

Web supplementary materials for “Informative Retesting”

For each reference to the web supplementary materials in the paper, we provide the materials here or references to where they can be found.

Section 3: The R programs are available on the Journal’s supplementary documents website and at www.chrisbilder.com/grouptesting.

Section 4: The technical report

Bilder, C., Black, M., and Tebbs, J. (2009), “Expected number of tests for halving and matrix pooling in heterogeneous populations,” Technical Report, University of Nebraska-Lincoln, Department of Statistics

is included here on pages 2–9.

Expected number of tests for halving and matrix pooling in heterogeneous populations

Technical report prepared by

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1. INTRODUCTION

Most expected number of test derivations for retesting procedures make the assumption that each individual has the same probability of positivity. In a heterogeneous setting where individuals have different probabilities, new derivations are needed. The purpose of this document is to provide these derivations for the matrix pooling and halving retesting protocols. The results here are extensions to those in Sections 3 and 4 of Kim et al. (2007).

2. MATRIX POOLING

In the “SA1” testing protocol first proposed in Phatarfod and Sudbury (1994), specimens are arranged into a matrix-like grid. Specimens are pooled within each row and column separately. Individuals at the intersections of positive rows and positive columns are possible positives. These individuals are further tested individually to complete the decoding. Other matrix pooling testing protocols are discussed in Kim et al. (2007), but we will focus on this one only.

Let T be a random variable denoting the number of tests needed to decode one matrix of specimens. We can write the expected number of tests then as $E(T) = I + J + A$ where I is the number of rows, J is the number of columns, and A is the number of retests performed at the intersection of positive rows and columns. Note that $A = \sum_{i=1}^I \sum_{j=1}^J P(R_i = 1 \cap C_j = 1)$ where R_i and C_j are binary random variables denoting whether or not a row i and column j are positive, respectively (1 = positive, 0 = negative). Now,

$$\begin{aligned} P(R_i = 1 \cap C_j = 1) &= 1 - P(R_i = 0 \cup C_j = 0) \\ &= 1 - [P(R_i = 0) + P(C_j = 0) - P(R_i = 0 \cap C_j = 0)]. \end{aligned} \quad (1)$$

When there is no testing error, (1) becomes

$$P(R_i = 1 \cap C_j = 1) = 1 - \left[\prod_{j'=1}^J (1 - p_{ij'}) + \prod_{i'=1}^I (1 - p_{i'j}) - \frac{\left[\prod_{j'=1}^J (1 - p_{ij'}) \right] \left[\prod_{i'=1}^I (1 - p_{i'j}) \right]}{(1 - p_{ij})} \right] \quad (2)$$

where p_{ij} is the probability that the individual in row i and column j is positive. Note that the $(1 - p_{ij})$ divisor in (2) occurs because it is present twice in the numerator. When there is testing error, let \tilde{R}_i and \tilde{C}_j denote the true values of R_i and C_j , respectively, and let S_e and S_p denote the sensitivity and specificity, respectively, so that $S_e = P(R_i = 1 | \tilde{R}_i = 1)$ and $S_p = P(R_i = 0 | \tilde{R}_i = 0)$ (similarly for the columns). Expressions in (1) become the following:

$$\begin{aligned} P(R_i = 0) &= P(R_i = 0 \cap \tilde{R}_i = 0) + P(R_i = 0 \cap \tilde{R}_i = 1) \\ &= P(R_i = 0 | \tilde{R}_i = 0)P(\tilde{R}_i = 0) + P(R_i = 0 | \tilde{R}_i = 1)P(\tilde{R}_i = 1) \\ &= S_p \prod_{j'=1}^J (1 - p_{ij'}) + (1 - S_e) \left[1 - \prod_{j'=1}^J (1 - p_{ij'}) \right] \end{aligned}$$

$$\begin{aligned} P(C_j = 0) &= P(C_j = 0 \cap \tilde{C}_j = 0) + P(C_j = 0 \cap \tilde{C}_j = 1) \\ &= P(C_j = 0 | \tilde{C}_j = 0)P(\tilde{C}_j = 0) + P(C_j = 0 | \tilde{C}_j = 1)P(\tilde{C}_j = 1) \\ &= S_p \prod_{i'=1}^I (1 - p_{i'j}) + (1 - S_e) \left[1 - \prod_{i'=1}^I (1 - p_{i'j}) \right] \end{aligned}$$

$$\begin{aligned} P(R_i = 0 \cap C_j = 0) &= P(R_i = 0 \cap C_j = 0 \cap \tilde{R}_i = 0 \cap \tilde{C}_j = 0) \\ &\quad + P(R_i = 0 \cap C_j = 0 \cap \tilde{R}_i = 0 \cap \tilde{C}_j = 1) \\ &\quad + P(R_i = 0 \cap C_j = 0 \cap \tilde{R}_i = 1 \cap \tilde{C}_j = 0) \\ &\quad + P(R_i = 0 \cap C_j = 0 \cap \tilde{R}_i = 1 \cap \tilde{C}_j = 1) \\ &= P(R_i = 0 \cap C_j = 0 | \tilde{R}_i = 0 \cap \tilde{C}_j = 0) \times P(\tilde{R}_i = 0 \cap \tilde{C}_j = 0) \\ &\quad + P(R_i = 0 \cap C_j = 0 | \tilde{R}_i = 0 \cap \tilde{C}_j = 1) \times P(\tilde{R}_i = 0 \cap \tilde{C}_j = 1) \\ &\quad + P(R_i = 0 \cap C_j = 0 | \tilde{R}_i = 1 \cap \tilde{C}_j = 0) \times P(\tilde{R}_i = 1 \cap \tilde{C}_j = 0) \\ &\quad + P(R_i = 0 \cap C_j = 0 | \tilde{R}_i = 1 \cap \tilde{C}_j = 1) \times P(\tilde{R}_i = 1 \cap \tilde{C}_j = 1) \end{aligned}$$

$$\begin{aligned}
&= P(R_i = 0 \mid \tilde{R}_i = 0) \times P(C_j = 0 \mid \tilde{C}_j = 0) \times \frac{\left[\prod_{j'=1}^J (1 - p_{ij'}) \right] \left[\prod_{i'=1}^I (1 - p_{i'j}) \right]}{(1 - p_{ij})} \\
&\quad + P(R_i = 0 \mid \tilde{R}_i = 0) \times P(C_j = 0 \mid \tilde{C}_j = 1) \times \left[\prod_{j'=1}^J (1 - p_{ij'}) \right] \left[1 - \prod_{i'=1, i' \neq i}^I (1 - p_{i'j}) \right] \\
&\quad + P(R_i = 0 \mid \tilde{R}_i = 1) \times P(C_j = 0 \mid \tilde{C}_j = 0) \times \left[\prod_{i'=1}^I (1 - p_{i'j}) \right] \left[1 - \prod_{j'=1, j' \neq j}^J (1 - p_{ij'}) \right] \\
&\quad + P(R_i = 0 \mid \tilde{R}_i = 1) \times P(C_j = 0 \mid \tilde{C}_j = 1) \\
&\quad \times \left\{ 1 - \left[\prod_{i'=1}^I (1 - p_{i'j}) + \prod_{j'=1}^J (1 - p_{ij'}) - \frac{\left[\prod_{j'=1}^J (1 - p_{ij'}) \right] \left[\prod_{i'=1}^I (1 - p_{i'j}) \right]}{(1 - p_{ij})} \right] \right\} \\
&= S_p^2 \frac{\left[\prod_{j'=1}^J (1 - p_{ij'}) \right] \left[\prod_{i'=1}^I (1 - p_{i'j}) \right]}{(1 - p_{ij})} + S_p (1 - S_e) \left[\prod_{j'=1}^J (1 - p_{ij'}) \right] \left[1 - \prod_{i'=1, i' \neq i}^I (1 - p_{i'j}) \right] \\
&\quad + S_p (1 - S_e) \left[\prod_{i'=1}^I (1 - p_{i'j}) \right] \left[1 - \prod_{j'=1, j' \neq j}^J (1 - p_{ij'}) \right] \\
&\quad + (1 - S_e)^2 \times \left\{ 1 - \left[\prod_{i'=1}^I (1 - p_{i'j}) + \prod_{j'=1}^J (1 - p_{ij'}) - \frac{\left[\prod_{j'=1}^J (1 - p_{ij'}) \right] \left[\prod_{i'=1}^I (1 - p_{i'j}) \right]}{(1 - p_{ij})} \right] \right\}
\end{aligned}$$

where we use the standard assumption that test outcomes are conditionally independent given the true outcomes (see Litvak et al. 1994 for discussion). Putting the above expressions into (1) leads to the desired result.

3. HALVING

The halving testing protocol involves successively splitting positive groups into two equal sized halves. This halving of positive groups continues until all groups test negative or until individual testing occurs. For example, 3-stage halving for a group of size $I = 16$ begins by testing the whole group. If this group tests positive, the second stage involves splitting it into two groups of size 8. If either of these groups test positive, a third stage occurs where each individual is tested rather than halving again. A 4-stage halving protocol would continue with halving into groups of size 4 before individual testing.

Let $G_{s,j} = 1(0)$ be a positive (negative) test result for the j^{th} ordered sub-group of the s^{th} stage in the group of interest for $j = 1, \dots, 2^{s-1}$ and $s = 1, \dots, S$. In the last example, $G_{1,1}$ represents the test result of the initial group of size 16, and $G_{2,1}$ represents the test result for the first group of size 8 halved from an initial positive group. In a 3-stage testing example, we can write the expected number of tests as

$$E(T) = 1 + 2P(G_{1,1} = 1) + I_{2,1}P(G_{1,1} = 1 \cap G_{2,1} = 1) + I_{2,2}P(G_{1,1} = 1 \cap G_{2,2} = 1)$$

where T is the number of tests and $I_{s,j}$ is the number of items remaining in the j^{th} ordered sub-group at stage s . Adding a fourth stage leads to an expected number of tests of

$$\begin{aligned} E(T) = & 1 + 2P(G_{1,1} = 1) + 2P(G_{1,1} = 1 \cap G_{2,1} = 1) + 2P(G_{1,1} = 1 \cap G_{2,2} = 1) + \\ & I_{3,1}P(G_{1,1} = 1 \cap G_{2,1} = 1 \cap G_{3,1} = 1) + I_{3,2}P(G_{1,1} = 1 \cap G_{2,1} = 1 \cap G_{3,2} = 1) + \\ & I_{3,3}P(G_{1,1} = 1 \cap G_{2,2} = 1 \cap G_{3,3} = 1) + I_{3,4}P(G_{1,1} = 1 \cap G_{2,2} = 1 \cap G_{3,4} = 1). \end{aligned}$$

These results can be generalized to

$$E(T) = 1 + 2 \sum_{s=1}^{S-2} \sum_{j=1}^{2^{s-1}} P \left(\bigcap_{\{(t,k):G_{s,j}=1\}} \{G_{t,k} = 1\} \right) + \sum_{j=1}^{2^{S-2}} I_{S-1,j} P \left(\bigcap_{\{(t,k):G_{S-1,j}=1\}} \{G_{t,k} = 1\} \right) \quad (3)$$

for an appropriate number of stages S given the initial group size.

In situations where an odd-sized group is being “halved”, final stage group sizes $I_{S,j}$ can be set equal to 0. For example, consider a 4-stage halving with $I = 7$ tested in the following stages:

- 1) Test a group of size 7. If positive, go to stage 2.
- 2) Test in groups of size 4 and 3. If a group tests positive, go to stage 3 with those individuals.
- 3) For the group of size 4, split it into two groups of size 2. If a group tests positive, go to stage 4 with those individuals. For the group of size 3, split it into one group of size 2 and one group of size 1. If the group of size 2 tests positive, go to stage 4.

4) Individually test items in any group that tested positive.

The expected number of tests are

$$\begin{aligned} E(T) = & 1 + 2P(G_{1,1} = 1) + 2P(G_{1,1} = 1 \cap G_{2,1} = 1) + 2P(G_{1,1} = 1 \cap G_{2,2} = 1) + \\ & 2P(G_{1,1} = 1 \cap G_{2,1} = 1 \cap G_{3,1} = 1) + 2P(G_{1,1} = 1 \cap G_{2,1} = 1 \cap G_{3,2} = 1) + \\ & 2P(G_{1,1} = 1 \cap G_{2,2} = 1 \cap G_{3,3} = 1) + 0P(G_{1,1} = 1 \cap G_{2,2} = 1 \cap G_{3,4} = 1) \end{aligned}$$

where we have assumed $G_{2,2}$ was the group test outcome for three individuals and $G_{3,3}$ was the group test outcome for two individuals. Note that the group for $G_{3,4}$ could not actually be tested here, but its corresponding probability is removed from the above expression due to its 0 coefficient.

Each of the probabilities in the above expressions is found by taking into account the true group test outcomes. Let $\tilde{G}_{s,j}$ be the true response for $G_{s,j}$, and let S_e and S_p denote the sensitivity and specificity, respectively, so that $S_e = P(G_{s,j} = 1 | \tilde{G}_{s,j} = 1)$ and $S_p = P(G_{s,j} = 0 | \tilde{G}_{s,j} = 0)$. For the first group,

$$\begin{aligned} P(G_{1,1} = 1) &= P(G_{1,1} = 1 \cap \tilde{G}_{1,1} = 0) + P(G_{1,1} = 1 \cap \tilde{G}_{1,1} = 1) \\ &= P(G_{1,1} = 1 | \tilde{G}_{1,1} = 0)P(\tilde{G}_{1,1} = 0) + P(G_{1,1} = 1 | \tilde{G}_{1,1} = 1)P(\tilde{G}_{1,1} = 1) \\ &= (1 - S_p) \left[\prod_{i=1}^I (1 - p_i) \right] + S_e \left[1 - \prod_{i=1}^I (1 - p_i) \right]. \end{aligned}$$

Probabilities for groups from later stages become more complicated to find because past stages need to be taken into account. For example, the probability of positivity for the first stage 2 group after the initial group tests positive is

$$\begin{aligned} P(G_{1,1} = 1 \cap G_{2,1} = 1) &= P(G_{1,1} = 1 \cap G_{2,1} = 1 \cap \tilde{G}_{1,1} = 0 \cap \tilde{G}_{2,1} = 0) + \\ &\quad P(G_{1,1} = 1 \cap G_{2,1} = 1 \cap \tilde{G}_{1,1} = 1 \cap \tilde{G}_{2,1} = 0) + \\ &\quad P(G_{1,1} = 1 \cap G_{2,1} = 1 \cap \tilde{G}_{1,1} = 1 \cap \tilde{G}_{2,1} = 1), \end{aligned}$$

which takes into account the three ways that $G_{1,1} = 1 \cap G_{2,1} = 1$ can occur with respect to the true responses. Continuing, we obtain

$$\begin{aligned} P(G_{1,1} = 1 \cap G_{2,1} = 1) &= (1 - S_p)^2 \left[\prod_{i=1}^I (1 - p_i) \right] + S_e(1 - S_p) \left[\prod_{i \in G_{2,1}} (1 - p_i) \right] \left[1 - \prod_{i \in G_{2,2}} (1 - p_i) \right] \\ &\quad + S_e^2 \left[1 - \prod_{i \in G_{2,1}} (1 - p_i) \right] \end{aligned}$$

where the $i \in G_{s,j}$ shorthand notation denotes the set of individuals who appear in the j^{th} order group at the s^{th} stage. These results can be generalized for $s > 1$ to

$$P\left(\bigcap_{\{(t,k):G_{s,j}=1\}} \{G_{t,k} = 1\}\right) = (1 - S_p)^s \left[\prod_{i=1}^I (1 - p_i) \right] + \\ \sum_{a=1}^{s-1} S_e^a (1 - S_p)^{s-a} \left[\prod_{i \in G_{a+1,\ell}} (1 - p_i) \right] \left[1 - \prod_{i \in \bar{G}_{a+1,\ell}} (1 - p_i) \right] + \\ S_e^s \left[1 - \prod_{i \in G_{s,j}} (1 - p_i) \right]$$

where $\ell = \lceil j/2^{s-1-a} \rceil$ and $i \in \bar{G}_{s,j}$ denotes the individuals within the parent group of $G_{s,j}$ excluding those in $G_{s,j}$ itself (e.g., $i \in \bar{G}_{3,3}$ denotes all individuals in $G_{3,4}$). Substituting the $P\left(\bigcap_{\{(t,k):G_{s,j}=1\}} \{G_{t,k} = 1\}\right)$ expressions into (3) gives the expected number of tests for halving.

4. CALCULATING THE EXPECTED NUMBER OF TESTS

For both matrix pooling and halving, the expected number of tests are functions of the individual probabilities. The ordering of these individual probabilities can change these expected values. In cases where all of the individual probabilities differ, there could be $I!$ different expected values. Therefore, we recommend computing the expected values over a large number of permutations for these individual probabilities. These expected values can be averaged to compute one estimated expected number of tests not dependent on the individual probability orderings. In cases where only a few individual probabilities differ, all possible permutations for these individual probabilities can be found leading to the expected values. The expected number of tests without order dependency is then the sum of these expected values weighted by the inverse of the number of possible permutations.

REFERENCES

Kim, H., Hudgens, M., Dreyfuss, J., Westreich, D., and Pilcher, C. (2007), “Comparison of group testing algorithms for case identification in the presence of test error,”

Biometrics, 63, 1152-1163.

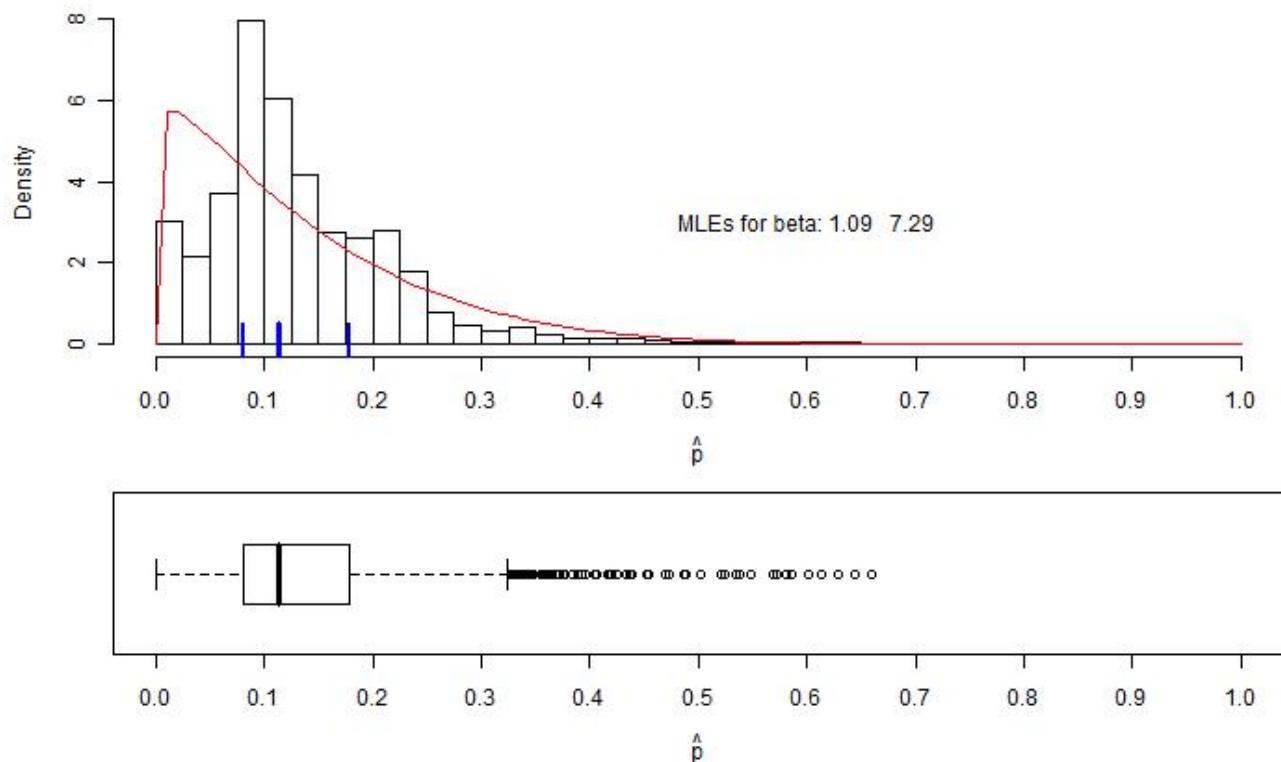
Litvak, E., Tu, X., and Pagano, M. (1994), "Screening for the presence of a disease by pooling sera samples," *Journal of the American Statistical Association*, 89, 424-434.

Phatarfod, R. and Sudbury, A. (1994), "The use of a square array scheme in blood testing," *Statistics in Medicine*, 13, 2337-2343.

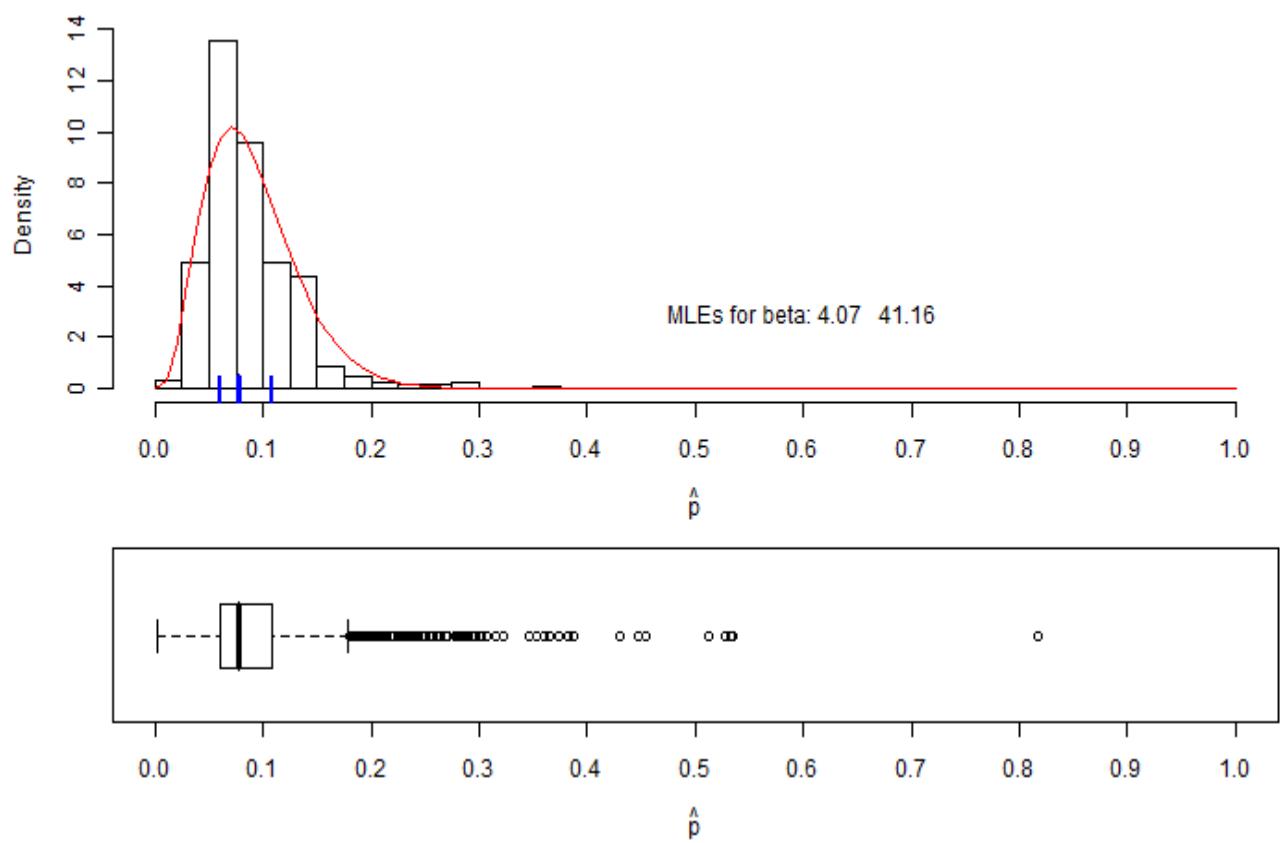
Section 5.1: Pages 11-14 contain histograms and box plots for the estimated individual probabilities.

Fitted beta(α, β) distributions are included on each histogram.

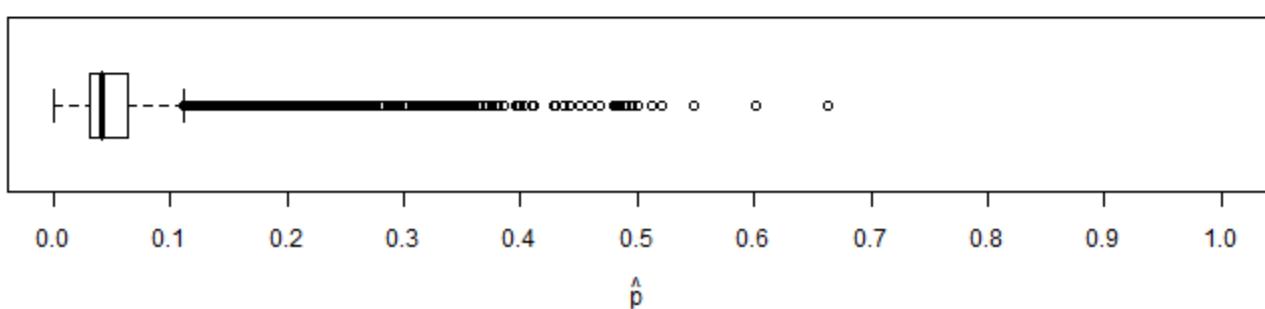
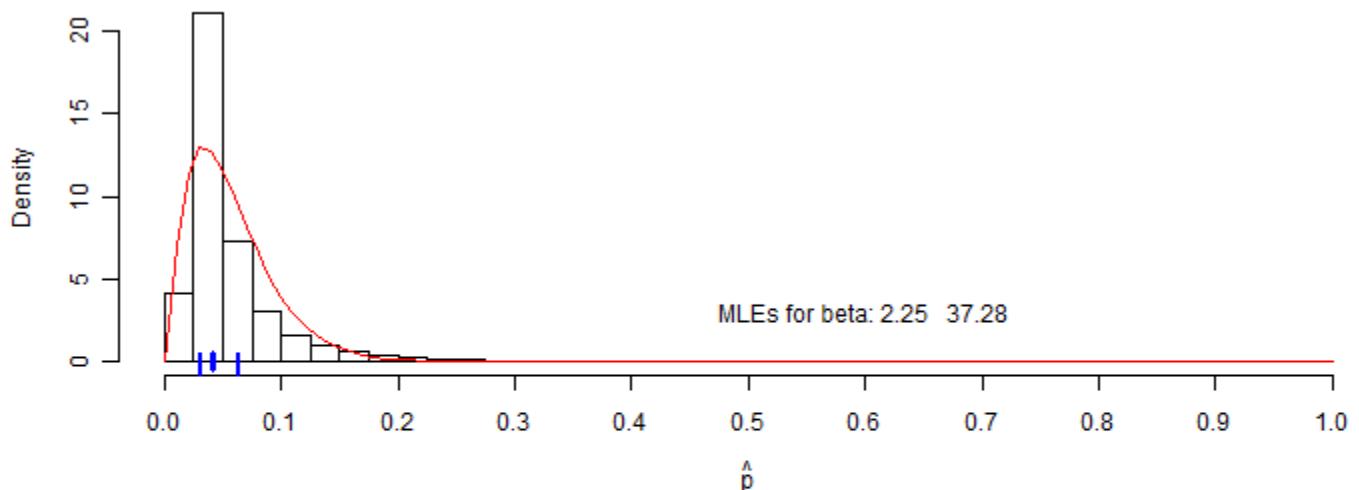
Estimated probabilities for 2005 chlamydia (female, urine)



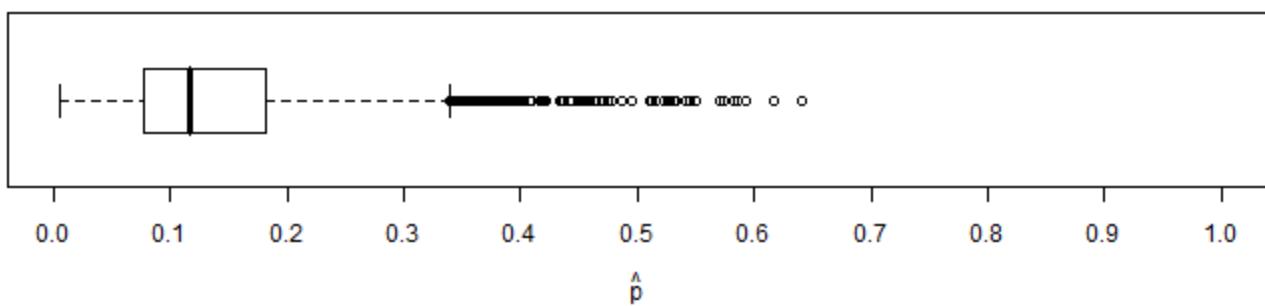
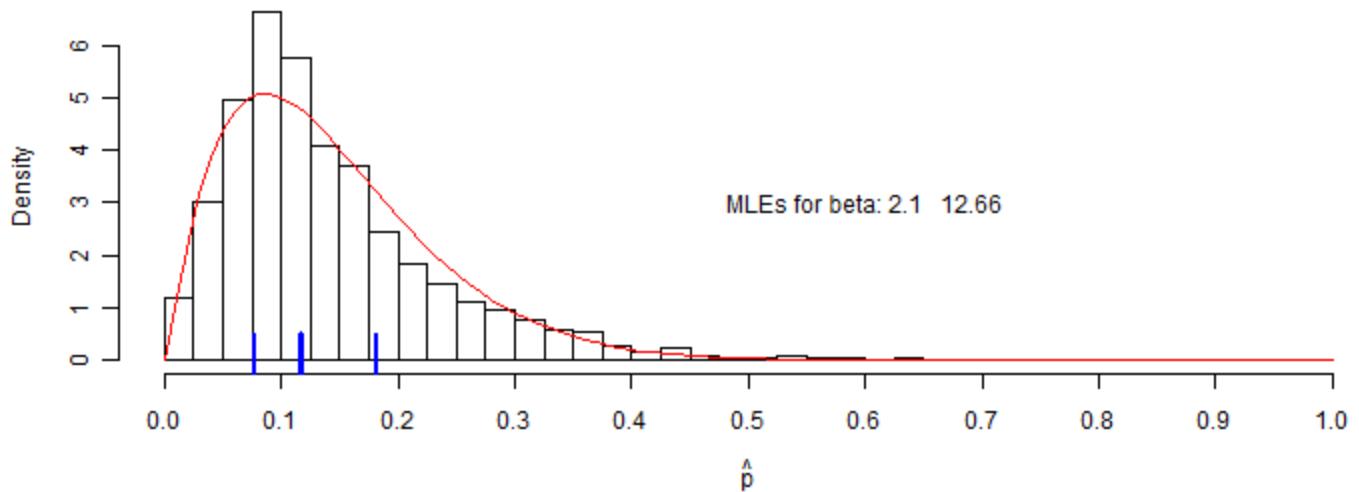
Estimated probabilities for 2005 chlamydia (male, urine)



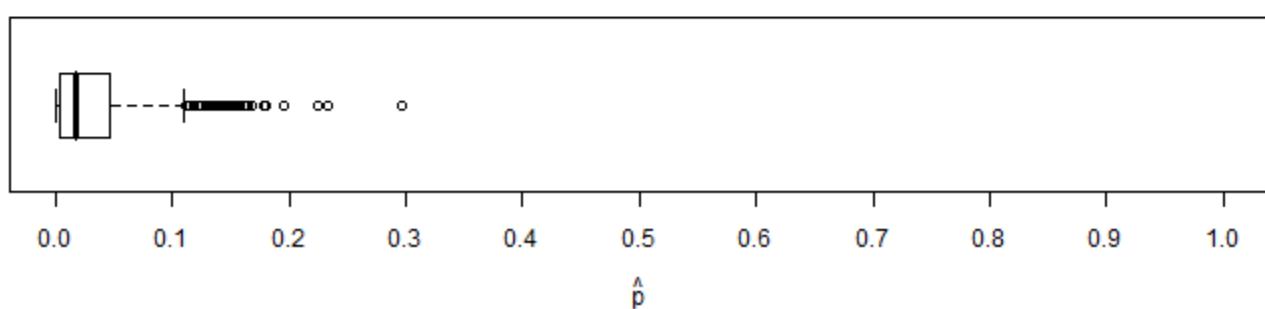
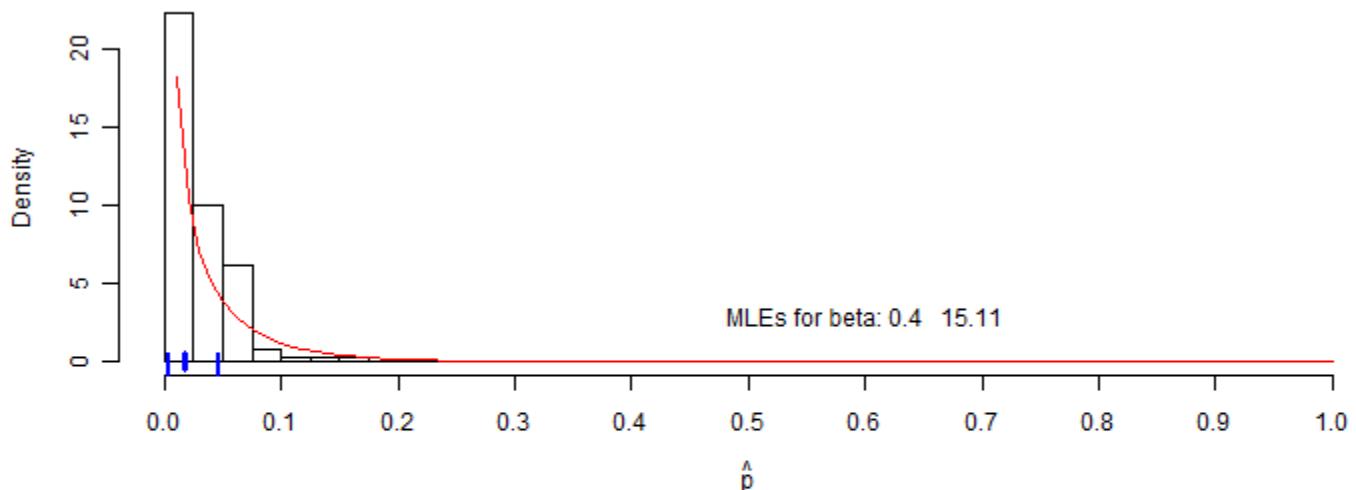
Estimated probabilities for 2005 chlamydia (female, swab)



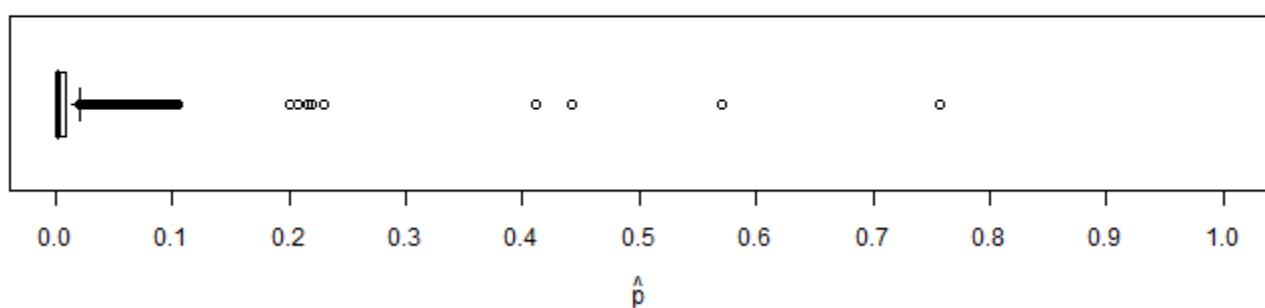
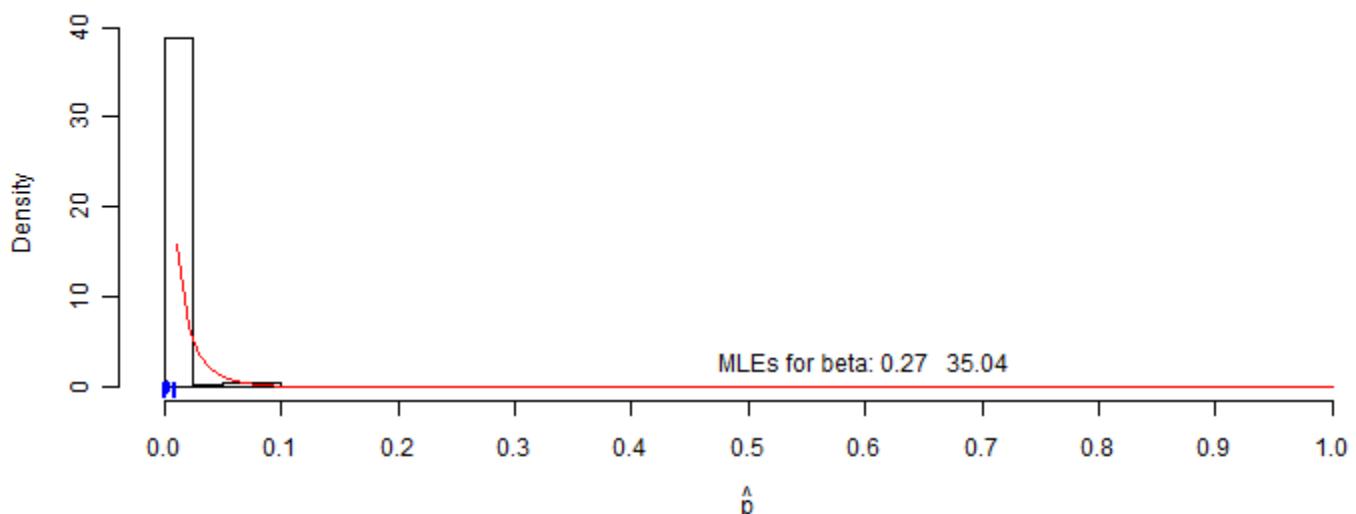
Estimated probabilities for 2005 chlamydia (male, swab)



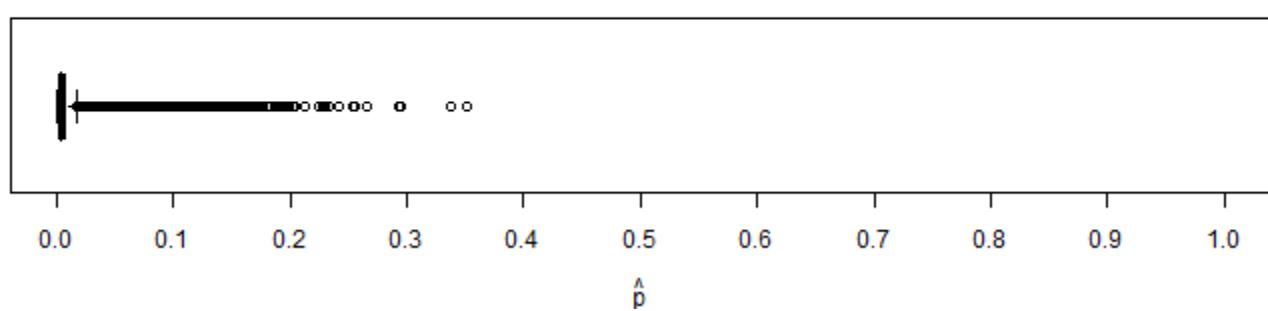
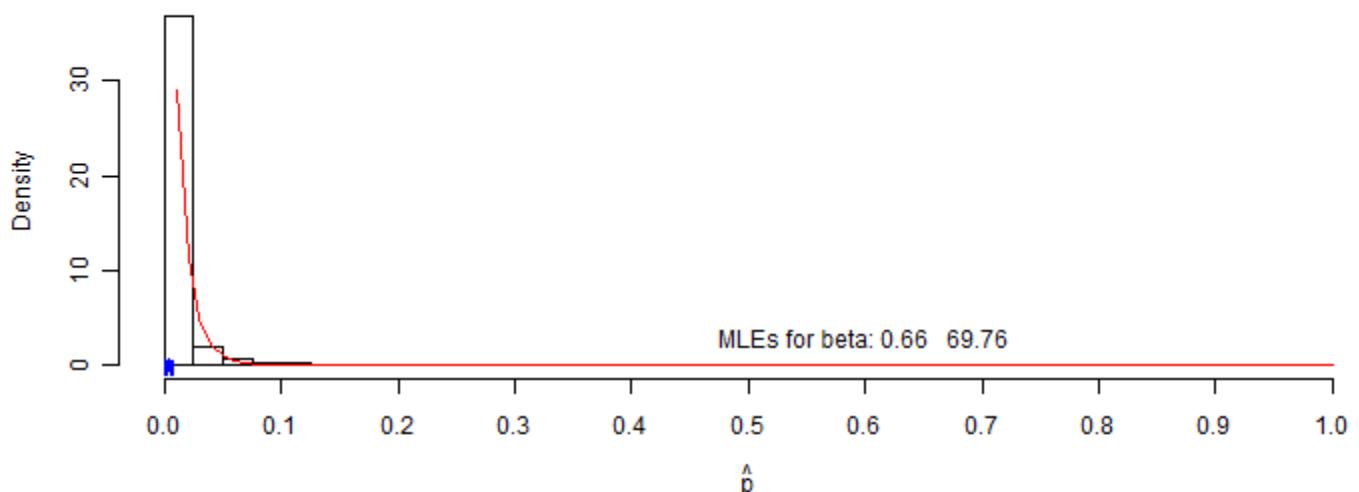
Estimated probabilities for 2005 gonorrhea (female, urine)



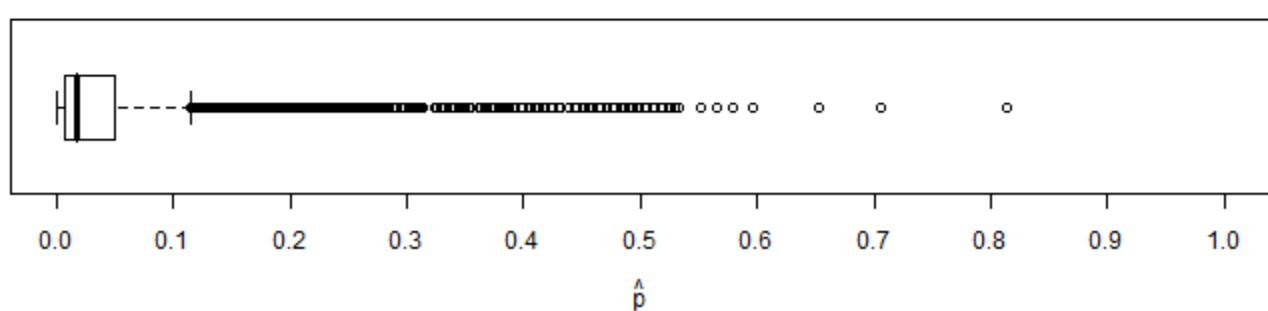
Estimated probabilities for 2005 gonorrhea (male, urine)



Estimated probabilities for 2005 gonorrhea (female, swab)



Estimated probabilities for 2005 gonorrhea (male, swab)



Section 5: Pages 16-19 contain all of the results for groups of size 5, 10, and 20. Note that these pages are 11×17 inch in size.

Disease/specimen/gender	Procedure	Group size	Means over 10 implementations				
			# of tests	PS _e	PS _p	PPPV	PNPV
Chlamydia/urine/female	Dorf	5	1473.6	0.6552	0.9873	0.8539	0.9620
	NIS	5	1355.9	0.6195	0.9926	0.9045	0.9585
	FIS	5	1316.9	0.6305	0.9931	0.9118	0.9596
	1SIS	5	1331.1	0.6221	0.9925	0.9033	0.9588
	2SIS	5	1325.6	0.6154	0.9925	0.9017	0.9581
	3H	5	1342.6	0.5360	0.9968	0.9501	0.9500
	4H	5	Full 4H can not be done with a group of size 5				
	MP	5	1449.5	0.5334	0.9969	0.9514	0.9498
	Dorf	10	1651.3	0.6680	0.9819	0.8068	0.9632
	NIS	10	1343.9	0.5812	0.9870	0.8350	0.9543
Chlamydia/urine/male	FIS	10	1249.8	0.5853	0.9900	0.8686	0.9548
	1SIS	10	1361.7	0.5949	0.9871	0.8397	0.9557
	2SIS	10	1288.6	0.6029	0.9885	0.8552	0.9566
	3H	10	1263.8	0.5371	0.9905	0.8651	0.9499
	4H	10	1174.1	0.4217	0.9967	0.9349	0.9385
	MP	10	1300.1	0.5184	0.9901	0.8560	0.9479
	Dorf	20	2029.3	0.6551	0.9732	0.7344	0.9615
	NIS	20	1473.6	0.5254	0.9832	0.7793	0.9483
	FIS	20	1355.9	0.5158	0.9861	0.8069	0.9474
	1SIS	20	1620.0	0.5772	0.9804	0.7690	0.9536
Chlamydia/swab/female	2SIS	20	1429.4	0.5331	0.9829	0.7791	0.9491
	3H	20	1466.1	0.5327	0.9838	0.7882	0.9491
	4H	20	1101.9	0.3945	0.9937	0.8769	0.9356
	MP	20	1603.8	0.5107	0.9806	0.7488	0.9467
	Dorf	5	2078.7	0.8638	0.9877	0.8645	0.9877
	NIS	5	1926.1	0.8366	0.9900	0.8835	0.9853
	FIS	5	1849.6	0.8494	0.9923	0.9091	0.9864
	1SIS	5	1863.8	0.8434	0.9907	0.8919	0.9859
	2SIS	5	1851.4	0.8422	0.9919	0.9042	0.9858
Chlamydia/swab/male	3H	5	1974.9	0.7960	0.9945	0.9286	0.9817
	4H	5	Full 4H can not be done with a group of size 5				
	MP	5	2144.3	0.8116	0.9956	0.9434	0.9831
	Dorf	10	2521.2	0.8635	0.9746	0.7550	0.9875
	NIS	10	2073.6	0.8335	0.9834	0.8207	0.9849
	FIS	10	1887.4	0.8316	0.9871	0.8540	0.9848
	1SIS	10	2059.7	0.8431	0.9831	0.8192	0.9857
	2SIS	10	1920.9	0.8406	0.9857	0.8427	0.9856
	3H	10	2022.7	0.8084	0.9874	0.8533	0.9827
	4H	10	1944.5	0.7509	0.9938	0.9177	0.9778
Chlamydia/swab/female	MP	10	2040.6	0.8091	0.9861	0.8407	0.9828
	Dorf	20	3165.8	0.8575	0.9609	0.6655	0.9868
	NIS	20	2435.9	0.7872	0.9758	0.7476	0.9806
	FIS	20	2256.1	0.8066	0.9797	0.7830	0.9824
	1SIS	20	2757.2	0.8247	0.9700	0.7139	0.9839
	2SIS	20	2488.3	0.8159	0.9760	0.7553	0.9832
	3H	20	2479.4	0.7997	0.9763	0.7536	0.9817
	4H	20	2008.8	0.7350	0.9874	0.8414	0.9763
	MP	20	2715.9	0.8184	0.9699	0.7120	0.9833
	Dorf	5	8903.5	0.8690	0.9914	0.8606	0.9920
Chlamydia/swab/male	NIS	5	8197.7	0.8529	0.9945	0.9045	0.9910
	FIS	5	7735.1	0.8551	0.9958	0.9254	0.9912
	1SIS	5	7810.8	0.8580	0.9954	0.9195	0.9913
	2SIS	5	7746.0	0.8512	0.9957	0.9233	0.9909
	3H	5	8337.7	0.7989	0.9966	0.9348	0.9878
	4H	5	Full 4H can not be done with a group of size 5				
	MP	5	9637.3	0.8042	0.9982	0.9636	0.9881
	Dorf	10	10192.0	0.8683	0.9844	0.7737	0.9919
	NIS	10	8245.3	0.8318	0.9903	0.8395	0.9897
	FIS	10	7142.9	0.8418	0.9934	0.8861	0.9904
Chlamydia/swab/male	1SIS	10	7787.4	0.8496	0.9909	0.8514	0.9908
	2SIS	10	7217.1	0.8426	0.9929	0.8791	0.9904
	3H	10	7976.7	0.8037	0.9927	0.8702	0.9880
	4H	10	7662.1	0.7423	0.9969	0.9361	0.9844
	MP	10	7835.2	0.8104	0.9935	0.8838	0.9884
	Dorf	20	13653.8	0.8666	0.9744	0.6749	0.9917
	NIS	20	10033.3	0.8180	0.9849	0.7683	0.9888
	FIS	20	8226.0	0.8265	0.9887	0.8169	0.9894
	1SIS	20	10273.1	0.8373	0.9833	0.7544	0.9900
	2SIS	20	8839.1	0.8324	0.9870	0.7963	0.9897
Chlamydia/swab/male	3H	20	9871.5	0.8068	0.9850	0.7675	0.9881
	4H	20	7872.9	0.7460	0.9930	0.8664	0.9846
	MP	20	10129.6	0.7978	0.9839	0.7521	0.9876
	Dorf	5	2661.5	0.8580	0.9786	0.8572	0.9788
	NIS	5	2517.4	0.8270	0.9873	0.9071	0.9745
	FIS	5	2324.4	0.8396	0.9907	0.9313	0.9764
	1SIS	5	2361.4	0.8362	0.9899	0.9251	0.9758
	2SIS	5	2325.1	0.8403	0.9912	0.9347	0.9765
	3H	5	2603.9	0.7880	0.9918	0.9352	0.9690
	4H	5	Full 4H can not be done with a group of size 5				
Chlamydia/swab/male	MP	5	2692.3	0.7906	0.9924	0.9396	0.9694
	Dorf	10	3171.0	0.8531	0.9661	0.7902	0.9778
	NIS	10	2744.4	0.8094	0.9791	0.8528	0.9717
	FIS	10	2291.7	0.8066	0.9856	0.8938	0.9715
	1SIS	10	2674.4	0.8183	0.9781	0.8479	0.9730
	2SIS	10	2383.2	0.8121	0.9844	0.8861	0.9722
	3H	10	2735.4	0.7998	0.9816	0.8667	0.9704
	4H	10	2671.1	0.7286	0.9918	0.9301	0.9607
	MP	10	2854.7	0.8006	0.9778	0.8438	0.9704</td

Disease/specimen/gender	Procedure	Group size	# of tests	Means over 10 implementations				Scale	Gonorrhea in Section 5.1	
				PS _e	PS _p	PPV	PNPV			
Gonorrhea/urine/female	Dorf	5	797.2	0.7170	0.9980	0.8773	0.9943	1	Gonorrhea in Section 5.1	
	NIS	5	754.6	0.7132	0.9991	0.9392	0.9942	2		
	FIS	5	746.8	0.7264	0.9992	0.9526	0.9945	3		
	1SIS	5	746.6	0.7472	0.9990	0.9370	0.9949	4		
	2SIS	5	749.1	0.7396	0.9992	0.9463	0.9948	5		
	3H	5	738.9	0.6038	0.9996	0.9704	0.9921	6		
	4H	5	Full 4H can not be done with a group of size 5							
	MP	5	1129.5	0.6019	1.0000	0.9970	0.9920	7		
	Dorf	10	737.0	0.7283	0.9969	0.8272	0.9945	8		
	NIS	10	608.5	0.7170	0.9981	0.8864	0.9943			
Gonorrhea/urine/male	FIS	10	575.1	0.7434	0.9985	0.9093	0.9948		Gonorrhea in Section 5.1	
	1SIS	10	595.3	0.7075	0.9976	0.8548	0.9941			
	2SIS	10	587.9	0.7094	0.9983	0.8982	0.9942			
	3H	10	559.2	0.6528	0.9984	0.8950	0.9931			
	4H	10	530.2	0.5396	0.9995	0.9577	0.9908			
	MP	10	639.2	0.6057	0.9995	0.9588	0.9921			
	Dorf	20	947.0	0.7340	0.9942	0.7234	0.9946			
	NIS	20	665.5	0.6887	0.9966	0.8030	0.9937			
	FIS	20	604.3	0.7302	0.9972	0.8462	0.9946			
	1SIS	20	660.0	0.7170	0.9964	0.8027	0.9943			
Gonorrhea/swab/female	2SIS	20	592.3	0.7453	0.9970	0.8333	0.9949		Gonorrhea in Section 5.1	
	3H	20	585.0	0.6358	0.9976	0.8452	0.9927			
	4H	20	453.0	0.5453	0.9989	0.9047	0.9909			
	MP	20	512.4	0.6019	0.9987	0.9017	0.9920			
	Dorf	5	1213.0	0.9328	0.9957	0.7796	0.9989			
	NIS	5	1146.7	0.9328	0.9973	0.8503	0.9989			
	FIS	5	1113.4	0.9410	0.9973	0.8516	0.9990			
	1SIS	5	1116.8	0.9377	0.9977	0.8689	0.9990			
	2SIS	5	1118.6	0.9295	0.9972	0.8444	0.9989			
Gonorrhea/swab/male	3H	5	1106.5	0.9131	0.9988	0.9225	0.9986		Gonorrhea in Section 5.1	
	4H	5	Full 4H can not be done with a group of size 5							
	MP	5	1638.4	0.9229	0.9995	0.9696	0.9988			
	Dorf	10	1082.0	0.9475	0.9931	0.6912	0.9992			
	NIS	10	901.7	0.9393	0.9964	0.8106	0.9990			
	FIS	10	810.6	0.9344	0.9968	0.8235	0.9989			
	1SIS	10	822.7	0.9393	0.9962	0.8033	0.9990			
	2SIS	10	818.9	0.9492	0.9966	0.8188	0.9992			
	3H	10	821.7	0.9246	0.9973	0.8464	0.9988			
	4H	10	793.8	0.8771	0.9991	0.9413	0.9980			
Gonorrhea/swab/male	MP	10	942.9	0.9082	0.9988	0.9225	0.9985		Gonorrhea in Section 5.1	
	Dorf	20	1385.0	0.9377	0.9880	0.5562	0.9990			
	NIS	20	954.0	0.9246	0.9932	0.6898	0.9988			
	FIS	20	768.8	0.9393	0.9955	0.7701	0.9990			
	1SIS	20	825.1	0.9213	0.9942	0.7227	0.9987			
	2SIS	20	787.0	0.9377	0.9953	0.7660	0.9990			
	3H	20	876.4	0.9066	0.9945	0.7267	0.9985			
	4H	20	704.2	0.8754	0.9982	0.8844	0.9980			
	MP	20	777.0	0.9147	0.9967	0.8176	0.9986			
	Dorf	5	5110.5	0.9335	0.9989	0.8906	0.9994			
Gonorrhea/swab/female	NIS	5	4916.2	0.9368	0.9992	0.9220	0.9994		Gonorrhea in Section 5.1	
	FIS	5	4756.4	0.9351	0.9995	0.9462	0.9994			
	1SIS	5	4765.7	0.9335	0.9994	0.9349	0.9994			
	2SIS	5	4756.2	0.9341	0.9994	0.9334	0.9994			
	3H	5	4837.7	0.9081	0.9997	0.9695	0.9991			
	4H	5	Full 4H can not be done with a group of size 5							
	MP	5	8015.1	0.9027	0.9999	0.9928	0.9991			
	Dorf	10	4001.0	0.9422	0.9980	0.8227	0.9994			
	NIS	10	3427.4	0.9400	0.9989	0.8873	0.9994			
	FIS	10	2994.0	0.9416	0.9992	0.9227	0.9994			
Gonorrhea/swab/male	1SIS	10	3059.4	0.9384	0.9993	0.9229	0.9994		Gonorrhea in Section 5.1	
	2SIS	10	2987.7	0.9389	0.9993	0.9281	0.9994			
	3H	10	3231.7	0.9173	0.9992	0.9143	0.9992			
	4H	10	3138.9	0.8708	0.9998	0.9724	0.9988			
	MP	10	4267.8	0.9011	0.9998	0.9777	0.9991			
	Dorf	20	4523.0	0.9313	0.9964	0.7156	0.9993			
	NIS	20	3251.6	0.9313	0.9981	0.8236	0.9993			
	FIS	20	2350.0	0.9384	0.9990	0.8960	0.9994			
	1SIS	20	2598.6	0.9324	0.9985	0.8559	0.9993			
	2SIS	20	2370.6	0.9249	0.9990	0.8968	0.9993			
Gonorrhea/urine/female	3H	20	3007.0	0.8897	0.9985	0.8523	0.9990		Gonorrhea in Section 5.1	
	4H	20	2502.3	0.8660	0.9993	0.9175	0.9987			
	MP	20	2770.2	0.9151	0.9993	0.9285	0.9992			
	Dorf	5	1808.5	0.9715	0.9923	0.8673	0.9985			
	NIS	5	1662.7	0.9650	0.9949	0.9063	0.9982			

Disease/specimen/gender	Procedure	Group size	Means over 10 implementations				
			# of tests	PS _e	PS _p	PPV	PNPV
Chlamydia/urine/female	Dorf	5	1504.2	0.6607	0.9871	0.8524	0.9626
	NIS	5	1379.6	0.6301	0.9924	0.9042	0.9596
	FIS	5	1346.5	0.6177	0.9928	0.9064	0.9583
	1SIS	5	1346.0	0.6346	0.9926	0.9065	0.9601
	2SIS	5	1338.7	0.6206	0.9920	0.8980	0.9586
	3H	5	1370.9	0.5302	0.9956	0.9316	0.9494
	4H	5	Full 4H can not be done with a group of size 5				
	MP	5	1456.7	0.5129	0.9969	0.9497	0.9477
	Dorf	10	1718.5	0.6478	0.9805	0.7901	0.9610
	NIS	10	1411.5	0.5827	0.9857	0.8221	0.9544
Chlamydia/urine/male	FIS	10	1333.7	0.5963	0.9877	0.8464	0.9559
	1SIS	10	1416.2	0.6033	0.9872	0.8427	0.9566
	2SIS	10	1361.9	0.5824	0.9884	0.8495	0.9544
	3H	10	1308.0	0.5206	0.9908	0.8640	0.9482
	4H	10	1203.6	0.4198	0.9964	0.9291	0.9383
	MP	10	1303.5	0.5261	0.9903	0.8598	0.9487
	Dorf	20	2029.3	0.6445	0.9726	0.7276	0.9604
	NIS	20	1502.6	0.5199	0.9824	0.7705	0.9477
	FIS	20	1500.3	0.5209	0.9845	0.7924	0.9479
	1SIS	20	1684.3	0.5706	0.9802	0.7649	0.9528
Chlamydia/swab/female	2SIS	20	1554.1	0.5364	0.9823	0.7741	0.9494
	3H	20	1469.3	0.5202	0.9847	0.7943	0.9478
	4H	20	1124.2	0.3930	0.9931	0.8666	0.9354
	MP	20	1624.3	0.5338	0.9804	0.7554	0.9490
	Dorf	5	2166.2	0.8669	0.9850	0.8408	0.9879
	NIS	5	1973.5	0.8525	0.9902	0.8875	0.9867
	FIS	5	1916.5	0.8485	0.9918	0.9038	0.9864
	1SIS	5	1936.2	0.8556	0.9906	0.8916	0.9870
	2SIS	5	1915.3	0.8588	0.9907	0.8930	0.9872
Chlamydia/swab/male	3H	5	2034.8	0.8088	0.9936	0.9201	0.9829
	4H	5	Full 4H can not be done with a group of size 5				
	MP	5	2131.8	0.7985	0.9954	0.9403	0.9820
	Dorf	10	2515.4	0.8553	0.9735	0.7462	0.9867
	NIS	10	2062.3	0.8322	0.9841	0.8257	0.9848
	FIS	10	1965.9	0.8294	0.9850	0.8336	0.9846
	1SIS	10	2085.0	0.8391	0.9818	0.8074	0.9854
	2SIS	10	1977.3	0.8372	0.9856	0.8411	0.9853
	3H	10	1996.7	0.8035	0.9854	0.8331	0.9823
	4H	10	1924.6	0.7356	0.9951	0.9319	0.9765
Chlamydia/urine/other	MP	10	2038.5	0.7972	0.9860	0.8376	0.9817
	Dorf	20	3183.4	0.8653	0.9600	0.6626	0.9875
	NIS	20	2483.6	0.7935	0.9759	0.7488	0.9812
	FIS	20	2394.9	0.7903	0.9754	0.7446	0.9809
	1SIS	20	2798.3	0.8184	0.9694	0.7078	0.9833
	2SIS	20	2582.4	0.8144	0.9739	0.7396	0.9830
	3H	20	2492.0	0.8119	0.9764	0.7574	0.9829
	4H	20	2009.1	0.7425	0.9871	0.8392	0.9769
	MP	20	2660.5	0.7994	0.9724	0.7249	0.9817
	Dorf	5	9065.0	0.8603	0.9912	0.8567	0.9914
Chlamydia/swab/other	NIS	5	8283.7	0.8479	0.9942	0.9001	0.9907
	FIS	5	7789.7	0.8495	0.9953	0.9178	0.9908
	1SIS	5	7863.0	0.8546	0.9953	0.9182	0.9911
	2SIS	5	7794.0	0.8467	0.9957	0.9238	0.9907
	3H	5	8455.0	0.7993	0.9965	0.9333	0.9878
	4H	5	Full 4H can not be done with a group of size 5				
	MP	5	9624.8	0.7984	0.9980	0.9609	0.9878
	Dorf	10	10522.0	0.8609	0.9838	0.7651	0.9914
	NIS	10	8453.0	0.8388	0.9903	0.8416	0.9901
	FIS	10	7454.6	0.8411	0.9928	0.8767	0.9903
Chlamydia/swab/female	1SIS	10	8042.8	0.8507	0.9903	0.8428	0.9909
	2SIS	10	7554.4	0.8409	0.9921	0.8662	0.9903
	3H	10	8158.7	0.8065	0.9921	0.8629	0.9882
	4H	10	7779.1	0.7420	0.9971	0.9390	0.9844
	MP	10	7830.5	0.8070	0.9937	0.8867	0.9883
	Dorf	20	13744.5	0.8563	0.9750	0.6770	0.9911
	NIS	20	10065.1	0.8045	0.9843	0.7577	0.9880
	FIS	20	9000.3	0.8092	0.9869	0.7908	0.9883
	1SIS	20	10735.7	0.8283	0.9824	0.7427	0.9894
	2SIS	20	9548.9	0.8135	0.9859	0.7792	0.9885
Chlamydia/swab/male	3H	20	9942.9	0.7910	0.9855	0.7699	0.9872
	4H	20	7937.8	0.7533	0.9929	0.8670	0.9850
	MP	20	10172.7	0.8050	0.9841	0.7564	0.9880
	Dorf	5	2813.0	0.8554	0.9788	0.8575	0.9784
	NIS	5	2576.9	0.8354	0.9857	0.8969	0.9757
	FIS	5	2388.3	0.8348	0.9891	0.9194	0.9757
	1SIS	5	2433.2	0.8394	0.9887	0.9174	0.9763
	2SIS	5	2393.4	0.8381	0.9896	0.9233	0.9761
	3H	5	2717.1	0.7983	0.9905	0.9264	0.9705
	4H	5	Full 4H can not be done with a group of size 5				
Chlamydia/urine/other	MP	5	2680.4	0.7859	0.9913	0.9309	0.9687
	Dorf	10	3295.5	0.8501	0.9682	0.8002	0.9774
	NIS	10	2804.2	0.8026	0.9787	0.8491	0.9708
	FIS	10	2522.6	0.8079	0.9816	0.8678	0.9716
	1SIS	10	2822.9	0.8249	0.9765	0.8399	0.9739
	2SIS	10	2599.0	0.8153	0.9800	0.8589	0.9726
	3H	10	2757.4	0.7814	0.9813	0.8622	0.9678
	4H	10	2715.8	0.7339	0.9920	0.9318	0.9615
	MP	10	2828.5	0.7960	0.9790	0.8499	0.9698

Disease/specimen/gender	Procedure	Group size	# of tests	Means over 10 implementations				Scale:	Gonorrhea in Section 5.2	
				PS _e	PS _p	PPPV	PNPV			
Gonorrhea/urine/female	Dorf	5	796.4	0.7245	0.9981	0.8905	0.9945	1	Gonorrhea in Section 5.2	
	NIS	5	755.6	0.7075	0.9990	0.9333	0.9941	2		
	FIS	5	743.9	0.6736	0.9986	0.9083	0.9935	3		
	1SIS	5	737.7	0.7151	0.9989	0.9268	0.9943	4		
	2SIS	5	740.6	0.6830	0.9988	0.9221	0.9937	5		
	3H	5	739.8	0.6226	0.9995	0.9630	0.9925	6		
	4H	5	Full 4H can not be done with a group of size 5							
	MP	5	1131.8	0.6453	0.9999	0.9909	0.9929	7		
	Dorf	10	728.7	0.7075	0.9968	0.8204	0.9941	8		
	NIS	10	615.4	0.6925	0.9984	0.8993	0.9938			
	FIS	10	577.0	0.7094	0.9986	0.9117	0.9941			
	1SIS	10	589.6	0.7094	0.9983	0.8931	0.9942			
	2SIS	10	574.9	0.7094	0.9985	0.9061	0.9942			
	3H	10	556.1	0.6132	0.9990	0.9308	0.9923			
	4H	10	519.5	0.4925	0.9996	0.9627	0.9898			
Gonorrhea/urine/male	MP	10	640.3	0.6283	0.9998	0.9849	0.9926			
	Dorf	20	899.6	0.7396	0.9948	0.7475	0.9948			
	NIS	20	642.3	0.6641	0.9979	0.8656	0.9933			
	FIS	20	605.2	0.6981	0.9976	0.8563	0.9939			
	1SIS	20	642.9	0.6925	0.9964	0.7958	0.9938			
	2SIS	20	619.9	0.6925	0.9970	0.8292	0.9938			
	3H	20	542.5	0.6038	0.9976	0.8395	0.9920			
	4H	20	431.1	0.5170	0.9989	0.9057	0.9903			
	MP	20	522.8	0.6264	0.9981	0.8659	0.9925			
	Dorf	5	1188.5	0.9475	0.9961	0.7972	0.9992			
	NIS	5	1123.5	0.9361	0.9973	0.8474	0.9990			
	FIS	5	1082.6	0.9360	0.9976	0.8640	0.9990			
	1SIS	5	1089.4	0.9246	0.9979	0.8733	0.9988			
	2SIS	5	1085.5	0.9361	0.9978	0.8715	0.9990			
	3H	5	1097.1	0.9180	0.9991	0.9434	0.9987			
	4H	5	Full 4H can not be done with a group of size 5							
	MP	5	1637.5	0.9180	0.9997	0.9826	0.9987			
Gonorrhea/swab/female	Dorf	10	1068.0	0.9295	0.9932	0.6880	0.9989		Gonorrhea in Section 5.2	
	NIS	10	867.2	0.9246	0.9959	0.7857	0.9988			
	FIS	10	796.7	0.9311	0.9969	0.8294	0.9989			
	1SIS	10	824.8	0.9311	0.9966	0.8155	0.9989			
	2SIS	10	804.4	0.9164	0.9969	0.8322	0.9986			
	3H	10	810.4	0.9082	0.9977	0.8650	0.9985			
	4H	10	781.7	0.8623	0.9991	0.9424	0.9978			
	MP	10	948.8	0.9098	0.9985	0.9108	0.9986			
	Dorf	20	1328.6	0.9361	0.9893	0.5869	0.9990			
	NIS	20	917.5	0.9213	0.9936	0.7013	0.9987			
	FIS	20	816.1	0.9180	0.9958	0.7798	0.9987			
	1SIS	20	925.1	0.9148	0.9933	0.6898	0.9986			
	2SIS	20	846.0	0.9246	0.9947	0.7398	0.9988			
	3H	20	858.0	0.9098	0.9951	0.7509	0.9986			
	4H	20	699.1	0.8885	0.9980	0.8774	0.9982			
	MP	20	778.1	0.9180	0.9963	0.8014	0.9987			
Gonorrhea/swab/male	Dorf	5	5137.0	0.9351	0.9988	0.8844	0.9994		Gonorrhea in Section 5.2	
	NIS	5	4938.8	0.9324	0.9994	0.9360	0.9993			
	FIS	5	4779.4	0.9416	0.9995	0.9434	0.9994			
	1SIS	5	4792.0	0.9303	0.9995	0.9432	0.9993			
	2SIS	5	4787.6	0.9378	0.9993	0.9312	0.9994			
	3H	5	4845.5	0.8946	0.9997	0.9701	0.9990			
	4H	5	Full 4H can not be done with a group of size 5							
	MP	5	8011.2	0.8957	0.9999	0.9940	0.9990			
	Dorf	10	4028.0	0.9378	0.9979	0.8148	0.9994			
	NIS	10	3442.5	0.9319	0.9987	0.8738	0.9994			
	FIS	10	3122.1	0.9324	0.9991	0.9088	0.9993			
	1SIS	10	3181.2	0.9265	0.9992	0.9146	0.9993			
	2SIS	10	3139.1	0.9254	0.9992	0.9166	0.9993			
	3H	10	3234.6	0.8978	0.9992	0.9141	0.9990			
	4H	10	3144.0	0.8768	0.9997	0.9703	0.9988			
	MP	10	4268.9	0.9076	0.9998	0.9796	0.9991			
Gonorrhea/swab/male	Dorf	20	4516.0	0.9232	0.9965	0.7158	0.9993		Gonorrhea in Section 5.2	
	NIS	20	3211.6	0.9151	0.9981	0.8254	0.9992			
	FIS	20	2670.2	0.9119	0.9984	0.8501	0.9992			
	1SIS	20	2854.6	0.9216	0.9983	0.8428	0.9993			
	2SIS	20	2669.6	0.9157	0.9986	0.8659	0.9992			
	3H	20	2997.9	0.8865	0.9984	0.8463	0.9989			
	4H	20	2477.1	0.8535	0.9993	0.9263	0.9986			
	MP	20	2742.5	0.9043	0.9994	0.9363	0.9991			
	Dorf	5	1837.0	0.9725	0.9910	0.8483	0.9986			
	NIS	5	1679.0	0.9645	0.9944	0.8995	0.9982			
	FIS	5	1482.6	0.9720	0.9969	0.9411	0.9986			
	1SIS	5	1514.7							

Section 6: The R programs are available on the Journal's supplementary documents website and at
www.chrisbilder.com/grouptesting.

Appendix: $I_k = 4$ example

We provide additional details here on the algorithm used to compute the PMF for the number of tests under FIS. The notation in the paper will be used here with the exception that the subscript k is dropped for convenience.

Define $y_{(1,2)} = 1$ if there is at least one diagnosed positive among $y_{(1)}$ and $y_{(2)}$, and define $y_{(1,2)} = 0$ if both $y_{(1)}$ and $y_{(2)}$ are diagnosed as negative. This notation is useful because $G_{12} = 1$ always leads to two more tests and $G_{12} = 0$ leads to no more tests, so the individual responses are not necessarily important when examining T . Define $\tilde{y}_{(1,2)}$ in a similar manner for the true value of $y_{(1,2)}$. The left-side of Table 1 provides $P(\tilde{Y}_{(1,2)} = \tilde{y}_{(1,2)}, \tilde{Y}_{(3)} = \tilde{y}_{(3)})$, the true probabilities for the possible set of outcomes, where $\bar{p}_{(i)} = 1 - p_{(i)}$. The second column is $\mathbf{q}^{(3)}$ as defined in the paper. The right-side of the table gives $\mathbf{A}^{(3)}$ as defined in the paper with column headers representing the observed possible outcomes of $y_{(1,2)}$ and $y_{(3)}$ and the corresponding number of tests. As given in the paper, the PMF for T at $j = 3$ is $\mathbf{S}^{(3)} = \mathbf{A}^{(3)'} \mathbf{q}^{(3)}$. Therefore, taking each column as a vector, one can find the inner product of the second column of the left-side table with a column in the right-side table to find the corresponding $P(T = t)$. For example, the product of the gray cells in the table leads to

$$\begin{aligned} P(Y_{(1,2)} = 1, Y_{(3)} = 1, \tilde{Y}_{(1,2)} = 1, \tilde{Y}_{(3)} = 1) &= P(G_{123} = 1, G_3 = 1, G_{12} = 1, \tilde{G}_{123} = 1, \tilde{G}_3 = 1, \tilde{G}_{12} = 1) \\ &= S_e^3 (1 - \bar{p}_{(1)} \bar{p}_{(2)}) p_{(3)}. \end{aligned}$$

Multiplying out the other values in the same columns and summing these joint probabilities results in $P(T = 5) = (1 - S_p)^3 \bar{p}_{(1)} \bar{p}_{(2)} \bar{p}_{(3)} + S_e^2 (1 - S_p) (1 - \bar{p}_{(1)} \bar{p}_{(2)}) \bar{p}_{(3)} + S_e^2 (1 - S_p) \bar{p}_{(1)} \bar{p}_{(2)} p_{(3)} + S_e^3 (1 - \bar{p}_{(1)} \bar{p}_{(2)}) p_{(3)}$.

Table 2 is the extension of Table 1 to include a fourth individual in a group. The left-side table is set up the same way as before, but now $\mathbf{q}^{(4)} = [\bar{p}_{(4)}, p_{(4)}]'$ $\otimes \mathbf{q}^{(3)}$ is given. The right-side table is broken up into four parts as shown by the vertical and horizontal borderlines of wider point size. The last four columns correspond to $\{G_{1234} = 1, G_4 = 1\}$. This means that two additional tests are needed in order to reach G_{123} in the FIS tree for $j = 3$. These two additional tests are indicated in the “ $t =$ ” row of the table. In the body of the last four columns, we have the sensitivities and specificities that

would be needed for specific conditional probabilities. For example, the lower right hand corner cell corresponds to

$$\begin{aligned}
& P(Y_{(1,2)} = 1, Y_{(3)} = 1, Y_{(4)} = 1 \mid \tilde{Y}_{(1,2)} = 1, \tilde{Y}_{(3)} = 1, \tilde{Y}_{(4)} = 1) \\
&= P(G_{1234} = 1, G_4 = 1, G_{123} = 1, G_3 = 1, G_{12} = 1 \mid \tilde{G}_{1234} = 1, \tilde{G}_4 = 1, \tilde{G}_{123} = 1, \tilde{G}_3 = 1, \tilde{G}_{12} = 1) \\
&= P(G_{1234} = 1 \mid \tilde{G}_{1234} = 1) \times P(G_4 = 1 \mid \tilde{G}_4 = 1) \\
&\quad \times P(G_{123} = 1 \mid \tilde{G}_{123} = 1) \times P(G_3 = 1 \mid \tilde{G}_3 = 1) \times P(G_{12} = 1 \mid \tilde{G}_{12} = 1) \\
&= S_e^5.
\end{aligned}$$

There is an interesting pattern evident here. For the rows corresponding to $\tilde{y}_{(4)} = 1$, the cells (purple region) are simply $S_e^2 \mathbf{A}^{(3)}$. The S_e^2 arises from $P(G_{1234} = 1 \mid \tilde{G}_{1234} = 1) \times P(G_4 = 1 \mid \tilde{G}_4 = 1)$. For the rows of $\tilde{y}_{(4)} = 0$, the last three rows of $\mathbf{A}^{(3)}$ are multiplied by $S_e(1-S_p)$ (dark blue region), and the first row of $\mathbf{A}^{(3)}$ is multiplied by $(1-S_p)^2$ (light blue region). The $S_e(1-S_p)$ comes from $P(G_{1234} = 1 \mid \tilde{G}_{1234} = 1) \times P(G_4 = 1 \mid \tilde{G}_4 = 0)$, and $(1-S_p)^2$ comes from $P(G_{1234} = 1 \mid \tilde{G}_{1234} = 0) \times P(G_4 = 1 \mid \tilde{G}_4 = 0)$. The first four columns of the right-side table correspond to when $G_{1234} = 0$ or when (3) would be tested after $\{G_{1234} = 1, G_4 = 0\}$. Similar patterns occur for these as in the last four columns. Notice only one additional test over those for $j = 3$ would be needed when $\{G_{1234} = 1, G_4 = 0\}$. The G_{1234} test takes the place of the G_{123} test leaving the additional test for G_4 .

Computing each $P(T = t)$ for $j = 4$ can be done in a similar manner as for $j = 3$. For example, $P(T = 7)$ is found by taking the inner product of the last column of the right-side table with the $\mathbf{q}^{(4)}$ column of the left-side table. For the benefit of a simplified algorithmic approach, one can modify this by taking advantage of the commonalities found between $j = 3$ and $j = 4$. Then

$$\begin{aligned}
P(T = 7 \mid I = 4) &= S_e(1 - S_p)\bar{p}_{(4)}P(T = 5 \mid I = 3) + S_e^2 p_{(4)}P(T = 5 \mid I = 3) \\
&\quad + [(1 - S_p)^2 - S_e(1 - S_p)](1 - S_p)^3 \bar{p}_{(1)}\bar{p}_{(2)}\bar{p}_{(3)}\bar{p}_{(4)},
\end{aligned}$$

where we use the notation of $P(T = t \mid I)$ to emphasize the recursive connections between probabilities for $j = 3$ and $j = 4$. Using this recursive connection is essential in order to have software efficiently calculate the PMF without running out of memory for larger group sizes. Also, one can see the motivation behind Step 2c of the algorithm given in the paper. When $j = 4$, Step 2c becomes

$$\mathbf{S}_2^{(4)} = [S_e(1 - S_p)\bar{p}_{(4)} + S_e^2 p_{(4)}] \mathbf{S}^{(3)} + [(1 - S_p)^2 - S_e(1 - S_p)] \prod_{i=1}^4 \bar{p}_{(i)} \mathbf{W}^{(3)}$$

so that the last elements of $\mathbf{S}^{(3)}$, $\mathbf{W}^{(3)}$, and $\mathbf{S}_2^{(4)}$ are $P(T = 5 \mid I = 3)$, $(1 - S_p)^3$, and $P(T = 7 \mid I = 4)$, respectively. Finally, we can also see the need for the $\mathbf{W}^{(3)}$ vector. It is used to adjust probability calculations where the recursive relationship does not hold in the same ways as elsewhere.

The “ $t =$ ” row of Table 2 provides the number of tests, but there are sometimes two columns that have the same number of tests. Steps 1c and 2d of the algorithm sum these probabilities that correspond to the same t , while also properly ordering them for $t = 1, 3, 4, 5, 6, 7$. In the end, $\mathbf{S}^{(4)}$ gives all of the probabilities for the PMF of T at $j = 4$. Because larger group sizes follow the pattern of adding a $G_{1,\dots,j}$ and a G_j for each additional increment of the group size, we are able to formulate the general algorithm for any group size as given in the paper.

Table 1. An illustrative table for the $j = 3$ case.

$\tilde{y}_{(1,2)}, \tilde{y}_{(3)}$	$P(\tilde{Y}_{(1,2)} = \tilde{y}_{(1,2)}, \tilde{Y}_{(3)} = \tilde{y}_{(3)})$	$t =$	1	3	4	5
$y_{(1,2)}, y_{(3)}$			0,0	0,1	1,0	1,1
0,0	$\bar{p}_{(1)}\bar{p}_{(2)}\bar{p}_{(3)}$		S_p	$S_p(1-S_p)^2$	$S_p(1-S_p)$	$(1-S_p)^3$
0,1	$(1 - \bar{p}_{(1)}\bar{p}_{(2)})\bar{p}_{(3)}$		$1-S_e$	$S_e(1-S_p)(1-S_e)$	S_pS_e	$S_e^2(1-S_p)$
1,0	$\bar{p}_{(1)}\bar{p}_{(2)}p_{(3)}$		$1-S_e$	$S_e^2 S_p$	$S_e(1-S_e)$	$S_e^2(1-S_p)$
1,1	$(1 - \bar{p}_{(1)}\bar{p}_{(2)})p_{(3)}$		$1-S_e$	$S_e^2(1-S_e)$	$S_e(1-S_e)$	S_e^3

Table 2. An illustrative table for the $j = 4$ case; cells are colored to help readers see patterns.

$\tilde{y}_{(1,2)}, \tilde{y}_{(3)}, \tilde{y}_{(4)}$	$P(\tilde{Y}_{(1,2)}, \tilde{Y}_{(3)}, \tilde{Y}_{(4)})$	$t =$	1 + 0	3 + 1	4 + 1	5 + 1	1 + 2	3 + 2	4 + 2	5 + 2
$y_{(1,2)}, y_{(3)}, y_{(4)}$ =			0,0,0	0,1,0	1,0,0	1,1,0	0,0,1	0,1,1	1,0,1	1,1,1
0,0,0	$\bar{p}_{(1)}\bar{p}_{(2)}\bar{p}_{(3)}\bar{p}_{(4)}$		S_p	$S_p \times$ $S_p(1-S_p)^2$	$S_p \times$ $S_p(1-S_p)$	$S_p \times$ $(1-S_p)^3$	$(1-S_p)^2 \times$ S_p	$(1-S_p)^2 \times$ $S_p(1-S_p)^2$	$(1-S_p)^2 \times$ $S_p(1-S_p)$	$(1-S_p)^2 \times$ $(1-S_p)^3$
0,1,0	$(1 - \bar{p}_{(1)}\bar{p}_{(2)})\bar{p}_{(3)}\bar{p}_{(4)}$		$1-S_e$	$S_p \times$ $S_e(1-S_p)(1-S_e)$	$S_p \times$ $S_p S_e$	$S_p \times$ $S_e^2 (1-S_p)$	$S_e(1-S_p) \times$ $1-S_e$	$S_e(1-S_p) \times$ $S_e(1-S_p)(1-S_e)$	$S_e(1-S_p) \times$ $S_p S_e$	$S_e(1-S_p) \times$ $S_e^2 (1-S_p)$
1,0,0	$\bar{p}_{(1)}\bar{p}_{(2)}p_{(3)}\bar{p}_{(4)}$		$1-S_e$	$S_p \times$ $S_e^2 S_p$	$S_p \times$ $S_e(1-S_e)$	$S_p \times$ $S_e^2 (1-S_p)$	$S_e(1-S_p) \times$ $1-S_e$	$S_e(1-S_p) \times$ $S_e^2 S_p$	$S_e(1-S_p) \times$ $S_e(1-S_e)$	$S_e(1-S_p) \times$ $S_e^2 (1-S_p)$
1,1,0	$(1 - \bar{p}_{(1)}\bar{p}_{(2)})p_{(3)}\bar{p}_{(4)}$		$1-S_e$	$S_p \times$ $S_e^2 (1-S_e)$	$S_p \times$ $S_e(1-S_e)$	$S_p \times$ S_e^3	$S_e(1-S_p) \times$ $1-S_e$	$S_e(1-S_p) \times$ $S_e^2 (1-S_e)$	$S_e(1-S_p) \times$ $S_e(1-S_e)$	$S_e(1-S_p) \times$ S_e^3
0,0,1	$\bar{p}_{(1)}\bar{p}_{(2)}\bar{p}_{(3)}p_{(4)}$		$1-S_e$	$S_e(1-S_e)/(1-S_p) \times$ $S_p(1-S_p)^2$	$S_e(1-S_e)/(1-S_p) \times$ $S_p(1-S_p)$	$S_e(1-S_e)/(1-S_p) \times$ $(1-S_p)^3$	$S_e^2 \times$ S_p	$S_e^2 \times$ $S_p(1-S_p)^2$	$S_e^2 \times$ $S_p(1-S_p)$	$S_e^2 \times$ $(1-S_p)^3$
0,1,1	$(1 - \bar{p}_{(1)}\bar{p}_{(2)})\bar{p}_{(3)}p_{(4)}$		$1-S_e$	$(1-S_e) \times$ $S_e(1-S_p)(1-S_e)$	$(1-S_e) \times$ $S_p S_e$	$(1-S_e) \times$ $S_e^2 (1-S_p)$	$S_e^2 \times$ $1-S_e$	$S_e^2 \times$ $S_e(1-S_p)(1-S_e)$	$S_e^2 \times$ $S_p S_e$	$S_e^2 \times$ $S_e(1-S_p) S_e$
1,0,1	$\bar{p}_{(1)}\bar{p}_{(2)}p_{(3)}p_{(4)}$		$1-S_e$	$(1-S_e) \times$ $S_e^2 S_p$	$(1-S_e) \times$ $S_e(1-S_e)$	$(1-S_e) \times$ $S_e^2 (1-S_p)$	$S_e^2 \times$ $1-S_e$	$S_e^2 \times$ $S_e^2 S_p$	$S_e^2 \times$ $S_e(1-S_e)$	$S_e^2 \times$ $S_e^2 (1-S_p)$
1,1,1	$(1 - \bar{p}_{(1)}\bar{p}_{(2)})p_{(3)}p_{(4)}$		$1-S_e$	$(1-S_e) \times$ $S_e^2 (1-S_e)$	$(1-S_e) \times$ $S_e(1-S_e)$	$(1-S_e) \times$ S_e^3	$S_e^2 \times$ $1-S_e$	$S_e^2 \times$ $S_e^2 (1-S_e)$	$S_e^2 \times$ $S_e(1-S_e)$	$S_e^2 \times$ S_e^3