Bayesian inference of infected patients in group testing with prevalence estimation

Ayaka Sakata

1Institute of Statistical Mathematics, 10-3 Midori-cho, Tachikawa, Tokyo 190-8562, Japan
2Department of Statistical Science, The Graduate University for Advanced Science (SOKENDAI), Hayama-cho, Kanagawa 240-0193, Japan
3JST PRESTO, 4-1-8 Honcho, Kawaguchi, Saitama, 332-0012, Japan

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Group testing is a method of identifying infected patients by performing tests on a pool of specimens collected from patients. For the case in which the test returns a false result with finite probability, we propose Bayesian inference and a corresponding belief propagation (BP) algorithm to identify the infected patients from the results of tests performed on the pool. We show that the true-positive rate is improved by taking into account the credible interval of a point estimate of each patient. Further, the prevalence and the error probability in the test are estimated by combining an expectation-maximization method with the BP algorithm. As another approach, we introduce a hierarchical Bayes model to identify the infected patients and estimate the prevalence. By comparing these methods, we formulate a guide for practical usage.

I. INTRODUCTION

In clinical testing methods such as blood tests and polymerase chain reaction (PCR) tests, discovering infected patients from a large population requires significant operating costs. Because of limitations in the number of available devices, reagents, and technologists, a high demand exists for more efficient methods of testing. Group testing is one of the approaches for the reduction of the operating costs by performing tests on pools of specimens obtained from patients [1,2]. It is known that with the assumption that the rate of the infected patients in the population is sufficiently small, in principle, one can identify the infected patients from the tests on pools whose number is smaller than that of the population. Originally, group testing was developed for blood testing during World War II, and is now applied to various fields such as quality control in product testing [3], estimation of the content of genetically mutated organisms in maize grains [4], and multiple access communication [5].

The identification of the infected patients from the results of group test is mathematically formulated as a channel coding problem to reconstruct the original signal from a codeword transferred through noisy channel [6], where the original signal, codeword, and noisy channel correspond to the state of patients, states of the pools, and errors in the tests, respectively. Further, group testing can be regarded as a variant of compressed sensing [7,8] with discrete variables and logical sums. Hence, the progress in the last decade in sparse estimation including compressed sensing has revived interest in group testing, and information-theory approaches have achieved bound evaluation of group testing at a limiting case [9,10].

Recently, in response to the epidemic infection of COVID-19 that requires testing on large populations, the idea of group testing has attracted increasing attention [11,12] from the viewpoint of practical application rather than mathematics. In practice, clinical testing sometimes results in errors even when the operation is precise. For example, in PCR tests, false negative (FN) probabilities of up to 3% and false positive (FP) probabilities of up to 5% have been observed [13]. Moreover, the bacterial or viral load in the specimen depends on the specimen collection method and timing [14]. Therefore, a specimen sometimes does not contain a sufficient amount of the pathogen to exceed the detection limit, even when the patient is infected. Further, post-collection contamination of pathogens into a specimen can cause a positive result even when the patient is not infected. Statistical inference can contribute to the correction of errors by estimating the true state of patients from noisy test data, and quantifying the credibility of the estimation.

In this paper, we introduce Bayesian inference to identify the infected patients in the group testing problem considering the finite false probabilities in the test. The infection probability of each patient is approximately calculated by a belief propagation (BP) algorithm because of its low computational cost [15], although the BP algorithm does not achieve the information theoretic bound [16]. Our contributions with regard to the BP algorithm are as follows:

(i) The true positive (TP) ratio, namely the ratio of infected patients reconstructed as positive, is improved to be greater than the TP probability in the test by considering the confidence interval of the point estimate, which corresponds to the infection probability. We introduce a bootstrap method to construct the confidence interval.

(ii) In our framework, prevalence, which is the fraction of the infected patients in the population, is introduced into the prior distribution of the patients’ state. Prevalence is one of the fundamental measures in epidemiology, and group testing

*ayaka@ism.ac.jp
FIG. 1. Matrix representation of group testing, where each pool size is $N_G = 3$ and each overlap is $N_O = 2$. The summation in the usual matrix product is replaced with a logical sum.

has been applied to its estimation [17,19]. We construct the estimator of prevalence in addition to the identification of the infected patients by combining an expectation-maximization (EM) method with a BP algorithm. Following the same procedure, the TP and FP probabilities of the test are also estimated.

(iii) As another approach, we introduce the hierarchical Bayes model to identify the infected patients and estimate the prevalence. We apply the BP algorithm to the hierarchical Bayes model and evaluate the performance in comparison with the approach described in (ii), and find that the computational cost of the hierarchical Bayes approach is lesser than that required in (ii).

The remainder of the paper is organized as follows. In Section II, we explain the problem setting of group testing and introduce Bayesian inference. In Section III, we introduce the BP algorithm and show its reconstruction performance under finite false probabilities. In Section IV, we propose an estimator based on the confidence interval of the estimated infection probability. In Section V, we discuss the estimation of the unknown parameters in group testing by using the likelihood calculated by the BP algorithm. In Section VI, we introduce the hierarchical Bayes model for group testing and discuss the estimation of the prevalence by applying the BP algorithm to the hierarchical model. Section VII presents a summary and discussion, and supplementary comments are provided in Section VIII.

II. PROBLEM SETTING

We consider a population of $N$ patients and $M$ groups on which the test is performed. Let us denote the state of $N$-patients by $X^{(0)} \in \{0, 1\}^N$, where $X_i = 1$ and $X_i = 0$ means that $i$-th patient is infected and not infected, respectively. The grouping of the patients is determined by the pooling matrix $F \in \{0, 1\}^{M \times N}$, where $F_{\mu i} = 1$ and $F_{\mu i} = 0$ means that the $i$-th patient is in the $\mu$-th group and not, respectively. The true state of the $\mu$ ($= 1, \ldots, M$)-th group, denoted by $Y^{(0)}_\mu$, is given by

$$Y^{(0)}_\mu = \bigvee_{i=1}^N F_{\mu i} X_i^{(0)}, \tag{1}$$

where $\bigvee_{i=1}^N f_i = f_1 \lor f_2 \lor \cdots \lor f_N$ denotes the logical sum of $N$ components. Namely, when $\mu$-th pool contains at least one infected patient, the state of the $\mu$-th pool is 1 (positive), and 0 (negative) otherwise.

The test returns a false result with finite probability. We assume that the errors in the tests are independent from each other and model the observation (result of the test) as

$$Y_\mu = C(\bigvee_{i=1}^N F_{\mu i} X_i^{(0)}), \tag{2}$$
where $C(\cdot)$ is the probabilistic function whose behavior is given by [10]

$$P(C(a) = 1 | a = 1) = p_{TP}, \quad P(C(a) = 0 | a = 1) = 1 - p_{TP}$$

$$P(C(a) = 1 | a = 0) = p_{FP}, \quad P(C(a) = 0 | a = 0) = 1 - p_{FP}. \quad (3)$$

Here, $p_{TP}$ and $p_{FP}$ correspond to the TP and FP probabilities in the test, respectively, and these values are common for all tests. Fig. 1 shows matrix representation of the group testing, where we note that the summations in the usual matrix factorization are replaced with a logical sum. We focus on the case $\alpha \equiv M / N < 1$, where the number of tests is smaller than that of the patients. Hereafter, we consider that the size of group is fixed to $N_G$. Further, the overlap, which is the number of groups that each patient belongs to, is fixed at $N_G$; hence, the relationship $N_G = \alpha \times N_G$ holds.

### A. Bayesian inference

From the property of $C(\cdot)$, the generative model of $Y$ is given by

$$P(Y|X^{(0)}, p_{TP}, p_{FP}) = \prod_{\mu=1}^{M} P(Y_{\mu}|X^{(0)}, p_{TP}, p_{FP}) \quad (5)$$

where

$$P(Y_{\mu}|X, p_{TP}, p_{FP}) = p_{TP}Y_{\mu}T_{\mu}(X^{(0)}) + (1 - p_{TP})(1 - Y_{\mu})T_{\mu}(X^{(0)}) + p_{FP}Y_{\mu}(1 - T_{\mu}(X^{(0)))) + (1 - p_{FP})(1 - Y_{\mu})(1 - T_{\mu}(X^{(0)))) \quad (6)$$

and $T_{\mu}(X^{(0)}) = \vee_{i=1}^{N} F_{\mu i}X_{i}^{(0)}$. The purpose is to infer the true states of patients $X^{(0)}$ from the observation $Y$.

In general, the true generative process of $Y$ is unknown, but it is reasonable to assume that the process is expressed by the conditional Bernoulli distribution eq. (5), as the variables $Y$ and $X^{(0)}$ are binary, although the value of true parameters $p_{TP}$ and $p_{FP}$ are not known in advance. Bayesian inference is a preferred method in the presence of the reasonable model. As prior distribution of the patient states, we use following distribution:

$$P_{0}(X|\rho) = \prod_{i=1}^{N} (\rho X_{i} + (1 - \rho)(1 - X_{i})), \quad (7)$$

where $\rho \in [0, 1]$ is the prevalence, which is not known in advance. Following the Bayes rule, the posterior distribution is given by

$$P(X|Y) \propto P(Y|X, \hat{p}_{TP}, \hat{p}_{FP})P_{0}(X|\hat{\rho}), \quad (8)$$

where $\hat{p}_{TP}$, $\hat{p}_{FP}$, and $\hat{\rho}$ are the assumed TP probability, FP probability, and prevalence, respectively. The $i$-th patient’s state is identified on the basis of the marginal distribution given by

$$P(X_{i}|Y) = \sum_{X \backslash X_{i}} P(X|Y) \quad (9)$$

where $X \backslash X_{i}$ denotes components of $X$ other than $X_{i}$. As the variable $X_{i}$ is binary, we can represent the marginal distribution using a Bernoulli probability $\theta_{i}$ as

$$P(X_{i}|Y) = \theta_{i}X_{i} + (1 - \theta_{i})(1 - X_{i}), \quad (10)$$

and $\theta_{i}$ corresponds to the infection probability, namely, the probability that $X_{i} = 1$. The simplest estimate of $X_{i}^{(0)}$ is the maximum a posteriori (MAP) estimator given by

$$X_{i}^{(MAP)} = \mathbb{I}(\theta_{i} > 0.5), \quad (11)$$

where $\mathbb{I}(a)$ is the indicator function whose value is 1 when $a$ is true, and 0 otherwise.
The computation of the marginal distribution requires an exponential order of the sums, and thus is intractable. We approximately calculate the marginal distribution using the BP algorithm on the factor graph representation of the group testing [10,20]. Fig 2 shows the factor graph representation of the group testing for $N = 6, M = 4, N_G = 3$ and $N_O = 2$. Here, we denote $M(\mu)$ and $G(i)$ as the indices of the patients in the $\mu$-th pool, and that of the pools in which the $i$-th patient is included, respectively. The conditional probability $P(Y_\mu|X)$ depends on $X_i (i \in M(\mu))$; hence, the posterior distribution can be expressed as a bipartite graph, as shown in Fig 2. For the edge that connects the $\mu$-th factor (test) and the $i$-th variable (patient), two kinds of messages are defined as

$$\tilde{m}_{\mu \rightarrow i}(X_i) \propto \sum_{X_i \setminus X_i} P(Y_\mu|X, \hat{\theta}_{\mu \rightarrow i}, \hat{\rho}_{\mu \rightarrow i}) \prod_{j \in M(\mu) \setminus i} m_{j \rightarrow \mu}(X_i)$$

$$m_{i \rightarrow \mu}(X_i) \propto P_0(X_i|\hat{\rho}) \prod_{\nu \in G(i) \setminus \mu} \tilde{m}_{\nu \rightarrow i}(X_i),$$

which correspond to posterior information and output information, respectively. Intuitively, the messages $m_{i \rightarrow \mu}(X_i)$ and $\tilde{m}_{\mu \rightarrow i}(X_i)$ represent marginal distributions of $X_i$ before and after the $\mu$-th test is performed, respectively. As $\hat{X}_i \in \{0,1\}$, these messages are represented by one parameter as

$$\tilde{m}_{\mu \rightarrow i}(X_i) = \tilde{\theta}_{\mu \rightarrow i} X_i + (1 - \tilde{\theta}_{\mu \rightarrow i})(1 - X_i)$$

$$m_{i \rightarrow \mu}(X_i) = \theta_{i \rightarrow \mu} X_i + (1 - \theta_{i \rightarrow \mu})(1 - X_i),$$

where $\tilde{\theta}_{\mu \rightarrow i}$ and $\theta_{i \rightarrow \mu}$ are given by

$$\tilde{\theta}_{\mu \rightarrow i} = \frac{U_\mu}{Z_{\mu \rightarrow i}}$$

$$\theta_{i \rightarrow \mu} = \frac{\hat{\rho} \prod_{\nu \in G(i) \setminus \mu} \tilde{\theta}_{\nu \rightarrow i}}{Z_{i \rightarrow \mu}}$$

and

$$U_\mu = p_{TP} Y_\mu + (1 - p_{TP})(1 - Y_\mu)$$

$$W_\mu = p_{FP} Y_\mu + (1 - p_{FP})(1 - Y_\mu)$$

$$Z_{\mu \rightarrow i} = U_\mu \left(2 - \prod_{j \in M(\mu) \setminus i} (1 - \theta_{j \rightarrow \mu})\right) + W_\mu \prod_{j \in M(\mu) \setminus i} (1 - \theta_{j \rightarrow \mu})$$

$$Z_{i \rightarrow \mu} = \hat{\rho} \prod_{\nu \in G(i) \setminus \mu} \tilde{\theta}_{\nu \rightarrow i} + (1 - \hat{\rho}) \prod_{\nu \in G(i) \setminus \mu} (1 - \tilde{\theta}_{\nu \rightarrow i}).$$
Using these messages, we can approximate the marginal distribution as

\[ P(X_i) \propto \{
\begin{array}{l}
\hat{\rho} X_i + (1 - \hat{\rho})(1 - X_i) \\
\prod_{\mu \in \mathcal{G}(i)} \tilde{m}_{\mu-i}(X_i)
\end{array}
\] \]

\[
= \left( \hat{\rho} \prod_{\mu \in \mathcal{G}(i)} \tilde{m}_{\mu-i} \right) X_i + \left( 1 - \hat{\rho} \right) \prod_{\mu \in \mathcal{G}(i)} (1 - \tilde{m}_{\mu-i})(1 - X_i),
\]

and thus the infection probability is approximated as

\[
\hat{\theta}_i = \frac{\hat{\rho} \prod_{\mu \in \mathcal{G}(i)} \tilde{m}_{\mu-i} + (1 - \hat{\rho}) \prod_{\mu \in \mathcal{G}(i)} (1 - \tilde{m}_{\mu-i})}{\hat{\rho} \prod_{\mu \in \mathcal{G}(i)} \tilde{m}_{\mu-i}},
\]

and the MAP estimator is given by

\[
\hat{X}_i^{(MAP)} = \mathbb{1}(\hat{\theta}_i > 0.5).
\]

**Algorithm 1 BP for Bayesian Group Testing**

**Input:** \( Y \sim P(Y|X^{(0)}) \) and \( F \)

**Output:** \( \theta \in [0,1]^N \)

1: \( \{\theta^{(0)}_{\mu-i}\} \leftarrow \) initial values from \([0,1]^{N \times M}\)

2: \( \{\hat{\theta}^{(0)}_{\mu-i}\} \leftarrow \) initial values from \([0,1]^{M \times N}\)

3: \( U \leftarrow p_{TP} Y + (1 - p_{TP})(1_M - Y) \)

4: \( W \leftarrow p_{FP} Y + (1 - p_{FP})(1_M - Y) \)

5: for \( i = 1 \ldots T \) do

6: for all combinations of \((\mu,i)\) such that \( F_{\mu i} = 1 \) do

7: \( Z_{\mu-i}^{(t)} \leftarrow U_{\mu_i} \left[ 2 - \prod_{j \in \mathcal{M}(\mu) \setminus i} \left( 1 - \theta_{j-i}^{(t-1)} \right) \right] + W_{\mu_i} \prod_{j \in \mathcal{M}(\mu) \setminus i} \left( 1 - \theta_{j-i}^{(t-1)} \right) \)

8: \( Z_{\mu-i}^{(t)} \leftarrow \hat{\rho} \prod_{\nu \in \mathcal{G}(i) \setminus \mu} \theta_{\nu-i}^{(t-1)} + (1 - \hat{\rho}) \prod_{\nu \in \mathcal{G}(i) \setminus \mu} \left( 1 - \theta_{\nu-i}^{(t-1)} \right) \)

9: \( \hat{\theta}^{(t)}_{\mu-i} \leftarrow \frac{U_{\mu_i}}{Z_{\mu-i}^{(t)}} \)

10: \( \theta_{\mu-i}^{(t)} \leftarrow \frac{\rho \prod_{\nu \in \mathcal{G}(i) \setminus \mu} \theta_{\nu-i}^{(t-1)}}{Z_{\mu-i}^{(t)}} \)

11: end for

12: end for

13: for \( i = 1 \ldots N \) do

14: \( \hat{\theta}_i \leftarrow \frac{\rho \prod_{\mu \in \mathcal{G}(i)} \theta_{\mu-i}^{(T_i)}}{\rho \prod_{\mu \in \mathcal{G}(i)} \theta_{\mu-i}^{(T_i)} + (1 - \rho) \prod_{\mu \in \mathcal{G}(i)} (1 - \theta_{\mu-i}^{(T_i)})} \)

15: end for

First, we consider the case where we know the correct parameters; \( \hat{\rho}_{TP} = p_{TP}, \hat{\rho}_{FP} = p_{FP} \), and \( \hat{\rho} = \rho \). The pseudocode of the BP algorithm for group testing with known parameters is shown in Algorithm 1. We check the performance of BP algorithm for randomly constructed pooling matrix under the constraint as \( \sum_{i} F_{\mu i} = N_G \forall \mu \) and \( \sum_{\mu} F_{\mu i} = N_O \forall i \). The true state of patients \( X^{(0)} \) is also randomly generated under the constraint that \( \sum_{i} X_{i}^{(0)} = N \rho \). The accuracy of the MAP estimator is measured by the TP rate and FP rate given by

\[
TP = \frac{1}{N} \sum_{i} X_{i}^{(0)} \hat{X}_i^{(MAP)}
\]

\[
FP = \frac{1}{1 - \frac{1}{N} \sum_{i} X_{i}^{(0)}} - \frac{1}{N} \sum_{i} (1 - X_{i}^{(0)}) \hat{X}_i^{(MAP)}
\]

respectively. A TP value larger than \( p_{TP} \) and an FP value smaller than \( p_{FP} \) indicates that the performance of the BP-based identification is better than the parallel test of \( N \)-patients. Fig. 5 shows \( \rho \)-dependence of (a) TP and (b) FP at \( N = 1000, N_G = 10, p_{TP} = 0.95 \) and \( p_{FP} = 0.02 \), respectively. Each data point represents the averaged value with respect to 100 realizations of \( Y \) and \( X^{(0)} \). The horizontal lines in (a) and (b) indicate 0.95 and 0.02, which are the TP and FP probabilities of the test, respectively. As
FIG. 3. \( \rho \)-dependence of (a) TP and (b) FP at \( N = 1000 \) and \( N_G = 10 \) for various \( \alpha = M/N \). Error probabilities on the test are fixed at \( p_{TP} = 0.95 \) and \( p_{FP} = 0.02 \). The horizontal lines in (a) and (b) represent \( p_{TP} \) and \( p_{FP} \), respectively.

FIG. 4. \( \rho \)-dependence of (a) TP and (b) FP at \( N = 1000 \) and \( N_G = 10 \) for various \( \alpha \). Error rates are fixed at \( p_{TP} = 0.95 \) and \( p_{FP} = 0.1 \). The horizontal line in (a) represents \( p_{TP} \). Note that the FP region shown in (b) is below \( p_{FP} \).

\( \alpha \) increases, that is, as the number of tests increases, TP increases and the \( \rho \) region where TP is larger than \( p_{TP} \) extends. FP also has a smaller value than \( p_{FP} \) for small values of \( \rho \), and this success region extends as \( \alpha \) increases. For large \( \rho \), \( \hat{X}^{(MAP)} \) converges to 0 because \( \hat{\theta}_i < 0.5 \) \( \forall \) \( i \), and both TP and FP decrease to zero. A similar tendency is shown for different values of \( p_{TP} \) and \( p_{FP} \). As an example, we show TP and FP for \( N = 1000, N_G = 10, p_{TP} = 0.95, \) and \( p_{FP} = 0.1 \) in Fig. 4. The FP probability \( p_{FP} \) has large influence on TP, which is obvious from the comparison of Figs. 3 and 4. Intuitively, an increase in \( p_{FP} \) (or decrease in \( p_{TP} \)) causes uncertainty of the identification and decreases \( \hat{\theta}_i \); hence, the MAP estimator tends to be zero.

The dependence of TP on \( p_{TP} \) and \( p_{FP} \) is shown in Fig. 5(a) at \( N = 1000, N_G = 10 \) \((N_O = 5)\), and \( \rho = 0.01 \). The solid line indicates TP = \( p_{TP} \), and a TP value over the solid line means the reconstruction by the BP algorithm achieves a higher TP than the parallel test of \( N \)-patients, and this situation is achieved at a sufficiently small FP probability \( p_{FP} < 0.05 \) in this parameter region. The reconstruction performance also depends on \( N_G \). Fig. 5(b) shows the \( N_G \)-dependence of TP at \( N = 1000, M = 500, p_{TP} = 0.95, \) and \( p_{FP} = 0.05 \). TP increases as \( N_G \) increases without increasing the number of tests.

In practical testing, one of the objective is to identify the infected patients in order to prevent spreading of the disease. Therefore, increasing TP is a priority issue, and we mainly focus on the improvement of TP using the BP algorithm.

### A. BP algorithm needs “decision threshold”

Before proceeding to the improvement of TP, we discuss the trivial fixed points of the BP algorithm and introduce the idea of “decision threshold” for the identification of infected patients.
From eq. (23), when $\hat{\theta}_{j-\mu} = 1$ for $\mu \in \mathcal{G}(i)$, we obtain $\hat{\theta}_i = 1$ irrespective of the value of $\hat{\rho}$. This situation arises when $\theta_j = 0$ for $j \in \mathcal{M}(\mu)\setminus i$ at $p_{TP} = 0$. Therefore, $\hat{\theta}_i = 1$ is achieved when the patients $j \in \mathcal{M}(\mu)$ are estimated as negative before $\mu$-th test is performed, where $\mu \in \mathcal{G}(i)$. This is the case in which the $i$-th patient is trivially identified as positive. In other words, the BP algorithm does not return $\hat{\theta}_i = 1$ for general cases; hence, to determine the infected patients $X_i^{(0)} \in \{0, 1\}$ from an estimate at the BP fixed point $\hat{\theta}_i \in [0, 1]$, we need a “decision threshold” such as a MAP estimator, where $\hat{\theta}_i = 0.5$ is the threshold for determining the infected patients. TP and FP depend on this threshold, and our strategy for the improvement of TP is the appropriate choice of the threshold as discussed in next section.

The threshold at $\hat{\theta}_i = 0$ is expected to lead conservative result, but it is not appropriate for general value of $p_{TP}$. Following similar logic, $\hat{\theta}_i = 0$ is obtained when at least one of the components of $\hat{\theta}_{\mu-\mu}$ among $\mu \in \mathcal{G}(i)$ takes the value 0, which is achieved at $p_{TP} = 1$ and $Y_\mu = 0$ or $p_{TP} = 0$ and $Y_\mu = 1$. The former case means that all patients belong to the $\mu$-th test are negative when $Y_\mu = 0$ and $p_{TP} = 1$. In the latter case, $Y_\mu = 1$ means $Y_\mu^{(0)} = 0$ because $p_{TP} = 0$; Hence, all patients belonging to the positive test are negative. In other words, $\hat{\theta}_i$ is always larger than zero when $p_{TP}$ is less than 1 or larger than 1. Therefore, all of the patients are judged as positive under the threshold at $\hat{\theta}_i = 0$, which corresponds to FP = 1.

IV. IMPROVEMENT OF TRUE-POSITIVE RATE CONSIDERING FLUCTUATION OF THE ESTIMATES

The estimated Bernoulli probability $\hat{\theta}$ is a function of $Y$, and fluctuates depending on the probabilistic observation. The quantification of the credibility of $\hat{\theta}$ helps in determining the infected patients under conditions of noisy observation data. The confidence interval is one of the guides in inference considering the input fluctuation [21]. For convenience, we introduce the following statistic:

$$\hat{\tau}_i \equiv \log \frac{\hat{\theta}_i}{1 - \hat{\theta}_i},$$

which gives the MAP estimator as

$$X_i^{\text{MAP}} = \mathbb{I}(\hat{\tau}_i > 0).$$

Here, we assume that the generative model has the corresponding “true value” $\tau_i$. Following the normal theory, the 95% confidence interval of the true value of $\tau_i$ is constructed as

$$\tau_i \in [\hat{\tau}_i - 1.96\hat{\sigma}_i, \hat{\tau}_i + 1.96\hat{\sigma}_i],$$

where 1.96 is the 97.5% quantile of the standard normal distribution, and $\hat{\sigma}_i$ is the estimate of the standard error. We resort to the nonparametric bootstrap method to estimate the standard error [22]. We generate $b = 1, \cdots, N_B$ bootstrap samples $Y^{(b)} \in \{0, 1\}^M$ and $F^{(b)} \in \{0, 1\}^{M \times N}$ as

$$\{y^{(b)}_\mu, F^{(b)}_\mu\} \sim \hat{P}(y, \hat{F}),$$

FIG. 5. (a) $p_{TP}$-dependence of TP at $N = 1000, M = 500, N_G = 10$ ($N_O = 5$), and $\rho = 0.01$ for different values of $p_{TP}$. (b) $N_G$-dependence of TP at $N = 1000, M = 500$ and $p_{TP} = 0.95, p_{FP} = 0.05$. The solid line indicates $0.95(p_{TP})$. 

[raw]

From eq. (23), when $\hat{\theta}_{j-\mu} = 1$ for $\mu \in \mathcal{G}(i)$, we obtain $\hat{\theta}_i = 1$ irrespective of the value of $\hat{\rho}$. This situation arises when $\theta_j = 0$ for $j \in \mathcal{M}(\mu)\setminus i$ at $p_{TP} = 0$. Therefore, $\hat{\theta}_i = 1$ is achieved when the patients $j \in \mathcal{M}(\mu)\setminus i$ are estimated as negative before $\mu$-th test is performed, where $\mu \in \mathcal{G}(i)$. This is the case in which the $i$-th patient is trivially identified as positive. In other words, the BP algorithm does not return $\hat{\theta}_i = 1$ for general cases; hence, to determine the infected patients $X_i^{(0)} \in \{0, 1\}$ from an estimate at the BP fixed point $\hat{\theta}_i \in [0, 1]$, we need a “decision threshold” such as a MAP estimator, where $\hat{\theta}_i = 0.5$ is the threshold for determining the infected patients. TP and FP depend on this threshold, and our strategy for the improvement of TP is the appropriate choice of the threshold as discussed in next section.

The threshold at $\hat{\theta}_i = 0$ is expected to lead conservative result, but it is not appropriate for general value of $p_{TP}$. Following similar logic, $\hat{\theta}_i = 0$ is obtained when at least one of the components of $\hat{\theta}_{\mu-\mu}$ among $\mu \in \mathcal{G}(i)$ takes the value 0, which is achieved at $p_{TP} = 1$ and $Y_\mu = 0$ or $p_{TP} = 0$ and $Y_\mu = 1$. The former case means that all patients belong to the $\mu$-th test are negative when $Y_\mu = 0$ and $p_{TP} = 1$. In the latter case, $Y_\mu = 1$ means $Y_\mu^{(0)} = 0$ because $p_{TP} = 0$; Hence, all patients belonging to the positive test are negative. In other words, $\hat{\theta}_i$ is always larger than zero when $p_{TP}$ is less than 1 or larger than 1. Therefore, all of the patients are judged as positive under the threshold at $\hat{\theta}_i = 0$, which corresponds to FP = 1.

IV. IMPROVEMENT OF TRUE-POSITIVE RATE CONSIDERING FLUCTUATION OF THE ESTIMATES

The estimated Bernoulli probability $\hat{\theta}$ is a function of $Y$, and fluctuates depending on the probabilistic observation. The quantification of the credibility of $\hat{\theta}$ helps in determining the infected patients under conditions of noisy observation data. The confidence interval is one of the guides in inference considering the input fluctuation [21]. For convenience, we introduce the following statistic:

$$\hat{\tau}_i \equiv \log \frac{\hat{\theta}_i}{1 - \hat{\theta}_i},$$

which gives the MAP estimator as

$$X_i^{\text{MAP}} = \mathbb{I}(\hat{\tau}_i > 0).$$

Here, we assume that the generative model has the corresponding “true value” $\tau_i$. Following the normal theory, the 95% confidence interval of the true value of $\tau_i$ is constructed as

$$\tau_i \in [\hat{\tau}_i - 1.96\hat{\sigma}_i, \hat{\tau}_i + 1.96\hat{\sigma}_i],$$

where 1.96 is the 97.5% quantile of the standard normal distribution, and $\hat{\sigma}_i$ is the estimate of the standard error. We resort to the nonparametric bootstrap method to estimate the standard error [22]. We generate $b = 1, \cdots, N_B$ bootstrap samples $Y^{(b)} \in \{0, 1\}^M$ and $F^{(b)} \in \{0, 1\}^{M \times N}$ as

$$\{y^{(b)}_\mu, F^{(b)}_\mu\} \sim \hat{P}(y, \hat{F}),$$
where $\bar{F}^{(b)}_\mu$ is the $\mu$-th row vector of $F^{(b)}$ and $\hat{P}(Y, \tilde{F})$ is the empirical distribution of given $Y$ and $\tilde{F}$ defined by

$$\hat{P}(Y, \tilde{F}) = \frac{1}{M} \sum_{\nu=1}^M \delta(y_{\nu})\delta(\tilde{F} - \tilde{F}_\nu).$$

(31)

We perform the BP algorithm for every bootstrap sample $^\ast\ast$, and denote the estimate under the $b$-th bootstrap sample as $\hat{\tau}^{(b)}$. Using $\tau_i^{(b)}$ ($b = 1, \ldots, N_B$), the estimate of the standard error of $\hat{\tau}_i$ is given by

$$\hat{\sigma}_i = \sqrt{\frac{1}{N_B-1} \sum_{b=1}^{N_B} (\hat{\tau}_i^{(b)} - \bar{\tau}_i)^2},$$

(32)

where $\bar{\tau}_i = \frac{1}{N_B} \sum_{b=1}^{N_B} \hat{\tau}_i^{(b)}$ is the average over the bootstrap samples.

We define the bootstrap estimate of the $i$-th patient’s state as

$$\hat{X}_i^{(Boot)} = I(\hat{\tau}_i + 1.96\hat{\sigma}_i > 0),$$

(33)

which means that patients whose confidence interval runs over the region $\tau > 0$ are regarded as infected. In comparison with the MAP estimator eq. (28), the decision threshold over which the patients are estimated as infected is lower by $1.96\hat{\sigma}_i$. Further, when $\hat{X}^{(MAP)} = 1$, $\hat{X}^{(Boot)} = 1$ always; Hence, eq. (33) can change the result of patients who are judged by the MAP estimator as non-infected. Fig. 6 shows the (a) TP and (b) FP of the bootstrap estimate at $\hat{\tau}$ in Fig. 8 at $N = 1000$, $M = 500$, $N_G = 10$, $p_{TP} = 0.95$, $p_{FP} = 0.1$. We generate $N_B = 1000$ bootstrap samples for each set of sample $\{Y, F, X^{(0)}\}$, and each point is averaged over 100 samples. The MAP estimator cannot achieve a higher TP than $p_{TP}$ for any $\rho$, but the bootstrap estimator improves TP to be greater than $p_{TP}$. Meanwhile, FP of the bootstrap estimator is higher than that of the MAP estimator, which is caused by the reduced decision threshold compared with that of the MAP estimator. However, FP is smaller than $p_{FP}$ for sufficiently small $\rho$; hence, we consider the bootstrap estimator as practicable. The situation is the same for other parameter region. As an example, we show TP and FP of bootstrap estimator at $N = 1000$, $M = 400$, $N_G = 20$, $p_{TP} = 0.95$, $p_{FP} = 0.1$ in Fig. 7.

For the intuitive understanding of the bootstrap estimator, we show examples of the bootstrap distributions of $\tau$ in Fig. 8 at $N = 1000$, $M = 500$, $N_G = 10$, $p_{TP} = 0.95$, and $p_{FP} = 0.1$, where the solid line represents $\hat{\tau}$ and the two dashed lines indicate the confidence interval. This histogram was obtained from 1000 bootstrap samples; note that the confidence interval eq. (29) is not that for the bootstrap distribution. Fig. 8(a) shows the bootstrap distribution of an infected patient who is judged as non-infected by the MAP estimator and as infected by the bootstrap estimator. Fig. 8(b) shows the same for a non-infected patient. The patients shown in Fig. 8(a) and (b) contribute to the increase of TP and FP of bootstrap estimate, respectively.
V. ESTIMATION OF UNKNOWN PARAMETERS BY EXPECTATION MAXIMIZATION

In this section, we consider the estimation of the unknown parameters: prevalence $\rho$, TP probability $p_{TP}$, and FP probability $p_{FP}$. We construct their estimator by the maximum likelihood method, where the likelihood is given by

$$\sum_X P(Y|X, p_{TP}, p_{FP}) P(X|\rho) = P(Y|\rho, p_{TP}, p_{FP}),$$

and the estimators are given by

$$\hat{\rho} = \arg\max_{\rho} \ln P(Y|\rho, p_{TP}, p_{FP})$$

$$\hat{p}_{TP} = \arg\max_{p_{TP}} \ln P(Y|\rho, p_{TP}, p_{FP})$$

$$\hat{p}_{FP} = \arg\max_{p_{FP}} \ln P(Y|\rho, p_{TP}, p_{FP}).$$
An approximation of the log-likelihood is given by the BP algorithm as Bethe free entropy \([20]\), defined as

\[
S = \sum_{\mu=1}^{M} \ln Z_{\mu} + \sum_{i=1}^{N} \ln Z_{i} - \sum_{\mu} \sum_{i \in \mathcal{M}(\mu)} \ln Z_{\mu i},
\]

(38)

where

\[
Z_{\mu} \equiv \sum_{X} \prod_{i \in \mathcal{M}(\mu)} m_{i-\mu}(X_{i}) P(Y_{\mu}|X)
\]

\[
= U_{\mu} (1 - \tilde{q}_{\mu}) + W_{\mu} \tilde{q}_{\mu}
\]

(39)

\[
Z_{i} \equiv \sum_{X_{i}} \prod_{\mu \in \mathcal{G}(i)} \tilde{m}_{\mu-\mu}(X_{i}) \{ \rho X_{i} + (1 - \rho)(1 - X_{i}) \}
\]

\[
= \rho \prod_{\mu \in \mathcal{G}(i)} (1 - \tilde{\theta}_{\mu-\mu}) + (1 - \rho) \prod_{\mu \in \mathcal{G}(i)} (1 - \tilde{\theta}_{\mu-\mu})
\]

(40)

\[
Z_{\mu i} \equiv \sum_{X_{i}} m_{i-\mu}(X_{i}) \tilde{m}_{\mu-\mu}(X_{i})
\]

\[
= \theta_{i \rightarrow \mu} \tilde{\theta}_{\mu-\mu} + (1 - \theta_{i \rightarrow \mu})(1 - \tilde{\theta}_{\mu-\mu}),
\]

(41)

and

\[
\tilde{q}_{\mu} = \prod_{i \in \mathcal{M}(\mu)} (1 - \theta_{i \rightarrow \mu}).
\]

(42)

We derive the maximum-likelihood estimator by the stationary condition of the Bethe free entropy \([23]\). After the calculation shown in the appendix, we obtain

\[
\hat{\rho} = \frac{1}{N} \sum_{i=1}^{N} \hat{\theta}_{i}
\]

(43)

\[
\hat{\rho}_{TP} = \frac{1}{M} \sum_{\mu=1}^{M} \langle \langle Y_{\mu} = 1, T_{\mu}(X(\mu)) = 1 \rangle \rangle_{\mu}
\]

\[
= \frac{1}{M} \sum_{\mu=1}^{M} \langle \langle T_{\mu}(X(\mu)) = 1 \rangle \rangle_{\mu}
\]

(44)

\[
\hat{\rho}_{FP} = \frac{1}{M} \sum_{\mu=1}^{M} \langle \langle Y_{\mu} = 1, T_{\mu}(X(\mu)) = 0 \rangle \rangle_{\mu}
\]

\[
= \frac{1}{M} \sum_{\mu=1}^{M} \langle \langle T_{\mu}(X(\mu)) = 0 \rangle \rangle_{\mu}
\]

(45)

where \(\langle \cdot \rangle_{\mu}\) denotes the expectation of \(X(\mu) \equiv \{ X_{i} | i \in \mathcal{M}(\mu) \}\) according to the posterior distribution with respect to the \(\mu\)-th test defined by

\[
P_{\mu}(X(\mu)|Y_{\mu}) = \frac{1}{Z_{\mu}} P(Y_{\mu}|X(\mu)) \prod_{i \in \mathcal{M}(\mu)} m_{i-\mu}(X_{i}).
\]

(46)

and

\[
\langle \langle Y_{\mu} = 1, T_{\mu}(X(\mu)) = 1 \rangle \rangle_{\mu} = \frac{p_{TP} Y_{\mu} (1 - \tilde{q}_{\mu})}{Z_{\mu}}
\]

(47)

\[
\langle \langle Y_{\mu} = 1, T_{\mu}(X(\mu)) = 0 \rangle \rangle_{\mu} = \frac{p_{FP} Y_{\mu} \tilde{q}_{\mu}}{Z_{\mu}}
\]

(48)

\[
\langle \langle T_{\mu}(X(\mu)) = 1 \rangle \rangle_{\mu} = \frac{U_{\mu} (1 - \tilde{q}_{\mu})}{Z_{\mu}}
\]

(49)

\[
\langle \langle T_{\mu}(X(\mu)) = 0 \rangle \rangle_{\mu} = \frac{W_{\mu} \tilde{q}_{\mu}}{Z_{\mu}}
\]

(50)

Eqs. \((44)-(45)\) always have trivial fixed points at 0 and 1, and to avoid these solutions, we solve following expressions:

\[
f(u, v) \equiv \sum_{\mu} \frac{(2Y_{\mu} - 1)(1 - \tilde{q}_{\mu})}{Z_{\mu}} = 0
\]

(51)

\[
g(u, v) \equiv \sum_{\mu} \frac{(2Y_{\mu} - 1)\tilde{q}_{\mu}}{Z_{\mu}} = 0
\]

(52)
We calculate the infected probability of patients and the estimators of the unknown parameters by the expectation-maximization (EM) method; in the E-step, the fixed point of BP, \{\hat{\theta}_{\mu^{-i}}\} and \{\hat{\theta}_{i^{-\mu}}\}, is achieved by recursive updating under a fixed \(\hat{\rho}_{\text{FP}}\), \(\hat{\rho}_{\text{TP}}\) and \(\hat{\rho}\); in the M-step, these parameters are updated according to the extremization conditions of eqs. (43)-(45). We term this method the BP+EM algorithm, which is summarized in Algorithm 2.\[\text{Algorithm 2}^\dagger\]

Fig. 9 show the comparison between estimated parameters and true parameters at \(N = 1000, M = 500\), and \(N_G = 10\) for (a) \(\rho\) at \(p_{\text{TP}} = 0.95\) and \(p_{\text{FP}} = 0.1\), (b) \(p_{\text{TP}}\) at \(\rho = 0.1\) and \(p_{\text{FP}} = 0.1\), and (c) \(p_{\text{FP}}\) at \(\rho = 0.1\) and \(p_{\text{TP}} = 0.95\). The gradient of the diagonal lines is 1; Hence, the point on this line indicates that accurate estimation of the unknown parameters is achieved. In all of the figures, parameters that are not shown in the figure are also estimated at the same time. For the whole parameter region, the M-step converges to the true parameter. TP rate and FP rate of the BP+EM algorithm are the same as those of BP algorithm where the parameters are known.

We note that the behavior of the BP+EM algorithm heavily depends on the initial condition of \(\hat{\rho}_{\text{TP}}\) and \(\hat{\rho}_{\text{FP}}\). When the initial conditions of \(\hat{\rho}_{\text{TP}}\) and \(\hat{\rho}_{\text{FP}}\) are close to their true values, the BP+EM algorithm are stable; hence, the proposed method should be treated as a correction of the experimentally estimated values. Meanwhile, the estimation of \(\hat{\rho}\) is insensitive to the initial condition, which is smaller than \(\alpha\).
Algorithm 2 BP+EM for Bayesian group testing

Input: \( Y \sim P(Y | X^{(0)}) \) and \( F \)
Output: \( \theta \in [0, 1]^N \)

1: \textbf{Initialize:}
2: \( \{ \theta_i^{(0)} \} \leftarrow \text{initial value from } [0, 1]^{N \times M} \)
3: \( \{ \theta_{i,i}^{(0)} \} \leftarrow \text{initial value from } [0, 1]^{M \times N} \)
4: \( \{ \theta_{\mu,i}^{(0)} \} \leftarrow \text{initial value from } [0, 1]^3 \)
5: \( U[0] \leftarrow \rho_{\mu,i}^{[0]} + (1 - \rho_{\mu,i}^{[0]})(1_M - Y), \quad W[0] \leftarrow \rho_{FP}^{[0]} Y + (1 - \rho_{FP}^{[0]})(1_M - Y) \)
6: for \( s = 1 \ldots S \) do
7: for \( i = 1 \ldots I \) do
8: for all combinations of \( (\mu, i) \) such that \( F_{\mu,i} = 1 \) do
9: \( \hat{\theta}_{i,i}^{(s)} \leftarrow U_{\mu,i}^{[s-1]} \left( 2 - \Pi_{j \in \mathcal{M}(\mu) \setminus i} \left( 1 - \hat{\theta}_{j,i}^{(t-1)} \right) \right) + W_{\mu,i}^{[s-1]} \Pi_{j \in \mathcal{M}(\mu) \setminus i} \left( 1 - \hat{\theta}_{j,i}^{(t-1)} \right) \)
10: \( \hat{\theta}_{\mu,i}^{(s)} \leftarrow U_{\mu,i}^{[s-1]} \Pi_{j \in \mathcal{M}(\mu) \setminus i} \left( 1 - \hat{\theta}_{j,i}^{(t-1)} \right) \)
11: end for
12: end for
13: end for
14: end for
15: end for
16: for \( \mu = 1 \ldots M \) do
17: \( \hat{\rho}_{\mu}^{[s]} \leftarrow U_{\mu}^{[s-1]} (1 - \hat{g}_{\mu}^{[s]}) + W_{\mu}^{[s-1]} \hat{g}_{\mu}^{[s]} \)
18: \( Z_{\mu}^{[s]} \leftarrow \Pi_{i \in \mathcal{M}(\mu)} (1 - \hat{\theta}_{\mu,i}^{(T)}) \)
19: end for
20: \( f[x] \leftarrow \sum_{\mu} \left( Y_{\mu} - (1 - Y_{\mu}) (1 - \hat{g}_{\mu}^{[s]}) \right) / Z_{\mu}^{[s]}, \quad s[x] \leftarrow \sum_{\mu} (Y_{\mu} - (1 - Y_{\mu}) \hat{g}_{\mu}^{[s]}) / Z_{\mu}^{[s]} \)
21: \( G[x] \leftarrow \left[ \sum_{\mu} (2Y_{\mu} - 1) \hat{g}_{\mu}^{[s]} \right] Z_{\mu}^{[s]} + \left[ \sum_{\mu} (2Y_{\mu} - 1) (1 - \hat{g}_{\mu}^{[s]}) \right] Z_{\mu}^{[s]} \)
22: \( \hat{F}_{\mu,i}^{[s]} \leftarrow [f[x]^T \hat{P}_{FP}^{[s]}] + G[x]^T (f[x], s[x]) \)
23: \( U[x] \leftarrow \hat{P}_{FP}^{[s]} Y + (1 - \hat{F}_{FP}^{[s]})(1_M - Y), \quad W[x] \leftarrow \hat{P}_{FP}^{[s]} Y + (1 - \hat{F}_{FP}^{[s]})(1_M - Y) \)
24: end for

VI. HIERARCHICAL BAYES APPROACH

As another approach to estimating prevalence, we introduce the hierarchical Bayes model, where the prevalence is regarded as a hyperparameter distributed according to the hyperprior distribution

\[
\phi(\rho; a, b) = \frac{\rho^{a-1}(1 - \rho)^{b-1}}{B(a, b)}, \tag{53}
\]

which is the beta distribution with hyperhyperparameters \( a \) and \( b \), and \( B(a, b) \) is the beta function. The beta distribution is the conjugate of the Bernoulli distribution. A graphical representation of group testing for the hierarchical Bayes model is shown in Fig[10] The prior distribution of \( X_i \) under a given \( \rho \) is regarded as an "interaction" that is represented by a factor node \( I_i \). We introduce additional messages \( \pi_{i,i}, \tilde{I}_{i,i}, \tilde{I}_{i,i}, \text{and} f_{i,i} \) for all \( i \), that are propagated from \( X_i \) to \( I_i \), \( I_i \) to \( X_i \), \( I_i \) to \( \rho \), and \( \rho \) to \( I_i \), respectively, as shown in Fig[10]
FIG. 10. Graphical representation and messages of the hierarchical Bayes model for the group testing at $N = 6$, $M = 4$, $N_G = 3$ and $N_O = 2$.

The messages propagated between the bipartite graph of $Y$ and $X$ are given by

$$
\tilde{m}_{\mu \rightarrow i}(X_i) \propto \sum_{X_i/X_i} P(Y_{\mu} \mid X) \prod_{j \in M(\mu) \setminus i} m_{j \rightarrow \mu}(X_i)
$$  \hspace{1cm} (54)

$$
m_{i \rightarrow \mu}(X_i) = \tilde{\pi}_{i \rightarrow \mu}(x_i) \prod_{\nu \in G(i) \setminus \mu} \tilde{m}_{\nu \rightarrow i}(x_i),
$$  \hspace{1cm} (55)

where $\tilde{\pi}_{i \rightarrow \mu}$ carries the prior information to $X_i$. Here, we express $\tilde{\pi}_{i \rightarrow \mu}(x_i)$ by one parameter $\tilde{\rho}_i$, which is derived later, as

$$
\tilde{\pi}_{i \rightarrow \mu}(x_i) = \tilde{\rho}_i + (1 - \tilde{\rho}_i)(1 - X_i).
$$  \hspace{1cm} (56)

Using eq.(56), the parameters $\tilde{\theta}_{\mu \rightarrow i}$ and $\theta_{i \rightarrow \mu}$ that express the messages as Eqs. (14)-(15), are given by

$$
\tilde{\theta}_{\mu \rightarrow i} = \frac{U_{\mu}}{Z_{\mu \rightarrow i}}
$$  \hspace{1cm} (57)

$$
\theta_{i \rightarrow \mu} = \frac{\theta_{\rho_i} \prod_{\nu \in G(i) \setminus \mu} \tilde{\theta}_{\nu \rightarrow i}}{Z_{i \rightarrow \mu}},
$$  \hspace{1cm} (58)

where

$$
Z_{\mu \rightarrow i} = U_{\mu} \left(2 - \prod_{j \in M(\mu) \setminus i} (1 - \theta_{j \rightarrow \mu})\right) + W_{\mu} \prod_{j \in M(\mu) \setminus i} (1 - \theta_{j \rightarrow \mu}),
$$  \hspace{1cm} (59)

$$
Z_{i \rightarrow \mu} = \tilde{\rho}_i \prod_{\nu \in G(i) \setminus \mu} \tilde{\theta}_{\nu \rightarrow i} + (1 - \tilde{\rho}_i) \prod_{\nu \in G(i) \setminus \mu} (1 - \tilde{\theta}_{\nu \rightarrow i}),
$$  \hspace{1cm} (60)

and $U_{\mu}$ and $W_{\mu}$ are given by eqs.(18)-(19). The messages between variables and priors are given by

$$
\pi_{i \rightarrow \mu}(X_i) \propto \prod_{\mu \in G(i)} \tilde{m}_{\mu \rightarrow i}(X_i)
$$  \hspace{1cm} (61)

$$
\tilde{\pi}_{i \rightarrow \mu}(x_i) = \int_0^1 d\rho \rho X_i + (1 - \rho)(1 - X_i) r_{\mu \rightarrow i}(\rho),
$$  \hspace{1cm} (62)

and we obtain

$$
\tilde{\rho}_i = \int_0^1 d\rho \rho r_{\mu \rightarrow i}(\rho).
$$  \hspace{1cm} (63)
Further, by setting

$$\pi_{i \rightarrow i}(X_i) = \pi_i X_i + (1 - \pi_i)(1 - X_i),$$  \hspace{1cm} (64)$$

we obtain

$$\pi_i = \frac{\prod_{\mu \in G(i)} \hat{\theta}_{\mu \rightarrow i}}{\prod_{\mu \in G(i)} \hat{\theta}_{\mu \rightarrow i} + \prod_{\mu \in G(i)} (1 - \hat{\theta}_{\mu \rightarrow i})},$$  \hspace{1cm} (65)$$

which corresponds to the infection probability when the prior is ignored. The messages between prior $$I_i$$ and the hyperparameter $$\rho$$ are given by

$$\tilde{r}_{i \rightarrow p}(\rho) \propto \sum_{X_i} \{\rho X_i + (1 - \rho)(1 - X_i)\} \pi_{i \rightarrow i}(X_i)$$

$$= \rho \pi_i + (1 - \rho)(1 - \pi_i)$$  \hspace{1cm} (66)$$

$$r_p \rightarrow i(\rho) \propto \phi(\rho) \prod_{j \neq i} \tilde{r}_{j \rightarrow p}(\rho).$$  \hspace{1cm} (67)$$

Using these messages, we can approximate the marginal distribution as

$$P(X_i) \propto \pi_{i \rightarrow i}(X_i) \prod_{\mu \in G(i)} \tilde{m}_{\mu \rightarrow i}(X_i),$$  \hspace{1cm} (68)$$

and the infection probability of $$X_i$$ is estimated as

$$\hat{\theta}_i = \frac{\tilde{\rho}_i \prod_{\mu \in G(i)} \tilde{\theta}_{\mu \rightarrow i} + (1 - \tilde{\rho}_i) \prod_{\mu \in G(i)} (1 - \tilde{\theta}_{\mu \rightarrow i})}{\tilde{\rho}_i \prod_{\mu \in G(i)} \tilde{\theta}_{\mu \rightarrow i} + (1 - \tilde{\rho}_i) \prod_{\mu \in G(i)} (1 - \tilde{\theta}_{\mu \rightarrow i})}.$$  \hspace{1cm} (69)$$

We call the BP algorithm for the hierarchical Bayes model the hierarchical BP (HBP) algorithm; its pseudocode is summarized in Algorithm 3.

**Algorithm 3 HBP for group testing**

**Input:** $$Y \sim P(Y|X^{(0)})$$ and $$F$$

**Output:** $$\theta \in [0, 1]^N$$

1: Initialize:

1.1: \{$$g_{i \rightarrow i}^{(0)}$$\} ← initial value from $$[0, 1]^{N \times M}$$

1.2: \{$$G_{i \rightarrow i}^{(0)}$$\} ← initial value from $$[0, 1]^{M \times N}$$

1.3: $$\pi^{(0)}$$ ← initial value from $$[0, 1]^N$$

1.4: $$\tilde{\rho}^{(0)}$$ ← initial value from $$[0, 1]^N$$

3: $$U \leftarrow uY + (1 - u)(1_M - Y)$$  \hspace{1cm} $$W \leftarrow wY + (1 - w)(1_M - Y)$$

4: for $$t = 1, \ldots, T$$ do

5: for all combinations of ($$\mu, i$$) such that $$F_{\mu i} = 1$$ do

6: $$Z_{i \rightarrow i}^{(t)} \leftarrow U_{\mu} \left[2 - \prod_{\nu \in G(i) \mu} \left(1 - \theta_{\nu \rightarrow \mu}^{(t-1)}\right)\right] + W_{\mu} \prod_{j \in M(\mu) \setminus i} \left(1 - \tilde{\theta}_{j \rightarrow \mu}^{(t-1)}\right)$$

7: $$Z_{i \rightarrow i}^{(t)} \leftarrow P^{(t-1)}_{i} \prod_{\nu \in G(i) \mu} \theta_{\nu \rightarrow i}^{(t-1)} + (1 - P^{(t-1)}_{i}) \prod_{\nu \in G(i) \mu} (1 - \theta_{\nu \rightarrow i}^{(t-1)})$$

8: $$\tilde{\theta}_{i \rightarrow i}^{(t)} \leftarrow U_{\mu} \frac{Z_{i \rightarrow i}^{(t-1)}}{Z_{i \rightarrow i}^{(t-1)}}$$

9: $$\tilde{\theta}_{i \rightarrow i}^{(t)} \leftarrow U_{\mu} \frac{Z_{i \rightarrow i}^{(t-1)}}{Z_{i \rightarrow i}^{(t-1)}}$$

10: end for

11: for $$i = 1, \ldots, N$$ do

12: $$\pi_{i}^{(t)} \leftarrow \prod_{\mu \in G(i)} \theta_{\mu \rightarrow i}^{(t-1)} + \prod_{\mu \in G(i)} (1 - \theta_{\mu \rightarrow i}^{(t-1)})$$

13: $$\tilde{\pi}_{i}^{(t)} \leftarrow \int_{0}^{1} d\rho \rho^{(t)} \prod_{j \in I_i} \left(\rho_{j}^{(t)} + (1 - \rho)(1 - \pi_{j}^{(t)})\right)$$

14: $$\tilde{\rho}_{i}^{(t)} \leftarrow \int_{0}^{1} d\rho \rho^{(t)} \prod_{j \in I_i} \left(\rho_{j}^{(t)} + (1 - \rho)(1 - \pi_{j}^{(t)})\right)$$

15: end for

16: end for

17: for $$i = 1, \ldots, N$$ do

18: $$\hat{\theta}_{i} \leftarrow \tilde{\rho}_{i}^{(T)} \prod_{\mu \in G(i)} \theta_{\mu \rightarrow i}^{(T)} + (1 - \tilde{\rho}_{i}^{(T)}) \prod_{\mu \in G(i)} (1 - \theta_{\mu \rightarrow i}^{(T)})$$

19: end for
Fig. 11. Comparison of the BP+EM algorithm and HBP algorithm for (a) TP and (b) FP at $N = 1000$, $M = 500$, $N_G = 10$, $p_{TP} = 0.95$, and $p_{FP} = 0.05$. The horizontal line in (a) indicates $TP = p_{TP}$.

Fig. 11 shows the comparison between the BP+EM algorithm and HBP algorithm for (a) TP and (b) FP obtained by the MAP estimator at $N = 1000$, $M = 500$, $N_G = 10$, $p_{TP} = 0.95$, and $p_{FP} = 0.05$. Here, $p_{TP}$ and $p_{FP}$ are fixed at their true values. As shown in this figure, TP and FP by the HBP algorithm has almost the same values as those of the BP+EM algorithm. Further, the hyperhyperparameter in the beta distribution has a small influence on the TP and FP.

A. Comparison of BP+EM and HBP for finite system size

In this section, we discuss the difference between the BP+EM algorithm and HBP algorithm as estimation methods for prevalence. First, we consider the $N \to \infty$ limit, where the saddle point method can be applied to the integral of $\rho$ in eq.(63).

After the calculation shown in Appendix B, we obtain

$$\hat{\rho}_i = \rho_i^*, \quad (70)$$

where $\rho_i^*$ satisfies

$$\rho_i^* = \frac{1}{N - 1} \sum_{j \neq i} \tilde{\theta}_j(\rho_i^*), \quad (71)$$

$$\tilde{\theta}_j(\rho) = \frac{\rho \prod_{\mu \in G(j)} \tilde{\theta}_{\mu \to j} (1 - \rho) \prod_{j \neq i} (1 - \tilde{\theta}_{\mu \to j})}{\rho \prod_{j \neq i} \tilde{\theta}_{\mu \to j} + (1 - \rho) \prod_{j \neq i} (1 - \tilde{\theta}_{\mu \to j})}. \quad (72)$$

We note that eq.(71) does not depend on the hyperprior, and the prevalence is estimated as $\hat{\rho} = \frac{1}{N} \sum_{i=1}^{N} \hat{\rho}_i$. Comparing the estimated prevalence in the HBP algorithm with that of the BP+EM algorithm eq.(43) shows that the difference between the two estimators is negligible at $N \to \infty$. Therefore, we compared BP+EM and HBP focusing on the following points.

(I) Accuracy as an estimator of the prevalence for finite $N$

As mentioned previously, the difference between the two estimators is negligible at $N \to \infty$. However, the two estimators do not coincide with each other at finite $N$. We quantify the accuracy of the estimator at finite $N$ using bias defined by

$$bias = E_{Y,F}[|\hat{\rho}(Y,F) - \rho|], \quad (73)$$

where $\hat{\rho}(Y,F)$ denotes the estimates under given $Y$ and $F$. An accurate estimator results in a low bias value.

(II) Computational time

Although the mathematical forms of the estimator of prevalence are similar, the update rules in BP+EM algorithm and HBP algorithm differ from each other. The BP+EM algorithm consists of a double loop, namely the E-step for BP and the M-step for updating $\hat{\rho}$. In the HBP algorithm, the messages and the estimator are updated at the same time. The difference between these update rules influences the computational time.
Fig. 12 (a) and Fig. 13 (a) show $N$-dependence of the bias for the BP+EM and HBP algorithm at $\alpha = 0.5$, $\rho = 0.05$, $p_{TP} = 0.99$, and $p_{FP} = 0.01$ (Fig. 12), and $\alpha = 0.5$, $\rho = 0.05$, $p_{TP} = 0.95$, $p_{FP} = 0.05$ (Fig. 13). In these algorithms, the same 100-realization of $X^0$, $F$, and $Y$ were used for comparing these methods. The mean of the beta distribution is given by $a/(a+b)$; hence, the mean of the hyperprior at $a = 0.5$, $b = 0.95$ matches the true value of $\rho$. BP+EM and HBP at $\alpha = 0.5$, $b = 0.95$ show almost the same dependency on $N$ in bias. When $a$ and $b$ are not chosen to match the mean of the hyperprior, bias becomes large in finite $N$, but the difference in bias vanishes as $N \to \infty$.

Fig. 12 (b) and Fig. 13 (b) show $N$-dependence of the computation time, where we fixed our experimental environment to use a single 3.5 GHz Intel Core i7 CPU. The computational time of the HBP algorithm is less than that of the BP+EM algorithm, and this priority stands out for the high-noise case, which is obvious from the comparison between Fig. 12 (b) and Fig. 13 (b).

From these results, we consider that the choice of using BP+EM or HBP depends on the purpose. When precise estimation of prevalence is required and one has no conception of the appropriate hyperprior in small system size, BP+EM algorithm should be used. For quick identification of the infected patients, in particular for large system size, the HBP algorithm is well suited to the demand.
VII. SUMMARY AND DISCUSSION

In this study, we investigated the group testing problem where the test possess finite false probabilities. We introduced the BP algorithm to infer the infected patients under the Bayesian inference settings. The performance of the BP algorithm, in particular for the TP rate, was improved by considering the credible interval of the point estimate assigned to each patient. Our approach used bootstrap distribution to estimate the interval. The unknown parameters in the model, in particular prevalence, can be estimated using the EM method and hierarchical Bayes modeling. We compared these methods and formulated a guide for practical usage.

We concentrated on the pooling matrix randomly constructed under the column-wise and row-wise constraint specified by \( N_G \) and \( N_O \). The adaptive procedure of group testing was also examined, where the pooling for the next stage was sequentially designed by taking into account the output of the test in the previous stage \( \text{[26–28]} \). Extension of our BP and HBP algorithm to the adaptive setting is a promising way to explore more efficient pooling and test scheduling.

The MATLAB code used in this study is distributed on GitHub \( \text{https://github.com/AyakaSakata/GroupTesting} \).

VIII. COMMENTS AND NOTES

† The prevalence of the population does not necessarily match an individual’s infection probability; hence, the prior distribution is an assumption. We consider that this form of prior information is appropriate for the estimation of the prevalence in the sense that prevalence of the population generated by \( \text{Bernoulli}(\rho) \) converges to \( \rho \) for sufficiently large \( N \).

When the infection probability of each patient can be guessed from symptoms before performing the test and has different values for each patient, one can apply the information into the prior as \( \rho_i \). The BP algorithm for this case is obtained from HBP method by fixing the value of \( \tilde{\rho}_i \) at \( \rho_i \).

‡ We introduce a damping factor \( d \in (0, 1] \) for the stabilization of the algorithm as

\[
\tilde{\theta}_{\mu-i}^{(t)} \leftarrow d\tilde{\theta}_{\mu-i}^{(t)} + (1 - d)\tilde{\theta}_{\mu-i}^{(t-1)} \quad (74)
\]

\[
\theta_{i-\mu}^{(t)} \leftarrow d\theta_{i-\mu}^{(t)} + (1 - d)\theta_{i-\mu}^{(t-1)} \quad (75)
\]

For HBP, we introduce additional damping as

\[
\pi_i^{(t)} \leftarrow d\pi_i^{(t)} + (1 - d)\pi_i^{(t-1)} \quad (76)
\]

\[
\tilde{\rho}_i^{(t)} \leftarrow d\tilde{\rho}_i^{(t)} + (1 - d)\tilde{\rho}_i^{(t-1)} \quad (77)
\]

In all the numerical simulations performed in this study, we set \( d = 0.1 \) conservatively, but this choice extends the time for convergence. To achieve faster and stable convergence, an adaptive setting of the damping factor for group testing is worth studying \( \text{[29]} \).

§ Here, \( \mathbf{1}_M \) denotes an \( M \)-dimensional vector whose components take the value 1.

¶ For the construction of the confidence interval for Bayesian point estimate, the parametric bootstrap method is another approach \( \text{[30, 31]} \), where the bootstrap samples are generated according to the posterior distribution with the point estimate.

∥ Another construction method of the credible interval uses the bootstrap percentile as

\[
\tau \in [G_B^{-1}(0.025), G_B^{-1}(0.975)] \quad (78)
\]

where \( G_B^{-1}(\alpha) \) is the \( \alpha \)-percentile of the bootstrap distribution. We tried this interval for determining the infected patients. The obtained TP is comparable with the normal theory, but FP tends to be large compared with the interval determined by the normal theory.

∗∗ The bootstrap sample contains the same row vector of \( \mathbf{F} \) with high probability. We omit the overlapped rows to stabilize the BP algorithm.

†† We solve eq.\( \text{[51]} \) and eq.\( \text{[52]} \) by the Newton method in the M-step; however, the optimization at each M-step induces algorithmic instability. Hence, we update \( \hat{\rho}_{\text{TP}} \) and \( \hat{\rho}_{\text{FP}} \) for only one step following the Newton method.
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Appendix A: Derivation of maximum-(approximated) likelihood estimator

The derivative of $S$ with respect to $\rho$, $p_{TP}$, and $p_{FP}$ is given by

$$\frac{\partial}{\partial \rho} S = \sum_i \frac{\partial}{\partial \rho} \ln Z_i = \sum_i \prod_{\mu \in G(i)} \tilde{\theta}_{\mu-i} - \prod_{\mu \in G(i)} (1 - \hat{\theta}_{\mu-i}) \frac{\sum_i \theta_i}{\rho} - \frac{\sum_i (1 - \theta_i)}{1 - \rho} (A1)$$

$$\frac{\partial}{\partial p_{TP}} S = \sum_{\mu} \frac{\partial}{\partial p_{TP}} \ln Z_{\mu} = \sum_{\mu} \frac{Y_{\mu}(1 - \tilde{q}_{\mu}) - (1 - Y_{\mu})(1 - \tilde{q}_{\mu})}{Z_{\mu}} = \frac{\sum_{\mu} (I(Y_{\mu} = 1, T_{\mu}(X) = 1))_{\mu}}{p_{TP}} - \frac{\sum_{\mu} (I(Y_{\mu} = 0, T_{\mu}(X) = 1))_{\mu}}{1 - p_{TP}} (A2)$$

$$\frac{\partial}{\partial p_{FP}} S = \sum_{\mu} \frac{\partial}{\partial p_{FP}} \ln Z_{\mu} = \sum_{\mu} \frac{Y_{\mu}\tilde{q}_{\mu} - (1 - Y_{\mu})\tilde{q}_{\mu}}{Z_{\mu}} = \frac{\sum_{\mu} (I(Y_{\mu} = 1, T_{\mu}(X) = 0))_{\mu}}{p_{FP}} - \frac{\sum_{\mu} (I(Y_{\mu} = 0, T_{\mu}(X) = 0))_{\mu}}{1 - p_{FP}} \times (A3),$$

respectively. Solving eqs. (A1)–(A3) under the condition that they are zero, we obtain the extremization conditions in eqs. (43)–(45).

Appendix B: Estimated value of the prevalence in hierarchical Bayes model at $N \to \infty$

Substituting eq.(67) into eq.(63), we obtain the following expression.

$$\tilde{p}_i = \frac{\int d\rho \rho \phi(\rho) \exp \left[ N \left\{ \frac{1}{N} \sum_{j \neq i} \log \left\{ \rho \pi_i + (1 - \rho)(1 - \pi_i) \right\} \right\} \right]}{\int d\rho \phi(\rho) \exp \left[ N \left\{ \frac{1}{N} \sum_{j \neq i} \log \left\{ \rho \pi_i + (1 - \rho)(1 - \pi_i) \right\} \right\} \right]} (B1)$$

Applying the saddle point method, we obtain

$$\tilde{p}_i = \rho_i^*, (B2)$$

where $\rho_i^*$ satisfies

$$\frac{1}{N} \sum_{j \neq i} \frac{\pi_i - (1 - \pi_i)}{\rho_i^* \pi_i + (1 - \rho_i^*)(1 - \pi_i)} = 0. (B3)$$
From eqs. (65) and (72), eq. (B3) is transformed as

\[
\frac{1}{N} \sum_{j \neq i} \tilde{\theta}_j (\rho^*_{i,j}) = \frac{1}{N} \sum_{j \neq i} \frac{1 - \tilde{\theta}_j (\rho^*_{i,j})}{1 - \rho^*_{i,j}},
\]

and we obtain eq. (71) by transforming eq. (B4) with respect to \( \rho^*_{i,j} \).