n}{\sqrt{n}} - \sqrt{n} \frac{2-q^2}{1+q} < -\gamma \ln n\right),$$

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

$$P\left(\frac{T_n}{\sqrt{n}} - \sqrt{n} \frac{2-q^2}{1+q} > \gamma \ln n\right) \leq e^{-\gamma^2 \frac{2-q^2}{1+q} - \gamma \ln n} E e^{\frac{T_n}{\sqrt{n}}} = e^{-\gamma^2 \frac{2-q^2}{1+q} - \gamma \ln n} M_{T_n}\left(\frac{1}{\sqrt{n}}\right).$$

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

$$M_{T_n}\left(\frac{1}{\sqrt{n}}\right) = \left(1 + O\left(\frac{1}{\sqrt{n}}\right)\right) e^{c_{01} \sqrt{n} + c_{12} - \frac{c_{11}^2}{2} + O\left(\frac{1}{\sqrt{n}}\right)}$$

$$(-1)^n e^{c_{11} \sqrt{n} + c_{12} - \frac{c_{11}^2}{2} + n \ln q + O\left(\frac{1}{\sqrt{n}}\right)}.$$

Since,

$$c_{01} = \frac{2-q^2}{1+q} \quad \text{and} \quad c_{11} \sqrt{n} - \frac{2-q^2}{1+q} \sqrt{n} + c_{12} - \frac{c_{11}^2}{2} + n \ln q = n \ln q \left(1 + O\left(\frac{1}{\sqrt{n}}\right)\right),$$
we obtain that
\[ e^{-\sqrt{n} \frac{2 - q^2}{1 + q} - \gamma \ln n M_{T_n} \left( \frac{1}{\sqrt{n}} \right)} = e^{-\gamma \ln n} O(1) \leq \frac{C_q}{n^\gamma} \]
for some constant \( C_q \in (0, \infty) \) independent of \( \gamma \). In the same way,
\[ P \left( \left| \frac{T_n}{n} - 2 - q^2 \right| < -\gamma \frac{\ln n}{\sqrt{n}} \right) \leq e^{\sqrt{n} \frac{2 - q^2}{1 + q} - \gamma \ln n M_{T_n} \left( -\frac{1}{\sqrt{n}} \right)} \leq \frac{C_q}{n^\gamma} \]
provided \( C_q \) in the previous inequality was chosen large enough. Taking \( \gamma > 1 \), we then have that
\[ \sum_{n=2}^{\infty} P \left( \left| \frac{T_n}{n} - 2 - q^2 \right| > \gamma \frac{\ln n}{\sqrt{n}} \right) \leq 2C_q \sum_{n=1}^{\infty} \frac{1}{n^\gamma} < \infty. \]
Hence (A.20) and the claim.

**Step 3: CLT.** It suffices to show that
\[ M \sqrt{n} \left( \frac{T_n}{n} - 2 - \frac{q^2}{q + q} \right) \xrightarrow{n \to \infty} M_{\xi}(t), \quad \xi \sim N(0, \sigma^2) \]
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 that
\[ M \sqrt{n} \left( \frac{T_n}{n} - 2 - \frac{q^2}{q + q} \right) = e^{-t \sqrt{n} \frac{2 - q^2}{1 + q} + O\left( \frac{1}{\sqrt{n}} \right)} \]
\[ \left( 1 + O \left( \frac{1}{\sqrt{n}} \right) \right) \left( e^{tc_{01} \sqrt{n} + t^2 \left( c_{02} - \frac{q^2}{q + q} \right)} + O\left( \frac{1}{\sqrt{n}} \right) \right) \] 
\[ (-1)^n e^{tc_{11} \sqrt{n} + t^2 \left( c_{12} - \frac{q^2}{q + q} + n \ln q + O\left( \frac{1}{\sqrt{n}} \right) \right)} = \]
\[ \left( 1 + O \left( \frac{1}{\sqrt{n}} \right) \right) e^{t^2 \left( c_{02} - \frac{q^2}{q + q} \right) + O\left( \frac{1}{\sqrt{n}} \right)} + O\left( q^n \right) \xrightarrow{n \to \infty} t^2 \left( c_{02} - \frac{q^2}{q + q} \right). \]

Direct calculations show that \( c_{01} = \frac{-q^2}{2} = \frac{x^2}{2} \).

**Step 4: LDP.** To prove the final claim, we apply Gärtner-Ellis (GE) Theorem (see [5], Section 2.3) to \( Z_n = \frac{T_n}{n} \). First, note that, for any fixed \( \lambda \in \mathbb{R} \),
\[ \alpha_0(\lambda) > \alpha_1(\lambda) \Rightarrow \lim_{n \to \infty} \frac{\kappa_{n-2}(\lambda)}{\kappa_{n-1}(\lambda)} = \frac{1}{\alpha_0(\lambda)} \Rightarrow \]
\[ \Lambda(\lambda) := \lim_{n \to \infty} \frac{1}{n} \ln M_{Z_n}(n\lambda) = \lim_{n \to \infty} \frac{1}{n} \ln M_{T_n}(\lambda) = \]
\[ \lim_{n \to \infty} \frac{1}{n} \ln \alpha_0^n(\lambda) = \ln \alpha_0(\lambda) \in \mathbb{R}. \]
Since \( \mathbb{R} \ni \lambda \mapsto \Lambda(\lambda) \) is differentiable at every \( \lambda \in \mathbb{R} \), it follows that all GE assumptions hold and \( T_n \) satisfies LDP with a good rate function \( I \) equal to the Legendre transform of \( \Lambda \).
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