

Supplementary material to *The Efficient Design of Nested Group Testing Algorithms for Disease Identification in Clustered Data*

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A1: Group testing algorithms:

The generalized group testing problem (GGTP) arises when designing a group testing procedure for w individuals, with corresponding probabilities $\mathbf{p} = p_1, \dots, p_w$ of being positive ($q_i = 1 - p_i$). Under this scenario, Equations A1.1-A1.3 give the expected number of tests per individual under D, D', and S respectively for any subset of size $k \geq 1$. [1, 2]

$$\mathbb{E}_D(T|k, \mathbf{p}) = 1 + \left(\frac{1}{k} - \prod_{i=1}^k q_i\right) \mathbb{I}(k \geq 2) \quad (\text{S1})$$

$$\mathbb{E}_{D'}(T|k, \mathbf{p}) = 1 + \left(\frac{1}{k} - \prod_{i=1}^k q_i - \frac{1}{k} p_k \prod_{i=1}^{k-1} q_i\right) \mathbb{I}(k \geq 2) \quad (\text{S2})$$

$$\mathbb{E}_S(T|k, \mathbf{p}) = \frac{1}{k} \{2k - 1 - [(q_1 + \dots + q_{k-1}) + q_{k-1}q_k + q_{k-2}q_{k-1}q_k + \dots + q_1q_2 \dots q_k]\}. \quad (\text{S3})$$

A2: Group testing with dilution:

Hwang's dilution function, representing the probability of correctly identifying a positive group, as a function of the group size k , disease prevalence p , and a dilution parameter d ranging from $d = 0$ (no dilution) to $d = 1$ (complete dilution)

$$D(k, p, d) = p/(1 - q^{k^d}). \quad (\text{S4})$$

Hwang's expected-cost function for the Dorfman procedure in a no-residual setting:

$$C_D(k, p, c, d) = \frac{1}{k} + \frac{(1-q^k)p}{1-q^{k^d}} + cp - \frac{cp^2}{1-q^{k^d}}. \quad (\text{S5})$$

If p is close to 0 and k is not too large, this may be optimized numerically by finding the roots of

$$f(k) = -1 + (1 - d)k^{2-d}p + cd k^{1-d}p. \quad (\text{S6})$$

Assuming that all group members share a common p_i , we may calculate the ratio of the expected number of correct classifications per individual to the total expected number of tests per individual ($\mathbb{E}(T_C)/\mathbb{E}(T_T)$) and the ratio of the expected number of missed cases to the total expected number of cases ($\mathbb{E}[M]/\mathbb{E}[D]$) using these quantities:

$$\begin{aligned} \mathbb{E}_D(T_C|k, p_i, d) &= \frac{1}{k} \left\{ q_i^k \times k + (1 - q_i^k)D(k, p_i, d) \times k + (1 - q_i^k)[1 - D(k, p_i, d)] \times \left(k - \frac{kp_i}{1 - q_i^k} \right) \right\} \\ &= k - [1 - D(k, p_i, d)]kp_i \end{aligned} \quad (\text{S7})$$

$$\begin{aligned} \mathbb{E}_D(T_T|k, p_i, d) &= \frac{1}{k} \{ 1 \times q_i^k + 1 \times [1 - D(k, p_i, d)](1 - q_i^k) + (k + 1) \times D(k, p_i, d)(1 - q_i^k) \} \\ &= \frac{1}{k} \{ q_i^k + [1 - D(k, p_i, d) - q_i^k + q_i^k D(k, p_i, d)] + D(k, p_i, d)(1 + k - kq_i^k - q_i^k) \} \\ &= D(k, p_i, d) - D(k, p_i, d)q_i^k + \frac{1}{k} \end{aligned} \quad (\text{S8})$$

$$\begin{aligned} \mathbb{E}_D(M|k, p_i, d) &= k - (\mathbb{E}_D[C|k, p_i, d]) \\ &= [1 - D(k, p_i, d)]kp_i \end{aligned} \quad (\text{S9})$$

$$\mathbb{E}(D|k, p_i) = kp_i. \quad (\text{S10})$$

A3: Optimal choice of l_i when using \hat{p} :

An optimal choice of l_i s for cluster-specific prevalence estimation is not optimal for a single prevalence estimate $\hat{p}_i = \hat{p}$ (Eq. 2.4) across all clusters. Using \hat{p} , we may obtain an accurate and precise estimate of the mean prevalence $p = \frac{\alpha}{\alpha+\beta}$ using a much smaller l_i , at the cost of no longer distinguishing cluster prevalences.

To investigate the optimal choice of l_i in this scenario, we assume there to be n clusters, each of size $m_i = m$, with a single $l_i = l$ (and optimum l^*) across all clusters. We generate 10,000 simulated data sets each consisting of simulated prevalences $\{p_1, \dots, p_n\}$ and observed values of \hat{p} for $l = 1, \dots, 10, \{\hat{p}^1, \dots, \hat{p}^{10}\}$. For each data set, we calculate $\mathbb{E}(T)$ using Equations 2.8-2.10 and $\{p_1, \dots, p_n\}$, with group size \widehat{k}_l^* derived from \hat{p}^l . We then calculate the empirical average of the simulated $\mathbb{E}(T)$ for each l and take l^* to be the value that minimizes these averages. **Figure S3** illustrates these values of l^* by $n, m \in \{10, \dots, 200\}$, for $\alpha = 1, p \in \{0.01, 0.05, 0.1, 0.2, 0.3\}$, and Procedures D, D', and S. For computational tractability, n and m are restricted so $n \times m \leq 5000$.

Across all scenarios, l^* was highest for small values of n and high values of m ; with a small number of large clusters, more individuals may be evaluated per cluster for accurate estimation of p . For D, D', and S and $p \in \{0.05, 0.1\}$, $1 \leq l^* \leq 3$ was sufficient. For $p = 0.01, m > 50$, and $n < 50$, a l^* of 4 or 5 may be required to provide an accurate estimate, due to the lower bound on \hat{p} . Larger values of l^* may likewise be required for $p = 0.2$. Finally, for $p = 0.3$, much larger values of l^* are favored, particularly for Procedure D: if \hat{p} indicates that the optimal group size is 1, the number of tests per subject will be equal to 1 regardless of the value of l^* .

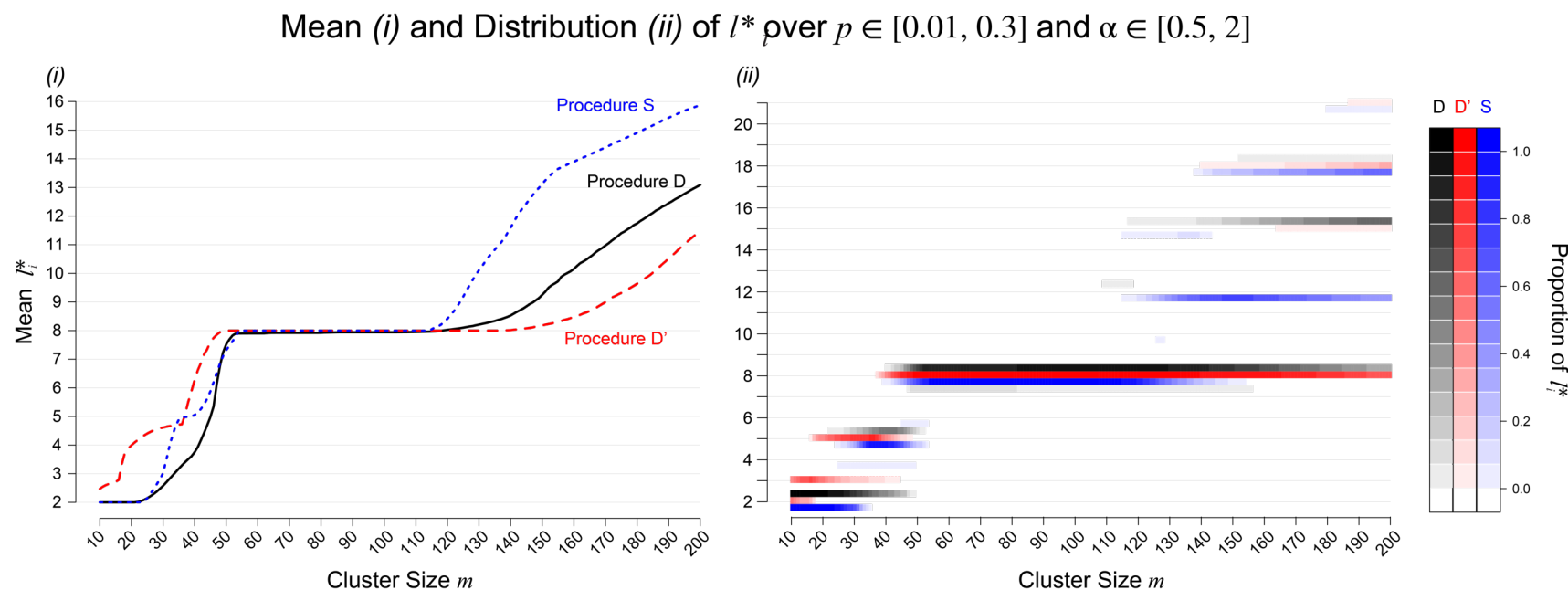
A4: Dilution Simulation Methods

We used simulations similar to those described in Section 4.1 to evaluate the impact of dilution on Dorfman group testing designs with clustering. As in the previous simulations, we varied the prevalence estimation method ($p_i, \hat{p}, \hat{p}_i, \tilde{p}_i$), the mean prevalence (0.01, 0.05, 0.1), the number of clusters n and individuals per cluster m ($\{n, m\} \in \{10, 100\}, \{31, 32\}, \{100, 10\}$), and the shape parameter α (0.5, 0.75, 1, 1.5, 2). We also varied the dilution factor d (0, 0.05, 0.1, 0.2, 0.3, 0.5) and cost parameter c (50, 100, 200) and averaged the results for each set of parameters over 50,000 simulated cohorts. The simulation steps followed those of Section 4.1.2, with several changes:

- Groups were strictly formed within clusters; superclusters were not used.
- Step 2b was omitted.
- In Step 2c, the estimated optimum group size was obtained from both the standard results for Procedure D (dilution is present but not accounted for) and Equation S5 under the cluster estimated prevalence.

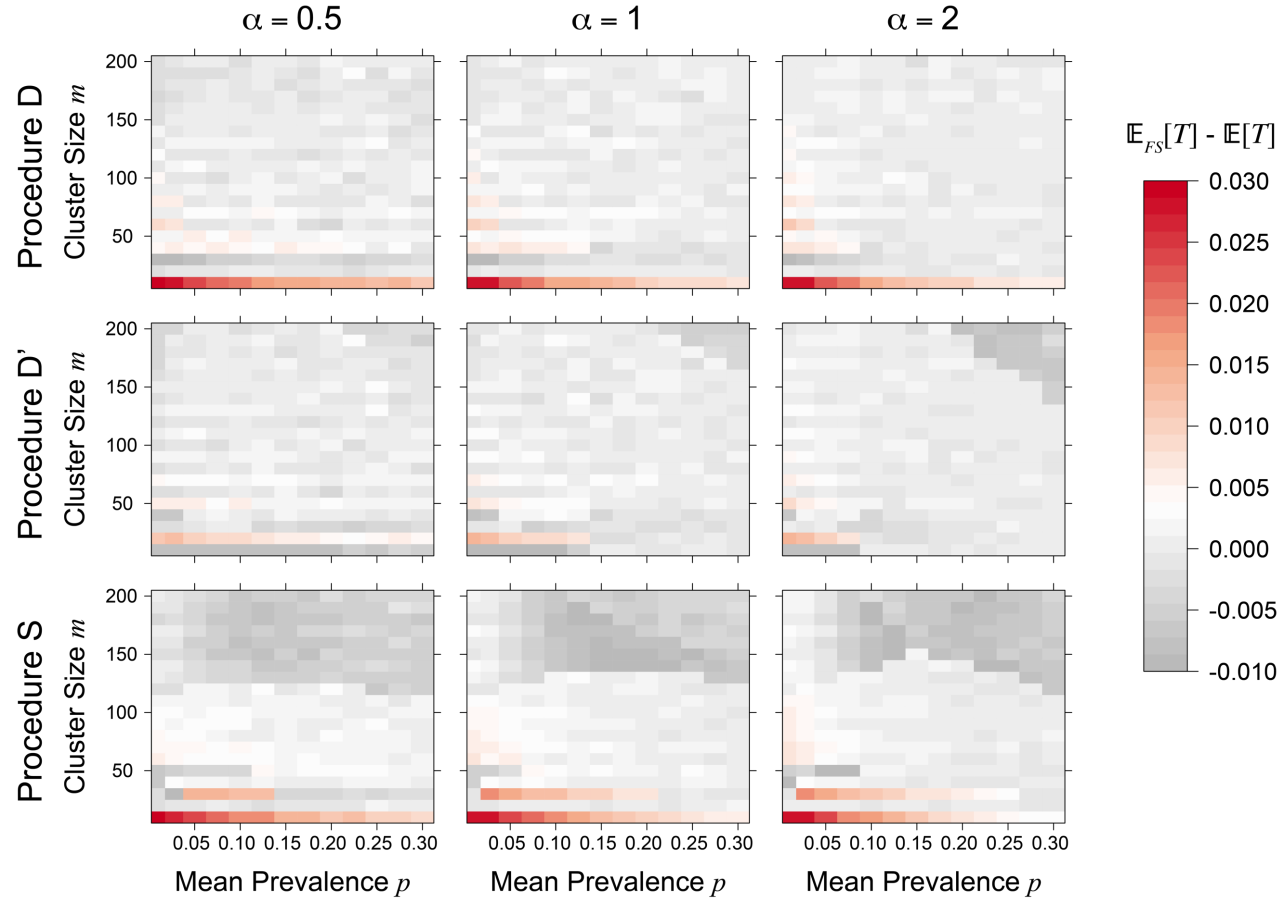
Under Step 2d, we evaluated $\mathbb{E}_D(T_C|\widehat{\mathbf{k}}^*(\mathbf{x}), \mathbf{p}_j)$, $\mathbb{E}_D(M|\widehat{\mathbf{k}}^*(\mathbf{x}), \mathbf{p}_j)$, $\mathbb{E}(D|\widehat{\mathbf{k}}^*(\mathbf{x}), \mathbf{p}_j)$, and $\mathbb{E}_D(T_T|\widehat{\mathbf{k}}^*(\mathbf{x}), \mathbf{p}_j)$ using Equations S7 through S10.

Figure S1: (i) Sample mean values of optimum number of individuals to test per cluster, l_i^* , for $m \in \{10, \dots, 200\}$, across 200 equally spaced values of each of $\alpha \in [0.5, 2]$ and $p \in [0.01, 0.3]$, by cluster size m . (ii) Proportion of l_i^* calculated over this region equal to 2, ..., 21, by cluster size m .



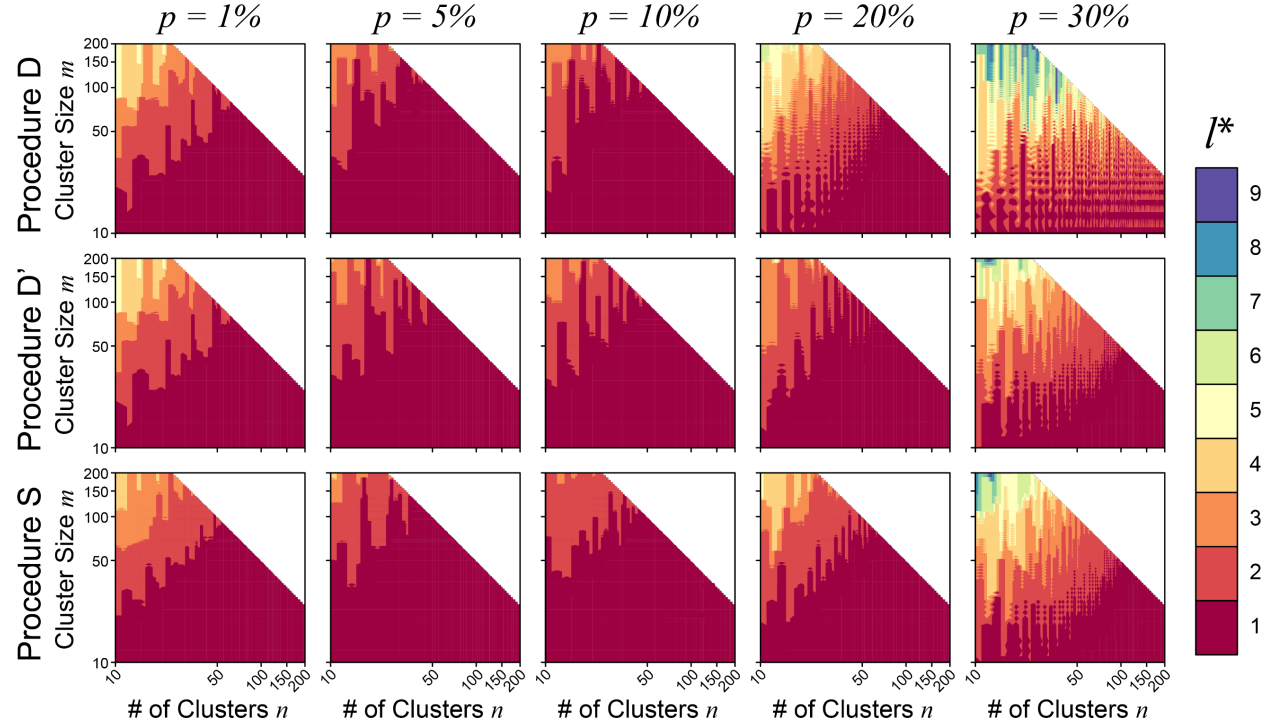
For clusters of size ≤ 50 , l_i^* is highest on average for Procedure D', followed by Procedures S and D. For $m \geq 120$, l_i^* is highest for Procedure S. When $50 < m < 120$, the average l_i^* for all three procedures is approximately equal to 8; almost all (α, p) pairs produced $l_i^* = 8$ over this region. The intuition for this involves the trade-off between improved prevalence estimation with increasing l_i vs increased number of tests. Small increases in l_i do not necessarily correspond to substantially improved prevalence estimation. For example, under Procedure D, l_i values between 8 and 11 have the same number of possible values of \hat{p}_i corresponding to a group size greater than 1, and have the same distribution of group sizes between the estimates. It is not until $l_i = 12$ that the number of possible \hat{p}_i values increases, and only at $l_i = 15$ does the corresponding maximum group size change. For larger cluster sizes, correspondingly larger values of l_i may improve the expected number of tests overall, particularly if the overall prevalence is low and there's a higher chance of a \hat{p}_i corresponding to a larger group size in the rest of the cluster. However, for moderate cluster sizes $l_i^* = 8$ provides a reasonable amount of possible values of \hat{p}_i , without a substantial cost in number of tests. Simulations for \tilde{p}_i and $\hat{\tilde{p}}_i$ produced similar results.

Figure S2: Heatmap of $\mathbb{E}_{FS}(T) - \mathbb{E}(T)$ using l_i^* optimized with regard to $\mathbb{E}(T)$. ($\mathbb{E}_{FS}(T)$: Expected number of tests under finite sample adjustment; $\mathbb{E}(T)$: Expected number of tests without adjustment) for 13 equally spaced values of the mean prevalence $p = \frac{\alpha}{\alpha+\beta} \in [0.001, 0.3]$ and 20 equally spaced values of the cluster size $m \in [10, 200]$. Simulations are under Procedures D, D', and S, for $\alpha \in \{0.5, 1, 2\}$.



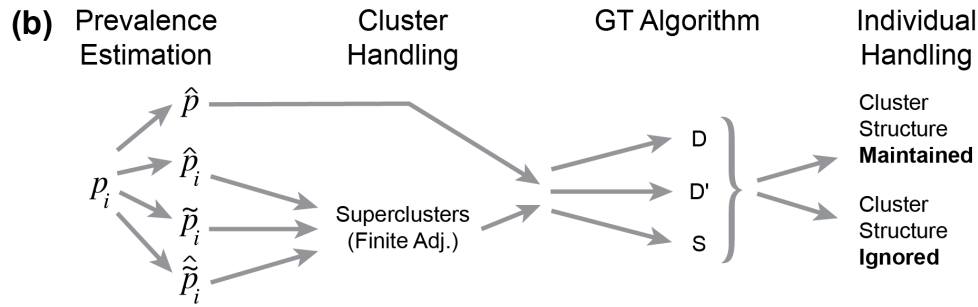
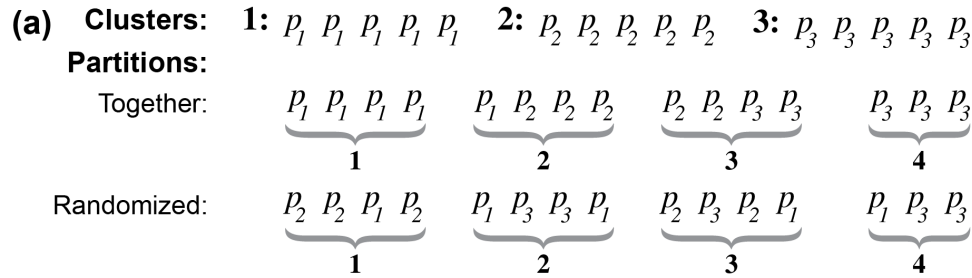
The largest differences are seen for small clusters ($m = 10$). Overall, however, the differences were small, with a maximum of 0.032 across all scenarios. Simulations for \hat{p}_i and $\hat{\tilde{p}}_i$ produced similar results.

Figure S3: Filled contour plot of optimum number of individuals to test per cluster, l^* , when using a common \hat{p} , by number of clusters $n \in \{10, \dots, 200\}$, cluster size $m \in \{10, \dots, 200\}$, for $p = \frac{\alpha}{\alpha+\beta} = \{0.01, 0.05, 0.1, 0.2, 0.3\}$ (columns) and Procedures D, D', and S (rows) ($\alpha = 1$).



In this scenario, $n \times l^*$ observations are used to calculate \hat{p} , thus a minimum of n individuals from separate clusters will be used, and the number of individuals used in the calculation is necessarily a multiple of n . Therefore, l^* for n clusters of size m is not anticipated to equal l_i^* for a single cluster of size $n \times m$. Additionally, even for sets of n, m , and l such that $n \times m$ and $n \times l$ are equal across sets, variability in the distribution of \hat{P} may differ. In each panel, for a fixed n smaller than approximately 50, as m increases l^* correspondingly increases, reflecting the benefit of improved prevalence estimation when a larger overall pool of individuals is available.

Table S1: (a) Illustration of cluster randomization for group construction. ‘Maintained’ prioritizes keeping cluster members together when forming the group testing partition. ‘Ignored’ randomizes cluster members with a common \hat{p}_i (or \tilde{p}_i , $\hat{\hat{p}}_i$, or \hat{p}) prior to forming the group testing partition. **(b)** Diagram of 24 group testing algorithms examined through simulations. “Superclusters” are sets of individuals with a shared estimated prevalence \hat{p}_i , \tilde{p}_i , or $\hat{\hat{p}}_i$. **(c)** Table of 24 group testing algorithms examined through simulations.



(c)	Prevalence Estimate	Group-Testing Procedure	Individual Handling
1	\hat{p}	D	Cluster members kept together during construction of the group testing partition
2		D'	
3		S	
4		D	All individuals randomized prior to the construction of the group testing partition (equivalent to testing naïve to cluster structure)
5		D'	
6		S	
7	\hat{p}_i	D, within superclusters	Cluster members kept together during construction of the group testing partition
8	\tilde{p}_i		
9	$\hat{\hat{p}}_i$		
10	\hat{p}_i	D', within superclusters	
11	\tilde{p}_i		
12	$\hat{\hat{p}}_i$		
13	\hat{p}_i	S, within superclusters	
14	\tilde{p}_i		
15	$\hat{\hat{p}}_i$		
16	\hat{p}_i	D, within superclusters	Within each supercluster, individuals are randomized prior to the construction of the group testing partition
17	\tilde{p}_i		
18	$\hat{\hat{p}}_i$		
19	\hat{p}_i	D', within superclusters	
20	\tilde{p}_i		
21	$\hat{\hat{p}}_i$		
22	\hat{p}_i	S, within superclusters	
23	\tilde{p}_i		
24	$\hat{\hat{p}}_i$		

Table S2: Expectation $\mathbb{E}(T)$ and standard deviation $\sigma(T)$ of the number of tests per subject **using the true value of p** by $\{n, m\}$ and mean prevalence p , for group testing procedures $\in \{D, D', S\}$, and $\alpha = 1$. Values calculated **(a)** *not* including or **(b)** including l^* in the overall number of tests; for **(a)**, values are calculated using only the $m - l^*$ remaining individuals for each cluster. The number of initial individual tests l^* is optimized for each m, p , and procedure (D, D' , or S).

(a)	GT Algorithm	n	m	$p = \frac{\alpha}{\alpha + \beta}$									
				0.01		0.05		0.1		0.2		0.3	
				$\mathbb{E}(T)$	$\sigma(T)$	$\mathbb{E}(T)$	$\sigma(T)$	$\mathbb{E}(T)$	$\sigma(T)$	$\mathbb{E}(T)$	$\sigma(T)$	$\mathbb{E}(T)$	$\sigma(T)$
D	10	100	0.190	0.028	0.410	0.054	0.558	0.071	0.762	0.086	0.896	0.095	
D'			0.190	0.026	0.403	0.052	0.544	0.068	0.730	0.083	0.880	0.079	
S			0.147	0.023	0.347	0.054	0.500	0.074	0.720	0.088	0.880	0.079	
D	31	32	0.191	0.016	0.408	0.030	0.561	0.041	0.762	0.048	0.896	0.053	
D'			0.191	0.015	0.402	0.029	0.546	0.039	0.731	0.046	0.882	0.045	
S			0.145	0.013	0.345	0.030	0.500	0.042	0.721	0.049	0.880	0.045	
D	100	10	0.193	0.009	0.413	0.018	0.558	0.023	0.771	0.028	0.911	0.030	
D'			0.193	0.009	0.406	0.017	0.550	0.023	0.738	0.027	0.881	0.024	
S			0.138	0.007	0.342	0.017	0.498	0.024	0.719	0.028	0.881	0.024	

We observe the established efficiency rankings between Procedures D, D' , and S ($\mathbb{E}_D(T) \geq \mathbb{E}_{D'}(T) \geq \mathbb{E}_S(T)$)

(b) GT Algorithm	n	m	$p = \frac{\alpha}{\alpha + \beta}$									
			0.01		0.05		0.1		0.2		0.3	
			E(T)	$\sigma(T)$	E(T)	$\sigma(T)$	E(T)	$\sigma(T)$	E(T)	$\sigma(T)$	E(T)	$\sigma(T)$
D	10	100	0.247	0.026	0.457	0.049	0.594	0.065	0.781	0.080	0.905	0.087
D'			0.255	0.024	0.451	0.048	0.580	0.063	0.752	0.076	0.890	0.073
S			0.215	0.021	0.399	0.050	0.540	0.068	0.742	0.081	0.890	0.073
D	31	32	0.242	0.015	0.445	0.028	0.588	0.038	0.777	0.045	0.912	0.045
D'			0.267	0.013	0.458	0.027	0.617	0.033	0.773	0.039	0.901	0.038
S			0.252	0.011	0.447	0.026	0.531	0.039	0.765	0.041	0.899	0.038
D	100	10	0.355	0.007	0.530	0.014	0.646	0.018	0.817	0.022	0.929	0.024
D'			0.435	0.006	0.584	0.012	0.685	0.016	0.790	0.021	0.905	0.020
S			0.310	0.005	0.473	0.014	0.598	0.019	0.775	0.022	0.905	0.020

Once the $n \times l^*$ additional tests from the prevalence estimation are added, Procedure D occasionally outperforms D' , particularly for small cluster sizes; As discussed in Section 3.1 of the main text, \hat{p}_i is bounded from below by $p^* = \frac{1}{l^*+2}$, and for small p this bound is smaller than each p_i with high probability (for $p = 0.05, \alpha = 1, P[P_i < 0.1] = 0.86$). Therefore, $k_D^* \geq k_{D'}^* > \widehat{k_D^*} \geq \widehat{k_{D'}^*}$, for such p , and during the selection of $l_{D'}$, an optimal $l_{D'}^* > l_D^*$, with consequent $p_{D'}^* < p_D^*$ and $k_{D'}^* \geq k_D^*$, may minimize the $\mathbb{E}_{D'}(T)$ overall despite $\mathbb{E}_{D'}(T) > \mathbb{E}_D(T)$.

Table S3: Expectation $E(T)$ and standard deviation $\sigma(T)$ of the number of tests per subject **using the true and estimated prevalence values**, by $\{n, m\}$ and mean prevalence p , for group testing procedures $\in \{D, D', S\}$, and $\alpha = 1$. Values calculated including l^* in the overall number of tests; l^* is optimized for each m, p , and procedure (D, D', or S).

GT Algorithm	n	m	Prevalence Used	$p = \frac{\alpha}{\alpha + \beta}$									
				0.01		0.05		0.1		0.2		0.3	
				$\mathbb{E}(T)$	$\sigma(T)$	$\mathbb{E}(T)$	$\sigma(T)$	$\mathbb{E}(T)$	$\sigma(T)$	$\mathbb{E}(T)$	$\sigma(T)$	$\mathbb{E}(T)$	$\sigma(T)$
D	10	100	p	0.247	0.026	0.457	0.049	0.594	0.065	0.781	0.080	0.905	0.087
			\hat{p}	0.262	0.030	0.461	0.053	0.597	0.070	0.785	0.095	0.920	0.090
D'			p	0.255	0.024	0.451	0.048	0.580	0.063	0.752	0.076	0.890	0.073
			\hat{p}	0.267	0.028	0.456	0.051	0.587	0.065	0.764	0.081	0.890	0.080
S			p	0.215	0.021	0.399	0.050	0.540	0.068	0.742	0.081	0.890	0.073
			\hat{p}	0.225	0.023	0.403	0.052	0.542	0.072	0.740	0.092	0.883	0.088
D	31	32	p	0.242	0.015	0.445	0.028	0.588	0.038	0.777	0.045	0.912	0.045
			\hat{p}	0.260	0.023	0.453	0.032	0.596	0.041	0.784	0.061	0.939	0.062
D'			p	0.267	0.013	0.458	0.027	0.617	0.033	0.773	0.039	0.901	0.038
			\hat{p}	0.281	0.019	0.466	0.030	0.621	0.034	0.786	0.046	0.903	0.044
S			p	0.252	0.011	0.447	0.026	0.531	0.039	0.765	0.041	0.899	0.038
			\hat{p}	0.259	0.014	0.451	0.027	0.537	0.043	0.765	0.047	0.899	0.048
D	100	10	p	0.355	0.007	0.530	0.014	0.646	0.018	0.817	0.022	0.929	0.024
			\hat{p}	0.360	0.009	0.532	0.015	0.650	0.021	0.817	0.023	0.956	0.043
D'			p	0.435	0.006	0.584	0.012	0.685	0.016	0.790	0.021	0.905	0.020
			\hat{p}	0.439	0.008	0.586	0.013	0.689	0.017	0.801	0.026	0.905	0.022
S			p	0.310	0.005	0.473	0.014	0.598	0.019	0.775	0.022	0.905	0.020
			\hat{p}	0.316	0.010	0.477	0.015	0.601	0.020	0.775	0.025	0.904	0.024

Comparing to the same algorithms using \hat{p} or \hat{p}_i , estimating the prevalence increases both $E(T)$ and $\sigma(T)$ slightly for Procedures D, D', and S.

Table S4: Expectation $\mathbb{E}(T)$ and standard deviation $\sigma(T)$ of the number of tests per subject for group testing procedures $\in \{\mathbf{D}, \mathbf{D}', \mathbf{S}\}$ using prevalence estimates \hat{p} and \hat{p}_i , by $\{n, m\}$ and mean prevalence p , $\alpha = 1$. For common parameters, results for \hat{p} and \hat{p}_i share a common l^* , and l^* is optimized for each m, p , and procedure (D, D', or S). For each set of parameters, the lower $\mathbb{E}(T)$ and $\sigma(T)$ values between prevalence estimators are indicated in **bold**.

GT Algorithm	n	m	Prevalence Estimate	$p = \frac{\alpha}{\alpha + \beta}$									
				0.01		0.05		0.1		0.2		0.3	
				E(T)	σ(T)	E(T)	σ(T)	E(T)	σ(T)	E(T)	σ(T)	E(T)	σ(T)
D	10	100	\hat{p}	0.263	0.030	0.460	0.053	0.598	0.070	0.785	0.093	0.921	0.089
\hat{p}_i			0.345	0.018	0.482	0.046	0.604	0.066	0.757	0.075	0.843	0.070	
D'			\hat{p}	0.267	0.028	0.456	0.051	0.587	0.065	0.764	0.081	0.890	0.080
\hat{p}_i			0.349	0.014	0.476	0.045	0.593	0.063	0.740	0.073	0.827	0.069	
S			\hat{p}	0.225	0.023	0.402	0.051	0.543	0.071	0.742	0.091	0.884	0.088
			\hat{p}_i	0.305	0.016	0.438	0.048	0.562	0.068	0.721	0.079	0.813	0.075
D	31	32	\hat{p}	0.261	0.023	0.453	0.033	0.595	0.041	0.784	0.063	0.938	0.062
\hat{p}_i			0.414	0.016	0.541	0.032	0.653	0.039	0.792	0.042	0.868	0.035	
D'			\hat{p}	0.281	0.019	0.466	0.030	0.621	0.034	0.786	0.046	0.903	0.044
\hat{p}_i			0.436	0.018	0.563	0.034	0.659	0.031	0.782	0.035	0.854	0.034	
S			\hat{p}	0.259	0.014	0.451	0.027	0.537	0.042	0.765	0.048	0.898	0.048
			\hat{p}_i	0.378	0.009	0.518	0.026	0.625	0.039	0.763	0.040	0.842	0.038
D	100	10	\hat{p}	0.359	0.009	0.532	0.015	0.650	0.021	0.817	0.023	0.956	0.044
\hat{p}_i			0.500	0.007	0.609	0.015	0.706	0.019	0.825	0.020	0.893	0.019	
D'			\hat{p}	0.439	0.008	0.586	0.013	0.689	0.017	0.801	0.026	0.905	0.022
\hat{p}_i			0.564	0.008	0.663	0.015	0.746	0.017	0.838	0.015	0.893	0.015	
S			\hat{p}	0.316	0.010	0.477	0.015	0.601	0.020	0.775	0.025	0.904	0.025
			\hat{p}_i	0.495	0.007	0.590	0.015	0.679	0.019	0.798	0.021	0.870	0.020

For moderate- to large-sized clusters, using \hat{p}_i improves $\mathbb{E}(T)$ only for high values of p ($p \geq 0.2$). For $p < 0.2$, the boundedness and imprecision of \hat{p}_i outweigh the ability to calculate group size based on clusters' individual estimated prevalences. Indeed, for $p = 0.01$ and $p = 0.05$, we may have only one or two superclusters; at these values of p and for $l = 10$, $P(X_i > 1) = 0.004$ and $= 0.086$ respectively. In most cases \hat{p}_i has equivalent or superior $\sigma(T)$ to \hat{p} for all mean prevalence values.

Table S5: Expectation $\mathbb{E}(T)$ and standard deviation $\sigma(T)$ of the number of tests per subject, by α and mean prevalence p , for Procedures D' and S and prevalence estimates \hat{p} and \hat{p}_i . $n = 31$ and $m = 32$. For each set of parameters, the lower $\mathbb{E}(T)$ and $\sigma(T)$ values between prevalence estimators are indicated in **bold**.

GT Algorithm	α	Prevalence Estimate	$p = \frac{\alpha}{\alpha + \beta}$									
			0.01		0.05		0.1		0.2		0.3	
			$\mathbb{E}(T)$	$\sigma(T)$	$\mathbb{E}(T)$	$\sigma(T)$	$\mathbb{E}(T)$	$\sigma(T)$	$\mathbb{E}(T)$	$\sigma(T)$	$\mathbb{E}(T)$	$\sigma(T)$
D'	0.5	\hat{p}	0.278	0.023	0.455	0.040	0.605	0.045	0.768	0.062	0.889	0.057
		\hat{p}_i	0.435	0.018	0.549	0.036	0.637	0.035	0.737	0.040	0.799	0.040
S		\hat{p}	0.257	0.018	0.442	0.036	0.567	0.049	0.747	0.062	0.882	0.064
		\hat{p}_i	0.377	0.011	0.508	0.030	0.598	0.040	0.710	0.045	0.779	0.045
D'	0.75	\hat{p}	0.280	0.021	0.462	0.034	0.616	0.038	0.779	0.052	0.911	0.034
		\hat{p}_i	0.436	0.018	0.558	0.035	0.651	0.033	0.764	0.038	0.897	0.027
S		\hat{p}	0.259	0.016	0.448	0.031	0.575	0.042	0.758	0.054	0.909	0.036
		\hat{p}_i	0.377	0.010	0.514	0.028	0.615	0.037	0.742	0.042	0.891	0.029
D'	1	\hat{p}	0.281	0.019	0.466	0.030	0.621	0.034	0.786	0.046	0.897	0.049
		\hat{p}_i	0.436	0.018	0.563	0.034	0.660	0.031	0.782	0.035	0.833	0.037
S		\hat{p}	0.259	0.014	0.450	0.027	0.537	0.043	0.765	0.048	0.892	0.054
		\hat{p}_i	0.378	0.009	0.518	0.026	0.626	0.039	0.763	0.040	0.817	0.041
D'	1.5	\hat{p}	0.281	0.018	0.470	0.025	0.628	0.028	0.794	0.037	0.908	0.038
		\hat{p}_i	0.436	0.018	0.568	0.034	0.669	0.028	0.803	0.032	0.881	0.030
S		\hat{p}	0.260	0.013	0.454	0.023	0.543	0.036	0.751	0.046	0.905	0.040
		\hat{p}_i	0.378	0.009	0.522	0.024	0.636	0.037	0.787	0.039	0.873	0.033
D'	2	\hat{p}	0.282	0.017	0.506	0.020	0.631	0.025	0.798	0.032	0.903	0.044
		\hat{p}_i	0.437	0.018	0.570	0.019	0.674	0.027	0.815	0.029	0.854	0.034
S		\hat{p}	0.261	0.012	0.456	0.020	0.546	0.032	0.755	0.041	0.898	0.048
		\hat{p}_i	0.378	0.009	0.524	0.023	0.641	0.036	0.800	0.037	0.842	0.038

For $p = 0.01, 0.05, 0.1$, and 0.2 , $\mathbb{E}(T)$ increases slightly with β ; for $p = 0.3$, both the overall shape of the Beta distribution and the corresponding $\mathbb{E}(T)$ vary with β , but once again differences in $\mathbb{E}(T)$ are small. This, reassuringly, indicates that, as with the calculation of l^* , the choice of group testing design can be made based on the overall p , which is much more likely to be known than precise values of α and β .

Table S6: Expectation $\mathbb{E}(T)$ and standard deviation $\sigma(T)$ of the number of tests per subject, **by handling of cluster structure during group construction ('Maintained' vs. 'Ignored')**, $\{n, m\}$ and mean prevalence p , for Procedures D' and S, prevalence estimates \hat{p} and \hat{p}_i , and $\alpha = 1$. For common parameters, results for \hat{p} and \hat{p}_i share a common l^* , which is optimized for each p, m , and procedure (D' or S). For each set of parameters, the lower $\mathbb{E}(T)$ and $\sigma(T)$ values between prevalence estimator/individual handling combinations are indicated in **bold**.

GT Algorithm	n	m	Prev. Estimate	Cluster Structure	$p = \frac{\alpha}{\alpha + \beta}$									
					0.01		0.05		0.1		0.2		0.3	
					$\mathbb{E}(T)$	$\sigma(T)$	$\mathbb{E}(T)$	$\sigma(T)$	$\mathbb{E}(T)$	$\sigma(T)$	$\mathbb{E}(T)$	$\sigma(T)$	$\mathbb{E}(T)$	$\sigma(T)$
D'	10	100	\hat{p}	Maintained	0.267	0.028	0.457	0.051	0.587	0.065	0.764	0.081	0.890	0.079
				Ignored	0.269	0.028	0.469	0.053	0.606	0.067	0.787	0.077	0.909	0.074
			\hat{p}_i	Maintained	0.349	0.013	0.476	0.045	0.593	0.064	0.740	0.073	0.826	0.069
				Ignored	0.349	0.014	0.480	0.046	0.600	0.065	0.748	0.073	0.832	0.068
S			\hat{p}	Maintained	0.225	0.023	0.402	0.051	0.543	0.072	0.742	0.090	0.883	0.088
				Ignored	0.219	0.023	0.398	0.053	0.542	0.071	0.734	0.082	0.866	0.086
			\hat{p}_i	Maintained	0.305	0.016	0.439	0.049	0.563	0.069	0.721	0.078	0.813	0.074
				Ignored	0.303	0.016	0.435	0.048	0.558	0.068	0.716	0.078	0.809	0.075
D'	31	32	\hat{p}	Maintained	0.280	0.019	0.466	0.030	0.621	0.034	0.786	0.046	0.903	0.044
				Ignored	0.282	0.019	0.478	0.031	0.641	0.035	0.810	0.039	0.921	0.042
			\hat{p}_i	Maintained	0.436	0.018	0.563	0.035	0.660	0.031	0.782	0.035	0.854	0.034
				Ignored	0.436	0.018	0.566	0.035	0.664	0.032	0.789	0.036	0.862	0.034
S			\hat{p}	Maintained	0.259	0.014	0.451	0.027	0.537	0.043	0.764	0.048	0.898	0.048
				Ignored	0.254	0.015	0.449	0.028	0.538	0.042	0.758	0.042	0.875	0.048
			\hat{p}_i	Maintained	0.378	0.009	0.518	0.027	0.625	0.039	0.763	0.040	0.842	0.038
				Ignored	0.376	0.009	0.514	0.026	0.618	0.040	0.756	0.040	0.837	0.038
D'	100	10	\hat{p}	Maintained	0.438	0.008	0.586	0.013	0.689	0.017	0.801	0.026	0.905	0.022
				Ignored	0.440	0.008	0.594	0.013	0.703	0.016	0.822	0.021	0.924	0.023
			\hat{p}_i	Maintained	0.564	0.008	0.663	0.015	0.746	0.017	0.838	0.015	0.893	0.015
				Ignored	0.564	0.008	0.664	0.015	0.751	0.018	0.842	0.016	0.898	0.015
S			\hat{p}	Maintained	0.316	0.010	0.477	0.015	0.601	0.020	0.775	0.025	0.904	0.025
				Ignored	0.316	0.009	0.478	0.015	0.604	0.019	0.771	0.022	0.878	0.023
			\hat{p}_i	Maintained	0.495	0.007	0.590	0.015	0.679	0.019	0.798	0.020	0.870	0.020
				Ignored	0.494	0.007	0.585	0.015	0.674	0.019	0.793	0.021	0.867	0.020

For $p \leq 0.1$, performance is roughly the same for both methods of construction, in terms of both $\mathbb{E}(T)$ and $\sigma(T)$. For $p \geq 0.2$, preserving clusters moderately improved the performance of Procedure D' (difference in $\mathbb{E}(T) \leq 0.023$), while Procedure S in most cases performed equivalently between methods, although occasionally better when cluster structure was ignored during group construction due to the asymmetry in the expected number of tests under this procedure.

Table S7: Expectation $\mathbb{E}(T)$ and standard deviation $\sigma(T)$ of the number of tests per subject **by the overall size of the data set** ($n \times m \approx \{500, 1000, 2000\}$) and mean prevalence p , for Procedures D' and S, prevalence estimates \hat{p} and \hat{p}_i , and $\alpha = 1$. For common parameters, results for \hat{p} and \hat{p}_i share a common l^* , which is optimized for each m, p , and procedure (D' or S).

GT Algorithm	n	m	Prevalence Estimate	$p = \frac{\alpha}{\alpha + \beta}$										
				0.01		0.05		0.1		0.2		0.3		
				$\mathbb{E}(T)$	$\sigma(T)$	$\mathbb{E}(T)$	$\sigma(T)$	$\mathbb{E}(T)$	$\sigma(T)$	$\mathbb{E}(T)$	$\sigma(T)$	$\mathbb{E}(T)$	$\sigma(T)$	
D'	10	50	\hat{p}	0.331	0.025	0.504	0.047	0.623	0.059	0.785	0.074	0.900	0.073	
			\hat{p}_i	0.406	0.012	0.522	0.041	0.628	0.058	0.764	0.066	0.842	0.063	
			S	\hat{p}	0.249	0.024	0.420	0.051	0.582	0.065	0.765	0.082	0.894	0.080
				\hat{p}_i	0.362	0.018	0.486	0.050	0.600	0.062	0.746	0.071	0.830	0.068
D'	22	23	\hat{p}	0.314	0.022	0.488	0.035	0.613	0.042	0.801	0.048	0.910	0.049	
			\hat{p}_i	0.459	0.020	0.580	0.039	0.684	0.046	0.798	0.039	0.865	0.037	
			S	\hat{p}	0.242	0.020	0.410	0.036	0.550	0.050	0.749	0.063	0.895	0.067
				\hat{p}_i	0.424	0.018	0.532	0.037	0.635	0.045	0.771	0.050	0.852	0.048
D'	50	10	\hat{p}	0.440	0.011	0.587	0.018	0.690	0.022	0.801	0.033	0.909	0.037	
			\hat{p}_i	0.564	0.011	0.663	0.021	0.746	0.025	0.838	0.022	0.893	0.021	
			S	\hat{p}	0.320	0.013	0.479	0.021	0.602	0.028	0.777	0.037	0.906	0.040
				\hat{p}_i	0.495	0.010	0.590	0.021	0.679	0.026	0.798	0.029	0.870	0.028
D'	10	100	\hat{p}	0.267	0.028	0.456	0.051	0.587	0.065	0.764	0.081	0.890	0.080	
			\hat{p}_i	0.349	0.013	0.476	0.045	0.593	0.064	0.741	0.073	0.826	0.069	
			S	\hat{p}	0.225	0.023	0.402	0.051	0.543	0.072	0.742	0.091	0.884	0.088
				\hat{p}_i	0.305	0.016	0.438	0.048	0.562	0.068	0.721	0.078	0.813	0.075
D'	31	32	\hat{p}	0.281	0.019	0.466	0.030	0.621	0.034	0.786	0.046	0.903	0.044	
			\hat{p}_i	0.436	0.018	0.563	0.034	0.660	0.031	0.782	0.035	0.854	0.034	
			S	\hat{p}	0.259	0.014	0.450	0.027	0.537	0.043	0.765	0.048	0.898	0.048
				\hat{p}_i	0.378	0.009	0.518	0.026	0.626	0.039	0.763	0.040	0.842	0.038
D'	100	10	\hat{p}	0.439	0.008	0.586	0.013	0.689	0.017	0.801	0.026	0.905	0.022	
			\hat{p}_i	0.564	0.008	0.663	0.015	0.746	0.017	0.838	0.015	0.893	0.015	
			S	\hat{p}	0.316	0.010	0.477	0.015	0.601	0.020	0.775	0.025	0.904	0.025
				\hat{p}_i	0.495	0.007	0.590	0.015	0.679	0.019	0.798	0.021	0.870	0.020
D'	10	200	\hat{p}	0.257	0.027	0.433	0.053	0.569	0.068	0.754	0.084	0.889	0.077	
			\hat{p}_i	0.315	0.018	0.453	0.047	0.575	0.066	0.729	0.076	0.813	0.069	
			S	\hat{p}	0.205	0.024	0.388	0.052	0.531	0.073	0.742	0.089	0.882	0.086
				\hat{p}_i	0.262	0.015	0.403	0.047	0.530	0.068	0.698	0.078	0.795	0.076
D'	44	45	\hat{p}	0.338	0.012	0.511	0.022	0.631	0.029	0.791	0.039	0.903	0.033	
			\hat{p}_i	0.418	0.006	0.532	0.019	0.636	0.027	0.769	0.031	0.845	0.030	
			S	\hat{p}	0.228	0.012	0.421	0.024	0.558	0.033	0.751	0.042	0.899	0.037
				\hat{p}_i	0.352	0.008	0.493	0.023	0.606	0.031	0.750	0.035	0.833	0.032
D'	200	10	\hat{p}	0.437	0.006	0.585	0.009	0.689	0.013	0.800	0.021	0.905	0.014	
			\hat{p}_i	0.564	0.006	0.663	0.011	0.746	0.012	0.838	0.011	0.893	0.011	
			S	\hat{p}	0.313	0.007	0.476	0.010	0.601	0.015	0.775	0.016	0.904	0.015
				\hat{p}_i	0.495	0.005	0.590	0.011	0.679	0.013	0.798	0.015	0.870	0.014

Increasing n for fixed $m = 10$ does not measurably improve $\mathbb{E}(T)$ but does reduce $\sigma(T)$, while increasing m for fixed $n = 10$ improves $\mathbb{E}(T)$ but not $\sigma(T)$.

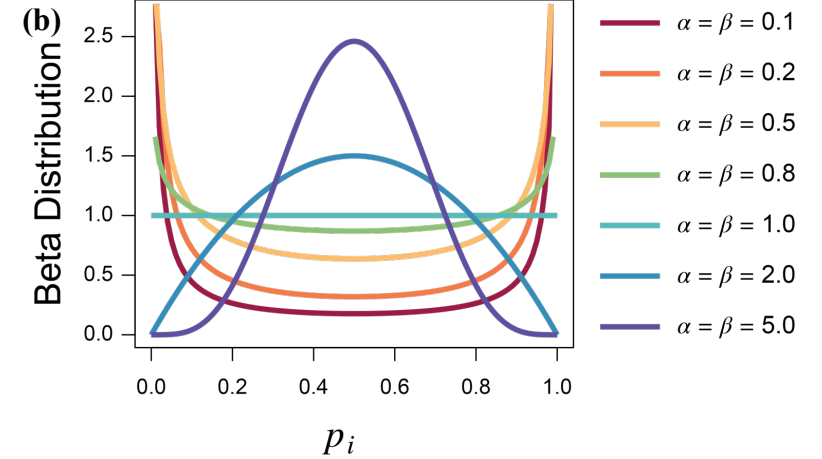
Table S8: Expectation $\mathbb{E}(T)$ and standard deviation $\sigma(T)$ of the number of tests per subject, by prevalence estimate (\hat{p}_i , \tilde{p}_i , and $\hat{\hat{p}}_i$), $\{n, m\}$ and mean prevalence p , for Procedures D' and S and $\alpha = 1$. For common parameters, results for \hat{p}_i , \tilde{p}_i and $\hat{\hat{p}}_i$ share a common l^* , which is optimized for each p , m , and procedure (D' or S).

GT Algorithm	n	m	Prevalence Estimate	$p = \frac{\alpha}{\alpha + \beta}$									
				0.01		0.05		0.1		0.2		0.3	
				$\mathbb{E}(T)$	$\sigma(T)$	$\mathbb{E}(T)$	$\sigma(T)$	$\mathbb{E}(T)$	$\sigma(T)$	$\mathbb{E}(T)$	$\sigma(T)$	$\mathbb{E}(T)$	$\sigma(T)$
D'	10	100	\hat{p}_i	0.349	0.013	0.476	0.045	0.593	0.064	0.741	0.073	0.826	0.069
			\tilde{p}_i	0.254	0.025	0.443	0.048	0.572	0.062	0.731	0.071	0.821	0.070
$\hat{\hat{p}}_i$			0.345	0.018	0.463	0.045	0.580	0.063	0.735	0.074	0.827	0.072	
S			\hat{p}_i	0.305	0.016	0.438	0.048	0.562	0.068	0.721	0.078	0.813	0.075
			\tilde{p}_i	0.216	0.021	0.393	0.049	0.530	0.066	0.705	0.080	0.808	0.075
			$\hat{\hat{p}}_i$	0.301	0.019	0.419	0.048	0.541	0.068	0.710	0.082	0.812	0.079
D'	31	32	\hat{p}_i	0.436	0.018	0.563	0.034	0.660	0.031	0.782	0.035	0.854	0.034
			\tilde{p}_i	0.266	0.015	0.457	0.026	0.612	0.031	0.758	0.039	0.849	0.035
$\hat{\hat{p}}_i$			0.433	0.025	0.531	0.052	0.622	0.036	0.764	0.040	0.850	0.038	
S			\hat{p}_i	0.378	0.009	0.518	0.026	0.626	0.039	0.763	0.040	0.842	0.038
			\tilde{p}_i	0.252	0.011	0.444	0.026	0.529	0.038	0.736	0.042	0.832	0.041
			$\hat{\hat{p}}_i$	0.373	0.022	0.475	0.039	0.591	0.052	0.740	0.043	0.835	0.043
D'	100	10	\hat{p}_i	0.564	0.008	0.663	0.015	0.746	0.017	0.838	0.015	0.893	0.015
			\tilde{p}_i	0.435	0.006	0.583	0.012	0.681	0.015	0.783	0.019	0.872	0.021
$\hat{\hat{p}}_i$			0.558	0.028	0.610	0.039	0.693	0.028	0.789	0.027	0.881	0.023	
S			\hat{p}_i	0.495	0.007	0.590	0.015	0.679	0.019	0.798	0.021	0.870	0.020
			\tilde{p}_i	0.310	0.005	0.473	0.013	0.596	0.018	0.762	0.022	0.863	0.022
			$\hat{\hat{p}}_i$	0.492	0.023	0.548	0.054	0.623	0.042	0.767	0.026	0.867	0.024

Using \tilde{p}_i reduces $\mathbb{E}(T)$ relative to both \hat{p}_i and $\hat{\hat{p}}_i$; this estimate uses the true α and β (although these values are rarely known in practice). The two purely data-driven estimates, \hat{p}_i and $\hat{\hat{p}}_i$, perform equivalently; in most cases, $\hat{\hat{p}}_i$ provides slightly lower values of $\mathbb{E}(T)$ but higher values of $\sigma(T)$. In addition, using $\hat{\hat{p}}_i$ explicitly assumes that the prevalences arise from a Beta distribution, while \hat{p}_i does not (although the optimization of l^* assumes a Beta distribution for all prevalence estimates).

Table S9: (a) Expectation $\mathbb{E}(T)$ and standard deviation $\sigma(T)$ of the number of tests per subject, by $\{n, m\}$, for Procedures D' and S, prevalence estimates \hat{p} and \hat{p}_i , and $\alpha = \beta \in \{0.1, 0.2, 0.5, 0.8, 1.0, 2.0, 5.0\}$ ($p = 0.5$). **(b)** Illustration of Beta distributions used in the simulation. For common parameters, results for \hat{p} and \hat{p}_i share a common l_i^* , which is optimized for each m , and procedure (D' or S). For each set of parameters, the lower $\mathbb{E}[T]$ and $\sigma[T]$ values between prevalence estimators are indicated in **bold**.

(a) GT Algorithm	$\alpha = \beta$	Prev. Estimate	n, m					
			10, 100		31, 32		100, 10	
			$E(T)$	$\sigma(T)$	$E(T)$	$\sigma(T)$	$E(T)$	$\sigma(T)$
D'	0.1	\hat{p}	0.965	0.081	0.991	0.032	1.000	0.005
		\hat{p}_i	0.723	0.102	0.762	0.051	0.817	0.022
S		\hat{p}	0.962	0.088	0.991	0.032	0.999	0.007
		\hat{p}_i	0.704	0.109	0.737	0.055	0.788	0.026
D'	0.2	\hat{p}	0.972	0.067	0.994	0.025	1.000	0.003
		\hat{p}_i	0.771	0.094	0.807	0.048	0.852	0.021
S		\hat{p}	0.970	0.072	0.994	0.024	1.000	0.004
		\hat{p}_i	0.755	0.101	0.790	0.050	0.826	0.024
D'	0.5	\hat{p}	0.985	0.042	0.998	0.012	1.000	0.001
		\hat{p}_i	0.855	0.075	0.880	0.036	0.912	0.017
S		\hat{p}	0.985	0.044	0.998	0.012	1.000	0.002
		\hat{p}_i	0.845	0.080	0.868	0.040	0.894	0.021
D'	0.8	\hat{p}	0.991	0.030	0.999	0.007	1.000	0.000
		\hat{p}_i	0.899	0.062	0.916	0.030	0.942	0.014
S		\hat{p}	0.991	0.029	0.999	0.007	1.000	0.001
		\hat{p}_i	0.889	0.065	0.909	0.033	0.931	0.018
D'	1.0	\hat{p}	0.994	0.025	1.000	0.005	1.000	0.000
		\hat{p}_i	0.917	0.055	0.932	0.027	0.954	0.012
S		\hat{p}	0.994	0.024	1.000	0.005	1.000	0.001
		\hat{p}_i	0.908	0.058	0.926	0.030	0.946	0.016
D'	2.0	\hat{p}	0.999	0.011	1.000	0.002	1.000	0.000
		\hat{p}_i	0.960	0.033	0.970	0.016	0.983	0.006
S		\hat{p}	0.999	0.011	1.000	0.002	1.000	0.000
		\hat{p}_i	0.956	0.036	0.968	0.018	0.982	0.007
D'	5.0	\hat{p}	1.000	0.004	1.000	0.001	1.000	0.000
		\hat{p}_i	0.990	0.015	0.996	0.008	1.000	0.002
S		\hat{p}	1.000	0.003	1.000	0.001	1.000	0.000
		\hat{p}_i	0.989	0.015	0.995	0.007	1.000	0.002

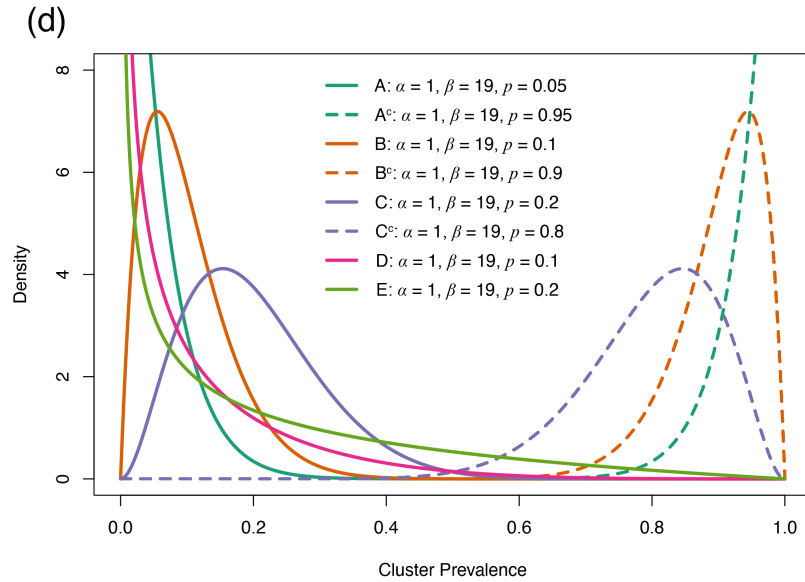


For $\alpha = \beta \geq 2$, and for group testing procedures using \hat{p} , group testing confers no benefits over simply testing each individual. For $\alpha = \beta \leq 1$, group testing using \hat{p}_i is more efficient than single-unit testing, and the efficiency gain increases with decreasing $\alpha = \beta$, with a minimum $\mathbb{E}_{D'}(T) = 0.723$ and $\mathbb{E}_S(T) = 0.704$ for $\alpha = \beta = 0.1$. **(b)** gives intuition for this result: for such low values of $\alpha = \beta$, our estimation of p_i allows us to categorize clusters as either very high prevalence, with individual testing for the remaining $m - l^*$

individuals, or very low prevalence, with group testing and a large \widehat{k}^* for the remaining $m - l^*$. This dichotomization is close to the ideal (pathological) example of using cluster structure in group testing, in which observing the first few individuals in a cluster tells us either that there are no cases in the remaining cluster and no further testing is needed or that the cluster is so full of cases that switching to individual testing is automatic. In most cases, $\sigma(T)$ is lower for \hat{p} than \hat{p}_i , as for most simulated data sets \hat{p} resulted in single-unit testing of all subjects.

Table S9: (c) Expected number of tests for mixtures of Beta distributions (illustrated in panel (d)), by mixture proportion and component distributions (with corresponding overall prevalence p), for Procedures D' and S, prevalence estimates \hat{p} and \hat{p}_i , and cluster handling during group construction (cluster structure maintained vs. ignored). l_i^* for each mixture distribution and procedure is calculated based on Beta $\hat{\alpha}$ and $\hat{\beta}$ estimated from 10,000 randomly generated observations from the mixture distribution. For each set of parameters, the lower $\mathbb{E}[T]$ between prevalence estimators is indicated in **bold**.

(c) Dist. 1	Dist. 2	Prop. Dist. 1	p	Procedure D'				Procedure S			
				Maintained		Ignored		Maintained		Ignored	
				\hat{p}	\hat{p}_i	\hat{p}	\hat{p}_i	\hat{p}	\hat{p}_i	\hat{p}	\hat{p}_i
A	A ^c	25%	0.725	1.000	0.910	1.000	0.911	1.000	0.880	1.000	0.879
		50%	0.5	0.991	0.817	0.998	0.818	0.991	0.747	0.990	0.744
		75%	0.275	0.803	0.724	0.876	0.725	0.798	0.619	0.815	0.616
B	B ^c	25%	0.7	1.000	0.919	1.000	0.920	1.000	0.911	1.000	0.910
		50%	0.5	0.995	0.861	0.999	0.864	0.995	0.822	0.994	0.819
		75%	0.3	0.857	0.790	0.908	0.792	0.861	0.733	0.857	0.728
C	C ^c	25%	0.65	1.000	0.960	1.000	0.961	1.000	0.957	1.000	0.956
		50%	0.5	0.999	0.916	1.000	0.919	0.999	0.911	0.998	0.907
		75%	0.35	0.944	0.873	0.964	0.877	0.942	0.864	0.925	0.859
A	B	25%	0.088	0.561	0.696	0.574	0.698	0.510	0.611	0.506	0.603
		50%	0.075	0.526	0.675	0.540	0.676	0.473	0.581	0.471	0.573
		75%	0.062	0.489	0.653	0.503	0.655	0.488	0.549	0.487	0.544
A	C	25%	0.162	0.714	0.791	0.731	0.795	0.682	0.741	0.674	0.732
		50%	0.125	0.635	0.738	0.659	0.741	0.596	0.667	0.595	0.660
		75%	0.088	0.548	0.685	0.572	0.687	0.546	0.593	0.553	0.588
B	C	25%	0.175	0.762	0.790	0.775	0.796	0.711	0.772	0.701	0.763
		50%	0.15	0.694	0.782	0.709	0.784	0.660	0.729	0.653	0.720
		75%	0.125	0.644	0.750	0.659	0.752	0.604	0.685	0.600	0.677
B	D	25%	0.1	0.573	0.698	0.603	0.700	0.573	0.610	0.581	0.605
		50%	0.1	0.579	0.704	0.603	0.707	0.534	0.621	0.537	0.613
		75%	0.1	0.586	0.711	0.604	0.713	0.540	0.631	0.539	0.623
C	E	25%	0.2	0.756	0.793	0.789	0.798	0.756	0.737	0.754	0.732
		50%	0.2	0.765	0.810	0.790	0.815	0.764	0.764	0.758	0.758
		75%	0.2	0.794	0.806	0.811	0.813	0.751	0.790	0.740	0.782



For the three strongly bimodal mixtures (A & A^c, B & B^c, C & C^c), \hat{p}_i is more efficient than \hat{p} , as estimating cluster-specific prevalences allows for identification of high- and low-prevalence clusters even when there is more heterogeneity than the Beta distributions in (a) or the low and high prevalence clusters are not narrowly distributed around 0% and 100% prevalence. The other scenarios represent increased heterogeneity relative to the Beta distributions examined in the other simulations. In nearly all of these cases, the increased heterogeneity does not cause \hat{p}_i to be more efficient than \hat{p} . For some mixtures with an overall prevalence of 20%, \hat{p}_i performs equivalently to or slightly better than \hat{p} , which is concordant with other simulations where $p = 0.2$.

Table S10: (a) Total expected number of tests per subject $\mathbb{E}(T_T)$. **(b)** Ratio of expected number of missed cases to total expected number of cases ($\mathbb{E}(M)/\mathbb{E}(D)$), by **prevalence estimator**, dilution factor d , mean prevalence p , and dilution handling (‘Miss.’ optimizing group size for Procedure D, ‘Acct.’ optimizing group size using Equation 2.13). For common parameters, results for all prevalence estimators share a common l^* , which is optimized for each p , and m for Procedure D.

(a)

		d										
		0	0.05		0.1		0.2		0.3		0.5	
			Dilution Handling									
p	Prev. Est.	-	Miss.	Acct.	Miss.	Acct.	Miss.	Acct.	Miss.	Acct.	Miss.	Acct.
0.01	\hat{p}	0.265	0.260	0.350	0.255	0.468	0.247	0.676	0.240	0.756	0.229	1.000
	\hat{p}_i	0.414	0.413	1.000	0.411	1.000	0.409	1.000	0.407	1.000	0.403	1.000
	\tilde{p}_i	0.242	0.233	0.248	0.225	0.243	0.211	0.288	0.200	0.320	0.185	0.403
	p_i	0.223	0.221	0.235	0.214	0.251	0.202	0.303	0.192	0.352	0.178	0.415
0.05	\hat{p}	0.452	0.437	0.734	0.423	0.918	0.400	0.976	0.381	0.982	0.350	1.000
	\hat{p}_i	0.541	0.535	1.000	0.530	1.000	0.521	1.000	0.512	1.000	0.498	1.000
	\tilde{p}_i	0.445	0.431	0.647	0.418	1.000	0.395	1.000	0.376	1.000	0.345	1.000
	p_i	0.418	0.405	0.534	0.392	0.631	0.369	0.734	0.349	0.784	0.318	0.828
0.1	\hat{p}	0.596	0.579	0.956	0.562	0.995	0.535	0.999	0.510	0.999	0.471	1.000
	\hat{p}_i	0.653	0.645	1.000	0.637	1.000	0.623	1.000	0.610	1.000	0.589	1.000
	\tilde{p}_i	0.584	0.567	1.000	0.551	1.000	0.522	1.000	0.496	1.000	0.455	1.000
	p_i	0.557	0.541	0.714	0.526	0.792	0.498	0.859	0.474	0.889	0.436	0.913

(b)		d									
		0.05		0.1		0.2		0.3		0.5	
		Dilution Handling									
p	Prev. Est.	Miss.	Acct.	Miss.	Acct.	Miss.	Acct.	Miss.	Acct.	Miss.	Acct.
0.01	\hat{p}	0.084	0.063	0.160	0.095	0.292	0.098	0.401	0.094	0.566	0.000
	\hat{p}_i	0.048	0.000	0.093	0.000	0.176	0.000	0.251	0.000	0.377	0.000
	\tilde{p}_i	0.101	0.088	0.190	0.168	0.341	0.250	0.461	0.317	0.633	0.377
	p_i	0.093	0.078	0.177	0.129	0.319	0.180	0.435	0.201	0.603	0.228
0.05	\hat{p}	0.068	0.023	0.130	0.014	0.242	0.008	0.336	0.008	0.486	0.000
	\hat{p}_i	0.040	0.000	0.077	0.000	0.146	0.000	0.208	0.000	0.313	0.000
	\tilde{p}_i	0.068	0.025	0.130	0.000	0.241	0.000	0.336	0.000	0.486	0.000
	p_i	0.065	0.022	0.124	0.023	0.230	0.019	0.321	0.017	0.465	0.016
0.1	\hat{p}	0.054	0.004	0.105	0.001	0.197	0.000	0.276	0.000	0.406	0.000
	\hat{p}_i	0.032	0.000	0.062	0.000	0.117	0.000	0.166	0.000	0.250	0.000
	\tilde{p}_i	0.055	0.000	0.107	0.000	0.200	0.000	0.281	0.000	0.412	0.000
	p_i	0.048	0.008	0.092	0.007	0.172	0.005	0.243	0.005	0.357	0.004

The presence of unaccounted-for dilution nominally increases efficiency; the total number of tests is reduced due to the possibility for false negative groups that do not receive subsequent per-unit testing. This comes at the cost of missed cases, however. Using \hat{p}_i rather than \hat{p} reduces group sizes and thus lowers the rate of missed cases. Using \tilde{p}_i , and thus the true α and β , or even the true p_i values themselves, further increases efficiency but still carries higher missed-case rates.

Table S11: (a) Total expected number of tests per subject $\mathbb{E}(T_T)$. **(b)** Ratio of expected number of missed cases to total expected number of cases ($\mathbb{E}(M)/\mathbb{E}(D)$) **by cost parameter c** , prevalence estimate \hat{p} or \hat{p}_i , dilution factor d , mean prevalence p , optimizing group size using Equation 2.13. $\alpha = 1$, $n = 31$, $m = 32$, and l^* is optimized for each p , and m for Procedure D; for common parameters, results for all prevalence estimators share a common l^* .

(a)			d					
c	p	Prev. Est.	0	0.05	0.1	0.2	0.3	0.5
50	0.01	\hat{p}	0.265	0.291	0.302	0.352	0.461	0.608
		\hat{p}_i	0.414	1.000	1.000	1.000	1.000	1.000
	0.05	\hat{p}	0.452	0.545	0.629	0.813	0.915	0.970
		\hat{p}_i	0.541	1.000	1.000	1.000	1.000	1.000
	0.1	\hat{p}	0.596	0.808	0.911	0.981	0.995	0.999
		\hat{p}_i	0.653	1.000	1.000	1.000	1.000	1.000
100	0.01	\hat{p}	0.265	0.350	0.468	0.676	0.756	1.000
		\hat{p}_i	0.414	1.000	1.000	1.000	1.000	1.000
	0.05	\hat{p}	0.452	0.734	0.918	0.976	0.982	1.000
		\hat{p}_i	0.541	1.000	1.000	1.000	1.000	1.000
	0.1	\hat{p}	0.596	0.956	0.995	0.999	0.999	1.000
		\hat{p}_i	0.653	1.000	1.000	1.000	1.000	1.000
200	0.01	\hat{p}	0.265	0.484	0.677	1.000	1.000	1.000
		\hat{p}_i	0.414	1.000	1.000	1.000	1.000	1.000
	0.05	\hat{p}	0.452	0.920	0.976	1.000	1.000	1.000
		\hat{p}_i	0.541	1.000	1.000	1.000	1.000	1.000
	0.1	\hat{p}	0.596	0.995	0.999	1.000	1.000	1.000
		\hat{p}_i	0.653	1.000	1.000	1.000	1.000	1.000

(b)			d				
c	p	Prev. Est.	0.05	0.1	0.2	0.3	0.5
50	0.01	\hat{p}	0.076	0.135	0.224	0.249	0.276
		\hat{p}_i	0.000	0.000	0.000	0.000	0.000
	0.05	\hat{p}	0.044	0.067	0.062	0.039	0.022
		\hat{p}_i	0.000	0.000	0.000	0.000	0.000
	0.1	\hat{p}	0.019	0.017	0.007	0.003	0.001
		\hat{p}_i	0.000	0.000	0.000	0.000	0.000
100	0.01	\hat{p}	0.063	0.095	0.098	0.094	0.000
		\hat{p}_i	0.000	0.000	0.000	0.000	0.000
	0.05	\hat{p}	0.023	0.014	0.008	0.008	0.000
		\hat{p}_i	0.000	0.000	0.000	0.000	0.000
	0.1	\hat{p}	0.004	0.001	0.000	0.000	0.000
		\hat{p}_i	0.000	0.000	0.000	0.000	0.000
200	0.01	\hat{p}	0.046	0.052	0.000	0.000	0.000
		\hat{p}_i	0.000	0.000	0.000	0.000	0.000
	0.05	\hat{p}	0.007	0.004	0.000	0.000	0.000
		\hat{p}_i	0.000	0.000	0.000	0.000	0.000
	0.1	\hat{p}	0.000	0.000	0.000	0.000	0.000
		\hat{p}_i	0.000	0.000	0.000	0.000	0.000

With increasing c , group sizes as obtained from Equation 2.13 decrease, increasing the total expected number of tests **(a)** but decreasing the proportion of cases that will be missed **(b)**. When using \hat{p}_i , single-unit testing is optimal for all scenarios. As d increases, more cases are missed despite accounting for dilution in group size optimization. For high c and d , single-unit testing is optimal.

Table S12: (a) Total expected number of tests per subject $\mathbb{E}(T_T)$. **(b)** Ratio of expected number of missed cases to total expected number of cases ($\mathbb{E}(M)/\mathbb{E}(D)$) **by number of clusters n and cluster size m** , prevalence estimate \hat{p} or \hat{p}_i , dilution factor d , mean prevalence p , and dilution handling ('Miss.' optimizing group size for Procedure D, 'Acct.' optimizing group size using Equation 2.13). $\alpha = 1$, $c = 100$, and l^* is optimized for each p , and m for Procedure D; for common parameters, results for all prevalence estimators share a common l^* .

(a)

				<i>d</i>										
				0	0.05		0.1		0.2		0.3		0.5	
				Dilution Handling										
<i>p</i>	Prev. Est.	<i>n</i>	<i>m</i>	-	Miss.	Acct.	Miss.	Acct.	Miss.	Acct.	Miss.	Acct.	Miss.	Acct.
0.01	\hat{p}	10	100	0.263	0.254	0.318	0.248	0.386	0.238	0.658	0.230	0.695	0.218	1.000
		31	32	0.265	0.260	0.350	0.255	0.468	0.247	0.676	0.240	0.756	0.229	1.000
		100	10	0.250	0.396	0.411	0.387	0.442	0.372	0.523	0.360	0.651	0.343	0.779
	\hat{p}_i	10	100	0.351	0.340	1.000	0.338	1.000	0.334	1.000	0.331	1.000	0.325	1.000
		31	32	0.414	0.413	1.000	0.411	1.000	0.409	1.000	0.407	1.000	0.403	1.000
		100	10	0.531	0.530	1.000	0.529	1.000	0.527	1.000	0.525	1.000	0.522	1.000
0.05	\hat{p}	10	100	0.460	0.445	0.665	0.432	0.873	0.408	0.945	0.389	0.983	0.358	0.987
		31	32	0.452	0.437	0.734	0.423	0.918	0.400	0.976	0.381	0.982	0.350	1.000
		100	10	0.536	0.530	0.669	0.522	0.887	0.507	0.990	0.494	0.999	0.472	1.000
	\hat{p}_i	10	100	0.482	0.473	1.000	0.465	1.000	0.451	1.000	0.439	1.000	0.419	1.000
		31	32	0.541	0.535	1.000	0.530	1.000	0.521	1.000	0.512	1.000	0.498	1.000
		100	10	0.631	0.627	1.000	0.623	1.000	0.616	1.000	0.610	1.000	0.599	1.000
0.1	\hat{p}	10	100	0.598	0.581	0.914	0.566	0.987	0.538	0.996	0.514	0.999	0.475	0.999
		31	32	0.596	0.579	0.956	0.562	0.995	0.535	0.999	0.510	0.999	0.471	1.000
		100	10	0.652	0.638	0.972	0.625	0.999	0.602	1.000	0.581	1.000	0.548	1.000
	\hat{p}_i	10	100	0.605	0.592	1.000	0.581	1.000	0.561	1.000	0.544	1.000	0.514	1.000
		31	32	0.653	0.645	1.000	0.637	1.000	0.623	1.000	0.610	1.000	0.589	1.000
		100	10	0.721	0.715	1.000	0.710	1.000	0.699	1.000	0.690	1.000	0.674	1.000

(b)

				<i>d</i>									
				0.05		0.1		0.2		0.3		0.5	
				Dilution Handling									
<i>p</i>	Prev. Est.	<i>n</i>	<i>m</i>	Miss.	Acct.	Miss.	Acct.	Miss.	Acct.	Miss.	Acct.	Miss.	Acct.
0.01	\widehat{p}	10	100	0.090	0.069	0.171	0.110	0.309	0.114	0.422	0.131	0.588	0.000
		31	32	0.084	0.063	0.160	0.095	0.292	0.098	0.401	0.094	0.566	0.000
		100	10	0.106	0.073	0.200	0.119	0.358	0.174	0.484	0.189	0.665	0.198
	\widehat{p}_i	10	100	0.060	0.000	0.117	0.000	0.218	0.000	0.307	0.000	0.451	0.000
		31	32	0.048	0.000	0.093	0.000	0.176	0.000	0.251	0.000	0.377	0.000
		100	10	0.037	0.000	0.072	0.000	0.137	0.000	0.196	0.000	0.297	0.000
0.05	\widehat{p}	10	100	0.068	0.030	0.131	0.022	0.242	0.017	0.336	0.008	0.484	0.008
		31	32	0.068	0.023	0.130	0.014	0.242	0.008	0.336	0.008	0.486	0.000
		100	10	0.051	0.028	0.099	0.018	0.185	0.003	0.260	0.000	0.381	0.000
	\widehat{p}_i	10	100	0.052	0.000	0.100	0.000	0.188	0.000	0.265	0.000	0.392	0.000
		31	32	0.040	0.000	0.077	0.000	0.146	0.000	0.208	0.000	0.313	0.000
		100	10	0.031	0.000	0.060	0.000	0.113	0.000	0.162	0.000	0.246	0.000
0.1	\widehat{p}	10	100	0.055	0.008	0.106	0.002	0.197	0.001	0.277	0.000	0.407	0.000
		31	32	0.054	0.004	0.105	0.001	0.197	0.000	0.276	0.000	0.406	0.000
		100	10	0.046	0.003	0.089	0.000	0.167	0.000	0.235	0.000	0.346	0.000
	\widehat{p}_i	10	100	0.041	0.000	0.080	0.000	0.151	0.000	0.213	0.000	0.317	0.000
		31	32	0.032	0.000	0.062	0.000	0.117	0.000	0.166	0.000	0.250	0.000
		100	10	0.024	0.000	0.048	0.000	0.090	0.000	0.129	0.000	0.195	0.000

For \hat{p}_i , the proportion of missed cases decreases (and expected number of tests increases) with cluster size, as l^* is smaller for smaller clusters, resulting in higher estimated cluster prevalences and smaller groups, which then suffer less dilution. This relationship holds for \hat{p} and $p = 0.1$ as well, but not for \hat{p} and lower values of p ; the relationship between cluster size, l^* , and the distribution of \hat{p} is more complex than that of \hat{p}_i .

Table S13: (a) Total expected number of tests per subject $\mathbb{E}(T_T)$. **(b)** Ratio of expected number of missed cases to total expected number of cases ($\mathbb{E}(M)/\mathbb{E}(D)$) by **Beta shape parameter α** , prevalence estimate \hat{p} or \hat{p}_i , dilution factor d , mean prevalence p , and dilution handling ('Miss.' optimizing group size for Procedure D, 'Acct.' optimizing group size using Equation 2.13). $n = 31$, $m = 32$, $c = 100$, and l^* is optimized for each p , and m for Procedure D; for common parameters, results for all prevalence estimators share a common l^* .

(a)			d										
			0	0.05		0.1		0.2		0.3		0.5	
			Dilution Handling										
α	p	Prev. Est.	-	Miss.	Acct.	Miss.	Acct.	Miss.	Acct.	Miss.	Acct.	Miss.	Acct.
0.5	0.01	\widehat{p}	0.264	0.258	0.349	0.254	0.465	0.246	0.674	0.239	0.755	0.229	1.000
		\widehat{p}_i	0.413	0.412	1.000	0.410	1.000	0.408	1.000	0.406	1.000	0.402	1.000
	0.05	\widehat{p}	0.440	0.425	0.729	0.412	0.915	0.391	0.975	0.374	0.981	0.346	1.000
		\widehat{p}_i	0.528	0.523	1.000	0.519	1.000	0.511	1.000	0.503	1.000	0.490	1.000
	0.1	\widehat{p}	0.575	0.559	0.952	0.543	0.994	0.519	0.999	0.498	0.999	0.463	1.000
		\widehat{p}_i	0.622	0.616	1.000	0.609	1.000	0.598	1.000	0.587	1.000	0.570	1.000
1	0.01	\widehat{p}	0.265	0.260	0.350	0.255	0.468	0.247	0.676	0.240	0.756	0.229	1.000
		\widehat{p}_i	0.414	0.413	1.000	0.411	1.000	0.409	1.000	0.407	1.000	0.403	1.000
	0.05	\widehat{p}	0.452	0.437	0.734	0.423	0.918	0.400	0.976	0.381	0.982	0.350	1.000
		\widehat{p}_i	0.541	0.535	1.000	0.530	1.000	0.521	1.000	0.512	1.000	0.498	1.000
	0.1	\widehat{p}	0.596	0.579	0.956	0.562	0.995	0.535	0.999	0.510	0.999	0.471	1.000
		\widehat{p}_i	0.653	0.645	1.000	0.637	1.000	0.623	1.000	0.610	1.000	0.589	1.000
2	0.01	\widehat{p}	0.266	0.261	0.350	0.256	0.465	0.247	0.676	0.240	0.756	0.229	1.000
		\widehat{p}_i	0.414	0.413	1.000	0.411	1.000	0.409	1.000	0.407	1.000	0.403	1.000
	0.05	\widehat{p}	0.460	0.444	0.737	0.429	0.922	0.405	0.977	0.385	0.983	0.352	1.000
		\widehat{p}_i	0.548	0.542	1.000	0.537	1.000	0.527	1.000	0.517	1.000	0.502	1.000
	0.1	\widehat{p}	0.610	0.593	0.959	0.575	0.996	0.545	0.999	0.519	1.000	0.477	1.000
		\widehat{p}_i	0.674	0.664	1.000	0.656	1.000	0.640	1.000	0.626	1.000	0.602	1.000

(b)			d									
			0.05		0.1		0.2		0.3		0.5	
			Dilution Handling									
α	p	Prev. Est.	Miss.	Acct.	Miss.	Acct.	Miss.	Acct.	Miss.	Acct.	Miss.	Acct.
0.5	0.01	\hat{p}	0.083	0.063	0.159	0.095	0.291	0.099	0.399	0.094	0.564	0.000
		\hat{p}_i	0.047	0.000	0.091	0.000	0.172	0.000	0.246	0.000	0.370	0.000
	0.05	\hat{p}	0.066	0.023	0.128	0.015	0.236	0.008	0.328	0.008	0.474	0.000
		\hat{p}_i	0.036	0.000	0.070	0.000	0.133	0.000	0.189	0.000	0.285	0.000
	0.1	\hat{p}	0.052	0.004	0.100	0.001	0.188	0.000	0.263	0.000	0.386	0.000
		\hat{p}_i	0.027	0.000	0.053	0.000	0.100	0.000	0.142	0.000	0.213	0.000
1	0.01	\hat{p}	0.084	0.063	0.160	0.095	0.292	0.098	0.401	0.094	0.566	0.000
		\hat{p}_i	0.048	0.000	0.093	0.000	0.176	0.000	0.251	0.000	0.377	0.000
	0.05	\hat{p}	0.068	0.023	0.130	0.014	0.242	0.008	0.336	0.008	0.486	0.000
		\hat{p}_i	0.040	0.000	0.077	0.000	0.146	0.000	0.208	0.000	0.313	0.000
	0.1	\hat{p}	0.054	0.004	0.105	0.001	0.197	0.000	0.276	0.000	0.406	0.000
		\hat{p}_i	0.032	0.000	0.062	0.000	0.117	0.000	0.166	0.000	0.250	0.000
2	0.01	\hat{p}	0.084	0.063	0.160	0.095	0.293	0.099	0.402	0.094	0.568	0.000
		\hat{p}_i	0.048	0.000	0.094	0.000	0.178	0.000	0.254	0.000	0.382	0.000
	0.05	\hat{p}	0.069	0.024	0.132	0.014	0.244	0.008	0.340	0.007	0.491	0.000
		\hat{p}_i	0.042	0.000	0.081	0.000	0.154	0.000	0.219	0.000	0.329	0.000
	0.1	\hat{p}	0.056	0.004	0.108	0.001	0.201	0.000	0.283	0.000	0.417	0.000
		\hat{p}_i	0.035	0.000	0.068	0.000	0.128	0.000	0.182	0.000	0.274	0.000

The proportion of missed cases **(b)** is consistent across various shapes of Beta distribution, for the same mean prevalence, while the expected number of tests goes up slightly with increasing α .

Table S14: (a) Total expected number of tests per subject $\mathbb{E}(T_T)$. **(b)** Ratio of expected number of missed cases to total expected number of cases ($\mathbb{E}(M)/\mathbb{E}(D)$) for selected values of Beta shape parameters such that $\alpha = \beta$ ($p = 0.5$), prevalence estimate \hat{p} or \hat{p}_i , dilution factor d , and dilution handling ('Miss.' optimizing group size for Procedure D, 'Acct.' optimizing group size using Equation 2.13). $n = 31$, $m = 32$, $c = 100$, and l^* is optimized for each p , and m for Procedure D; for common parameters, results for all prevalence estimators share a common l^* .

(a)			d										
			0	0.05		0.1		0.2		0.3		0.5	
			Dilution Handling										
α	β	Prev. Est.	-	Miss.	Acct.	Miss.	Acct.	Miss.	Acct.	Miss.	Acct.	Miss.	Acct.
0.1	0.1	\hat{p}	0.997	0.997	1.000	0.997	1.000	0.997	1.000	0.997	1.000	1.000	0.997
		\hat{p}_i	0.755	0.753	1.000	0.752	1.000	0.749	1.000	0.746	1.000	1.000	0.741
0.2	0.2	\hat{p}	0.998	0.998	1.000	0.998	1.000	0.998	1.000	0.998	1.000	1.000	0.998
		\hat{p}_i	0.803	0.800	1.000	0.797	1.000	0.791	1.000	0.787	1.000	1.000	0.779
0.5	0.5	\hat{p}	1.000	0.999	1.000	0.999	1.000	0.999	1.000	0.999	1.000	1.000	0.999
		\hat{p}_i	0.886	0.881	1.000	0.876	1.000	0.867	1.000	0.859	1.000	1.000	0.846
0.8	0.8	\hat{p}	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
		\hat{p}_i	0.925	0.919	1.000	0.914	1.000	0.905	1.000	0.897	1.000	1.000	0.883
1	1	\hat{p}	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
		\hat{p}_i	0.941	0.936	1.000	0.930	1.000	0.921	1.000	0.912	1.000	1.000	0.897

For Beta distributions such as $\alpha = \beta = 0.1$, as with the primary results, using \hat{p}_i can provide improved efficiency (smaller number of tests) compared to \hat{p} as we may distinguish between clusters that are either likely to be full of cases or have no cases. The proportion of missed cases is also low in these settings, as most cases are contained within clusters that will receive individual testing.

(b)			d									
			0.05		0.1		0.2		0.3		0.5	
			Dilution Handling									
α	β	Prev. Est.	Miss.	Acct.	Miss.	Acct.	Miss.	Acct.	Miss.	Acct.	Miss.	Acct.
0.1	0.1	\hat{p}	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000
		\hat{p}_i	0.002	0.000	0.003	0.000	0.006	0.000	0.009	0.000	0.013	0.000
0.2	0.2	\hat{p}	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.001	0.000
		\hat{p}_i	0.003	0.000	0.006	0.000	0.011	0.000	0.015	0.000	0.022	0.000
0.5	0.5	\hat{p}	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.001	0.000
		\hat{p}_i	0.005	0.000	0.010	0.000	0.018	0.000	0.026	0.000	0.038	0.000
0.8	0.8	\hat{p}	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
		\hat{p}_i	0.005	0.000	0.010	0.000	0.018	0.000	0.026	0.000	0.039	0.000
1	1	\hat{p}	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
		\hat{p}_i	0.005	0.000	0.010	0.000	0.019	0.000	0.028	0.000	0.041	0.000

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