Decision Theoretic Cutoff and ROC Analysis for Bayesian Optimal Group Testing

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Abstract—We study the inference problem in the noisy group testing to identify defective items from the perspective of the decision theory. We introduce Bayesian inference and consider the Bayesian optimal setting in which the true generative process of the test results is known. We demonstrate the adequacy of the posterior marginal probability in the Bayesian optimal setting as a diagnostic variable based on the area under the curve (AUC). Using the posterior marginal probability, we derive the general expression of the optimal cutoff value that yields the minimum expected risk function. Furthermore, we evaluate the performance of the Bayesian group testing without knowing the true states of the items: defective or non-defective. By introducing an analytical method from statistical physics, we derive the receiver operating characteristics curve, and quantify the corresponding AUC under the Bayesian optimal setting. The obtained analytical results precisely describe the actual performance of the belief propagation algorithm defined for single samples when the number of items is sufficiently large.

Index Terms—Group testing, Bayes risk, cutoff, ROC curve.

I. INTRODUCTION

GROUP testing is an effective testing method to reduce the number of tests required for identifying defective items by performing tests on the pools of items [1]. In individual testing, identifying defective items, particularly in a noiseless test, is feasible. In this case, the number of tests needed to identify the states of the items grows in accordance with the number of the items being tested, which is computationally undesirable in large-scale testing scenarios. Meanwhile, group testing involves pooling multiple items, and performing tests on the resultant pools. Most research in group testing has been concentrated to the case where the number of the pools $M$ is smaller than the number of items $N$, to reduce the number of tests required relative to the number of items being tested. As with previous studies, we will focus on the cases where $M < N$. The identification of items’ states through group testing when $M < N$ is equivalent to solving an underdetermined problem. It is expected that when the prevalence (fraction of the defective items) is sufficiently small, the defective items can be accurately identified using an appropriate inference method, as with sparse estimation [2], [3], wherein an underdetermined problem is solved under the assumption that the number of nonzero (defective in the context of group testing) components in the variables to be estimated is sufficiently small. The reduction in the number of tests reduces the testing costs; hence, the application of group testing to various diseases such as HIV [4] and hepatitis virus [5], [6] has been discussed. In addition, the need to detect elements in heterogeneous states from a large population is common not only in medical tests but also in various other fields. The group testing matches such demands and is applied to the detection of rare mutations in genetic populations [7] and the monitoring of exposure to chemical substances [8].

The accuracy of group testing depends on the pooling method; that is, how the items are assigned to their respective pools. Pooling methods can be categorized as either non-adaptive, where pools are fixed in advance, or adaptive, where pools are sequentially determined based on the test results. Examples of non-adaptive pooling methods include regular-random pooling, wherein every item is included in the same number of pools randomly assigned, and Bernoulli pooling, wherein every item is independently prescribed a probability to be included in each pool [9], [10]. The original group testing proposed by Dorfman [1] uses an adaptive pooling method called two-stage testing. Developing on the two-stage testing, the binary splitting method has been proposed, where the defective pools are sequentially divided into subpools, which are themselves tested and divided, and so on [11], [12]. From an experimental point of view, a method called shifted transversal for high-throughput screening has been proposed [13]. In addition, a pooling method using a paper-like device for multiple malaria infections has been developed for effective testing [14]. Recently, a pooling method using active learning has also been proposed [15], [16].

The estimation of the items’ states under the given pools has been theoretically studied, largely based on the mathematical
correspondence between the group testing and information theoretic problems [10], [17]. Within a sublinear regime, where the number of the defective item is $\sim N^\gamma$ with $0 < \gamma < 1$, sharp phase transition phenomena have been observed at the same information-theoretic threshold when using both Bernoulli pooling [18], [19] and regular-random pooling [20]. Given these information-theoretic bounds, recent attempts to understand the computational-statistical gaps have been made [20], [21], [22]. It has been suggested that a polynomial-time Markov Chain Monte Carlo (MCMC) method can achieve approximate recovery under Bernoulli pooling using the number of tests given by the information-theoretic bound [21].

Most previous studies have focused on the sublinear regime. However, the fraction of the defective items in the population can easily increase due to the sampling bias known as Berkson’s bias [23], [24]. Considering such situations, theoretical and algorithmic attempts at linear regime, where the fraction of the defective items is proportional to $N$, expand the availability of the group testing.

In this study, we examine the problem of estimating the items’ states in noisy group testing under regular-random and non-adaptive pooling within the linear regime, where the prevalence is $O(1)$. We introduce belief propagation (BP) algorithm and corresponding replica analysis in statistical physics, which are valid in the linear regime. Because errors are inevitable in realistic testing scenarios [25], Bayesian inference has been incorporated into the estimation process in group testing to model probabilistic errors [26], [27]. With appropriate modeling, the estimation of the items’ states using Bayesian inference is superior to binary splitting-based methods in the case of finite error probability, although its theoretical understanding is still lacking. We introduce the Bayesian optimal setting for conducting a theoretical analysis, wherein the true generative process of the test results is known. The statistical model considered here describes an idealized group testing, and there are no practical tests that completely match this setting. However, as explained in the main text, the Bayesian optimal setting considered here can provide a practical guide for group testing.

The basis for applying Bayesian inference to estimate the items’ states, which are discrete, is the posterior distribution, which has a continuous value $[0, 1]$ defined on the items’ states (defective or non-defective). In a previous study, it has been suggested that the Bayesian group testing cannot achieve perfect identification of items’ states, in the sense that the marginal posterior distribution in the linear regime does not assign a value of 1 to the true states [27]. In this study, we theoretically demonstrate that the perfect identification is impossible in Bayesian optimal group testing under the linear regime, even in the noiseless case. Therefore, the items’ states should be determined on the basis of the posterior distribution with values in $(0, 1)$. This problem setting is like those found in medical diagnosis based on continuous test values [28]. We proceed to quantify the performance of the Bayesian group testing as a diagnostic classifier.

We consider two quantification methods used in medical tests that output continuous values. The first is the cutoff-dependent property. In prior studies on Bayesian group testing, the maximum posterior marginal (MPM) estimator, which is equivalent to the cutoff of 0.5, was used for the mapping to determine the items’ states from the posterior distribution [26], [27]. However, there is no mathematical background behind the use of the MPM estimator. Appropriately determine the cutoff in Bayesian group testing using a risk function from the view point of decision theory [29] or utility theory [30], and understand the MPM estimator and the maximization of Youden index in the unified framework of the Bayesian decision theory. We show that usage of the MPM estimator in group testing, where a sufficiently low prevalence of defective is expected, leads to a decision prioritizing the decrease of false positives over false negatives.

The second characterization is the cutoff-independent property using the receiver operating characteristic (ROC) curve [31], [32]. More quantitatively, the area under the curve (AUC) of the ROC curve is used as an indicator of the usefulness of a test [33]. Generally, evaluating the AUC of a diagnostic classifier requires a gold standard for diagnosing true items’ states with certainty. In cases where there is no specific and sensitive test to detect the target disease, that is, the no-gold standard case, the ROC curve and AUC must first be estimated using statistical models [34], [35]. Bayesian methods have been developed for these estimation, either parametric [36], or non-parametric [37], and semiparametric [38] models depending on the experimental situations. We demonstrate that an analytical method originating from statistical physics can be used to derive ROC curve and measure the corresponding AUC in the Bayesian optimal setting even in the no-gold-standard case. Although the Bayesian optimal setting is not realistic, we show that using AUC in the Bayesian optimal setting provides the maximum value of the AUC among any other estimation methods.

The main contributions of our study are as follows.

- We show that the expected AUC is maximized under the Bayesian optimal setting when we use diagnostic variables that have the same order of magnitude as marginal posterior probability, where the diagnostic variable is the (possibly continuous-valued) statistic used to determine the items’ states from the test outcomes.

- We show that in the Bayesian optimal setting, Bayes risk function defined by the false positive rate and false negative rate is minimized using the marginal posterior probability and appropriate cutoff. The form of the cutoff derived indicates that the MPM estimator is not necessarily appropriate for the group testing problems in the linear regime, particularly when the correction of the false negatives is a practical demand.

- We derive the distribution of the marginal posterior probability for defective and non-defective items under the Bayesian optimal setting without knowing which items are defective. Using this distribution, we obtain the ROC curve and quantify the AUC without gold-standard. Then, we identify the parameter region in which the group testing with smaller number of tests yields a better
We introduce the following assumptions in our model of the dependence on \( \alpha \).

We demonstrate that the analytical results obtained can accurately describe the behavior of the BP algorithm employed on a single sample when the number of items is sufficiently large. Using the analytical expression, we show that Bayesian optimal group testing cannot achieve perfect identification of items’ states in the linear regime. Additionally, we suggest the absence of the first order transition, which indicates the absence of a statistical-computational gap.

The remainder of this paper is organized as follows. In Sec. II, we describe our model for the group testing and Bayesian optimal setting. In Sec. III, we introduce several propositions hold in the Bayesian optimal setting, and derive a general expression for the cutoff corresponding to the risk function. In Sec. IV, the performance evaluation method based on the replica method for the group testing is summarized and the results are presented. In Sec. V, the correspondence between the replica method and the BP algorithm is explained. Sec. VI summarizes this study and explains the considerations regarding the assumptions used in this paper.

II. MODEL AND SETTINGS

Let us denote the number of items as \( N \). We consider pools under the constraint that the number of items in each pool is \( K \), and the number of pools each item belongs to is \( C \). Here, we refer to \( K \) and \( C \) as the pool size and overlap, respectively, and set them to be sufficiently smaller than \( N \). There are \( N^\nu = \frac{N^\nu}{K(N-K)^\nu} \) pools that satisfy the condition. We label them as \( \nu = 1, 2, \ldots, N^\nu \) and prepare the corresponding variable \( c = \{c_1, c_2, \ldots, c_N\} \in \{0,1\}^{N^\nu} \), which represents pooling method: \( c_0 \in \{0\} \) indicates that the \( \nu \)-th pool is tested, whereas \( c_0 = 0 \) indicates that it is not tested. We consider that each pool is not tested more than once, and \( M \)-tests are performed in total; hence, \( \sum \nu c_\nu = M \) and \( C = KM/N \) hold. As we are focusing on the case when \( M < N \), we set \( \alpha = M/N \) (<1). The set of labels of the items in the \( \nu \)-th pool is \( L(\nu) \), and the number of labels in \( L(\nu) \) is \( K \) without dependence on \( \nu \). The true state of all items is denoted by \( x^{(0)} \in \{0,1\}^N \), and that of the items in the \( \nu \)-th pool is denoted by \( x^{(0)}(\nu) \in \{0,1\}^K \). For instance, when the 1st pool contains the 1st, 2nd, and 3rd items, \( x^{(0)}(1) = \{x_1^{(0)}, x_2^{(0)}, x_3^{(0)} \} \).

We introduce the following assumptions in our model of the group testing.

- A1 The pools that contain at least one defective item are regarded as positive.
- A2 Each test result independently obeys the identical distribution.

In addition, we consider that the test property is characterized by the true positive probability \( p_{TP} \) and false positive probability \( p_{FP} \). We denote the \( \nu \)-th pool’s test result as \( y_\nu \), and consider the case \( y_\nu \in \{0,1\} \). Hence, the true generative process of the test result \( y_\nu \) performed on the \( \nu \)-th pool is given by

\[
\begin{align*}
  p(y_\nu | c_\nu, x^{(0)}(\nu)) &= (1 - c_\nu) \\
  &+ c_\nu \left( (p_{TP} y_\nu + (1 - p_{TP})(1 - y_\nu)) T(x^{(0)}(\nu)) \\
  &+ (p_{FP} y_\nu + (1 - p_{FP})(1 - y_\nu)) (1 - T(x^{(0)}(\nu))) \right),
\end{align*}
\]

and the joint distribution of the \( M \)-test results is given by

\[
  p(y|c,x) = \prod_{\nu=1}^{N^\nu} p(y_\nu|c_\nu, x^{(0)}(\nu)).
\]

- A3 The true positive probability \( p_{TP} \) and false positive probability \( p_{FP} \) are known in advance.

Following this assumption, the assumed model for the inference is set as \( p(y|c,x) \), where \( x = \{0,1\}^N \) is the items’ states correspond to the model parameter.

As the prior knowledge, we introduce the following model assumptions.

- A4 The prevalence, the fraction of defective items, \( \theta \) is known.
- A5 The pretest probability of all items is set to the prevalence \( \theta \), and we consider the items to be independently and identically distributed under a Bernoulli prior with Bernoulli parameter \( \theta \).

\[
\phi(x) = \prod_{i=1}^N \{(1 - \theta)(1 - x_i) + \theta x_i\}.
\]

Following the Bayes’ theorem, the posterior distribution is given by

\[
P(x|y,c) = \frac{1}{P_y(y|c)} f(y|x,c) \phi(x),
\]

where \( P_y(y|c) \) is the normalization constant given by

\[
P_y(y|c) = \sum_{x \in \{0,1\}^N} f(y|x,c) \phi(x).
\]

We note that \( P_y(y|c) \) corresponds to the true generative process of the test results in the Bayesian optimal setting. In the problem setting considered here, the assumed model used in the inference matches the true generative process of the test results. We refer to such a setting as \textit{Bayes optimal}.

III. APPROPRIATE DIAGNOSTIC VARIABLE AND CUTOFF

In this section, we present a discussion based on Bayesian decision theory for the setting of the diagnostic variable and cutoff.

A. Diagnostic Variable for Decision

First, we consider the statistic that should be used as a diagnostic variable to determine the items’ states. In this study, we adopt the statistic that is expected to maximize the AUC. We denote the arbitrary statistic \( s_i(y,c) = \mathbb{R} \) for the \( i \)-th item, which characterizes the estimated item’s state under the pooling method \( c \) and the test result \( y \). The statistic \( s \) does not need to be evaluated in the framework of Bayesian
estimation but can be defined based on other methods. We use
the following expression for the AUC, which is equivalent to
the Wilcoxon–Mann–Whitney test statistic [33]:
\[
\text{AUC}(x^{(0)}, s(y, c)) = \frac{1}{N^2\theta(1-\theta)} \times \sum_{i \neq j} x_i^{(0)}(1-x_j^{(0)}) \left\{ \mathbb{I}(s_i(y, c) > s_j(y, c)) + \frac{1}{2} \mathbb{I}(s_i(y, c) = s_j(y, c)) \right\}.
\]
(5)
Furthermore, we define the expected AUC as
\[
\text{AUC}[s] = \mathbb{E}[X^{(0)} \left| y, c \right.] \mathbb{E}[AUC(X^{(0)}, s(Y, c))],
\]
where \( \mathbb{E}[X^{(0)} \left| y, c \right.] \) and \( \mathbb{E}[y, c] \) denote the expectations according to the prior \( \phi(x^{(0)}) \) and the likelihood \( f(y|x^{(0)}, c) \), respectively, and \( \text{AUC}[s] \) refers to the expected AUC as a function of \( s \). In the Bayesian optimal setting, the expected AUC is given by
\[
\text{AUC}[s] = \sum_y P_y(y,c) \hat{\text{AUC}}_S(y, c),
\]
where \( \hat{\text{AUC}}_S(y, c) \) is the posterior AUC defined by
\[
\hat{\text{AUC}}_S(y, c) = \frac{\rho_s^2}{N^2\theta(1-\theta)} \times \sum_{i \neq j} E_X|x_i \left| y, c \right. \left[ x_i(1-x_j) \right] \left\{ \mathbb{I}(s_i(y, c) > s_j(y, c)) + \frac{1}{2} \mathbb{I}(s_i(y, c) = s_j(y, c)) \right\}.
\]
(7)
Here, \( E_X|x_i \left| y, c \right. \left[ x_i(1-x_j) \right] \) denotes the expectation with respect to the posterior distribution \( P(x|y, c) \). We denote the marginal posterior probability under the Bayesian optimal setting as \( \rho_s(y, c) = \sum_x X \rho_s(x, y, c) \). For simplicity, we consider the case where \( E_X|x_i \left| y, c \right. \left[ x_i(1-x_j) \right] \sim \rho_s(y, c)(1-\rho_j(y, c)) \) holds, which means that correlations among the components of \( X \) are negligible in \( P(x|y, c) \); hence,
\[
\hat{\text{AUC}}_S(y, c) = \frac{\rho_s^2}{N^2\theta(1-\theta)} \sum_{i > j} \rho_s^2(y, c),
\]
(8)
where
\[
\rho_s^2(y, c) = \left\{ \rho_s(y, c)(1-\rho_j(y, c)) \mathbb{I}(s_i(y, c) > s_j(y, c)) + \rho_j(y, c)(1-\rho_i(y, c)) \mathbb{I}(s_i(y, c) > s_j(y, c)) + \frac{1}{2} \rho_i(y, c)(1-\rho_j(y, c)) \mathbb{I}(s_i(y, c) > s_j(y, c)) \right\}.
\]
(9)
As a diagnostic variable, we adopt the statistic that yields
the largest \( \hat{\text{AUC}}(y, c) \). The following proposition suggests the
statistic appropriate for the purpose.

**Proposition 1:** We introduce the order statistic of \( \rho \) as
\( \rho_{\sigma(1)} \leq \rho_{\sigma(2)} \leq \cdots \leq \rho_{\sigma(N)} \), where \( \sigma(j) \in \{1, 2, \ldots, N\} \) denotes the index of the component in \( \rho \) whose value is
the \( j \)-th smallest. The maximum of the posterior AUC \( 8 \) is achieved when \( s \) is aligned in the same order as \( \rho \); namely
\( s_{\sigma(i)} > s_{\sigma(j)} \) for \( \rho_{\sigma(i)} > \rho_{\sigma(j)} \) and \( s_{\sigma(i)} = s_{\sigma(j)} \) for \( \rho_{\sigma(i)} = \rho_{\sigma(j)} \).

**Proof:** Using the order statistics, the posterior AUC for
\( s = \rho \) is given by
\[
\hat{\text{AUC}}_\rho(y, c) = \frac{1}{N^2\theta(1-\theta)} \sum_{i > j} \rho_s(i)(1-\rho_s(j)).
\]
(10)
When \( i > j \), the difference between \( \rho_s(i)(1-\rho_s(j)) \) and \( \rho_s(i)(1-\rho_s(j)) \) under an arbitrary statistics \( s \) is given by
\[
\rho_s(i)(1-\rho_s(j)) - \rho_s(i)(1-\rho_s(j)) \geq 0
\]
(11)
where we used the identity \( \mathbb{I}(s_i > s_j) = 1 - \mathbb{I}(s_i < s_j) - \mathbb{I}(s_i = s_j) \). Therefore, we obtain
\[
\hat{\text{AUC}}_\rho(y, c) - \hat{\text{AUC}}_s(y, c) = \frac{1}{N^2\theta(1-\theta)} \sum_{i > j} \rho_s(i)(1-\rho_s(j)) - a_{\rho(i)}(1-\rho_s(j)) \geq 0.
\]
(12)
The equality holds when \( s \) is aligned in the same order as \( \rho \), for which \( 9 \) guarantees \( a_{\rho(i)}(1-\rho_s(j)) = \rho_s(i)(1-\rho_s(j)) \) for any pair where \( i > j \).

In principle, any statistic \( s \) can achieve a maximum of \( \hat{\text{AUC}} \) when it satisfies the aforementioned condition. The simplest example is \( s = \rho \). Furthermore, \( s_i = \rho_i^k \) for \( k > 0 \) also
yields a maximal value of \( \hat{\text{AUC}} \). Proposition 1 is similar to the
Bayes optimal scoring function for the multilabel classifier
using rank-loss [39]. Although AUC maximization and rank-
loss minimization are based on different principles, the current
problem setting of group testing can be regarded as an \( N \)-label
classification problem, where \( x^{(0)} = 1 \) indicates that the \( i \)-th
label is relevant. We further show that the arguments based on
Bayes optimality also provide a guideline for appropriately
determining cutoff in the following section.

**B. Determination of Cutoff**

AUC maximization does not uniquely specify the optimal
estimator. Here, we further introduce another criterion, that of
the utility function, for cutoff determination, and show that
the posterior marginal is adequate under the utility function.
We define the utility function for the use of an arbitrary
estimator \( \hat{x}(y, c) \in \{0, 1\}^N \) as follows [30]:
\[
U(x^{(0)}, \hat{x}(y, c); u) = \theta(\text{TP}) + \theta(\text{FP}) \text{FN} + (1-\theta)(\text{FP})u_{\text{FP}} + (1-\theta)(\text{TN})u_{\text{TN}}
\]
\[
= \theta(\text{TP}) + (1-\theta)(\text{FP})u_{\text{FP}} + \theta(\text{FN} - \text{TP}) + (1-\theta)(\text{FP})u_{\text{FP}} + (1-\theta)(\text{TN})u_{\text{TN}}
\]
(13)
where \( u = \{\text{TP}, \text{FP}, \text{FP}, \text{FP}, \text{TP} \} \), and \( \text{TP}, \text{FN} = 1 - \text{TP}, \text{FP} = 1 - \text{TN}, \text{and TN} \) are the true positive rate, false negative rate,
false positive rate, and true negative rate, respectively.
Following our notations, \( \text{FN} \) and \( \text{FP} \) are given by
\[
\text{FN}(x^{(0)}, \hat{x}(y, c)) = \sum_{i=1}^N x_i^{(0)}(1-\hat{x}_i(y, c)) \frac{N}{N \theta}
\]
(14)
\[
\text{FP}(x^{(0)}, \hat{x}(y, c)) = \sum_{i=1}^N (1-x_i^{(0)})\hat{x}_i(y, c) \frac{N}{N \theta}
\]
(15)
The first and second terms of (13) are constants given by the model parameters; hence, for convenience, we define the risk function $R(x^{(0)}, \hat{x}(y, c); \lambda)$ from the third and fourth terms of (13) as

$$R(x^{(0)}, \hat{x}(y, c); \lambda) = \lambda_{FN} FN + \lambda_{FP} FP,$$

(16)

where $\lambda = \{\lambda_{FN}, \lambda_{FP}\}$ is the set of parameters given by $\lambda_{FN} = -\theta (u_{FN} - u_{TP}) > 0$ and $\lambda_{FP} = -(1 - \theta) (u_{FP} - u_{TN}) > 0$, respectively. The risk function evaluates the detrimental effect of the incorrectly estimated results. The maximization of the utility function is equivalent to the minimization of the risk function; hence, we consider the risk minimization. We define an expected risk as $E_c \{R(x^{(0)}, \hat{x}(y, c); \lambda)\}$. Under the Bayesian optimal setting, the expected risk known as Bayes risk is given by

$$\hat{R}(\hat{x}; \lambda) = \sum_y P_y(y|c) \hat{R}(\hat{x}(y, c); \lambda),$$

(17)

where $\hat{R}(\hat{x}(y, c); \lambda)$ is the posterior risk defined as

$$\hat{R}(\hat{x}(y, c); \lambda) = \lambda_{FN} \hat{FN}(\hat{x}(y, c)) + \lambda_{FP} \hat{FP}(\hat{x}(y, c)),$$

(18)

and $\hat{FN}$ and $\hat{FP}$ are the posterior FN and posterior FP defined as

$$\hat{FN}(\hat{x}(y, c)) = E_{X|y, c} \left[ \sum_{i=1}^N X_i (1 - \hat{x}_i(y, c)) / N \theta \right]$$

$$= \sum_{i=1}^N \rho_i(y, c) (1 - \hat{x}_i(y, c)), \quad (19)$$

$$\hat{FP}(\hat{x}(y, c)) = E_{X|y, c} \left[ \sum_{i=1}^N (1 - X_i) \hat{x}_i(y, c) / N \theta \right]$$

$$= \sum_{i=1}^N (1 - \rho_i(y, c)) \hat{x}_i(y, c), \quad (20)$$

respectively. Here, the following relationship holds:

$$E_{X^{(0)}} \left[ E_{Y|X^{(0)}, c} \{ \hat{FN}(\hat{x}(Y, c)) \} \right] = E_{X^{(0)}} \left[ E_{Y|X^{(0)}, c} \{ \hat{FN}(X^{(0)}, \hat{x}(Y, c)) \} \right]$$

$$E_{X^{(0)}} \left[ E_{Y|X^{(0)}, c} \{ \hat{FP}(\hat{x}(Y, c)) \} \right] = E_{X^{(0)}} \left[ E_{Y|X^{(0)}, c} \{ \hat{FP}(X^{(0)}, \hat{x}(Y, c)) \} \right], \quad (21)$$

$$E_{X^{(0)}} \left[ E_{Y|X^{(0)}, c} \{ \hat{FN}(X^{(0)}, \hat{x}(Y, c)) \} \right] = E_{X^{(0)}} \left[ E_{Y|X^{(0)}, c} \{ \hat{FN}(X^{(0)}, \hat{x}(Y, c)) \} \right]$$

$$E_{X^{(0)}} \left[ E_{Y|X^{(0)}, c} \{ \hat{FP}(X^{(0)}, \hat{x}(Y, c)) \} \right]. \quad (22)$$

We define the optimal estimator as that minimizes the posterior risk $\hat{R}(\hat{x}(y, c); \lambda)$ for any $y$ and $c$ at a given $\lambda$. The optimal estimator yields the minimum expected risk, and the estimator corresponds to the Bayes estimator in the decision theory [29]. The following proposition represents the basis for the cutoff determination.

**Proposition 2:** The optimal estimator is given by a cutoff-based function using the marginal posterior probability in the Bayesian optimal setting $\rho$ as

$$\hat{x}_i(y, c) = \mathbb{I} \left( \rho_i(y, c) > \frac{\theta \lambda_{FP}}{\lambda_{FN}(1 - \theta) + \theta \lambda_{FP}} \right). \quad (23)$$

**Proof:** Transforming the R.H.S. of (18), we obtain

$$\hat{R}(\hat{x}(y, c); \lambda)$$

$$= \frac{1}{N} \sum_{i=1}^N \left\{ \frac{\lambda_{FN} \rho_i(y, c)}{\theta} + \hat{x}_i(y, c) \left( \frac{\lambda_{FP}(1 - \rho_i(y, c))}{1 - \theta} \right) \right\},$$

The component-wise minimization of (24) with respect to $\hat{x}_i$ under the constraint $\hat{x}_i \in \{0, 1\}$ leads to (23).

In general, any function that maps $[0, 1]$-continuous values to $\{0, 1\}$-discrete values can be an estimator for the items’ states, but (23) indicates that the optimal estimator is defined by the cutoff given by the prevalence $\theta$ and the parameters of the risk function $\lambda_{FN}$ and $\lambda_{FP}$. Furthermore, the form of (23) indicates that the marginal posterior probability is appropriate for the evaluation of the test performance using AUC.

Let us consider the maximization of the Youden index as an example of risk minimization. The Youden index is expressed as follows:

$$J_Y(x^{(0)}, y, c) = TP(x^{(0)}, y, c) - FP(x^{(0)}, y, c). \quad (25)$$

Hence, $J_Y(x^{(0)}, y, c) = 1 - R(x^{(0)}, y, c; \lambda_{FN} = \lambda_{FP} = 1/2)$. Thus, the maximization of the Youden index corresponds to equal reductions in the false negative and false positive. By following Proposition 2, we immediately obtain Corollary 1 by substituting $\lambda_{FN} = \lambda_{FP} = 1/2$ into (23).

**Corollary 1:** Setting the cutoff value to equal the prevalence $\theta$ maximizes the posterior Youden index, as given by (25).

Next, let us consider the MPM estimator corresponding to the cutoff of 0.5. Following (23), 0.5 is the optimal cutoff at $\lambda_{FN} = \theta$ and $\lambda_{FP} = 1 - \theta$, where the risk is equivalent to the mean squared error

$$\frac{1}{N} E_{X^{(0)}} \left[ E_{Y|X^{(0)}, c} \left( \sum_{i=1}^N (X_i^{(0)} - \hat{x}_i(Y, c))^2 \right) \right].$$

This fact is consistent with previous studies in which the optimality of the MPM estimator is supported in terms of the minimization of the expected mean squared error [40], [41], [42]. The risk at $\lambda_{FN} = \theta$ and $\lambda_{FP} = 1 - \theta$ implies that the priority of the decision is determined by the prevalence $\theta$; when $\theta < 0.5$, the priority is to reduce false positives, and when $\theta > 0.5$, the priority is to reduce false negatives. In other words, the use of the MPM estimator indicates that the priority of the decision is to avoid identification errors in larger populations of the non-defective and defective populations. Group testing is effective when the prevalence is sufficiently small; hence, the usage of the MPM estimator in the group testing decreases the false positives rather than the false negatives. If we need to reduce the false negative rate in group testing rather than the false positive rate, such as a test where a low false positive probability is considered, the usage of the MPM estimator may not achieve the purpose; hence, the setting of the appropriate cutoff under the risk is important.

**C. Optimal Cutoff and Bayes Factor**

The expression of the estimator with the appropriate cutoff (23) has correspondence with the Bayes factor [43]. The Bayes factor is defined as the ratio of the marginal likelihoods of
two competing models. Here, we focus on the $i$-th item and consider $x_i^{(0)} = 0$ and $x_i^{(0)} = 1$ as the competing ‘models.’

We denote the Bayes factor for the $i$-th item $\text{BF}_i^{(0)}$ and define it as [44] and [45]

$$\text{BF}_i^{(0)}(y, c) = \frac{f_i(y|c, x_i = 1)}{f_i(y|c, x_i = 0)},$$

(26)

where $\hat{f}_i(y|c, x_i) = \frac{1}{\varphi_i(y|c)} \sum_{x \neq x_i} f(y|x, c) \prod_{j \neq i} \phi(x_j)$ is the marginalized likelihood under the constraint on $x_i$. The Bayes factor can be expressed using the posterior odds $O_i^{\text{post}}(y, c)$ and the prior odds $O_i^{\text{pri}}(y, c)$ as

$$\text{BF}_i^{(0)}(y, c) = \frac{O_i^{\text{post}}(y, c)}{O_i^{\text{pri}}(y, c)},$$

(27)

where

$$O_i^{\text{post}}(y, c) = \frac{\rho_i(y, c)}{1 - \rho_i(y, c)},$$

(28)

$$O_i^{\text{pri}}(y, c) = \frac{\theta}{1 - \theta}.$$

(29)

Based on the expressions (28) and (29), the optimal estimator with the appropriate cutoff (23) is expressed using the Bayes factor as follows:

$$\widehat{x}_i(y, c) = 1 \left( \text{BF}_i^{(0)}(y, c) > \frac{\lambda_{\text{FP}}}{\lambda_{\text{FN}}} \right).$$

(30)

In particular, in the maximization of the expected Youden index, which corresponds to $\lambda_{\text{FP}} = \lambda_{\text{FN}}$, the $i$-th item is considered defective when $\text{BF}_i^{(0)} > 1$, and considered non-defective when $\text{BF}_i^{(0)} < 1$. Following the conventional interpretation of the Bayes factor, $\text{BF}_i^{(0)} = 1$ indicates that the evidence against $x_i^{(0)} = 0$ is ‘not worth more than a bare mention’ [44], [46]. Hence, the maximization of the posterior Youden index provides a loose criterion for deciding $x_i^{(0)} = 1$. Meanwhile, the MPM estimator, which corresponds to $\lambda_{\text{FP}} = 1 - \theta$ and $\lambda_{\text{FN}} = \theta$ with a small prevalence provides a strict criterion for deciding $x_i^{(0)} = 1$. For instance, at $\theta = 0.01$, the $i$-th item is regarded as defective when $\text{BF}_i^{(0)} > 99$. In the conventional interpretation, $\text{BF}_i^{(0)} = 99$ indicates that the evidence against $x_i^{(0)} = 0$ is ‘Strong’ [44] or ‘Very Strong’ [46]. Hence, the usage of the MPM estimator at small values of $\theta$ indicates that strong evidence is required to identify the defective items.

As explained in Sec.V, in the BP algorithm, the Bayes factor can be expressed by using the probabilities appearing in the algorithm.

IV. ROC ANALYSIS BY REPLICA METHOD

As discussed in the previous section, the Bayesian optimal setting maximizes the expected AUC, and hence, minimizes the expected risk. In this section, we evaluate the expected AUC under the Bayesian optimal setting. The procedure explained herein has been introduced for the analysis of error-correcting codes such as low-density-parity-check codes [47] and compressed sensing [48], which have mathematical similarities with the group testing. For deriving the ROC curve and the associated AUC, we restrict our discussion to pooling method $c$, with pools generated according to the uniform distribution under the constraints of pool size $K$ and overlap $C$; that is,

$$\text{Pr}[C = c] = \frac{1}{D} \prod_{i=1}^{N} \delta \left( \sum_{\mu \in G(i)} c_{\mu} - C \right) =: P_c(c).$$

(31)

Here, $G(i)$ is the set of pool indices containing the $i$-th item, and $D$ is the normalization constant. We need to obtain the distributions of the marginal posterior probability of the non-defective items $P_{\rho}^-(\rho|y, x^{(0)}, c)$ and the defective items $P_{\rho}^+(\rho|y, x^{(0)}, c)$ under the realization of test result $y$, pooling methods $c$, and items’ state $x^{(0)}$. These are respectively defined as

$$P_{\rho}^-(\rho|y, x^{(0)}, c) = \frac{1}{N(1 - \theta)} \sum_{i=1}^{N} (1 - x_i^{(0)}) \delta (\rho - \rho_i(y, c)), $$

(32)

and

$$P_{\rho}^+(\rho|y, x^{(0)}, c) = \frac{1}{N \theta} \sum_{i=1}^{N} x_i^{(0)} \delta (\rho - \rho_i(y, c)). $$

(33)

We can define an ensemble of the distributions $P_{\rho}^\pm(\rho|y, x^{(0)}, c)$ associated with the joint distribution given by

$$\text{Pr}[Y = y, C = c, X^{(0)} = x^{(0)}] = P_C(c) f(y|c, x^{(0)}) \phi(x^{(0)}),$$

(34)

We assume that the distributions $P_{\rho}^\pm(\rho|y, x^{(0)}, c)$ under the fixed set of $(y, c, x^{(0)})$, generated according to (34), converge to their averaged distributions at sufficiently large values of $N$; that is,

$$P_{\rho}^-(\rho) = \frac{1}{N(1 - \theta)} \times \sum_{i=1}^{N} E_{Y, C, X^{(0)}} \left[ (1 - X_i^{(0)}) \delta (\rho - \rho_i(Y, C)) \right],$$

(35)

$$P_{\rho}^+(\rho) = \frac{1}{N \theta} \sum_{i=1}^{N} E_{Y, C, X^{(0)}} \left[ X_i^{(0)} \delta (\rho - \rho_i(Y, C)) \right].$$

(36)

where $E_{Y, C, X^{(0)}} [\cdot]$ denotes the expectation according to the joint distribution (34).

For further calculations, we introduce the integral representation of the delta function in (35) and (36).

$$\delta (\rho - \rho_i(Y, C)) = \int d\tilde{\rho} \exp \left\{-\tilde{\rho} (\rho - \rho_i(Y, C))\right\} = \int d\tilde{\rho} e^{-\tilde{\rho} \sum_{k=0}^{\infty} \frac{1}{k!} (\tilde{\rho} \rho_i(Y, C))^k}. $$

(37)

We define the conditional expectation of the $k$-th power of the posterior marginal probability as follows:

$$m_{ik}^- = E_{Y, C, X^{(0)}} \left[ (1 - X_i^{(0)}) \rho_i^k(Y, C) \right],$$

(38)

$$m_{ik}^+ = E_{Y, C, X^{(0)}} \left[ X_i^{(0)} \rho_i^k(Y, C) \right].$$

(39)
Using (39), the distribution of the marginal posterior probability is given by
\[
P^+_o(\rho) = \frac{1}{N\theta} \sum_{i=1}^{N} \int d\tilde{\rho} \ e^{-\tilde{\rho} \sum_{k=0}^{\infty} \frac{\rho^k}{k!} m^+_{ik}}, \tag{40}
\]
\[
P^-_o(\rho) = \frac{1}{N(1-\theta)} \sum_{i=1}^{N} \int d\tilde{\rho} \ e^{-\tilde{\rho} \sum_{k=0}^{\infty} \frac{\rho^k}{k!} m^-_{ik}}. \tag{41}
\]
The strategy for obtaining the distributions is based on the reconstruction of the distribution by the moments \(m^+_{ik}, m^-_{ik}\) for \(i \in \{1, \ldots, N\}, k \in \{0, 1, \ldots, \infty\}\), as shown in (40)-(41). The calculation methods for \(m^+_{ik}\) and \(m^-_{ik}\) are the same; hence, we mainly explain the calculation of \(m^+_{ik}\).

For the expectation with respect to \(X, C, X^{(0)}\), we introduce the following identity that generalizes function \(g(x)\) and \(k \in N:\)
\[
E_{X|y,c}[g(X)]^k = \lim_{n \to 0} P^n_y(y|c) E_{X|y,c}[g(X)]^k
= \lim_{n \to 0} P^{n-k}_y(y|c) \prod_{\alpha=1}^{k} \sum_{X^{(\alpha)}} g(x^{(\alpha)}) f(y|x^{(\alpha)}, c) \phi(x^{(\alpha)}), \tag{42}
\]
where we express the \(k\)-th power by introducing \(k\)-replicated systems \(x^{(\alpha)} \in \{0, 1\}^N, \alpha \in \{1, \ldots, k\}\). Using the identity (42), we obtain
\[
m^+_{ik} = \lim_{n \to 0} M^+_{ik}(n) \tag{43}
M^+_{ik}(n) = E_{X,Y,C}(X^{(0)}) \left[ P^{n-k}_y(Y|C) X_i \right.
\times \prod_{\alpha=1}^{k} \sum_{X^{(\alpha)}} f(y|C, X^{(\alpha)}) \phi(x^{(\alpha)}) \right]. \tag{44}
\]
We introduce a calculation method known as the replica method for the evaluation of (44). First, assume that \(n \in N\) and \(n > k\); hence, \(n-k \in N\). We obtain the following expressions:
\[
M^+_{ik}(n) = E_{X,Y,C}(X^{(0)}) \left[ \sum_{X^{(0)}} \cdots \sum_{X^{(k)}} X_1^{(1)} X_2^{(2)} \cdots X_k^{(k)} \right.
\times \prod_{\alpha=1}^{k} f(y|C, X^{(\alpha)}) \phi(x^{(\alpha)}) \right]. \tag{45}
\]
\[
\sum_{\alpha=1}^{k} P_c(c) \sum_{x^{(1)}} \cdots \sum_{x^{(k)}} x_1^{(1)} x_2^{(2)} \cdots x_k^{(k)} \times \prod_{\alpha=1}^{k} f(y|c, x^{(\alpha)}) \phi(x^{(\alpha)}), \tag{46}
\]
where \(P^{n-k}_y(y|C)\) is expressed using the \(n-k\)-replicas \(\{x^{(k+1)}, \ldots, x^{(n)}\}\) in (45). We combine \(X^{(0)}\) with other replica variables; hence, (46) is represented by the \(n+1\)-replica variables \(X^{(0)}, X^{(1)}, \ldots, X^{(n)}\). The analytical expression of (46) for the integer \(n\) is analytically continued to the real values of \(n\) to take the limit \(n \to 0\) in (43). The detailed calculation is presented in the Appendix; here, we briefly explain the basic approach for the calculations.

Owing to the statistical uniformity of the current system, the unnormalized weight in (46) can be decomposed into the factorized form
\[
\sum_{y, c} P_c(c) \prod_{a=0}^{n} f(y|x^{(a)}) \phi(x^{(a)}) \simeq Z_n \prod_{i=1}^{N} B_n(\bar{x}_i) \tag{47}
\]
as \(N\) tends toward infinity, where \(\bar{x}_i = \{x_1^{(i)}, x_2^{(i)}, \ldots, x_n^{(i)}\} \in \{0, 1\}^{n+1}\) represent the replicated variables, and \(B_n(\bar{x}_i)\) is a joint distribution with \(\lim_{n \to 0} Z_n = 1\). The joint distribution \(B_n(\bar{x}_i)\) is expressed as
\[
B_n(\bar{x}_i) = \frac{Q^C_n(\bar{x}_i) \prod_{a=0}^{n} \phi(x^{(a)})}{\sum_{\bar{x}} Q^C_n(\bar{x}) \prod_{a=0}^{n} \phi(x^{(a)})} \tag{48}
\]
using the auxiliary function \(Q^C_n(\bar{x}_i)\) determined by a pair of functional equations:
\[
\bar{Q}_n(\bar{x}) = \frac{N^K}{(K-1)!} \prod_{i=1}^{K-1} W_n(\bar{x}, \bar{x}_1, \ldots, \bar{x}_{K-1}) \prod_{k=1}^{K-1} Q_n(\bar{x}_k) \tag{49}
\]
\[
Q_n(\bar{x}) = C \bar{Q}^C_n(\bar{x}) \prod_{a=0}^{n} \phi(x^{(a)}) / \sum_{\bar{x}} \bar{Q}^C_n(\bar{x}) \prod_{a=0}^{n} \phi(x^{(a)}), \tag{50}
\]
where
\[
W_n(\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_K) = \prod_{a=0}^{n} \left\{ p_{\text{TP}} T(x_1^{(a)}, \ldots, x_K^{(a)}) + p_{\text{FP}} (1 - T(x_1^{(a)}, \ldots, x_K^{(a)})) \right\}
\]
\[
\prod_{a=0}^{n} \left\{ (1 - p_{\text{TP}}) T(x_1^{(a)}, \ldots, x_K^{(a)})
\quad + (1 - p_{\text{FP}}) (1 - T(x_1^{(a)}, \ldots, x_K^{(a)})) \right\}. \tag{51}
\]
where we made an exception for \(x^{(0)}\) to explicitly extract the dependence of the solution on the true state \(x^{(0)}\). Similarly, we express \(\bar{Q}_n(\bar{x})\) and \(B_n(\bar{x})\) as

\[
\bar{Q}_n(\bar{x}) = \bar{Q}_n \left\{ (1 - \tilde{\rho}_n) \left( 1 - x^{(0)} \right) + \tilde{\rho}_n x^{(0)} \right\} \\
\times \int_0^1 d\mu \tilde{\pi}(\mu|x^{(0)}) \prod_{a=1}^n \left\{ (1 - \mu) \left( 1 - x^{(a)} \right) + \mu x^{(a)} \right\}
\]

(53)

and

\[
B_n(\bar{x}) = \left\{ (1 - \rho_n) \left( 1 - x^{(0)} \right) + \rho_n x^{(0)} \right\} \\
\times \int_0^1 d\rho \rho^p_p \left( \rho(x^{0}) \right) \prod_{a=1}^n \left\{ (1 - \rho) \left( 1 - x^{(a)} \right) + \rho x^{(a)} \right\}.
\]

(54)

Here, \(\pi(\cdot|x^{(0)})\), \(\tilde{\pi}(\cdot|x^{(0)})\), and \(\rho^p_p(\cdot|x^{0})\) denote distributions over \([0, 1]\) conditional on the true state \(x^{(0)}\).

Inserting these expressions into eqs. (48)-(50) results in a set of equations for determining \(Q_n\), \(\bar{Q}_n\), \(\rho_n\), \(\tilde{\rho}_n\), \(\pi(\cdot|x^{(0)})\), \(\tilde{\pi}(\cdot|x^{(0)})\), and \(\rho^p_p(\cdot|x^{0})\), which are likely to hold not only for \(n \in \mathbb{N}\) but also to all \(n \in \mathbb{R}\). Therefore, we employ the resultant expressions to take the limit as \(n \to 0\), which provides

\[
Q_0 = \left( C \frac{(K - 1)!}{NK - 1} \right)^{1/K},
\]

(55)

\[
\bar{Q}_0 = \frac{2C}{Q_0},
\]

(56)

\[
\rho_0 = \theta,
\]

(57)

\[
\tilde{\rho}_0 = \frac{1}{2}.
\]

(58)

Conditional distributions \(\pi(\cdot|x^{(0)})\) and \(\tilde{\pi}(\cdot|x^{(0)})\) are determined by the functional equations

\[
\tilde{\pi}(\mu|1) = \int_{k=1}^{K-1} d\mu_k \sum_{u_k^{(0)}} \phi(u_k^{(0)}) \pi(\mu_k|u_k^{(0)}) \\
\times \left[ p_{TP} \delta(\tilde{\mu} - \tilde{\mu}(p_{TP}, p_{FP}, \mu(K-1))) \\
+ (1 - p_{TP}) \delta(\tilde{\mu} - \tilde{\mu}(1 - p_{TP}, 1 - p_{FP}, \mu(K-1))) \right],
\]

(59)

\[
\tilde{\pi}(\mu|0) = \tilde{\pi}(\mu|1) - \int_{k=1}^{K-1} d\mu_k \pi(\mu_k|0)(1-\theta)^{K-1}(p_{TP} - p_{FP}) \\
\times \left[ \delta(\tilde{\mu} - \tilde{\mu}(p_{TP}, p_{FP}, \mu(K-1))) \\
- \delta(\tilde{\mu} - \tilde{\mu}(1 - p_{TP}, 1 - p_{FP}, \mu(K-1))) \right],
\]

(60)

respectively, where \(\mu(K-1) = [\mu_1, \cdots, \mu_{K-1}]^\top\) and

\[
\tilde{\mu}(p_{TP}, p_{FP}, \mu(K-1)) = \frac{p_{TP}}{p_{TP} + p_{FP}(1 - q(\mu(K-1))) + p_{FP}q(\mu(K-1))}.
\]

(61)

We set \(q(\mu(K-1)) = \prod_{k=1}^{K} (1 - \mu_k)\). Using the conjugate distribution \(\tilde{\pi}(\mu|x^{(0)})\), the distribution \(\pi(\mu|x^{(0)})\) is given by

\[
\pi(\mu|x^{(0)}) = \int_{\gamma=1}^{C-1} d\mu_\gamma \tilde{\pi}(\mu_\gamma|x^{(0)}) \delta(\mu - \mu(\mu(C-1), \theta))
\]

(62)

where \(\mu(C) = [\mu_1, \cdots, \mu_C]^\top\), and

\[
\mu(\mu(C), \theta) = \frac{\theta \prod_{\gamma=1}^C (1 - \mu_\gamma) + \theta \prod_{\gamma=1}^C \mu_\gamma}{(1 - \theta) \prod_{\gamma=1}^C (1 - \mu_\gamma) + \theta \prod_{\gamma=1}^C \mu_\gamma},
\]

(63)

and

\[
P_\rho(\rho|x^{0}) = \int_{\gamma=1}^C d\mu_\gamma \tilde{\pi}(\mu_\gamma|x^{(0)}) \delta(\rho - \mu(\mu(C), \theta)).
\]

(64)

Finally, we evaluate

\[
m^+_n = \lim_{n \to 0} \sum_{x^{(0)}_i, x^{(1)}_i, \cdots, x^{(n)}_i} x^{(0)}_i x^{(1)}_i \cdots x^{(k)}_i B_n(\bar{x}_i)
\]

(65)

\[
m^-_n = \lim_{n \to 0} \sum_{x^{(0)}_i, x^{(1)}_i, \cdots, x^{(n)}_i} (1 - x^{(0)}_i) x^{(1)}_i \cdots x^{(k)}_i B_n(\bar{x}_i).
\]

(66)

By inserting (47) into eqs. (48)-(50) and utilizing the trivial identity \(\lim_{n \to 0} Z_n = 1\), we have that

\[
m^+_n = \theta \int_0^1 d\rho p_p(\rho|1)
\]

(67)

\[
m^-_n = (1 - \theta) \int_0^1 d\rho p_p(\rho|0).
\]

(68)

for any \(i \in \{1, \ldots, N\}\). These expressions imply that \(P_\rho(\rho|x^{0})\) represents something more than the distributions for the marginal posterior probabilities, denoted in (40) and (41) as \(P^+_\rho(\rho = 1)\) and \(P^-_\rho(\rho = 0)\). We emphasize that in deriving the distributions, we did not apply any knowledge about which items are defective or nondefective.

A. Absence of the Perfect Identification Solution in the Linear Regime

Here, we define the perfect identification solution as the case where both \(P^+_\rho(\rho = 1) = 1\) and \(P^-_\rho(\rho = 0) = 1\) are satisfied; that is, the case where the posterior marginal probability takes the value 1 for the true state, and otherwise 0. We can show that the perfect identification solution does not appear as a solution of the saddle point equation, even in the noiseless case.

For simplicity, here we consider the noiseless case, where \(p_{TP} = 1\) and \(p_{FP} = 0\). From the forms of the posterior marginal probability given by (64) at \(p_{TP} = 1\) and \(p_{FP} = 0\), \(\tilde{\pi}(\mu|x^{0}) = \delta(\mu - x^{0})\) should hold, in order to satisfy \(P^+_{\rho}(\rho = 1) = P^-_{\rho}(\rho = 0) = 1\). We show that this solution does not appear for both \(x^{(0)} \in \{0, 1\}\) in a contradictory manner.

First, we assume that \(\tilde{\pi}(\mu|x^{0}) = \delta(\mu - x^{0})\) is a solution of the set of saddle point equations (59), (60) and (62).
In this case, from (62), \( \pi(\mu|x^{(0)}) = \delta(\mu - x^{(0)}) \) should hold. By substituting \( \pi(\mu|x^{(0)}) = \delta(\mu - x^{(0)}) \) into (59) and (60), we obtain

\[
\hat{\pi}(\hat{\mu}|x^{(0)}) = (1 - \theta)^{K-1}\delta(\hat{\mu} - x^{(0)}) + (1 - (1 - \theta)^{K-1}) \delta(\hat{\mu} - \frac{1}{2}). \tag{69}
\]

This form contradicts the assumption that \( \hat{\pi}(\hat{\mu}|x^{(0)}) = \delta(\hat{\mu} - x^{(0)}) \) for general \( K \) and \( \theta \). Eq. (69) holds only when \( K = 1 \) or \( \theta \to 0 \), cases where under these conditions the estimation problem in group testing is trivial.

Expression (69) under the assumption \( \pi(\mu|x^{(0)}) = \delta(\mu - x^{(0)}) \) can be understood using the following consideration. Let us focus on an item, say, the \( i \)-th item, and one of the pools including the item. Let us denote this as the \( \mu \)-th pool. Intuitively, the first term of (69) describes the case in which \( K - 1 \) items in the \( \mu \)-th pool, other than the \( i \)-th item, are non-defective. In the noiseless case, the observation of the \( \mu \)-th pool enables us to perfectly identify the state of the \( i \)-th item, using the knowledge that the other \( K - 1 \) items in the pool are non-defective. The second term of (69) describes the case when at least one item in the \( \mu \)-th pool, other than the \( i \)-th item, is defective. In this case, the observation of the \( \mu \)-th pool cannot uniquely determine the state of the \( i \)-th item, since the state of the \( \mu \)-th pool is defective irrespective of the \( i \)-th item’s state. It can be understood that this uncertainty arising due to the OR function prevents perfect identification.

The absence of the perfect identification in the linear regime indicates the need for a cutoff in deciding items’ states.

**B. Numerical Calculation of the Distributions by Population Dynamics**

To obtain the distributions (64) for \( x^{(0)} \in \{0, 1\} \), we need to calculate the distributions \( \pi(\hat{\mu}_\gamma|x^{(0)}) \) and \( \pi(\mu_k|x^{(0)}) \) to satisfy (59), (60), and (62). Here, we numerically obtain these distributions using a sampling method known as population dynamics (PD) [50]; the procedure is shown in Algorithm 1.

PD considers the recursive updating of (59), (60), and (62) as

\[
\tilde{\pi}^{(t)}(\tilde{\mu}|1) = \int \prod_{k=1}^{K-1} d\mu_k \sum_{u_k} \phi(u_k)\pi^{(t-1)}(\mu_k|u_k) \nonumber
\]

\[
\times \left[p_{TP}\delta\left(\tilde{\mu} - \tilde{\mu}(TP, FP, C_{K-1})\right) + (1-p_{TP})\delta\left(\tilde{\mu} - (1-p_{TP}, 1-p_{FP}, C_{K-1})\right)\right] \tag{70}
\]

\[
\tilde{\pi}^{(t)}(\tilde{\mu}|0) = \tilde{\pi}^{(t)}(\tilde{\mu}|1) - \int \prod_{k=1}^{K-1} d\mu_k \pi^{(t-1)}(\mu_k|0)(1-\theta)^{K-1}(p_{TP} - p_{FP}) \nonumber
\]

\[
\times \left[\delta\left(\tilde{\mu} - \tilde{\mu}(TP, FP, C_{K-1})\right) - \delta\left(\tilde{\mu} - (1-p_{TP}, 1-p_{FP}, C_{K-1})\right)\right] \tag{71}
\]

\[
\pi^{(t)}(\mu|x) = \int \prod_{\gamma=1}^{C-1} d\mu_{\gamma} \tilde{\pi}^{(t-1)}(\mu_{\gamma}|x) \delta\left(\mu - \mu(\mu_{C-1}, \theta)\right) \nonumber
\]

\[
(x \in \{0, 1\}), \tag{72}
\]

where \( t \) in the superscript denotes the iteration step. For updating the distributions, we prepare four populations of random variables \( \pi^-, \pi^+, \pi^-, \pi^+ \) corresponding to the four distributions \( \pi(\mu|0), \pi(\mu|1), \pi(\tilde{\mu}|0), \pi(\tilde{\mu}|1) \), respectively.

The number of components in the populations are set to be a sufficiently large value, which we denote as \( N_\pi \). For instance, let us consider the population dynamics corresponding to (72). In updating the population \( \pi^+ \), we select \( C - 1 \) components from the population \( \pi^\pm \); this operation mimics \( C - 1 \)-times-sampling according to \( \pi(\mu|0) \) or \( \pi(\mu|1) \). Using the selected \( C - 1 \)-components, we compute \( \mu(\mu_{C-1}, \theta) \), and replace a randomly chosen component in \( \mu^\pm \) with \( \mu(\mu_{C-1}, \theta) \). The same procedure is repeated for updating (59) and (60). After updating sufficient time steps \( T \) according to (62), (59), and (60), we approximately calculate the distribution (64) by sampling the components of the populations \( \hat{\mu}^\pm \) a sufficient number of times \( R \).

Fig. 1 shows the examples of \( P^{\pm}_\rho(\rho) \) calculated by the population dynamics, where the parameters are set as \( N_\pi = 10^3 \), \( T = 10^5 \), and \( R = 10^5 \). Distribution (a) is for \( \alpha = 0.5 \).
Algorithm 1 Population Dynamics for Evaluation of $P^\pm_{\rho}(\rho)$

Input: $p_{\text{TP}}, p_{\text{FP}}, \theta, K, C, N_{\pi}, T, R$
Output: $P^\pm_{\rho}(\rho)$ for $x \in \{0, 1\}$

1: Initialize:
2: $\pi^\pm, \hat{\pi}^\pm \leftarrow$ Initial values from $[0, 1]^{N_{\pi}}$
3: for $t = 1 \ldots T$ do  $	riangleright$ Start: Evaluate cavity distributions
4: for $\gamma = 1 \ldots C - 1$ do
5: $i^+ \sim [1, N_{\pi}]$ and $\hat{\mu}_\gamma \leftarrow \hat{\pi}^+_{i^+}$
6: $i^- \sim [1, N_{\pi}]$ and $\hat{\mu}_\gamma \leftarrow \hat{\pi}^-_{i^-}$
7: end for
8: $\gamma^+ \sim [1, N_{\pi}]$ and $\pi^+_{\gamma^+} \leftarrow \mu(\hat{\mu}(\gamma^-), \theta)$
9: $\gamma^- \sim [1, N_{\pi}]$ and $\pi^-_{\gamma^-} \leftarrow \mu(\hat{\mu}(\gamma^+), \theta)$
10: end for
11: $j^+ \sim [1, N_{\pi}], b^+ \sim [0, 1]$
12: $\mu_j^+ \leftarrow \pi^+_{j^+} I(b^+ \leq \theta) + \pi^-_{j^+} I(b^+ > \theta)$
13: $u_j^- \leftarrow I(b^- \leq \theta)$ and $\mu_j^- \leftarrow \pi^+_{j^-} u_j^+ + \pi^-_{j^-} (1 - u_j^-)$
14: end for
15: $\ell^+ \sim [1, N_{\pi}], \pi^+ \sim [0, 1]$
16: if $\tau^+ \leq p_{\text{TP}}$ then
17: $\hat{\pi}^+(\rho) \leftarrow \hat{\mu}(p_{\text{TP}}, p_{\text{FP}}, \mu^+_{(K-1)})$
18: else
19: $\hat{\pi}^+(\rho) \leftarrow \hat{\mu}(1 - p_{\text{TP}}, 1 - p_{\text{FP}}, \mu^+_{(K-1)})$
20: end if
21: $v \leftarrow (p_{\text{FP}} - p_{\text{TP}}) I\left(\sum_{\ell=1}^{K-1} u_\ell^- = 0\right) + p_{\text{TP}}$
22: if $\tau^- \leq v$ then
23: $\hat{\pi}^-(\rho) \leftarrow \hat{\mu}(p_{\text{TP}}, p_{\text{FP}}, \mu^-_{(K-1)})$
24: else
25: $\hat{\pi}^-(\rho) \leftarrow \hat{\mu}(1 - p_{\text{TP}}, 1 - p_{\text{FP}}, \mu^-_{(K-1)})$
26: end if
27: end for
28: for $r = 1 \ldots R$ do  $	riangleright$ Start: Evaluation of $P^\pm_{\rho}(\rho)$
29: for $\gamma = 1 \ldots C$ do
30: $i^+ \sim [1, N_{\pi}]$ and $\hat{\mu}_\gamma \leftarrow \pi^+_{i^+}$
31: $i^- \sim [1, N_{\pi}]$ and $\hat{\mu}_\gamma \leftarrow \pi^-_{i^-}$
32: end for
33: $P^\pm_{\rho} \leftarrow \mu(\hat{\mu}^\pm_{(K)}, \theta)$
34: end for
35: $P^\pm_{\rho}(\rho) \leftarrow$ Histogram of $\{P^\pm_{\rho}\}$

$d = 0.05$, $p_{\text{TP}} = 0.98$, and $p_{\text{FP}} = 0.01$, which is an example for small prevalence and small error probabilities, and (b) is for $\alpha = 0.5$, $\theta = 0.1$, $p_{\text{TP}} = 0.9$, and $p_{\text{FP}} = 0.05$, which is an example for relatively large prevalence and large error probabilities. In the case of (a), the peaks of the two distributions are far apart, and the two populations can be separated with high accuracy. Meanwhile, in case (b), the posterior probability for the defective items is widely distributed.

C. Absence of the First Order Transition

The population dynamics converges to a unique solution for any parameter region we examined. This means that Bayesian optimal group testing in the linear regime does not exhibit the first-order phase transition. In general, first-order transition can lead to a computational-statistical gap, where local-search algorithms cannot achieve the theoretical performance limits. Although proving the absence of first order transitions is difficult under the current framework, our observations suggest that the same property holding in the sublinear regime holds in the linear regime [20], [21].

D. Comparison With the BP Algorithm

We have imposed some assumptions in our analysis so far. Here, we confirm the adequacy of these assumptions by comparing the analytical results with those obtained using the BP algorithm [27], [51]. The details of the BP algorithm and its correspondence with the replica analysis are discussed in Sec. V. When the set of $(y, c, x^{(0)})$ is generated according to the distribution assumed in replica analysis, it is known that the posterior marginals obtained by the BP algorithm converge to their exact respective values as $N$ and $M$ tend to infinity, while setting the ratio $\alpha = M/N \sim O(1)$ [52].

In the numerical simulation using BP, we set the number of items to $N = 1000$. We generated 1000 samples of the set of test results $y$, pooling method $c$, and items’ state $x^{(0)}$ according to (34), and ran the BP algorithm for each sample. The results shown in following figures are averages over the samples.

In Fig. 2(a), the AUC derived using the replica method and the associated population dynamics are compared with that calculated using the BP algorithm at $\alpha = 0.5, K = 10, p_{\text{TP}} = 0.95, p_{\text{FP}} = 0.1$. TP and FP for each cutoff are calculated using the true state of the items and the posterior probability by BP. As shown in 2(a), the theoretical result, denoted by ‘Replica,’ coincides with the algorithmic result of BP, denoted by ‘BP,’ where the result of BP is averaged over 100 samples of $y$, $c$, and $x^{(0)}$. In Fig. 2(b), the dependence on the prevalence of the cutoff, which maximizes the expected Youden index calculated by the replica method, is shown. For comparison, we show the diagonal dashed line with gradient 1. As discussed in Sec. III, the cutoff that maximizes the expected Youden index is coincident with the prevalence. This observation also supports the adequacy of our analysis.
Fig. 3. Comparison of (a) TP and (b) FP under the cutoff of \( \theta \) (Youden) and 0.5 (MPM) for \( \alpha = 0.5, p_{TP} = 0.95, \) and \( p_{FP} = 0.1 \). The dashed horizontal lines represent the characteristics of the original test; \( p_{TP} \) for (a) and \( p_{FP} \) for (b).

Fig. 4. Our criterion for the effectiveness of group testing. As shown in (a), when the original test property (dot at \( \text{(Fig. 4)} \)) is an example of the ROC curve obtained with the criterion shown in Fig. 4 for the quantitative comparison setting is superior to that of the original test. We introduce the performance of the group testing under the Bayesian optimal setting as a guide to interpret which parameter region is appropriate for the group testing.

In Fig. 3, the cutoff-dependent properties, (a) true positive rate (TP) and (b) false positive rate (FP), are shown in comparison with the results of the replica method and BP algorithm, where the lines with labels ‘Youden’ and ‘MPM’ indicate the TP and FP under the cutoff of \( \theta \) and 0.5, respectively. The cutoff-dependent property evaluated by the replica method also matches with that calculated by the BP algorithm. The horizontal dashed lines represent the original test properties, (a) \( p_{TP} \), (b) \( p_{FP} \), and TP > \( p_{TP} \) and FP < \( p_{FP} \) indicate that a part of the test errors are corrected by the group testing. As discussed in Sec. III, the MPM estimator prefers to decrease FP, and as a tradeoff, the TP obtained using the MPM estimator is lower than that in the Youden index maximization. In the case of Youden index maximization, the false positive and false negative can be corrected simultaneously when \( \theta < 0.06 \). This result also matches the behavior of the BP algorithm.

E. Effectiveness of the Group Testing Measured by ROC Curve

We discuss the parameter region in which the identification performance of the group testing under the Bayesian optimal setting is superior to that of the original test. We introduce the criterion shown in Fig. 4 for the quantitative comparison between the original test and the group testing. The solid line in Fig. 4 is an example of the ROC curve obtained with Bayesian group testing, and the dot located at \( (p_{TP}, p_{FP}) \) represents an example of the original test property. The better test method approaches the ROC curve toward the point (FP = 0, TP = 1); hence, we consider the group test under the Bayesian optimal setting superior to the original test when the dot is below the ROC curve, as shown in Fig. 4 (a). In the contrasting situation, the dot is over the ROC curve, as shown in Fig. 4 (b), and we consider that the group test cannot exceed the original test performance. The ROC curve is obtained with the distributions of the posterior marginal probabilities derived by the replica method under the Bayesian optimal setting \( P_{\text{Bayes}}(\rho) \).

Fig. 5 shows the phase diagrams based on the criterion at \( \alpha = 0.5 \) and \( K = 10 \) for (a) \( \theta = 0.05 \) and (b) \( \theta = 0.07 \), where the shaded area represents the region where the group testing under the Bayesian optimal setting is effective. Here, we do not consider the region \( p_{TP} < 0.5 \) and \( p_{FP} > 0.5 \), where the test performance is worse than the random decision on the items’ states. The effective region shrinks as the prevalence increases, and extends as the number of tests increases. As \( p_{TP} \) decreases, the group testing performance becomes inferior to that of the original test for a small region \( p_{FP} \). This is because a part of the true negatives is erroneously changed to positive while correcting the false negatives, and the fraction of false results is larger than \( p_{FP} \).

As discussed in Sec. III, the Bayesian optimal setting yields the largest value of the expected AUC when the correlation between the items’ states is ignored. Therefore, in the model mismatch case, the effective regions shown in Fig. 5 are smaller than that in the Bayesian optimal setting. In the parameter region where the group testing under the Bayesian optimal setting is inferior to the original test, it is expected that the group testing under any other setting is also inferior to the original test. We can utilize the phase diagrams of the Bayes optimal setting as a guide to interpret which parameter region is appropriate for the group testing.

V. INTERPRETATION OF THE REPLICA ANALYSIS FROM THE CORRESPONDENCE WITH THE BP ALGORITHM

A. BP Algorithm

The meaning of the distributions \( \pi \) and \( \bar{\pi} \) in the replica method and the corresponding population dynamics can be interpreted by utilizing the correspondence between the replica method and BP algorithm. The derivation of the BP algorithm for the group testing can be referred from [9], [26], [27], [51], and is briefly explained here. Fig. 6(a) illustrates a graphical representation of the posterior distribution (3) for the group testing, where the pools on which the tests are not performed
(ν-th pool with cν = 0) are not depicted. The variable nodes (□) and factor nodes (□) represent the items’ states and the test results performed on the pools, respectively. The edges represent the pooling method; the edge between the 1st factor node and 1st item indicates that the 1st item is contained in the 1st pool. The degrees of factor nodes and variable nodes correspond to the pool size K and overlap C. In the derivation of the BP algorithm, we locally impose a tree approximation as shown in Fig. 6(b), and define two messages pν→i(xν) and ˜pν→i(xν) on the edge that connects ν-th factor node and i-th variable node. Intuitively, these messages correspond to the marginal posterior distributions of xν before and after performing the ν-th test under the tree approximation. The BP algorithm describes the constructive manner of the joint distribution on the tree as

$$p_{ν→i}(x_{ν}) \propto \phi(x_{ν}) \prod_{\eta \in \mathcal{G}(i) \cup ν} \tilde{p}_{η→i}(x_{ν})$$

(74)

where we denote $\tilde{f}(y_{ν}|x_{ν}) = f(y_{ν}|c_{ν} = 1, x_{ν})$ for conciseness. As mentioned earlier, L(ν) and $\mathcal{G}(i)$ are the set of item labels in the ν-th pool and the set of pool labels i-th item is contained, respectively. Using these messages, the marginalized posterior distribution is given by

$$p_i(x_i) \propto \phi(x_i) \prod_{\eta \in \mathcal{G}(i)} \tilde{p}_{η→i}(x_i).$$

(75)

On the tree graphs, (75) describes the exact marginal distribution, and to obtain (75), we need to propagate the messages on the tree once starting from the arbitrary root. For the general graphs, we need to recursively update the messages for sufficient time steps until convergence; hence, hereafter, the messages are represented by the F-cavity fields and V-cavity fields, respectively, as

$$p_{ν→i}(x_{ν}) = (1 - m_{ν→i})\big(1 - x_{ν}\big) + m_{ν→i}x_{ν}$$

(76)

$$\tilde{p}_{ν→i}(x_{ν}) = (1 - \tilde{m}_{ν→i})\big(1 - x_{ν}\big) + \tilde{m}_{ν→i}x_{ν}.$$  

(77)

The time evolution of these Bernoulli parameters are derived from (73)–(74) as

$$m_{ν→i}^{(t)} = \frac{\theta}{\nu} \prod_{\eta \in \mathcal{G}(i) \cup ν} \tilde{m}_{η→i}^{(t-1)} \big(1 - \theta\big) \prod_{\eta \in \mathcal{G}(i) \cup ν} \tilde{m}_{η→i}^{(t-1)} + \theta \prod_{\eta \in \mathcal{G}(i) \cup ν} \tilde{m}_{η→i}^{(t-1)} \big(1 - \tilde{m}_{ν→i}^{(t-1)}\big)$$

(78)

$$\tilde{m}_{ν→i}^{(t)} = \frac{U_ν}{U_ν \big(2 - \prod_{j \in L(ν) \setminus i} (1 - m_{j→ν}^{(t-1)})\big) + W_ν \prod_{j \in L(ν) \setminus i} (1 - m_{j→ν}^{(t-1)})}.$$  

(79)

where

$$U_ν = p_{TP} y_ν + (1 - p_{TP})(1 - y_ν),$$  

(80)

$$W_ν = p_{FP} y_ν + (1 - p_{FP})(1 - y_ν).$$  

(81)

We denote the obtained cavity fields after sufficient updates as $\{m_{ν→i}\}$ and $\{\tilde{m}_{ν→i}\}$. The marginal posterior distribution (75) is expressed using the Bernoulli parameter $m_i$, which is given by the F-cavity fields as

$$m_i = \frac{\theta \prod_{\eta \in \mathcal{G}(i)} \tilde{m}_{η→i} \big(1 - \tilde{m}_{η→i}\big) + \theta \prod_{\eta \in \mathcal{G}(i)} \tilde{m}_{η→i} \big(1 - \tilde{m}_{η→i}\big)}{\big(1 - \theta\big) \prod_{\eta \in \mathcal{G}(i)} \tilde{m}_{η→i} \big(1 - \tilde{m}_{η→i}\big) + \theta \prod_{\eta \in \mathcal{G}(i)} \tilde{m}_{η→i} \big(1 - \tilde{m}_{η→i}\big)}.$$  

(82)

The decision based on the Bayes factor (30) can be easily implemented by the BP algorithm using the expression (83).

Fig. 6. (a) Factor graph representation of the posterior distribution for pools on which the tests are performed. (b) Tree approximation of the graph and messages defined on the edges.

An advantage of the BP algorithm is that the updating of the messages is implemented using the matrix products. In Algorithm 2, the BP algorithm using the matrix representation is summarized, where the messages are represented in the matrix forms $M \in \mathbb{R}^{N \times M}$ and $\tilde{M} \in \mathbb{R}^{M \times N}$, where $M_{si} = m_{i→ν}$ and $\tilde{M}_{si} = \tilde{m}_{ν→i}$.
In Algorithm 2, we introduce the matrix $F \in \{0, 1\}^{M \times N}$ representing the pooling method $c$, whose components are 1. The notations $\circ$ and $\odot$ represent the Hadamard product and Hadamard division, respectively, namely \( (\circ)_{ij} = x_i \odot y_j \) and \( (\odot)_{ij} = x_i / y_j \), where $A$ and $B$ are matrices of the same size.

### B. Expectation of BP Trajectory and Replica Analysis

The cavity fields in the BP algorithm are random variables that depend on the realization of the randomness $y$ and $c$, where $y$ is generated by the true items' states $x^{(0)}$. Let us define the probability distribution of the F-cavity fields for defective and non-defective items at step $t$ as

$$
\pi_{BP}^{(t)}(m|1) = E_{y,c,x^{(0)}|x^{(0)} = 1}[\delta(m_{i=\nu}^{(t)} - m)]
$$

(84)

$$
\pi_{BP}^{(t)}(m|0) = E_{y,c,x^{(0)}|x^{(0)} = 0}[\delta(m_{i=\nu}^{(t)} - m)],
$$

(85)

and that of the V-cavity fields as

$$
\tilde{\pi}_{BP}^{(t)}(\tilde{m}|1) = E_{y,c,x^{(0)}|x^{(0)} = 1}[\delta(\tilde{m}_{\nu-i}^{(t)} - m)]
$$

(86)

$$
\tilde{\pi}_{BP}^{(t)}(\tilde{m}|0) = E_{y,c,x^{(0)}|x^{(0)} = 0}[\delta(\tilde{m}_{\nu-i}^{(t)} - m)],
$$

(87)

where $E_{y,c,x^{(0)}|x^{(0)} = 1}[\cdot]$ and $E_{y,c,x^{(0)}|x^{(0)} = 0}[\cdot]$ denote the expectation with respect to randomness under the constraint that $x_i^{(0)} = 1$ and $x_i^{(0)} = 0$, respectively. Here, we assume that (84)–(87) do not depend on $i$, and the dependency between the messages can be ignored. Under this assumption, we can show that the time evolution equations of the distributions (84)–(87) correspond to the recursive updating of the distributions derived by the replica method as follows. Assuming the independence of $\tilde{m}_{\eta-i}$ for $\eta \in G(i)$, (86) is transformed as

$$
\pi_{BP}^{(t)}(m|1) = E_{y,c,x^{(0)}|x^{(0)} = 1}[\delta(m_{i=\nu}^{(t)} - m)]
$$

(84)

$$
= \int d\tilde{m}_{\nu-i} \tilde{\pi}_{BP}^{(t-1)}(\tilde{m}_{\nu-i}|1) \delta(m - \mu(\tilde{m}_{(C-1)})),
$$

(88)

where $\tilde{m}_{(C-1)} = [\tilde{m}_{1}, \cdots, \tilde{m}_{C-1}]^T$ and $\mu(\tilde{m}_{(C-1)}, \theta)$ is given by (63). Equation (88) corresponds to the recursive relationship of the distribution derived using the replica method (72) at $x = 1$. The same relationship holds for $\pi_{BP}^{(t)}(m|0)$ based on the above discussion.
For the derivation of the V-cavity field distribution, we need to consider the generative process of $y$. When $x_i = 1$, the test result on the $\nu$-th pool $y_\nu$, which contains the $i$-th item, is 1 with probability $p_{TP}$ and 0 with probability $1 - p_{TP}$, irrespective of the states of the other items in the pool. Therefore, under the assumption of independency of the V-cavity fields, (86) is given by

$$
\hat{\pi}_{\text{BF}}^{(t)}(\tilde{m}|1) = \int \prod_{\nu=1}^{K-1} dm_{\nu} \sum_{x_1 \cdots x_{K-1}} \prod_{\nu=1}^{K-1} \phi(x_\nu) \pi^{(t-1)}_{\text{BF}}(m_\nu|x_\nu) \times \begin{align*}
&\left\{ p_{TP} \delta(\tilde{m} - \hat{\mu}(p_{TP}, p_{FP}, m_{(K-1)})) \right. \\
&\left. + (1 - p_{TP}) \delta(\tilde{m} - \hat{\mu}(1-p_{TP}, 1-p_{FP}, m_{(K-1)})) \right\},
\end{align*}
$$

(89)

Equation (89) is equivalent to the analytical expression derived using the replica method (70). Meanwhile, when $x_i^{(0)} = 0$, the test result $y_\nu$ is governed by the other items in the pool. When all items are non-defective, $y_\nu = 1$ and $y_\nu = 0$ are realized with probability $p_{TF}$ and $1 - p_{TF}$, respectively. If there is at least one defective item in the $\nu$-th pool, $y_\nu = 1$ and $y_\nu = 0$ are realized with probability $p_{TF}$ and $1 - p_{TF}$, respectively. Thus, only the all-zero case differs from the distribution $\hat{\pi}_{\text{BF}}^{(t)}(\tilde{m}|1)$.

In summary, we obtain

$$
\hat{\pi}_{\text{BF}}^{(t)}(\tilde{m}|0) = \hat{\pi}_{\text{BF}}^{(t)}(\tilde{m}|1) + \int \prod_{\nu=1}^{K-1} dm_{\nu} \pi^{(t)}_{\text{BF}}(m_\nu|0)(1-\theta)^{K-1} \times \left\{ (p_{FP} - p_{TP}) \delta(\tilde{m} - \hat{\mu}(p_{TP}, p_{FP}, m_{(K-1)})) + p_{TP} \delta(\tilde{m} - \hat{\mu}(1-p_{TP}, 1-p_{FP}, m_{(K-1)})) \right\}
$$

(90)

Equation (90) is equivalent to (71) in the replica method.

In fact, the BP algorithm is defined for one realization of the randomness $y, c$, and $x^{(0)}$. However, because of the law of large numbers, it is expected that the empirical distributions of the cavity fields for a single typical samples of $y, c, x^{(0)}$ converge in probability as

$$
\frac{1}{N\theta C} \sum_{i=1}^{N} \sum_{1, \nu \in \mathcal{G}(i)} x_i^{(0)} \delta(m_i^{(t)} - m) \overset{N \to \infty}{\rightarrow} \pi_{\text{BF}}^{(t)}(m|1)
$$

(91)

$$
\frac{1}{N\theta C} \sum_{i=1}^{N} \sum_{1, \nu \in \mathcal{G}(i)} (1-x_i^{(0)}) \delta(m_i^{(t)} - m) \overset{N \to \infty}{\rightarrow} \pi_{\text{BF}}^{(t)}(m|0)
$$

(92)

$$
\frac{1}{MK \theta} \sum_{\nu=1}^{M} \sum_{1 \in \mathcal{M}(\nu)} x_{\nu}^{(0)} \delta(\tilde{m}_{\nu^{(t)}} - \tilde{m}) \overset{N \to \infty}{\rightarrow} \hat{\pi}_{\text{BF}}^{(t)}(\tilde{m}|1)
$$

(93)
In this study, we analyzed a group testing model under the Bayesian optimal setting. We demonstrated that the posterior AUC takes the maximum value when the marginal posterior probability under the Bayesian optimal setting is used as the diagnostic variable. Furthermore, we derived an optimal cutoff based on the expected risk; in particular, the estimator defined by the cutoff that equals the prevalence maximizes an unbiased estimator of the expected Youden index. The derived cutoff can be interpreted by using the Bayes factor. To understand the performance of the group testing under the Bayesian optimal setting, we applied the replica method in statistical physics to the group testing model. The obtained result matched the result of the algorithm, which supports our analysis. Based on the consideration of the Bayesian optimal setting, the obtained results are expected to provide an estimation of the upper bound for the group testing performance.

In the following, we summarize the assumptions introduced in our problem setting, and explain how we can approach these assumptions to achieve realistic settings in the future.

- **A1** The pools containing at least one defective item are regarded as positive.

When we consider the clinical testing where the specimens of the patients are pooled, the dilution effect is negligible. To consider this effect, a group testing model that has a detection limit is proposed [53]. Furthermore, in applying the group testing to the genome sequence processing, semi-quantitative group testing is a realistic setting rather than the logical sum rule [54].

- **A2** Independence of the tests.

When the specimens collected from the defected patients do not contain sufficient amounts of the pathogen to exceed the detection threshold, the results of the test performed on the pools that contain insufficient specimen quantity can be non-defective with a high probability when compared with other pools. This is an example that violates the assumption of the independence and identicality of the tests. In the case of the diagnostic test for intrathoracic tuberculosis in children, a multiple sampling and pooling method for specimens collected using different methods such as gastric aspirate, nasopharyngeal aspirate, and induced sputum has been discussed to obtain greater specimen volume [55]. The combinatorial formulation of the collection method of the specimen and the subsequent group testing are expected to provide more realistic models.

- **A3-4** Prior knowledge of the true positive probability, false positive probability, and prevalence.

The test properties \(p_{TP} \) and \(p_{FP} \) and the prevalence \(\theta\) are generally unknown; hence, an estimation procedure is required. There are various methods to estimate the true positive probability and false positive probability in a diagnostic test, and the utilization of these methods before performing the group testing is straightforward. For instance, in previous studies, the...
estimation of parameters was studied by introducing Bayesian inference [56]. To simultaneously estimate these parameters and the items’ states in the group testing, the expectation-maximization method and hierarchical Bayes approach [27] can be combined with the BP algorithm. When accurate parameter estimation fails, corresponding to a model mismatch, the calculation of estimators under the assumption of replica symmetry breaking may be required [52].

- **A5** Pretest probabilities being independently and identically distributed

When applying group testing to infectious diseases identification, the item (patient) state can be dependent on one another. Factors potentially contributing to this dependency include attributes of the patients relating to their susceptibility to the diseases, and the community to which the patients belong to. In order to model this dependency, mixed-effects modeling [57] to take into account for regional-dependencies of the prevalence, and SIR stochastic network models [58] associated with the group testing have been proposed. In the BP algorithm described in Sec.IV-B, the evaluation of the marginal posterior probability under the item-dependent prior distribution is possible. In addition, hierarchical Bayes modeling for group testing [27] considering the factors that induce dependency between the items is within the scope of the BP algorithm. Revealing cutoff dependence in such a realistic setting is one of the future issues we present for future study and discussion.

**APPENDIX**

**DETAILS OF THE REPLICA METHOD**

We introduce the following expression of the Kronecker’s delta:

\[ \delta(a, b) = \delta_{|z| = 1} \frac{dz}{2\pi\sqrt{-1}z^{b+1}} e^a. \]  

(95)

By applying (95) to the distribution for the c (31), we obtain:

\[ P_c(c) = \frac{1}{D} \prod_{j=1}^{N} \int_{|z_j| = 1} \frac{dz_j}{2\pi\sqrt{-1}z_j^{c_j+1}} \sum_{z \in \mathbb{C}^n} e^{\sum_{a \in \mathbb{C}} c_{a} z_{a}}. \]  

(96)

where the integral representation of the Kronecker’s delta is introduced. The procedure for calculating (46) is summarized in three steps.

- **1** Summation of y and c
- **2** Integration of z, which appears in the integral representation of Kronecker’s delta in (96)
- **3** Derive saddle point equations and apply RS assumption

The procedures are described below.

**A. Summation of y and c**

Here, we denote

\[ W(\{\bar{x}\}) = \sum_{y, c} P_c(c) \prod_{a=0}^{n} f(y|c, x^{(a)}) \phi(x^{(a)}). \]  

(97)

Summation over y and c leads to the following expression:

\[ W(\{\bar{x}\}) = \frac{1}{D} \int \prod_{j=1}^{N} \frac{dz_j z_j^{-(C+1)}}{(2\pi\sqrt{-1})^N} \times \phi(\{x^{(a)}\}) \prod_{\nu=1}^{N_p} \left[ 1 + \prod_{j \in \mathcal{E} (\nu)} z_j W_n(\bar{x}_{(\nu)}) \right]. \]  

(98)

Here, \( \bar{x}_j = \{x^{(0)}_i, x^{(1)}_i, \ldots, x^{(n)}_i\} \in \{0, 1\}^{n+1} \) is the replica vector of the i-th variable, and \( \bar{x}_{(\nu)} = \{\bar{x}^{(0)}_1, \ldots, \bar{x}^{(n)}_K\} \). We set \( \phi(\{x^{(a)}\}) = \prod_{a=0} \phi(x^{(a)}) \), and \( W_n(\bar{x}_{(\nu)}) \) is defined as

\[ W_n(\bar{x}_{(\nu)}) = \prod_{a=0} \left\{ p_{TP} T(\bar{x}^{(a)}_{(\nu)}) + p_{FP} (1 - T(\bar{x}^{(a)}_{(\nu)}) \right\} + \prod_{a=0} \left\{ (1 - p_{TP}) T(\bar{x}^{(a)}_{(\nu)}) + (1 - p_{FP}) (1 - T(\bar{x}^{(a)}_{(\nu)}) \right\}. \]  

(99)

Furthermore, we introduce the dummy variables \( \tilde{u}_j = \{u^{(0)}_j, u^{(1)}_j, \ldots, u^{(n)}_j\} \in \{0, 1\}^{n+1} \) for \( j = 1, \ldots, K \), and substitute the identity \( \sum_{\tilde{u}_j} \delta(\bar{x}_j, \tilde{u}_j) = 1 \) for every \( j \in \{1, \ldots, K\} \) as

\[ W(\{\bar{x}\}) = \frac{1}{D} \int \prod_{j=1}^{N} \frac{dz_j z_j^{-(C+1)}}{(2\pi\sqrt{-1})^N} \phi(\{x^{(a)}\}) \times \exp \left[ \sum_{\nu=1}^{N_p} \prod_{u \in \mathcal{E} (\nu)} \left\{ z_j \sum_{\tilde{u}_j} \delta(\bar{x}_{(\nu)}, \tilde{u}_j) W_n(\{\tilde{u}_j\}) \right\} \right] \times \exp \left[ \frac{N K}{K!} \sum_{\tilde{u}_j} \prod_{j=1}^{K} Q_n(\tilde{u}_j) W_n(\{\tilde{u}_j\}) \right]. \]  

(100)

In deriving (100), we used the relationship \( \sum_{K+1}^{N} 1 \sim 1 \) for \( K! \sum_{i=1}^{N} 1 \sum_{j=1}^{N} (\sum_{K=1}^{N} 1) \), which is valid for sufficiently large values of N. Here, we set \( \{\tilde{u}_i\} = \{\tilde{u}_1, \ldots, \tilde{u}_K\} \), and define the function \( Q_n(\tilde{u}) \) as follows:

\[ Q_n(\tilde{u}) = \frac{1}{N} \sum_{i=1}^{N} z_i \prod_{a=0}^{n} \delta\left(x^{(a)}_i, u^{(a)}\right). \]  

(101)

(101) is a function of \( \tilde{z}, \{\tilde{x}\}, \) and \( \tilde{u} \), but, for typical \( z \) and \( \{x^{(a)}\} \) in the integrand of (98), it is expected that \( \frac{1}{N} \sum_{i=1}^{N} E_{z}(x^{(a)}) |z| \prod_{a=0}^{n} \delta(x^{(a)}_i, u^{(a)}) \) holds for sufficiently large values of N; hence, we consider \( Q_n \) as a function of \( \tilde{u} \).
B. Integration of $z$

We introduce the identity for all possible $\hat{u} \in \{0,1\}^{n+1}$:

$$1 = \int d\mathbf{Q}_n(\hat{u}) \delta \left( \frac{1}{N} \sum_{i=1}^{N} z_i \prod_{a=0}^{n} \delta(x_i^{(a)}, u_i^{(a)}) - \mathbf{Q}_n(\hat{u}) \right)$$

$$= \int \frac{d\mathbf{Q}_n(\hat{u})d\mathbf{Q}_n(\hat{u})}{2\pi}$$

$$\times \exp \left\{ \mathbf{Q}_n(\hat{u}) \left( \sum_{i=1}^{N} z_i \prod_{a=0}^{n} \delta(x_i^{(a)}, u_i^{(a)}) - N\mathbf{Q}_n(\hat{u}) \right) \right\},$$

(102)

where $\mathbf{Q}_n(\hat{u})$ is the conjugate of $\mathbf{Q}_n(\hat{u})$. Substituting this into (100) and integrating $z$, we obtain

$$\mathbb{W}(\{\mathbf{x}\}) = \frac{1}{D} \int d\mathbf{Q}_n d\mathbf{Q}_n \exp \left( N\psi(\mathbf{Q}_n, \mathbf{Q}_n) \prod_{i=1}^{N} \mathcal{B}_n(\mathbf{x}_i), \right)$$

(103)

where $\mathcal{B}_n(\mathbf{x}_i)$ is given by (48), $\mathbf{Q}_n = \{\mathbf{Q}_n(\hat{u}) | \hat{u} \in \{0,1\}^{n+1}\}$, and $\mathbf{Q}_n = \{\mathbf{Q}_n(\hat{u}) | \hat{u} \in \{0,1\}^{n+1}\}$. The function $\psi(\mathbf{Q}_n, \mathbf{Q}_n)$ is given by

$$\psi(\mathbf{Q}_n, \mathbf{Q}_n) = S_n(\mathbf{Q}_n) - \mathbb{V}(\mathbf{Q}_n, \mathbf{Q}_n) + \mathcal{E}_n(\mathbf{Q}_n),$$

(104)

where

$$\mathbb{V}(\mathbf{Q}_n, \mathbf{Q}_n) = \sum_{\hat{u}} \mathbf{Q}_n(\hat{u}) \mathbf{Q}_n(\hat{u})$$

(105)

$$S_n(\mathbf{Q}_n) = \ln \prod_{\mathbf{x}_i} \phi(\mathbf{x}_i)(\mathbf{Q}_n(\mathbf{x}_i))^C$$

(106)

$$\mathcal{E}_n(\mathbf{Q}_n) = \frac{N^{K-1}}{K!} \sum_{\mathbf{u}_k, \ldots, \mathbf{u}_k} \prod_{k=1}^{K} \mathbf{Q}_n(\mathbf{u}_k) W_n(\{\mathbf{u}_k\}).$$

(107)

C. Saddle Point Method and RS Assumption

Considering sufficiently large $N$, we introduce the saddle point method for the integrals in (103). Thus, we obtain

$$\mathbb{W}(\{\mathbf{x}\}) = \frac{1}{D} \exp \left( N\psi(\mathbf{Q}_n^*, \mathbf{Q}_n^*) \right)$$

$$\times \prod_{i=1}^{N} \frac{\phi(\mathbf{x}_i) \left( \mathbf{Q}_n^*(\mathbf{x}_i) \right)^C}{\sum_{\mathbf{x}_i} \phi(\mathbf{x}_i) \left( \mathbf{Q}_n^*(\mathbf{x}_i) \right)^C},$$

(108)

where $\mathbf{Q}_n^*$ and $\mathbf{Q}_n^*$ denote the saddle points defined as

$$\{\mathbf{Q}_n^*, \mathbf{Q}_n^*\} = \arg \max \psi(\mathbf{Q}_n, \mathbf{Q}_n),$$

(109)

where $\max \mathbf{Q}_n, \mathbf{Q}_n$ represents the extremization with respect to $\mathbf{Q}_n$ and $\mathbf{Q}_n$. From the extremization conditions $\frac{\partial \psi}{\partial \mathbf{Q}_n} = 0$ and $\frac{\partial \psi}{\partial \mathbf{Q}_n} = 0$, we obtain the saddle point equations (49) and (50).

Substituting (52) and (53) into (50), we obtain

$$Q_n \{ (1 - \rho_n)(1 - x^{(0)}) + \rho_n x^{(0)} \}$$

$$\times \int d\mu \pi(\mu|x^{(0)}) \prod_{a=1}^{n} \left\{ (1 - \mu)(1 - x^{(a)}) + \mu x^{(a)} \right\}$$

$$= \frac{C}{\kappa_n} \left\{ (1 - \theta)(1 - \hat{\rho}_n)^{C-1}(1 - x^{(0)}) + \theta \hat{\rho}_n^{C-1} x^{(0)} \right\}$$

$$\times \int \prod_{\gamma=1}^{C-1} \left\{ d\hat{\mu}_\gamma \pi(\hat{\mu}_\gamma|x^{(0)}) \right\}$$

$$\times \prod_{a=1}^{n} \left\{ (1 - \theta) \prod_{\gamma=1}^{C-1} (1 - \hat{\mu}_\gamma)(1 - x^{(a)}) + \theta \prod_{\gamma=1}^{C-1} \hat{\mu}_\gamma x^{(a)} \right\},$$

(110)

where

$$\kappa_n = \sum_{x^{(0)}} \left\{ (1 - \theta)(1 - \hat{\rho}_n)^{C-1}(1 - x^{(0)}) + \theta \hat{\rho}_n^{C-1} x^{(0)} \right\}$$

$$\times \int \prod_{\gamma=1}^{C} \left\{ d\hat{\mu}_\gamma \pi(\hat{\mu}_\gamma|x^{(0)}) \right\}$$

$$\times \left\{ (1 - \theta) \prod_{\gamma=1}^{C-1} (1 - \hat{\mu}_\gamma) + \theta \prod_{\gamma=1}^{C-1} \hat{\mu}_\gamma \right\}.$$ (111)

This yields

$$Q_n = C \left\{ (1 - \theta)(1 - \hat{\rho}_n)^{C-1} + \theta \hat{\rho}_n^{C-1} \right\},$$

(112)

$$\rho_n = \frac{Q_n \kappa_n}{(1 - \theta)(1 - \hat{\rho}_n)^{C-1} + \theta \hat{\rho}_n^{C-1}},$$

(113)

and

$$\pi(\mu|x^{(0)}) = \frac{1}{\zeta_n(x^{(0)})} \int \prod_{\gamma=1}^{C-1} \left\{ d\hat{\mu}_\gamma \pi(\hat{\mu}_\gamma|x^{(0)}) \right\}$$

$$\times \left\{ (1 - \theta) \prod_{\gamma=1}^{C-1} (1 - \hat{\mu}_\gamma) + \theta \prod_{\gamma=1}^{C-1} \hat{\mu}_\gamma \right\}$$

$$\times \delta(\mu - \mu(\hat{\mu}_{C-1}, \theta)),$$

(114)

where

$$\zeta_n(x^{(0)}) = \int \prod_{\gamma=1}^{C-1} \left\{ d\hat{\mu}_\gamma \pi(\hat{\mu}_\gamma|x^{(0)}) \right\}$$

$$\times \left\{ (1 - \theta) \prod_{\gamma=1}^{C-1} (1 - \hat{\mu}_\gamma) + \theta \prod_{\gamma=1}^{C-1} \hat{\mu}_\gamma \right\}.$$ (115)

In addition, we compute $\sum_{\mathbf{x}_i} x^{(a)} \ldots \mathbf{Q}_n(\mathbf{x})$ for arbitrary subsets $\{a_1, \ldots, a_m\} \subseteq \{1, \ldots, n\}$ (0 $\leq m \leq n$) using the expressions on both sides of (49) keeping $x^0$ fixed as 1 or 0 under the replica symmetric assumption (52) and (53). This provides

$$\hat{\mathbf{Q}}_n \hat{\rho} \int d\hat{\mu}_1 \hat{\pi} = \frac{N^{K-1}}{(K-1)!} Q_n^{K-1}$$

$$\times \prod_{k=1}^{K} d\mu_k \left\{ \sum_{\gamma=0}^{n} \left( (1 - \rho_n)(1 - u_k^{(0)}) + \rho_n u_k^{(0)} \right) \pi(\mu_k|u_k^{(0)}) \right\}$$

$$\times \left\{ (p_{TP} + p_{TP}(1 - q(\mu_{K-1}))) + p_{TP} q(\mu_{K-1}) \right\}^{n-m} p_{TP} + (1 - p_{TP})(1 - p_{TP}(1 - q(\mu_{K-1})))$$

$$+ (1 - p_{TP}) q(\mu_{K-1}) \right\}^{n-m} (1 - p_{TP})^{m+1},$$

(116)
and
\[ \bar{Q}_n(1 - \bar{\rho}_n) \int d\bar{\mu}\pi(\bar{\mu}|0)\bar{\rho}^m = \frac{N^{K-1}}{(K-1)!} Q^{K-1}_n \]
\[ \times \prod_{k=1}^{K-1} d\mu_k \sum_{u_k(0)} \left\{ (1 - \mu_k)(1 - u_k(0)) + \rho \mu_k u_k(0) \right\} \pi(\mu_k|u_k(0)) \]
\[ \times \left\{ (p_{TP} + p_{FP}(1 - q(\mu_{K-1})) + p_{FP}q(\mu_{K-1})) \right\}^{n-m} p_{TP}^{m-1} \]
\[ + (1 - p_{TP} + (1 - p_{TP})(1 - q(\mu_{K-1}))) \]
\[ + (1 - p_{FP})q(\mu_{K-1}) \]}
\[ \times \left( p_{TP} + p_{FP}(1 - q(\mu_{K-1})) + p_{FP}q(\mu_{K-1}) \right) \]
\[ \times p_{TP}^{m}(p_{TP} - p_{FP}) \]
\[ + \left\{ (1 - p_{TP} + (1 - p_{TP})(1 - q(\mu_{K-1}))) \right\} \]
\[ + (1 - p_{FP})q(\mu_{K-1}) \]}
\[ \times (1 - p_{TP})^{m}(p_{TP} - p_{FP}) \].

Note that (112) – (117) can be defined not only for \( n \in \mathbb{N} \), but also for \( n \in \mathbb{R} \). Therefore, we can take the limit as \( n \to 0 \) for the expressions, directly reducing (114) to (62).

In addition, inserting \( m = 0 \) into (116) and (117), in conjunction with (112) and (113), leads to
\[ Q_0 = C \]
\[ \rho_0 = \frac{\theta_0^{C-1}}{(1 - \theta)(1 - \rho_0)^{C-1} + \theta_0^{C-1}} \]
\[ Q_0^3 = Q_0(1 - \rho_0) = \frac{N^{K-1}}{(K-1)!} Q^{K-1}_0 \].

These yield (55) – (58). Finally, comparing both sides of (116) and (117) offers (59) and (60). The form of (64) is derived by substituting (53) into (108) in the limit as \( n \to 0 \) after obtaining the above variables and distributions.

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