

Supporting information for “Objective functions for group testing”

Brianna D. Hitt^{a*}, Christopher R. Bilder^a, Joshua M. Tebbs^b, and Christopher S. McMahan^c

^aDepartment of Statistics, University of Nebraska-Lincoln, Lincoln, NE 68583

^bDepartment of Statistics, University of South Carolina, Columbia, SC 29208

^cDepartment of Mathematical Sciences, Clemson University, Clemson, SC 29634

*Corresponding author: Brianna D. Hitt, brianna.hitt@huskers.unl.edu

February 17, 2018

Contents

S1 Derivation of $E(C)$	2
S2 Additional results for Section 3.1	2
S3 Additional results for Section 3.2	2
S4 R programs	3

List of Tables

S1	OTC summary for $p = 0.01$ under non-informative group testing	5
S2	OTC summary for $p = 0.05$ under non-informative group testing	6
S3	OTC summary for $p = 0.10$ under non-informative group testing	7
S4	Largest differences for OTCs under non-informative group testing	8
S5	OTC summary for $E(P_i) = 0.01$ under informative group testing	9
S6	OTC summary for $E(P_i) = 0.05$ under informative group testing	10
S7	OTC summary for $E(P_i) = 0.10$ under informative group testing	11
S8	Largest differences for OTCs under informative group testing	12
S9	Full OTCs for $E(P_i) = 0.01$ under informative two-stage hierarchical group testing	13
S10	Full OTCs for $E(P_i) = 0.01$ under informative three-stage hierarchical group testing	14
S11	Full OTCs for $E(P_i) = 0.05$ under informative two-stage hierarchical group testing	15
S12	Full OTCs for $E(P_i) = 0.05$ under informative three-stage hierarchical group testing	16
S13	Full OTCs for $E(P_i) = 0.10$ under informative two-stage hierarchical group testing	17
S14	Full OTCs for $E(P_i) = 0.10$ under informative three-stage hierarchical group testing	18

S1 Derivation of $E(C)$

Because infectious disease testing is imperfect, define Y_i as the final diagnosis based on the group testing algorithm and \tilde{Y}_i as the true status of individual i , for $i = 1, \dots, I$. The probability that individual i is truly positive is denoted as $P(\tilde{Y}_i = 1) = p_i$. Also, define C as the number of correct classifications for a group of size I . The expected number of correct classifications for the group is

$$\begin{aligned} E(C) &= \sum_{i=1}^I P(Y_i = 0, \tilde{Y}_i = 0) + P(Y_i = 1, \tilde{Y}_i = 1) \\ &= \sum_{i=1}^I P(Y_i = 0 | \tilde{Y}_i = 0) P(\tilde{Y}_i = 0) + P(Y_i = 1 | \tilde{Y}_i = 1) P(\tilde{Y}_i = 1) \\ &= \sum_{i=1}^I PS_{p,i}(1 - p_i) + PS_{e,i}p_i \end{aligned}$$

where $PS_{p,i}$ and $PS_{e,i}$ are the pooling specificity and pooling sensitivity, respectively, for individual i .

S2 Additional results for Section 3.1

We provide additional results to coincide with our investigations in Section 3.1. Overall, these additional results continue to show that the OTCs have the same or very similar operating characteristics when using either objective function. We also include in our summaries the pooling positive predictive value, $PPPV$, and pooling negative predictive value, $PNPV$, as additional accuracy measures. The pooling positive (negative) predictive value is the probability that an individual who is determined to be positive (negative) by the testing algorithm is truly positive (negative). Predictive values simply provide an alternative way of looking at accuracy in comparison to the pooling sensitivity and pooling specificity. Expressions for all accuracy measures are available in [Kim et al. \(2007\)](#), [McMahan et al. \(2012a\)](#), [McMahan et al. \(2012b\)](#), and [Black et al. \(2015\)](#).

Table 1 in the paper provides a summary of the optimal testing configurations (OTCs) and their operating characteristics when $p = 0.01$. This table is reproduced here as Table [S1](#) with the addition of the predictive values. Similar tables for $p = 0.05$ and $p = 0.10$ are shown in Tables [S2](#) and [S3](#), respectively. The largest differences between operating characteristics for OTCs are shown in Table 2 of the main paper. Table [S4](#) displays the same results with the addition of the predictive values.

S3 Additional results for Section 3.2

S3.1 Tables

We provide additional results to coincide with our investigations in Section 3.2. Once again, these additional results show that the same or very similar operating characteristics are obtained regardless of which objective function is used. Table [S5](#) displays the same results as Table 3 in the paper but with the addition of the predictive values. Similar tables for $E(P_i) = 0.05$ and $E(P_i) = 0.10$ are provided in Tables [S6](#) and [S7](#), respectively. Table [S8](#) displays the same findings as Table 4 in the paper but with the addition of the predictive values.

Because informative group testing results in potentially different accuracy measures for each individual tested, we formed weighted averages across all individuals tested to present one overall value for each accuracy measure. These weighted averages are developed from accuracy definitions given by [Altman & Bland \(1994a\)](#) and [Altman & Bland \(1994b\)](#) and were used by [Black et al. \(2015\)](#). The pooling sensitivity is defined as

$$PS_e^W = \frac{\sum_i p_i PS_{e,i}}{\sum_i p_i}, \quad (1)$$

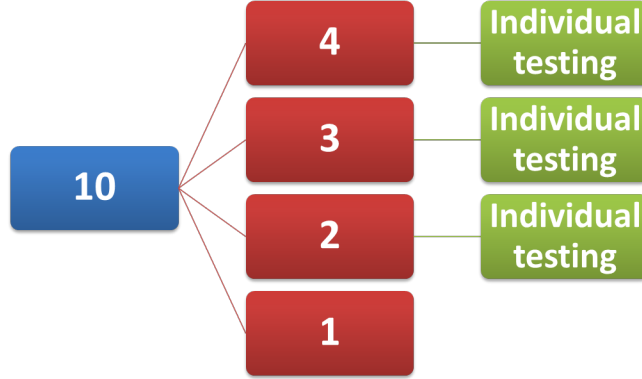


Figure S1: Diagram of the group testing algorithm described in Section S3.2. Group sizes are provided within nodes.

and the pooling specificity is defined as

$$PS_p^W = \frac{\sum_i (1 - p_i) PS_{p,i}}{\sum_i (1 - p_i)}. \quad (2)$$

Similarly, the pooling positive predictive value is defined as

$$PPPV^W = \frac{\sum_i p_i PS_{e,i}}{\sum_i p_i PS_{e,i} + (1 - p_i)(1 - PS_{p,i})}, \quad (3)$$

and the pooling negative predictive value is defined as

$$PNPV^W = \frac{\sum_i (1 - p_i) PS_{p,i}}{\sum_i (1 - p_i) PS_{p,i} + p_i(1 - PS_{e,i})}. \quad (4)$$

Expressions (1) through (4) represent weighted averages over all I individuals within the initial group for a hierarchical algorithm or all I^2 individuals within the array for an array-based algorithm.

S3.2 OTCs for informative group testing

Due to the lack of available space, Tables S5, S6, and S7 display at most only the initial (stage 1) group size for the informative hierarchical algorithms. We display their full algorithms in Tables S9 - S14. As described in Section 2, I_{sj} denotes the size of group j at stage s . For two-stage hierarchical testing, individuals are assembled into blocks (McMahan et al., 2012a), where we use a block size of 50. Thus, we have $\sum_j I_{1j} = 50$ by design.

To better understand the displayed OTCs in the tables, consider the OTC given in the first row of results in Table S12. The algorithm is performed over $S = 3$ stages with an initial group size of $I_{11} = 10$ individuals. If this initial group tests positively, four new groups are formed for the second stage of testing with sizes $I_{21} = 4$, $I_{22} = 3$, $I_{23} = 2$, and $I_{24} = 1$. Informative group testing always orders individuals by their probabilities of positivity. Therefore, the first group consists of the individuals with the four smallest probabilities, and the last group consists of the individual with the largest probability. If any of these groups test positively and has a size greater than 1, individual testing is performed upon its group members. For the first group in stage 2, this means that individual tests would be performed on each of its members in stage 3 ($I_{31} = I_{32} = I_{33} = I_{34} = 1$). For the last group in stage 2, no subsequent retesting would be performed. Figure S1 provides a pictorial representation of this group testing algorithm.

S4 R programs

Our research website at www.chrisbilder.com/grouptesting provides R programs to reproduce the research in this paper. In summary, we provide programs to

- Calculate $E(T)$ and the associated accuracy measures for several different objective functions, and
- Find the optimal testing configuration over a wide variety of settings.

All calculations for the paper were performed in version 3.4.1 of R (R Core Team, 2017).

References

- Altman, D & Bland, J (1994a), ‘Diagnostic tests 1: sensitivity and specificity,’ *BMJ*, **308**, p. 1552.
- Altman, D & Bland, J (1994b), ‘Diagnostic tests 2: predictive values,’ *BMJ*, **309**, p. 102.
- Black, MS, Bilder, CR & Tebbs, JM (2015), ‘Optimal retesting configurations for hierarchical group testing,’ *Journal of the Royal Statistical Society. Series C: Applied Statistics*, **64**(4), pp. 693–710, doi:10.1111/rssc.12097.
- Kim, HY, Hudgens, MG, Dreyfuss, JM, Westreich, DJ & Pilcher, CD (2007), ‘Comparison of group testing algorithms for case identification in the presence of test error,’ *Biometrics*, **63**(4), pp. 1152–1163, doi:10.1111/j.1541-0420.2007.00817.x.
- McMahan, CS, Tebbs, JM & Bilder, CR (2012a), ‘Informative Dorfman screening,’ *Biometrics*, **68**(1), pp. 287–296, doi:10.1111/j.1541-0420.2011.01644.x.
- McMahan, CS, Tebbs, JM & Bilder, CR (2012b), ‘Two-dimensional informative array testing,’ *Biometrics*, **68**(3), pp. 793–804, doi:10.1111/j.1541-0420.2011.01726.x.
- R Core Team (2017), *R: A language and environment for statistical computing*, R Foundation for Statistical Computing, Vienna, Austria, <https://www.R-project.org>.

Table S1: OTC summary for $p = 0.01$ under non-informative group testing. Equally sized groups are optimal at each stage; thus, an OTC of “24-6-1” means that stage 1 has a group of size 24, stage 2 has four groups of size 6, and stage 3 has twenty-four groups of size 1. Differences between O_{ET} and O_{MAR} are highlighted.

Algorithm	S_e	S_p	Objective		$E(T)/I$	PS_e	PS_p	$PPPV$	$PNPV$
			function	OTC					
2-stage hierarchical	0.99	0.99	O_{ET}	11-1	0.2035	0.9801	0.9990	0.9052	0.9998
			O_{MAR}	11-1	0.2035	0.9801	0.9990	0.9052	0.9998
	0.95	0.95	O_{ET}	11-1	0.2351	0.9025	0.9932	0.5727	0.9990
			O_{MAR}	11-1	0.2351	0.9025	0.9932	0.5727	0.9990
	0.90	0.90	O_{ET}	12-1	0.2742	0.8100	0.9816	0.3081	0.9980
			O_{MAR}	12-1	0.2742	0.8100	0.9816	0.3081	0.9980
3-stage hierarchical	0.99	0.99	O_{ET}	25-5-1	0.1354	0.9703	0.9996	0.9604	0.9997
			O_{MAR}	25-5-1	0.1354	0.9703	0.9996	0.9604	0.9997
	0.95	0.95	O_{ET}	24-6-1	0.1443	0.8574	0.9973	0.7634	0.9986
			O_{MAR}	24-6-1	0.1443	0.8574	0.9973	0.7634	0.9986
	0.90	0.90	O_{ET}	24-6-1	0.1562	0.7290	0.9938	0.5437	0.9973
			O_{MAR}	24-6-1	0.1562	0.7290	0.9938	0.5437	0.9973
Array w/o master pooling	0.99	0.99	O_{ET}	25-1	0.1378	0.9703	0.9995	0.9529	0.9997
			O_{MAR}	25-1	0.1378	0.9703	0.9995	0.9529	0.9997
	0.95	0.95	O_{ET}	25-1	0.1475	0.8575	0.9970	0.7456	0.9986
			O_{MAR}	24-1	0.1475	0.8575	0.9972	0.7566	0.9986
	0.90	0.90	O_{ET}	25-1	0.1611	0.7291	0.9926	0.4996	0.9973
			O_{MAR}	24-1	0.1611	0.7291	0.9930	0.5112	0.9973
Array w/ master pooling	0.99	0.99	O_{ET}	625-25-1	0.1364	0.9606	0.9995	0.9529	0.9996
			O_{MAR}	625-25-1	0.1364	0.9606	0.9995	0.9529	0.9996
	0.95	0.95	O_{ET}	625-25-1	0.1402	0.8146	0.9972	0.7458	0.9981
			O_{MAR}	576-24-1	0.1402	0.8146	0.9974	0.7569	0.9981
	0.90	0.90	O_{ET}	625-25-1	0.1450	0.6562	0.9934	0.4997	0.9965
			O_{MAR}	576-24-1	0.1450	0.6562	0.9937	0.5115	0.9965

Table S2: OTC summary for $p = 0.05$ under non-informative group testing. Equally sized groups are optimal at each stage; thus, a “24-6-1” means that stage 1 has a group of size 24, stage 2 has four groups of size 6, and stage 3 has twenty-four groups of size 1. There are no differences between the OTCs.

Algorithm	Objective		OTC	$E(T)/I$	PS_e	PS_p	PPPV	PNPV	
	S_e	S_p							function
2-stage hierarchical	0.99	0.99	O_{ET}	5-1	0.4317	0.9801	0.9981	0.9642	0.9990
			O_{MAR}	5-1	0.4317	0.9801	0.9981	0.9642	0.9990
	0.95	0.95	O_{ET}	5-1	0.4536	0.9025	0.9892	0.8141	0.9948
			O_{MAR}	5-1	0.4536	0.9025	0.9892	0.8141	0.9948
	0.90	0.90	O_{ET}	6-1	0.4786	0.8100	0.9719	0.6027	0.9898
			O_{MAR}	6-1	0.4786	0.8100	0.9719	0.6027	0.9898
3-stage hierarchical	0.99	0.99	O_{ET}	9-3-1	0.3773	0.9703	0.9990	0.9812	0.9984
			O_{MAR}	9-3-1	0.3773	0.9703	0.9990	0.9812	0.9984
	0.95	0.95	O_{ET}	9-3-1	0.3798	0.8574	0.9949	0.8993	0.9925
			O_{MAR}	9-3-1	0.3798	0.8574	0.9949	0.8993	0.9925
	0.90	0.90	O_{ET}	12-4-1	0.3806	0.7290	0.9853	0.7227	0.9857
			O_{MAR}	12-4-1	0.3806	0.7290	0.9853	0.7227	0.9857
Array w/o master pooling	0.99	0.99	O_{ET}	10-1	0.3809	0.9705	0.9986	0.9735	0.9984
			O_{MAR}	10-1	0.3809	0.9705	0.9986	0.9735	0.9984
	0.95	0.95	O_{ET}	10-1	0.3852	0.8581	0.9926	0.8597	0.9925
			O_{MAR}	10-1	0.3852	0.8581	0.9926	0.8597	0.9925
	0.90	0.90	O_{ET}	10-1	0.3907	0.7302	0.9842	0.7086	0.9858
			O_{MAR}	10-1	0.3907	0.7302	0.9842	0.7086	0.9858
Array w/ master pooling	0.99	0.99	O_{ET}	100-10-1	0.3772	0.9608	0.9986	0.9736	0.9979
			O_{MAR}	100-10-1	0.3772	0.9608	0.9986	0.9736	0.9979
	0.95	0.95	O_{ET}	100-10-1	0.3660	0.8152	0.9930	0.8600	0.9903
			O_{MAR}	100-10-1	0.3660	0.8152	0.9930	0.8600	0.9903
	0.90	0.90	O_{ET}	100-10-1	0.3517	0.6572	0.9858	0.7091	0.9820
			O_{MAR}	100-10-1	0.3517	0.6572	0.9858	0.7091	0.9820

Table S3: OTC summary for $p = 0.10$ under non-informative group testing. Equally sized groups are optimal at each stage; thus, a “24-6-1” means that stage 1 has a group of size 24, stage 2 has four groups of size 6, and stage 3 has twenty-four groups of size 1. There are no differences between the OTCs.

Algorithm	S_e	S_p	Objective		$E(T)/I$	PS_e	PS_p	$PPPV$	$PNPV$
			function	OTC					
2-stage hierarchical	0.99	0.99	O_{ET}	4-1	0.5970	0.9801	0.9972	0.9753	0.9978
			O_{MAR}	4-1	0.5970	0.9801	0.9972	0.9753	0.9978
	0.95	0.95	O_{ET}	4-1	0.6095	0.9025	0.9853	0.8722	0.9891
			O_{MAR}	4-1	0.6095	0.9025	0.9853	0.8722	0.9891
	0.90	0.90	O_{ET}	4-1	0.6251	0.8100	0.9683	0.7396	0.9787
			O_{MAR}	4-1	0.6251	0.8100	0.9683	0.7396	0.9787
3-stage hierarchical	0.99	0.99	O_{ET}	9-3-1	0.5836	0.9703	0.9981	0.9827	0.9967
			O_{MAR}	9-3-1	0.5836	0.9703	0.9981	0.9827	0.9967
	0.95	0.95	O_{ET}	9-3-1	0.5733	0.8574	0.9905	0.9091	0.9843
			O_{MAR}	9-3-1	0.5733	0.8574	0.9905	0.9091	0.9843
	0.90	0.90	O_{ET}	9-3-1	0.5619	0.7290	0.9808	0.8081	0.9702
			O_{MAR}	9-3-1	0.5619	0.7290	0.9808	0.8081	0.9702
Array w/o master pooling	0.99	0.99	O_{ET}	7-1	0.5821	0.9705	0.9978	0.9800	0.9967
			O_{MAR}	7-1	0.5821	0.9705	0.9978	0.9800	0.9967
	0.95	0.95	O_{ET}	7-1	0.5776	0.8585	0.9888	0.8950	0.9843
			O_{MAR}	7-1	0.5776	0.8585	0.9888	0.8950	0.9843
	0.90	0.90	O_{ET}	7-1	0.5722	0.7310	0.9772	0.7808	0.9703
			O_{MAR}	7-1	0.5722	0.7310	0.9772	0.7808	0.9703
Array w/ master pooling	0.99	0.99	O_{ET}	49-7-1	0.5767	0.9608	0.9978	0.9800	0.9957
			O_{MAR}	49-7-1	0.5767	0.9608	0.9978	0.9800	0.9957
	0.95	0.95	O_{ET}	49-7-1	0.5491	0.8156	0.9894	0.8952	0.9797
			O_{MAR}	49-7-1	0.5491	0.8156	0.9894	0.8952	0.9797
	0.90	0.90	O_{ET}	49-7-1	0.5154	0.6579	0.9795	0.7812	0.9626
			O_{MAR}	49-7-1	0.5154	0.6579	0.9795	0.7812	0.9626

Table S4: Largest differences between operating characteristics for OTCs under non-informative group testing. Values of p range from 0.005 to 0.150 by 0.005. The frequency column denotes the number of times a different OTC was found for O_{ET} and O_{MAR} among these values of p . Differences between operating characteristics are rounded to four decimal places. Note that operating characteristics are always smaller for O_{ET} than for O_{MAR} .

Algorithm	S_e	S_p	Frequency	Largest difference				
				$E(T)/I$	PS_e	PS_p	$PPPV$	$PNPV$
2-stage hierarchical	0.99	0.99	0	-	-	-	-	-
	0.95	0.95	3	0.0018	0.0000	0.0049	0.0262	0.0001
	0.90	0.90	4	0.0023	0.0000	0.0054	0.0345	0.0001
3-stage hierarchical	0.99	0.99	0	-	-	-	-	-
	0.95	0.95	1	0.0014	0.0000	0.0051	0.0296	0.0001
	0.90	0.90	5	0.0051	0.0000	0.0098	0.0575	0.0004
Array w/o master pooling	0.99	0.99	0	-	-	-	-	-
	0.95	0.95	5	0.0010	0.0018	0.0026	0.0195	0.0003
	0.90	0.90	8	0.0028	0.0022	0.0054	0.0305	0.0005
Array w/ master pooling	0.99	0.99	2	0.0005	0.0006	0.0008	0.0046	0.0001
	0.95	0.95	4	0.0012	0.0017	0.0026	0.0198	0.0003
	0.90	0.90	8	0.0015	0.0018	0.0051	0.0307	0.0005

Table S5: OTC summary for $E(P_i) = 0.01$ under informative group testing. Multiple initial group sizes for 2-stage hierarchical algorithms are found within a block size of 50, so they are not displayed here. The full OTCs are given in Tables S9 and S10. Differences between O_{ET} and O_{MAR} are highlighted.

Algorithm	α	S_e	S_p	Objective function	Initial group size for OTC	$E(T)/I$	PS_e^W	PS_p^W	$PPPV^W$	$PNPV^W$
2-stage hierarchical	0.99	0.99	0.99	O_{ET}	-	0.1947	0.9801	0.9991	0.9204	0.9998
				O_{MAR}	-	0.1947	0.9801	0.9991	0.9204	0.9998
	2	0.95	0.95	O_{ET}	-	0.2264	0.9025	0.9931	0.5687	0.9990
				O_{MAR}	-	0.2264	0.9025	0.9931	0.5687	0.9990
	0.90	0.90	0.90	O_{ET}	-	0.2657	0.8100	0.9822	0.3143	0.9981
				O_{MAR}	-	0.2657	0.8100	0.9822	0.3143	0.9981
	0.99	0.99	0.99	O_{ET}	-	0.1683	0.9801	0.9992	0.9245	0.9998
				O_{MAR}	-	0.1683	0.9801	0.9992	0.9245	0.9998
	0.5	0.95	0.95	O_{ET}	-	0.2019	0.9025	0.9943	0.6115	0.9990
				O_{MAR}	-	0.2019	0.9025	0.9943	0.6115	0.9990
	0.90	0.90	0.90	O_{ET}	-	0.2439	0.8100	0.9843	0.3389	0.9981
				O_{MAR}	-	0.2439	0.8100	0.9843	0.3389	0.9981
3-stage hierarchical	0.99	0.99	0.99	O_{ET}	26	0.1310	0.9703	0.9996	0.9629	0.9997
				O_{MAR}	26	0.1310	0.9703	0.9996	0.9629	0.9997
	2	0.95	0.95	O_{ET}	24	0.1400	0.8574	0.9975	0.7788	0.9986
				O_{MAR}	24	0.1400	0.8574	0.9975	0.7788	0.9986
	0.90	0.90	0.90	O_{ET}	27	0.1522	0.7290	0.9935	0.5324	0.9973
				O_{MAR}	26	0.1522	0.7290	0.9937	0.5408	0.9973
	0.99	0.99	0.99	O_{ET}	33	0.1197	0.9703	0.9996	0.9637	0.9997
				O_{MAR}	33	0.1197	0.9703	0.9996	0.9637	0.9997
	0.5	0.95	0.95	O_{ET}	28	0.1291	0.8574	0.9977	0.7883	0.9986
				O_{MAR}	28	0.1291	0.8574	0.9977	0.7883	0.9986
	0.90	0.90	0.90	O_{ET}	29	0.1422	0.7290	0.9942	0.5558	0.9973
				O_{MAR}	29	0.1422	0.7290	0.9942	0.5558	0.9973
Array w/o master pooling	0.99	0.99	0.99	O_{ET}	24	0.1351	0.9704	0.9996	0.9585	0.9997
				O_{MAR}	24	0.1351	0.9704	0.9996	0.9585	0.9997
	2	0.95	0.95	O_{ET}	24	0.1449	0.8575	0.9973	0.7652	0.9986
				O_{MAR}	24	0.1449	0.8575	0.9973	0.7652	0.9986
	0.90	0.90	0.90	O_{ET}	24	0.1586	0.7291	0.9932	0.5202	0.9973
				O_{MAR}	24	0.1586	0.7291	0.9932	0.5202	0.9973
	0.99	0.99	0.99	O_{ET}	30	0.1287	0.9703	0.9995	0.9493	0.9997
				O_{MAR}	30	0.1287	0.9703	0.9995	0.9493	0.9997
	0.5	0.95	0.95	O_{ET}	30	0.1389	0.8574	0.9968	0.7321	0.9985
				O_{MAR}	30	0.1389	0.8574	0.9968	0.7321	0.9985
	0.90	0.90	0.90	O_{ET}	30	0.1529	0.7290	0.9921	0.4844	0.9972
				O_{MAR}	30	0.1529	0.7290	0.9921	0.4844	0.9972

Table S6: OTC summary for $E(P_i) = 0.05$ under informative group testing. Multiple initial group sizes for 2-stage hierarchical algorithms are found within a block size of 50, so they are not displayed here. The full OTCs are given in Tables S11 and S12. There are no differences between the OTCs.

Algorithm	α	S_e	S_p	Objective function	Initial group size for OTC	$E(T)/I$	PS_e^W	PS_p^W	$PPPV^W$	$PNPV^W$
2-stage hierarchical	0.99	0.99	0.99	O_{ET}	-	0.4101	0.9801	0.9981	0.9645	0.9990
				O_{MAR}	-	0.4101	0.9801	0.9981	0.9645	0.9990
	2	0.95	0.95	O_{ET}	-	0.4321	0.9025	0.9892	0.8152	0.9948
				O_{MAR}	-	0.4321	0.9025	0.9892	0.8152	0.9948
	0.90	0.90	0.90	O_{ET}	-	0.4586	0.8100	0.9733	0.6149	0.9898
				O_{MAR}	-	0.4586	0.8100	0.9733	0.6149	0.9898
	0.99	0.99	0.99	O_{ET}	-	0.3584	0.9801	0.9984	0.9705	0.9990
				O_{MAR}	-	0.3584	0.9801	0.9984	0.9705	0.9990
	0.5	0.95	0.95	O_{ET}	-	0.3830	0.9025	0.9908	0.8371	0.9948
				O_{MAR}	-	0.3830	0.9025	0.9908	0.8371	0.9948
	0.90	0.90	0.90	O_{ET}	-	0.4124	0.8100	0.9761	0.6403	0.9899
				O_{MAR}	-	0.4124	0.8100	0.9761	0.6403	0.9899
3-stage hierarchical	0.99	0.99	0.99	O_{ET}	10	0.3687	0.9725	0.9990	0.9803	0.9986
				O_{MAR}	10	0.3687	0.9725	0.9990	0.9803	0.9986
	2	0.95	0.95	O_{ET}	11	0.3709	0.8574	0.9940	0.8821	0.9925
				O_{MAR}	11	0.3709	0.8574	0.9940	0.8821	0.9925
	0.90	0.90	0.90	O_{ET}	12	0.3724	0.7290	0.9862	0.7357	0.9857
				O_{MAR}	12	0.3724	0.7290	0.9862	0.7357	0.9857
	0.99	0.99	0.99	O_{ET}	11	0.3365	0.9757	0.9988	0.9768	0.9987
				O_{MAR}	11	0.3365	0.9757	0.9988	0.9768	0.9987
	0.5	0.95	0.95	O_{ET}	11	0.3433	0.8822	0.9934	0.8763	0.9938
				O_{MAR}	11	0.3433	0.8822	0.9934	0.8763	0.9938
	0.90	0.90	0.90	O_{ET}	10	0.3503	0.7582	0.9871	0.7560	0.9873
				O_{MAR}	10	0.3503	0.7582	0.9871	0.7560	0.9873
Array w/o master pooling	0.99	0.99	0.99	O_{ET}	10	0.3677	0.9705	0.9988	0.9761	0.9984
				O_{MAR}	10	0.3677	0.9705	0.9988	0.9761	0.9984
	2	0.95	0.95	O_{ET}	10	0.3731	0.8582	0.9933	0.8703	0.9925
				O_{MAR}	10	0.3731	0.8582	0.9933	0.8703	0.9925
	0.90	0.90	0.90	O_{ET}	11	0.3784	0.7295	0.9836	0.7004	0.9857
				O_{MAR}	11	0.3784	0.7295	0.9836	0.7004	0.9857
	0.99	0.99	0.99	O_{ET}	13	0.3372	0.9703	0.9986	0.9727	0.9985
				O_{MAR}	13	0.3372	0.9703	0.9986	0.9727	0.9985
	0.5	0.95	0.95	O_{ET}	13	0.3421	0.8575	0.9924	0.8551	0.9926
				O_{MAR}	13	0.3421	0.8575	0.9924	0.8551	0.9926
	0.90	0.90	0.90	O_{ET}	13	0.3484	0.7292	0.9837	0.7000	0.9859
				O_{MAR}	13	0.3484	0.7292	0.9837	0.7000	0.9859

Table S7: OTC summary for $E(P_i) = 0.10$ under informative group testing. Multiple initial group sizes for 2-stage hierarchical algorithms are found within a block size of 50, so they are not displayed here. The full OTCs are given in Tables S13 and S14. There are no differences between the OTCs.

Algorithm	α	S_e	S_p	Objective function	Initial group size for OTC	$E(T)/I$	PS_e^W	PS_p^W	$PPPV^W$	$PNPV^W$
2-stage hierarchical	0.99	0.99	0.99	O_{ET}	-	0.5674	0.9801	0.9975	0.9772	0.9978
				O_{MAR}	-	0.5674	0.9801	0.9975	0.9772	0.9978
	2	0.95	0.95	O_{ET}	-	0.5815	0.9025	0.9863	0.8798	0.9891
				O_{MAR}	-	0.5815	0.9025	0.9863	0.8798	0.9891
	0.90	0.90	0.90	O_{ET}	-	0.5973	0.8100	0.9681	0.7382	0.9787
				O_{MAR}	-	0.5973	0.8100	0.9681	0.7382	0.9787
	0.99	0.99	0.99	O_{ET}	-	0.4868	0.9833	0.9977	0.9793	0.9981
				O_{MAR}	-	0.4868	0.9833	0.9977	0.9793	0.9981
	0.5	0.95	0.95	O_{ET}	-	0.5054	0.9148	0.9873	0.8887	0.9905
				O_{MAR}	-	0.5054	0.9148	0.9873	0.8887	0.9905
	0.90	0.90	0.90	O_{ET}	-	0.5271	0.8333	0.9695	0.7522	0.9813
				O_{MAR}	-	0.5271	0.8333	0.9695	0.7522	0.9813
3-stage hierarchical	0.99	0.99	0.99	O_{ET}	5	0.5567	0.9764	0.9981	0.9824	0.9974
				O_{MAR}	5	0.5567	0.9764	0.9981	0.9824	0.9974
	2	0.95	0.95	O_{ET}	8	0.5550	0.8691	0.9891	0.8985	0.9855
				O_{MAR}	8	0.5550	0.8691	0.9891	0.8985	0.9855
	0.90	0.90	0.90	O_{ET}	8	0.5461	0.7500	0.9781	0.7916	0.9724
				O_{MAR}	8	0.5461	0.7500	0.9781	0.7916	0.9724
	0.99	0.99	0.99	O_{ET}	40	0.5074	0.9733	0.9976	0.9786	0.9970
				O_{MAR}	40	0.5074	0.9733	0.9976	0.9786	0.9970
	0.5	0.95	0.95	O_{ET}	40	0.5050	0.8711	0.9876	0.8863	0.9857
				O_{MAR}	40	0.5050	0.8711	0.9876	0.8863	0.9857
	0.90	0.90	0.90	O_{ET}	40	0.4994	0.7469	0.9739	0.7604	0.9719
				O_{MAR}	40	0.4994	0.7469	0.9739	0.7604	0.9719
Array w/o master pooling	0.99	0.99	0.99	O_{ET}	7	0.5585	0.9706	0.9981	0.9823	0.9967
				O_{MAR}	7	0.5585	0.9706	0.9981	0.9823	0.9967
	2	0.95	0.95	O_{ET}	7	0.5563	0.8587	0.9900	0.9050	0.9844
				O_{MAR}	7	0.5563	0.8587	0.9900	0.9050	0.9844
	0.90	0.90	0.90	O_{ET}	8	0.5494	0.7297	0.9757	0.7697	0.9701
				O_{MAR}	8	0.5494	0.7297	0.9757	0.7697	0.9701
	0.99	0.99	0.99	O_{ET}	8	0.5092	0.9704	0.9982	0.9837	0.9967
				O_{MAR}	8	0.5092	0.9704	0.9982	0.9837	0.9967
	0.5	0.95	0.95	O_{ET}	9	0.5076	0.8576	0.9892	0.8978	0.9843
				O_{MAR}	9	0.5076	0.8576	0.9892	0.8978	0.9843
	0.90	0.90	0.90	O_{ET}	9	0.5040	0.7294	0.9777	0.7842	0.9702
				O_{MAR}	9	0.5040	0.7294	0.9777	0.7842	0.9702

Table S8: Largest differences between operating characteristics for OTCs under informative group testing. Values of $E(P_i) = p$ range from 0.005 to 0.150 by 0.005. The frequency column denotes the number of times a different OTC was found among these values of p . Differences between operating characteristics are rounded to four decimal places. Note that the operating characteristic value for O_{ET} is always subtracted from the operating characteristic value for O_{MAR} . Thus, a negative value (indicated with parentheses) means that the value for O_{ET} was larger than the value for O_{MAR} .

Algorithm	α	S_e	S_p	Frequency	Largest difference				
					$E(T)/I$	PS_e^W	PS_p^W	$PPPV^W$	$PNPV^W$
2-stage hierarchical	2	0.99	0.99	0	-	-	-	-	-
		0.95	0.95	7	0.0006	(0.0023)	0.0011	0.0156	0.0004
		0.90	0.90	12	0.0010	(0.0052)	0.0023	0.0160	0.0007
	0.5	0.99	0.99	0	-	-	-	-	-
		0.95	0.95	3	0.0003	(0.0035)	0.0011	0.0102	0.0003
		0.90	0.90	15	0.0008	(0.0103)	0.0022	0.0277	0.0007
3-stage hierarchical	2	0.99	0.99	1	0.0000	(0.0019)	0.0002	0.0057	(0.0001)
		0.95	0.95	2	0.0035	0.0219	0.0033	0.0270	0.0034
		0.90	0.90	7	0.0044	0.0152	0.0062	0.0409	0.0023
	0.5	0.99	0.99	1	0.0000	0.0001	0.0001	0.0018	0.0000
		0.95	0.95	0	-	-	-	-	-
		0.90	0.90	3	0.0010	0.0250	0.0033	0.0296	0.0025
Array w/o master pooling	2	0.99	0.99	1	0.0003	0.0004	0.0005	0.0039	0.0001
		0.95	0.95	2	0.0011	0.0012	0.0027	0.0169	0.0002
		0.90	0.90	5	0.0016	0.0013	0.0040	0.0265	0.0003
	0.5	0.99	0.99	0	-	-	-	-	-
		0.95	0.95	3	0.0003	0.0004	0.0015	0.0129	0.0001
		0.90	0.90	11	0.0015	0.0004	0.0032	0.0194	0.0002

Table S9: Full OTCs for $E(P_i) = 0.01$ under informative two-stage hierarchical group testing. There are no differences in the OTCs for O_{ET} and O_{MAR} .

α	S_e	S_p	Objective function	Block size	$E(T)/I$	Group sizes				
						I_{11}	I_{12}	I_{13}	I_{14}	I_{15}
2	0.99	0.99	O_{ET}	50	0.1947	16	11	9	8	6
			O_{MAR}	50	0.1947	16	11	9	8	6
	0.95	0.95	O_{ET}	50	0.2264	18	13	11	8	
			O_{MAR}	50	0.2264	18	13	11	8	
	0.90	0.90	O_{ET}	50	0.2657	18	13	11	8	
			O_{MAR}	50	0.2657	18	13	11	8	
0.5	0.99	0.99	O_{ET}	50	0.1683	25	12	8	5	
			O_{MAR}	50	0.1683	25	12	8	5	
	0.95	0.95	O_{ET}	50	0.2019	25	12	8	5	
			O_{MAR}	50	0.2019	25	12	8	5	
	0.90	0.90	O_{ET}	50	0.2439	25	12	8	5	
			O_{MAR}	50	0.2439	25	12	8	5	

Table S10: Full OTCs for $E(P_i) = 0.01$ under informative three-stage hierarchical group testing. Differences between O_{ET} and O_{MAR} are highlighted.

α	S_e	S_p	Objective function	Group sizes						
				I_{11}	$E(T)/I$	I_{21}	I_{22}	I_{23}	I_{24}	I_{25}
2	0.99	0.99	O_{ET}	26	0.1310	8	6	5	4	3
			O_{MAR}	26	0.1310	8	6	5	4	3
	0.95	0.95	O_{ET}	24	0.1400	9	6	5	4	
			O_{MAR}	24	0.1400	9	6	5	4	
	0.90	0.90	O_{ET}	27	0.1522	10	7	6	4	
			O_{MAR}	26	0.1522	10	7	5	4	
0.5	0.99	0.99	O_{ET}	33	0.1197	15	6	5	4	3
			O_{MAR}	33	0.1197	15	6	5	4	3
	0.95	0.95	O_{ET}	28	0.1291	13	7	5	3	
			O_{MAR}	28	0.1291	13	7	5	3	
	0.90	0.90	O_{ET}	29	0.1422	14	7	5	3	
			O_{MAR}	29	0.1422	14	7	5	3	

Table S11: Full OTCs for $E(P_i) = 0.05$ under informative two-stage hierarchical group testing. There are no differences in the OTCs for O_{ET} and O_{MAR} .

α	S_e	S_p	Objective	Block	$E(T)/I$	Group sizes								
			function	size		I_{11}	I_{12}	I_{13}	I_{14}	I_{15}	I_{16}	I_{17}	I_{18}	I_{19}
2	0.99	0.99	O_{ET}	50	0.4101	9	7	6	6	5	5	4	4	4
			O_{MAR}	50	0.4101	9	7	6	6	5	5	4	4	4
	0.95	0.95	O_{ET}	50	0.4321	9	7	6	6	5	5	4	4	4
			O_{MAR}	50	0.4321	9	7	6	6	5	5	4	4	4
	0.90	0.90	O_{ET}	50	0.4586	10	8	7	6	5	5	5	4	
			O_{MAR}	50	0.4586	10	8	7	6	5	5	5	4	
0.5	0.99	0.99	O_{ET}	50	0.3584	16	9	6	5	4	4	3	3	
			O_{MAR}	50	0.3584	16	9	6	5	4	4	3	3	
	0.95	0.95	O_{ET}	50	0.3830	16	9	6	5	4	4	3	3	
			O_{MAR}	50	0.3830	16	9	6	5	4	4	3	3	
	0.90	0.90	O_{ET}	50	0.4124	17	9	7	5	5	4	3		
			O_{MAR}	50	0.4124	17	9	7	5	5	4	3		

Table S12: Full OTCs for $E(P_i) = 0.05$ under informative three-stage hierarchical group testing. There are no differences in the OTCs for O_{ET} and O_{MAR} .

α	S_e	S_p	Objective		Group sizes				
			function	I_{11}	$E(T)/I$	I_{21}	I_{22}	I_{23}	I_{24}
2	0.99	0.99	O_{ET}	10	0.3687	4	3	2	1
			O_{MAR}	10	0.3687	4	3	2	1
	0.95	0.95	O_{ET}	11	0.3709	5	3	3	
			O_{MAR}	11	0.3709	5	3	3	
	0.90	0.90	O_{ET}	12	0.3724	5	4	3	
			O_{MAR}	12	0.3724	5	4	3	
0.5	0.99	0.99	O_{ET}	11	0.3365	6	3	1	1
			O_{MAR}	11	0.3365	6	3	1	1
	0.95	0.95	O_{ET}	11	0.3433	6	3	1	1
			O_{MAR}	11	0.3433	6	3	1	1
	0.90	0.90	O_{ET}	10	0.3503	6	3	1	
			O_{MAR}	10	0.3503	6	3	1	

Table S13: Full OTCs for $E(P_i) = 0.10$ under informative two-stage hierarchical group testing. There are no differences in the OTCs for O_{ET} and O_{MAR} .

α	S_e	S_p	Objective function	Block size	$E(T)/I$	Group sizes																				
						I_{11}	I_{12}	I_{13}	I_{14}	I_{15}	I_{16}	I_{17}	I_{18}	I_{19}	$I_{1,10}$	$I_{1,11}$	$I_{1,12}$	$I_{1,13}$								
2	0.99	0.99	O_{ET}	50	0.5674	7	6	5	4	4	4	4	4	4	4	4	4	3	3	3	3	3	3	3		
			O_{MAR}	50	0.5674	7	6	5	4	4	4	4	4	4	4	4	4	4	3	3	3	3	3	3	3	
	0.95	0.95	O_{ET}	50	0.5815	7	6	5	4	4	4	4	4	4	4	4	4	4	3	3	3	3	3	3	3	
			O_{MAR}	50	0.5815	7	6	5	4	4	4	4	4	4	4	4	4	4	4	3	3	3	3	3	3	3
0.90	0.90	0.90	O_{ET}	50	0.5973	8	6	5	5	4	4	4	4	4	4	4	4	4	3	3	3	3	3	3	3	
			O_{MAR}	50	0.5973	8	6	5	5	4	4	4	4	4	4	4	4	4	4	3	3	3	3	3	3	3
	0.99	0.99	O_{ET}	50	0.4868	13	7	5	4	4	4	4	4	4	4	4	3	3	3	3	1	1	1	1	1	1
			O_{MAR}	50	0.4868	13	7	5	4	4	4	4	4	4	4	4	3	3	3	3	1	1	1	1	1	1
0.5	0.95	0.95	O_{ET}	50	0.5054	13	7	5	5	4	4	4	4	4	4	3	3	3	3	1	1	1	1	1	1	
			O_{MAR}	50	0.5054	13	7	5	5	4	4	4	4	4	4	4	3	3	3	3	1	1	1	1	1	1
0.90	0.90	0.90	O_{ET}	50	0.5271	14	7	6	5	4	4	4	4	4	4	4	4	3	3	1	1	1	1	1	1	
			O_{MAR}	50	0.5271	14	7	6	5	4	4	4	4	4	4	4	4	4	3	3	1	1	1	1	1	1

Table S14: Full OTCs for $E(P_i) = 0.10$ under informative three-stage hierarchical group testing. There are no differences in the OTCs for O_{ET} and O_{MAR} .

α	S_e	S_p	Objective	Group sizes											
			function	I_{11}	$E(T)/I$	I_{21}	I_{22}	I_{23}	I_{24}	I_{25}	I_{26}	I_{27}	I_{28}	I_{29}	$I_{2,10}$
2	0.99	0.99	O_{ET}	5	0.5567	3	1	1							
			O_{MAR}	5	0.5567	3	1	1							
	0.95	0.95	O_{ET}	8	0.5550	4	3	1							
			O_{MAR}	8	0.5550	4	3	1							
	0.90	0.90	O_{ET}	8	0.5461	4	3	1							
			O_{MAR}	8	0.5461	4	3	1							
0.5	0.99	0.99	O_{ET}	40	0.5074	12	6	5	4	4	3	3	1	1	1
			O_{MAR}	40	0.5074	12	6	5	4	4	3	3	1	1	1
	0.95	0.95	O_{ET}	40	0.5050	12	6	5	4	4	3	3	1	1	1
			O_{MAR}	40	0.5050	12	6	5	4	4	3	3	1	1	1
	0.90	0.90	O_{ET}	40	0.4994	12	7	5	4	4	3	3	1	1	
			O_{MAR}	40	0.4994	12	7	5	4	4	3	3	1	1	