

Optimal Group Testing: Structural Properties and Robust Solutions, with Application to Public Health Screening

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October 2018; Revised: March 2019; July 2019

Abstract

We provide a novel regret-based robust formulation of the Dorfman group size problem considering the realistic setting where the prevalence rate is uncertain, establish key structural properties of the optimal solution; and provide an exact algorithm. Our analysis also leads to exact closed-form expressions for the optimal Dorfman group size under a deterministic prevalence rate, which is the problem studied in the extant literature. Thus, our structural results not only unify existing, and mostly empirical, results on the Dorfman group size problem under a deterministic prevalence rate, but, more importantly, enable us to efficiently solve the robust version of this problem to optimality. We demonstrate the value of robust testing schemes with a case study on disease screening using realistic data. Our case study indicates that robust testing schemes can significantly outperform their deterministic counterparts, by not only substantially reducing the maximum regret value, but, in the majority of the cases, reducing testing costs as well. Our findings have important implications on public health screening practices.

Keywords: Group testing; Dorfman testing; robust optimization; regret minimization; screening

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1 Introduction and Motivation

Screening populations to classify individual subjects as *positive* or *negative* for a binary characteristic (e.g., the presence of an infectious disease or a genetic disorder) is essential in many settings. The most straightforward approach to this *classification problem* is to test each subject individually. However, for large populations and under limited resources, individual testing is often too costly. Consequently, testing facilities often use *group testing* in which specimens (e.g., blood, urine) collected from multiple subjects are grouped together and tested via a single test. We use the terms "specimen" and "subject," interchangeably, to refer to both the specimen collected for testing purposes and the corresponding subject. Group testing was first proposed by Dorfman [14] in the 1940's to screen military inductees for syphilis in an economical manner. Dorfman testing scheme has two stages: in the first stage, subjects are tested in groups; if the test outcome for a group is negative, then testing stops and all subjects in the group are classified as negative; if, on the other hand, the test outcome for a group is positive, indicating the presence of at least one positive subject in the group, then testing proceeds to the second stage, in which all subjects in the group are tested individually and classified based on their individual test outcome. A specimen typically contains sufficient material for multiple tests, therefore, such multi-stage testing schemes are possible. The choice of *group size* (i.e., the number of specimens in each group), which we refer to as the *Dorfman group size problem*, has a large impact on the efficiency and accuracy of Dorfman testing.

Since Dorfman's seminal work, various group testing schemes have been studied, ranging from multi-stage hierarchical group testing schemes, to array-based group testing schemes that take advantage of overlapping groups (e.g., [7, 24, 25]). For example, one multi-stage hierarchical group testing scheme divides each positive-testing group in half and tests the new, smaller groups, until either individual testing is reached, or a group tests negative (e.g., [7]). However, such complex multi-stage schemes can be difficult to implement, especially for high volume screening. Therefore, Dorfman testing scheme remains one of the most utilized group testing schemes, mainly because of its simplicity, efficiency, and effectiveness. For instance, an important application of group testing arises in public health screening, and two-stage Dorfman testing schemes are commonly used in this context. The American Red Cross uses Dorfman testing schemes, in groups of size 16, for screening the donated blood for HIV, hepatitis viruses B and C, and West Nile virus (WNV), all of which

can be transmitted through transfusion [12]. Many state public health laboratories utilize Dorfman testing schemes to screen higher risk populations for various infectious diseases. Group testing is also used in other fields; for example, in multi-access communication networks, to minimize conflict resolution time [3]; in industrial quality control, to identify defective products [39]; and in software testing, to detect software bugs or malware [8]. Consequently, in this paper, we study the two-stage Dorfman testing scheme, as our goal is to provide models and actionable guidelines for practitioners.

As discussed above, group testing is used to increase efficiency; thus, maximizing efficiency, or equivalently minimizing the expected number of tests, is integral to Dorfman testing design. Yet accuracy is still important, and a misclassification, in the form of a *false negative* classification (i.e., a true positive subject classified as negative) or a *false positive* classification (i.e., a true negative subject classified as positive), has undesirable consequences. For example, a false negative outcome in donated blood screening results in a potential infection in the transfusion recipient, while leading to a missed diagnosis (and hence to poor health outcomes and higher healthcare expenditures) in infectious disease screening. On the other hand, in many settings, including the examples discussed here, subjects classified as positive through screening are referred for confirmatory testing conducted via gold standard diagnostic tests (which are too costly to be used for screening) that typically correct the false positive outcomes. Thus, a false positive outcome contributes to the overall testing cost, but is less consequential than a false negative outcome. The relative importance of efficiency and accuracy metrics, and how they are modeled, depend on the setting. For example, for screening tests that are highly accurate (having almost perfect *sensitivity*, i.e., true positive probability, and *specificity*, i.e., true negative probability, i.e., *perfect tests*), group testing can maintain high levels of classification accuracy, while reducing testing costs substantially [28]. This is the main reason the efficiency of the Dorfman group size problem has received much attention in the literature (e.g., [14,22,24,28,36,37]). Conversely, for tests that are not highly accurate, a focus on classification accuracy may be appropriate, but this aspect has received very limited attention in the literature. Further, in a setting where a “hard” constraint on the testing budget exists (e.g., an annual screening budget), the objective of maximizing classification accuracy needs to be attained under a testing budget constraint, that is, the efficiency of the testing scheme restricts the accuracy of testing.

The prevalence rate of the binary characteristic (e.g., disease) in question is an important input

for the Dorfman group size problem. However, prevalence rates of many diseases are uncertain, and their estimates are often highly unreliable due to dynamically varying disease patterns (e.g., seasonal, vector-borne diseases, e.g., WNV, babesiosis, Lyme disease, Zika virus [16]), regional variations (e.g., the rate of HIV, per 100,000, in the United States (US) can vary anywhere from 1.8 to 54.4, depending on the state [19]), and surveillance studies that are often limited to small samples due to resource constraints [15, 26, 40]. Consider, for example, the case where prevalence rates vary dynamically over time. In response to such variation, testing facilities can, for instance, modify the testing scheme on a frequent basis, in an attempt to capture the current behavior of the disease. In other words, the testing facility can choose to solve the *deterministic* group size problem, i.e., under the assumption of a deterministic and known prevalence rate, every period (e.g., weekly or monthly). However, if the duration of the chosen period is small, then the testing facility must modify the scheme frequently, which may be infeasible or highly costly due to operational challenges and high set-up costs/time. On the other hand, if the duration of the period is large, then the prevalence rate during that period of time may vary substantially, and hence implementing a deterministic approach may be limiting. Therefore, a *robust* Dorfman testing design, which can take into account the variation in the prevalence rate, becomes important, as this can provide a single robust testing scheme that works *well* for a range of prevalence rate values, instead of just a point estimate.

Unfortunately, the robust version of the Dorfman group size problem is substantially more difficult than its deterministic counterpart, and to our knowledge, has not been studied in the literature. While a vast literature has studied the deterministic problem and its variations (e.g., [2, 14, 21, 22, 28, 37, 39]), this literature fails to provide structural properties of, and exact closed-form expressions for, the optimal deterministic Dorfman group size. Consequently, most of the extant literature solves the deterministic Dorfman group size problem through either enumeration or approximations, and does not offer insight on how the group size should be modified in response to prevalence rate uncertainty. As a note, an interesting variation of the deterministic Dorfman group size problem occurs in a heterogeneous population, i.e., subjects have potentially different risk (probability of positivity), and the tester needs to not only determine a set of Dorfman group sizes, but also assign the subjects to these groups based on their risk; this is the problem studied in a number of papers, e.g., [2, 22, 28, 37], but these analyses still rely on the assumption of a deterministic

and known prevalence rate.

Motivated by these gaps in the literature, we study both the deterministic and robust versions of the Dorfman group size problem, under both efficiency- and accuracy-based objectives. From this perspective, our research is also related to the robust optimization literature, which typically considers mini-max type of objective functions (in our setting, this implies minimizing the maximum expected number of tests, over *all possible* prevalence rate realizations) to produce robust solutions, but this type of objective can produce highly conservative solutions that deviate substantially from the expected value minimizing solutions, potentially leading to a high *price of robustness* [4, 5, 15]. *Regret* (see Section 4 for a formal definition) is an abstract construct that is designed to produce robust solutions that are not overly conservative, and mini-max regret objectives have been utilized in the Operations Research literature in many contexts, including inventory, revenue management, resource allocation, and online decision-making problems, e.g., [15, 32], but to our knowledge, it has not been used in the group testing literature. Both the traditional mini-max objective and the mini-max regret objective are desirable from a practitioner’s perspective, because they are *distribution-free*, that is, they do not require any distribution or moment information for the unknown random variable (in our case, the prevalence rate); all that is required is an uncertainty set (support) of the random variable, which is easier to estimate than its distribution or moments.

Our contributions in this paper correspond to both methodological and application aspects of the Dorfman group size problem. First, we establish key structural properties of the deterministic Dorfman group size problem that minimizes the expected number of tests, show that it follows a *threshold* policy, and provide exact closed-form expressions on the optimal group size as a function of key problem parameters. To our knowledge, this is the first analytical characterization of the optimal Dorfman group size under a deterministic prevalence rate. We then discuss how various empirical findings from the literature can be explained by our analytical characterization, and show that a commonly utilized approximation [36] corresponds to the first-order Taylor series expansion of our optimal solution. Thus, our analytical results *unify* and *extend* existing, and mostly empirical, results. While these results contribute to the literature, and are important in their own right, they are also essential for our study of the aforementioned *novel* variations of the Dorfman group size problem that consider classification accuracy or prevalence rate uncertainty. In our robust Dorfman

group size problem, we consider a mini-max regret objective, which leads to robust solutions with a low price of robustness, while requiring only minimal information on the unknown prevalence rate. We complement our analytical results with a case study on disease screening under dynamically varying prevalence rates. Our case study indicates that in more than 50% of all possible realizations of the prevalence rate, the robust model not only substantially reduces the maximum regret value over the deterministic model, but it also reduces the expected number of tests. In particular, when compared to the deterministic model that relies on an expected prevalence rate, the robust model is 28% more accurate, 16% less costly, and 71% more robust. In addition, the robust model reduces the expected number of tests and improves robustness over current screening practices. Such results demonstrate that robust testing schemes can offer strong protection against variations in the prevalence rate, and also have the potential to reduce testing costs.

Our characterization of the optimal Dorfman scheme, in both the deterministic and robust settings, should spur new analytical research. Further, our results have the potential to alter current screening practices. As discussed above, group testing is commonly utilized in public health screening. Consider, for example, chlamydia and gonorrhea, whose prevalence rates are on the rise in the US [10]: while several states test for these diseases in Dorfman groups of size four (e.g., Iowa and Idaho [27]), other states perform individual testing, but only on a small subset of the state’s adult population (e.g., North Carolina [30]), and there are no guidelines on how the group size should be selected for these screening effort. Consequently, our results can guide screening practices in public policy and other industrial settings. The robust solution aspect is especially relevant in practice, as prevalence rates are often uncertain in many of the settings discussed above. Further, the mini-max regret objective used in our robust formulation can be applied to the group size problem for other group testing schemes, providing a promising future research avenue.

The remainder of this paper is organized as follows. In Section 2, we introduce the notation and the decision problem. Then in Sections 3 and 4, we respectively study the deterministic and robust versions of the Dorfman group size problem, and in Section 5, we discuss our case study. We conclude, in Section 6, with a summary of our findings and directions for future research. For a concise presentation, all proofs are relegated to the online supplementary material.

2 The Notation, Assumptions, and the Decision Problem

Recall that the Dorfman testing scheme has two stages: in the first stage, subjects are tested in groups of size n ; if the test outcome for a group is negative, then testing stops and all subjects in the group are classified as negative for the binary characteristic; if, on the other hand, the test outcome for a group is positive, then testing proceeds to the second stage, in which all subjects in the group are tested individually and classified based on their individual test outcome.

Throughout, we use the terms *positive* and *negative* to refer both to the true status of a subject (i.e., the presence or absence of the binary characteristic) and to the test's outcome that classifies the subject in regard to the binary characteristic. In what follows, we assume that test outcomes are binary. While in some settings the test may measure a continuous-valued marker (e.g., the viral load in blood), continuous test outcomes are typically converted to binary outcomes via the use of predefined testing thresholds (cutoffs). In settings where the testing threshold is a constant, or cannot be modified by the testing facility, the assumption of a binary test outcome is a good modeling choice, and the analyses and results developed in this paper would hold. If, on the other hand, the testing facility can modify the testing threshold, then one must determine not only the optimal group sizes, but also optimal testing thresholds. This is an interesting research direction, but is beyond the scope of the present paper, and we discuss this extension in Section 6.

Let Se and Sp respectively denote the test's *sensitivity* (true positive probability) and *specificity* (true negative probability). We assume, without loss of generality, that the test's true negative probability is higher than its false negative probability, i.e., $Sp/(1 - Se) \geq 1$.¹ Then, $Se + Sp - 1 \in [0, 1]$. We assume that the test sensitivity and specificity are constants that are independent of group size. As discussed in Section 1, for certain tests, the sensitivity of group testing may start deteriorating once the group becomes "too large," due to what is known as the dilution effect of grouping, that is, the marker concentration from true positive subjects is diluted by the true negative subjects in the group. In such cases, test sensitivity values may depend on the group size. However, various studies indicate that the dilution effect is typically negligible when group sizes are within a certain limit [28, 38]. As such, towards the end of Section 3, we also examine the case where the

¹Any test not satisfying this assumption can be transformed into one that satisfies it by interpreting the test outcome in the opposite way.

group size is restricted by an upper limit. Let $P \in (0, 1)$ denote the prevalence rate of the binary characteristic under consideration. In the deterministic Dorfman group size problem (Section 3), we use p to denote the known and deterministic prevalence rate, and in the robust Dorfman group size problem (Section 4), we use P to denote the random prevalence rate. Finally, we let the random variable $T(n)$ denote the per subject number of tests for a Dorfman testing scheme with a group of size $n \geq 1$.

In the deterministic problem, the objective is to determine the group size, $n \in \mathbb{Z}^+$, that minimizes the per subject expected number of tests, that is, the objective is to minimize $\mathbb{E}[T(n)]$. On the other hand, in the robust problem, the objective is to minimize a regret-based function of the same objective function, as discussed subsequently. In the following, we first develop structural properties and closed-form expressions of an optimal solution in the deterministic problem (Section 3), and then study the robust problem (Section 4), which, without the results of Section 3, proves to be intractable.

3 The Deterministic Group Testing Problem

In the deterministic group testing problem, we assume that the prevalence rate is known with certainty and is a constant. As such, throughout this section, we set the prevalence rate to p , and, to simplify the subsequent notation, drop the conditioning on P . As mentioned in Section 2, the objective in the deterministic case is to determine an optimal group size, n_d^* , that minimizes the per subject expected number of tests (the extension to a classification accuracy based objective is discussed at the end of this section), that is, $n_d^* \equiv \operatorname{argmin}_{n \geq 1} \{\mathbb{E}[T(n)]\}$, where $\mathbb{E}[T(n)]$, for a given prevalence rate p , is given by:

$$\begin{aligned} \mathbb{E}[T(n)] &= \mathbb{E}[T(n) | N^+(n) = 0] P(N^+(n) = 0) + \mathbb{E}[T(n) | N^+(n) > 0] [1 - P(N^+(n) = 0)] \\ &= \left(\frac{1}{n} Sp + \frac{1+n}{n} (1 - Sp) \right) (1 - p)^n + \left(\frac{1}{n} (1 - Se) + \frac{1+n}{n} Se \right) [1 - (1 - p)^n] \\ &= \frac{1 + n [Se - (Se + Sp - 1)(1 - p)^n]}{n}, \end{aligned} \tag{1}$$

where $N^+(n) \sim \text{Binomial}(n, p)$ denotes the random number of true positive subjects in a group of size n for a prevalence rate of p . Observe that the expected number of tests for a group of n subjects,

given in the numerator of Eq. (1), is either 1, corresponding to the first test applied to the group in the first stage; or, if the group test outcome is positive, i.e., with probability $Se - (Se + Sp - 1)(1 - p)^n$, then the group test is augmented by n individual tests, one for each subject in the group, hence the multiplication of this probability with n (see the remaining part of the numerator). Lastly, the entire term (the expected number of tests for a group of n subjects) is divided by the group size, n , to determine the per subject expected number of tests. In what follows, we first study the properties of $\mathbb{E}[T(n)]$ and of its minimizer n_d^* , under the relaxation of the integrality constraint on n . These properties allow us to: (i) analytically characterize the optimal Dorfman group size, and (ii) identify the conditions under which Dorfman testing outperforms individual testing. From that perspective, the analytical results in this section provide a contribution to the extensive literature on Dorfman testing, which resorts to either enumeration or approximations to determine the optimal group size that minimizes the per subject expected number of tests. Towards this end, we first define the threshold points $\underline{p}$ and $\bar{p}$, and the group sizes n_0 and n_{-1} , which will be important in the subsequent analysis:

$$\underline{p} \equiv 1 - e^{-(Se + Sp - 1)e^{-1}}, \quad (2)$$

$$\bar{p} \equiv 1 - e^{-4(Se + Sp - 1)e^{-2}}, \quad (3)$$

and

$$n_0 \equiv \frac{2}{\ln(1 - p)} W_0 \left(-\frac{1}{2} \left(\frac{\ln \left(\frac{1}{1 - p} \right)}{Se + Sp - 1} \right)^{1/2} \right), \quad (4)$$

$$n_{-1} \equiv \frac{2}{\ln(1 - p)} W_{-1} \left(-\frac{1}{2} \left(\frac{\ln \left(\frac{1}{1 - p} \right)}{Se + Sp - 1} \right)^{1/2} \right), \quad (5)$$

where $\underline{p} \leq \bar{p}$ for all $Se, Sp \in [0, 1]: Se + Sp - 1 \in [0, 1]$, and $W(\cdot)$ is the Lambert W function, with $W_0(\cdot)$ denoting the principle Lambert branch, and $W_{-1}(\cdot)$ denoting the secondary Lambert branch [11].² The Lambert W function, $W(x)$, is defined by the following equation:

$$x = W(x)e^{W(x)}, \quad \forall x \in \mathbb{R}. \quad (6)$$

²Our notation, n_0 and n_{-1} , follows the commonly used notation for the Lambert W function.

In what follows, we review some properties of the Lambert W function that are utilized in the subsequent analysis; we refer the interested reader to [11] for a detailed discussion of the Lambert W function.

Property 1 (From [11]).

1. For $x < -1/e$, Eq. (6) does not have any real roots;
2. For $x \in (-1/e, 0)$, Eq. (6) has two real roots, given by $W_0(x)$ and $W_{-1}(x)$; and
3. For $x \geq 0$, Eq. (6) has only one real root, given by $W_0(x)$.

For reasons that will become clear in the sequel, we are mainly interested in the properties of function $W(x)$ when $x < 0$, summarized in the following result.

Property 2 (From [11]). For all $x \in [-1/e, 0]$, $W_0(x) \in [-1, 0]$ is increasing in x , while $W_{-1}(x) \in [-1, -\infty]$ is decreasing in x , where $W_0(x) \geq W_{-1}(x)$, with the equality attained at $-1/e$.

The following set of results characterize the optimal group size, and show how it critically depends on key problem parameters. In particular, we show that how function $\mathbb{E}[T(n)]$ (Eq. (1)) behaves in group size, n , depends on the prevalence rate, and therefore analyze this function in three mutually exclusive regions of the prevalence rate: $p \in (0, \underline{p}]$, $p \in (\underline{p}, \bar{p})$, and $p \in [\bar{p}, 1]$; and demonstrate our findings in Figure 1. To demonstrate how the behavior of function $\mathbb{E}[T(n)]$, hence the characteristics of an optimal group size, varies with the prevalence rate, consider first the case when the prevalence rate is low; smaller groups most likely contain no true positive subjects, but lead to higher testing costs. However, the probability of having at least one true positive subject in the group grows exponentially with group size, and hence it is not desirable to make the groups "too large." This behavior can be observed in Eq. (1) by setting $(1 - p)^n \approx 1 - np$, yielding $\mathbb{E}[T(n)] = 1/n + Se - (Se + Sp - 1)(1 - np)$, which is unimodal in n . On the other hand, when the prevalence rate is high, the probability that the group contains at least one true positive subject becomes high, making it likely that the group will test positive and hence individual testing will be required; as a result, making the group as large as possible reduces the per subject expected number of tests. We observe this behavior in Eq. (1) by setting $(1 - p)^n \approx 0$, yielding $\mathbb{E}[T(n)] = 1/n + Se$, which is decreasing in n . Because of such drastic differences in the behavior of $\mathbb{E}[T(n)]$, our analysis requires considering three mutually exclusive regions: (i) low prevalence rate, i.e., $(0, \underline{p}]$, (ii) high

prevalence rate, i.e., $[\bar{p}, 1)$, and (iii) all other cases, with a moderate prevalence rate, i.e., $(\underline{p}, \bar{p})$.

Lemma 1. *If $p < \bar{p}$, then $\mathbb{E}[T(n)]$ has exactly two stationary points, given by n_0 and n_{-1} , where n_0 is a local minimum and n_{-1} is a local maximum of $\mathbb{E}[T(n)]$, and $n_0 < n_{-1}$.*

Lemma 1 provides exact analytical expressions for the *unique* local minimum and *unique* local maximum of the $\mathbb{E}[T(n)]$ function when $p < \bar{p}$. Next, we fully characterize the optimal solution. In the following, we use the notation Se^+ to correspond to the limit approaching Se from above.

Theorem 1. *The optimal solution that minimizes $\mathbb{E}[T(n)]$ follows a threshold policy, with the following three cases fully characterizing the optimal solution:*

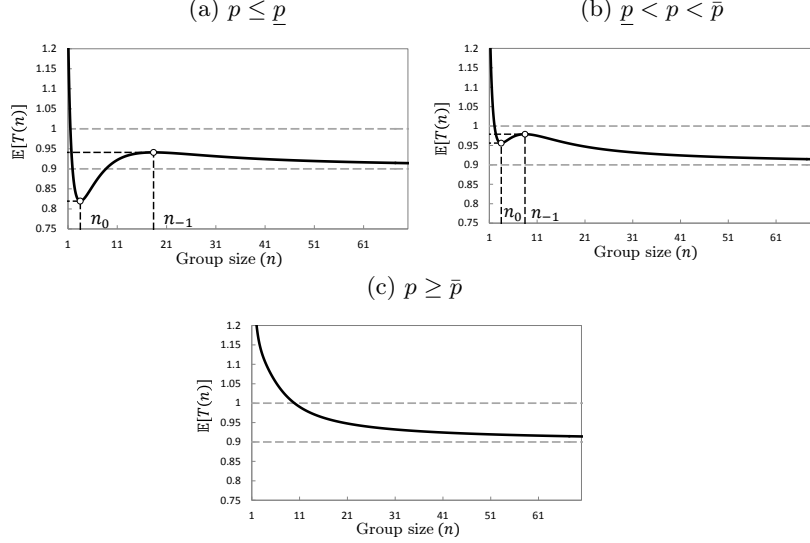
- (i) *If $p \geq \bar{p}$, then $\mathbb{E}[T(n)]$ is non-increasing in n for all $n > 0$. In this case, $n_d^* \rightarrow \infty$, with $\lim_{n \rightarrow \infty} \mathbb{E}[T(n)] \rightarrow Se^+$.*
- (ii) *If $\underline{p} < p < \bar{p}$, then n_0 is a local minimum, but not a global minimum, of $\mathbb{E}[T(n)]$, and the global minimum is attained at $n_d^* \rightarrow \infty$, with $\lim_{n \rightarrow \infty} \mathbb{E}[T(n)] \rightarrow Se^+$.*
- (iii) *If $p \leq \underline{p}$, then n_0 is a global minimum of $\mathbb{E}[T(n)]$, that is, $n_d^* = n_0$.*

Theorem 1 leads to several interesting insights, as we discuss below. For example, according to the first part of the theorem (part (i)), if the prevalence rate is sufficiently high, i.e., $p \geq \bar{p}$, then $\mathbb{E}[T(n)]$ is minimized by placing all the testing population into a single group; see Figure 1c. The following remark links this result to the empirical observations in the literature.

Remark 1. Theorem 1, part (i) provides an analytical justification for prior empirical work that states that for prevalence rates greater than 0.41, the per subject expected number of tests for a perfect test (i.e., $Se = Sp = 1$) is decreasing in n , e.g., [36]; this number can be obtained by setting $Se = Sp = 1$ in Eq. (3), leading to $\bar{p} = 1 - e^{-4e^{-2}} \approx 0.418$.

By parts (i) and (ii) of Theorem 1, when $p > \underline{p}$, $\mathbb{E}[T(n)]$ is minimized by placing all the testing population in a single group; see Figures 1b and 1c. Thus, part (ii) of the theorem expands the set of prevalence rates needed for the optimality of an infinite group size, from $\{p \geq \bar{p}\}$ to $\{p > \underline{p}\}$. Part (iii) of Theorem 1 provides the necessary condition, i.e., $p \leq \underline{p}$, for the local minimum n_0 to correspond to the global minimum. In fact, in most realistic settings, the prevalence rate is expected to satisfy this necessary condition, as the value of $\underline{p}$ is relatively high. In particular, while $\underline{p}$ is decreasing in each of Se and Sp , the condition, $p \leq \underline{p}$, is typically satisfied for realistic test efficacy

Figure 1: $\mathbb{E}[T(n)]$ as a function of group size, n , for different ranges of the prevalence rate, when $Se = Sp = 0.9$



values, e.g., when $Se = Sp = 0.95$, $\underline{p} = 1 - e^{-(Se+Sp-1)e^{-1}} \approx 28\%$ (see Eq. (2)). To put this condition into perspective, consider the prevalence rates of HIV, hepatitis viruses B and C, and WNV in the US, which respectively lie in the intervals $[0.500\%, 1.000\%]$, $[0.250\%, 0.440\%]$, $[1.300\%, 1.900\%]$, and $[0.008\%, 1.100\%]$ [15, 33]. Notice that the prevalence rates of all these infections are much smaller than $\underline{p} \approx 0.28$. Consequently, part (iii) of Theorem 1 is significant, because it provides the global optimal solution for a vast majority of realistic cases, without the need to solve an optimization problem. Interestingly, part (iii) also helps retrieve a commonly used approximation on the optimal group size for perfect tests.

Remark 2. The first-order Taylor series expansion of $n_0(p)$ around zero is given by:

$$n_0(p) \approx \sqrt{\frac{1}{p(Se + Sp - 1)}}, \quad (7)$$

which, for the special case of perfect tests ($Se = 1$, $Sp = 1$), further reduces to $1/\sqrt{p}$, a commonly utilized approximation in the literature, e.g., [36].

While the common approximation, $1/\sqrt{p}$, works relatively well when p is sufficiently small, its performance deteriorates quite rapidly as p becomes larger. For example, when $Se = Sp = 1$, the group size obtained by using the approximation, $1/\sqrt{p}$, can deviate from the optimal group size, $n_0(p)$, by as much as 32%, that is, the relative error, given by $|1/\sqrt{p} - n_0(p)|/n_0(p)$, can be as

high as 32%. More importantly, Theorem 1, and especially part (iii), removes the need for all such approximations, and provides the exact optimal solution for realistic values of p without the need to resort to enumeration. Such closed-form expressions also enable us to provide valuable insights on the characteristics of an optimal solution, as we discuss below.

Lemma 2. *If $p \leq \underline{p}$, then the following properties hold:*

- (i) *The global minimizer of $\mathbb{E}[T(n)]$, $n_0(p)$, is decreasing in both p and $Se + Sp$.*
- (ii) *The optimal objective function value, $\mathbb{E}[T(n_0(p))]$, is increasing in p .*

Lemma 2 states that: (a) for a given test, the optimal group size is smaller for “riskier” populations, i.e., populations with higher prevalence rate values; (b) for a given prevalence rate value, the optimal group size is smaller for more accurate tests; and (c) as the prevalence rate increases, the benefits of group testing are reduced, that is, the reductions in $\mathbb{E}[T(n)]$ are less drastic for riskier populations. More importantly, Lemma 2 leads to the following observation.

Corollary 1. For all $p \in (0, 1)$ and $Se, Sp \in [0, 1]: Se + Sp - 1 \in [0, 1]$, the optimal group size to the deterministic group size problem, n_d^* , satisfies the following condition:

$$n_d^* \geq \frac{e}{Se + Sp - 1}. \quad (8)$$

Corollary 1 is important, as it provides a *global* lower bound on the optimal group size for any prevalence rate value. Moreover, since $Se + Sp - 1 \in [0, 1]$, then the condition in Corollary 1 can also be represented as $n_d^* \geq e \approx 2.72$, implying that for any test and for any prevalence rate value, a group of size one or two will *never* be optimal.

Our characterization of the optimal group size under deterministic p trivially extends to the case where there is an upper limit on group size, which may arise due to technological limitations, or due to the dilution effect, as discussed in Section 1, e.g., [1, 41].

Corollary 2. Let $M \in \mathbb{Z}_+$ denote the upper limit on group size, that is, $n \leq M$. Then, from Theorem 1, we have the following:

1. If $p \leq \underline{p}$, then $n_d^* = \min\{n_0, M\}$.
2. If $\underline{p} < p < \bar{p}$, then $n_d^* = \min\{\arg \min \{\mathbb{E}[T(n_0)], \mathbb{E}[T(M)]\}, M\}$.

3. If $p \geq \bar{p}$, then $n_d^* = M$.

So far, we have determined the optimal Dorfman group size under the relaxation of the integrality constraint on n . However, using the structural properties of the relaxed problem, one can determine the optimal integral group size, as stated in the following result, which is an extension of Corollary 2.

Corollary 3. By Theorem 1, the optimal *integral* group size, n_d^* , can be obtained as follows:

1. If $p \leq \bar{p}$, $n_d^* = \min \left\{ \arg \min \left\{ \mathbb{E}[T(\lfloor n_0 \rfloor)], \mathbb{E}[T(\lceil n_0 \rceil)], \mathbb{E}[T(M)] \right\}, M \right\}$.
2. If $p > \bar{p}$, $n_d^* = M$.

If one is interested in the integral solution without an upper limit on group size, then setting M to infinity in Corollary 3 achieves this outcome. Moreover, Corollary 1 can be generalized to include both the integrality constraint and an upper limit on the group size. In such a case, the global lower bound will be given by the minimum of the floor of the right hand side of Eq. (8) and M , that is, $n_d^* \geq \min\{\lfloor e/(Se + Sp - 1) \rfloor, M\}$.

Next, we turn our attention to a much-discussed question in the literature, of when Dorfman testing outperforms individual testing, i.e., with one test per subject and without utilizing group testing. Our analytical results developed in this section enable us to answer this question, and, not surprisingly, the answer depends on the problem parameters, as we discuss in the subsequent analysis. Observe that in individual testing, the per subject expected number of tests is a constant, equal to 1, independent of the test outcome.

Lemma 3. When $Se < 1$, there always exists a group size, $n > 1$, such that $\mathbb{E}[T(n)] < 1 \forall p \in (0, 1)$.

Thus, when the test sensitivity is imperfect, one can always find a group size that makes Dorfman testing more efficient than individual testing. Interestingly, this result is independent of the prevalence rate, implying that group testing can offer savings even when the prevalence rate is high.

Corollary 4. When $Se = 1$, group testing outperforms individual testing if and only if $p \leq \underline{p}$ (see Theorem 1).

Lemma 3 and Corollary 4 fully characterize the behavior of Dorfman group testing when compared to an individual testing strategy. In general, whether or not group testing outperforms

individual testing heavily depends on the test efficacy values, Se and Sp , and the prevalence rate, p . Moreover, Corollary 4 links our findings to the empirical observations in the literature, as stated in the following remark.

Remark 3. Corollary 4 provides an analytical justification for Dorfman’s empirical observations, which indicate that for a perfect test ($Se = Sp = 1$), group testing outperforms individual testing, in terms of per subject expected number of tests, if and only if $p \leq 0.3$ [14]. According to Corollary 4, when $Se = 1$, group testing outperforms individual testing if and only if $p \leq \underline{p}$. Setting $Se = Sp = 1$ in Eq. (2), leads to $\underline{p} = 1 - e^{-e^{-1}} \approx 0.308$, coinciding with Dorfman’s empirical observations.

Model extensions to consider classification accuracy

So far, we have focused on minimizing the per subject expected number of tests, i.e., maximizing the efficiency of testing. As discussed in Section 1, however, both classification accuracy and testing efficiency may be important metrics in classification problems. Therefore, we next discuss a variation of the deterministic Dorfman group size problem that considers both metrics.

Towards this end, let $\mathbb{E}[FN(n)]$ and $\mathbb{E}[FP(n)]$ respectively denote the per subject expected number of false negatives (true positive subjects falsely classified as negative), and the per subject expected number of false positives (true negative subjects falsely classified as positive), when the group size is n . The expressions for $\mathbb{E}[FN(n)]$ and $\mathbb{E}[FP(n)]$ are given below (see the online supplementary material for derivations):

$$\begin{aligned}\mathbb{E}[FN(n)] &= (1 - Se^2)p, \\ \mathbb{E}[FP(n)] &= Se(1 - Sp)(1 - p) - (1 - Sp)(Se + Sp - 1)(1 - p)^n.\end{aligned}$$

Thus, the per subject expected number of false negatives, $\mathbb{E}[FN(n)]$, is independent of the group size, n , and hence, does not need to be considered for determining the optimal group size. This follows because the test sensitivity (Se) remains constant in group size (see Section 1); thus, the probability of a positive test outcome for a group containing at least one positive subject does *not* depend on the group size, leading to a constant $\mathbb{E}[FN(n)]$. As discussed in Sections 1 and 2,

from a classification accuracy perspective, practitioners are mainly concerned with false negatives, which represent the true positive subjects not detected by screening, and hence, can lead to severe consequences (e.g., potential infection in blood transfusion recipients, missed diagnosis). When the group size becomes “too large,” the sensitivity of group testing may deteriorate due to the dilution effect; in this case, one can either restrict the group size to an upper limit (see Corollary 2), or model the dilution effect of grouping and incorporate it in the optimization model, which is an interesting direction for future research (see Section 6).

In contrast, the per subject expected number of false positives, $\mathbb{E}[FP(n)]$, does depend on the group size, and is monotone increasing in n . To explain this result, consider a true negative subject, which is grouped with other subjects in the first stage of Dorfman. If the group size is small, then it is likely that the group will contain all true negative subjects and test negative, terminating the testing for all subjects in the group and classifying them as negative. On the other hand, the larger the first stage group size is, the larger the likelihood that the group will contain at least one true positive subject, and hence the larger the likelihood that the group will test positive in the first stage, leading to additional (individual) testing for each subject in the group, effectively giving each true negative subject another chance to (falsely) test positive. Thus, the false positive rate increases in group size. While the consequences of a false positive outcome (e.g., further confirmatory testing to resolve the false positive outcome) are much less severe than those of a false negative (see Section 1), the tester may still want to consider the false positives, in conjunction with the number of tests, for determining an optimal group size. The characterization of the structural properties of the $\mathbb{E}[T(n)]$ function, and of its optimal solution, discussed in the first part of this section, proves to be essential for various formulations that incorporate classification accuracy. To illustrate this point, we briefly discuss two relevant formulations that consider classification accuracy (i.e., false positives). The first model determines the group size that leads to the most accurate Dorfman testing scheme (i.e., minimum expected number of false positives), under a given testing budget, B , and may apply, for example, in a setting where the testing laboratory has a limited budget for screening efforts, but confirmatory testing, needed for all subjects classified as positive by screening, is conducted elsewhere and/or paid by another payer. On the other hand, the second formulation determines the group size that minimizes a weighted sum of the per subject expected number of false positives and the expected number of tests (based on the normalized weights w_{FP} and $w_T = 1 - w_{FP}$,

respectively), and may apply, for example, in a setting where the testing laboratory is responsible for (pays for) both screening and confirmatory testing.

$$\begin{aligned} \underset{n}{\text{minimize}} \quad & \mathbb{E}[FP(n)] \\ \text{subject to} \quad & \mathbb{E}[T(n)] \leq B. \end{aligned} \quad (9)$$

$$\underset{n}{\text{minimize}} \quad w_{FP}\mathbb{E}[FP(n)] + w_T\mathbb{E}[T(n)] \quad (10)$$

The results provided in this section can be readily adopted to determine the optimal solutions to both formulations, as we briefly discuss next (the details can be found in the online supplementary material). For example, for Model (9), it follows, by Theorem 1, that if $p \leq 1 - e^{-(Se+Sp-1)e^{-1}}$ and $\mathbb{E}[T(n_0(p))] \leq B \leq Se$, then the equation, $\mathbb{E}[T(n)] = B$, has exactly two solutions, and the interval between these two solutions represents the feasible region of (9). Moreover, the optimal solution will be attained at the lower bound of this interval, as $\mathbb{E}[FP(n)]$ is increasing in n . A similar analysis of Model (9) can be performed for all other regions of p ; see Table 2 in the online supplementary material. On the other hand, Model (10) can be solved by adopting straightforward modifications to the results obtained in this section. Specifically, the behavior of the new objective function, which is a weighted combination of the per subject expected number of false positives and number of tests, is similar to that of the per subject expected number of tests. Then, by following steps similar to the proof of Theorem 1(i), one can show that the optimal solution to Model (10) also follows a threshold policy and that the objective function can have at most two stationary points; see the online supplementary material for closed-form expressions for these new threshold values and stationary points (analogous to Eqs (2)-(5)). By utilizing such properties, many of the results developed in this section can be extended to also consider the expected number of false positives.

4 The Robust Group Testing Problem

In this section, we study the robust Dorfman group testing problem and discuss how the analytical solution to the deterministic problem (Section 3) can be utilized to obtain an optimal robust group size. In many settings, not only are prevalence rates uncertain, but their estimates are often highly unreliable, as discussed in Section 1. As such, determining robust testing schemes, i.e., testing schemes that work well under prevalence rate uncertainty, becomes important. Towards this end, we

formulate and study a *maximum regret minimization problem*, where regret, following the literature (e.g., [15, 29, 32]), corresponds to the deviation of the selected solution from the optimal solution had one known the true prevalence rate. More formally, the *Regret* function, for a given $n \geq 1$ and $p \in (0, 1)$, is given by:

$$\text{Regret}(n|P = p) = \mathbb{E}[T(n)|P = p] - \mathbb{E}[T(n_d^*(p))|P = p], \quad (11)$$

where $n_d^*(p)$ is the optimal group size to the deterministic problem (Section 3) for a given p . The *mini-max regret* function is developed in the literature as an alternative to the traditional mini-max type of objective functions commonly used in robust optimization (in our setting, this implies minimizing the maximum per subject expected number of tests, over *all possible* prevalence rate realizations), which can be overly conservative, leading to a high *price of robustness*, i.e., the relative change in the objective function value under the optimal robust solution compared to its expectation-based deterministic counterpart [5, 15, 32]. The related literature indicates that the mini-max regret objective can produce robust solutions, while reducing the price of robustness; as a result, mini-max regret objective has been utilized in many contexts, as discussed in Section 1, but to our knowledge, it has not been used in the group testing literature. A main motivation for choosing a mini-max type regret objective (over, for example, an expected regret type objective) is that it is *distribution-free*, that is, it only requires the range of values that the prevalence rate can take (also referred to as the uncertainty set in the robust optimization literature [4]), and does not require either the distribution or the moments of the unknown prevalence rate, which can be very difficult to estimate accurately. This is in direct contrast with other objectives, such as the minimization of an expected regret, that may require the distribution of the unknown prevalence rate. The use of a mini-max regret objective is not common within a healthcare setting (except for [15], which considers the blood screening setting), and one of our goals in this paper is to demonstrate the value of robust optimization in the group design setting under prevalence rate uncertainty.

We model the uncertainty around the unknown prevalence rate P using an interval type uncertainty set, i.e., $P \in [a, b]$, where $0 < a < b < 1$, similar to many studies, e.g., [4]. An interval type uncertainty set fits especially well with the epidemiology literature that reports prevalence rates of infectious or genetic diseases in terms of confidence intervals. Then, the objective in the

robust formulation is to find a group size, n_r^* , that minimizes the maximum regret over all possible realizations of the prevalence rate, P :

$$\underset{n \geq 1}{\text{minimize}} \quad \max_{p \in [a, b]} \{ \text{Regret}(n|P = p) \}.$$

This problem is difficult because for any given n , the maximum value of the *inner problem*, i.e., $\max_{p \in [a, b]} \{ \text{Regret}(n|P = p) \}$, is not necessarily attained at a boundary point, i.e., a or b . (See the online supplementary material for an example.) As such, one needs to solve the deterministic group size problem an infinite number of times, i.e., for all $p \in [a, b]$, in order to solve the robust group size problem, and without the closed-form expressions developed in Section 3, this problem becomes intractable. Therefore, in the following, we utilize the results of Section 3 and characterize key structural properties of the Regret function that enable us to optimally solve the inner problem.

Lemma 4. *The maximum value of the Regret function can be represented as:*

$$\max_{p \in [a, b]} \{ \text{Regret}(n|P = p) \} = \begin{cases} \max_{p \in [a, b]} \{ \mathbb{E}[T(n)|P = p] - \mathbb{E}[T(n_0(p))|P = p] \}, & \text{if } b \leq \underline{p}, \\ \max \left\{ \max_{p \in [a, \underline{p}]} \{ \mathbb{E}[T(n)|P = p] - \mathbb{E}[T(n_0(p))|P = p] \}, \frac{1}{n} - (Se + Sp - 1)(1 - b)^n \right\}, & \text{if } a \leq \underline{p} < b, \\ \frac{1}{n} - (Se + Sp - 1)(1 - b)^n, & \text{if } a > \underline{p}, \end{cases}$$

where $\underline{p}$ is as defined in Eq. (2).

Corollary 5. When $a > \underline{p}$, the optimal robust solution that minimizes the maximum regret always coincides with its deterministic counterpart for all $p \in [a, b]$, that is, the optimal maximum regret is equal to zero.

Corollary 5 directly follows from Lemma 4, because when $a > \underline{p}$, the group size that minimizes the per subject expected number of tests is equal to infinity for all $p \in [a, b]$ (see Theorem 1, parts (i) and (ii)). Hence, the optimal robust solution that minimizes the maximum regret is also equal to infinity, with the optimal maximum regret equal to zero, that is, in this case there is no regret, as the robust solution always coincides with its deterministic counterpart for all $p \in [a, b]$. However, the case considered in Corollary 5, i.e., $a > \underline{p}$, is unrealistic, as the lower estimate of the prevalence rate, a , is typically much lower than $\underline{p}$. As such, in what follows, we analyze the robust group testing problem when $a \leq \underline{p}$. Moreover, by Lemma 4, in all the remaining cases

(i.e., for all values of the parameters a and b such that $a \leq \underline{p}$), one needs to solve the problem: $\max_{p \in [a, \min\{b, \underline{p}\}]} \{\mathbb{E}[T(n)|P = p] - \mathbb{E}[T(n_d^*(p))|P = p]\}$. Hence, in what follows, we focus on the case when $a < b \leq \underline{p}$, and provide important structural properties of the $\text{Regret}(n|P = p)$ function. These properties enable us to find the global optimal solution to the maximum regret problem (the inner problem). To this end, we define:

$$h(p) \equiv n + \frac{1}{2 \ln(1-p) \left(1 + W_0 \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{(Se+Sp-1)} \right)^{1/2} \right) \right)},$$

with root $\tilde{p}(n)$, that is, $h(\tilde{p}(n)) = 0$.

Lemma 5. *For a given n , if $b \leq \underline{p}$, then:*

1. *if $h(a)h(b) > 0$, then $\text{Regret}(n|P = p)$ has at most one stationary point with respect to p ; and*
2. *if $h(a)h(b) \leq 0$, then $\text{Regret}(n|P = p)$ has at most two stationary points with respect to p .*

Lemma 6. *For a given n , if $\tilde{p}(n)$ exists, then it is unique.*

Recall that by Lemma 4, it is sufficient to analyze the Regret function in the range $b \leq \underline{p}$, as we do in Lemma 7.

Lemma 7. *For a given n , the following implications hold for all $b \leq \underline{p}$:*

- (i) *If $\tilde{p}(n) \in [a, b]$ and $\left. \frac{\partial \text{Regret}(n|P=p)}{\partial p} \right|_{p=\tilde{p}(n)} < 0$, then $\frac{\partial \text{Regret}(n|P=p)}{\partial p} < 0$ for all $p \in [a, b]$.*
- (ii) *If $\left. \frac{\partial \text{Regret}(n|P=p)}{\partial p} \right|_{p=a} > 0$ and $\left. \frac{\partial \text{Regret}(n|P=p)}{\partial p} \right|_{p=b} > 0$, then $\frac{\partial \text{Regret}(n|P=p)}{\partial p} > 0$ for all $p \in [a, b]$.*

Lemmas 5–7 enable us to construct an algorithm, which we refer to as *Regret Root-finding Algorithm (RRA)*, that finds **all** the stationary points, with respect to p , of the $\text{Regret}(n|P = p)$ function for each given n in a given interval of p , leading to the global maximum of the $\text{Regret}(n|P = p)$ function.

Theorem 2. *Algorithm **RRA** finds all stationary points of the $\text{Regret}(n|P = p)$ function with respect to p , for each given n .*

Algorithm 1: Regret Root-finding Algorithm (**RRA**)

Input : Se, Sp, a, b, n

Output: All stationary points of $Regret(n|P = p)$ (if any) with respect to p in $[a, b]$

```
if  $h(a)h(b) > 0$  then
    if  $(\partial Regret(n|P = p)/\partial p|_{p=a})(\partial Regret(n|P = p)/\partial p|_{p=b}) > 0$  then
        | No stationary points in  $[a, b]$ , STOP;
    else
        | One stationary point in  $[a, b]$ . Use a root-finding method to identify it, STOP;
    end
else
    Use a root-finding method to identify the single root of  $h(p)$  in  $[a, b]$ , denoted by  $\tilde{p}(n)$ ; if
     $\partial Regret(n|P = p)/\partial p|_{p=\tilde{p}(n)} < 0$  then
        | No stationary points in  $[a, b]$ , STOP;
    end
    if  $\partial Regret(n|P = p)/\partial p|_{p=\tilde{p}(n)} = 0$  then
        if  $(\partial Regret(n|P = p)/\partial p|_{p=a})(\partial Regret(n|P = p)/\partial p|_{p=\tilde{p}(n)-}) \leq 0$  then
            | Two stationary points in  $[a, b]$ , with one equal to  $\tilde{p}(n)$  and the other in  $[a, \tilde{p}(n))$ . Use a
            root-finding method to identify it, STOP;
        else
            if  $(\partial Regret(n|P = p)/\partial p|_{p=\tilde{p}(n)+})(\partial Regret(n|P = p)/\partial p|_{p=b}) \leq 0$  then
                | Two stationary points in  $[a, b]$ , with one equal to  $\tilde{p}(n)$  and the other in  $(\tilde{p}(n), b]$ . Use a
                root-finding method to identify it, STOP;
            else
                | One stationary point in  $[a, b]$  equal to  $\tilde{p}(n)$ , STOP;
            end
        end
    end
end
if  $\partial Regret(n|P = p)/\partial p|_{p=a} > 0$  and  $\partial Regret(n|P = p)/\partial p|_{p=b} > 0$  then
    | No stationary points in  $[a, b]$ , STOP;
else
    if  $\partial Regret(n|P = p)/\partial p|_{p=a} \leq 0$  then
        | A stationary point exists in  $[a, \tilde{p}(n)]$ , denoted by  $p^{*1}$ . Use a root-finding method to
        identify it;
    else
        | A stationary point exists in  $[\tilde{p}(n), b]$ , denoted by  $p^{*1}$ . Use a root-finding method to
        identify it;
    end
    if  $(\partial Regret(n|P = p)/\partial p|_{p=a})(\partial Regret(n|P = p)/\partial p|_{p=p^{*1}-}) \leq 0$  then
        | Two stationary points in  $[a, b]$ , with one equal to  $p^{*1}$  and the other in  $[a, p^{*1})$ . Use a
        root-finding method to identify it, STOP;
    else
        if  $(\partial Regret(n|P = p)/\partial p|_{p=p^{*1}+})(\partial Regret(n|P = p)/\partial p|_{p=b}) \leq 0$  then
            | Two stationary points in  $[a, b]$ , with one equal to  $p^{*1}$  and the other in  $(p^{*1}, b]$ . Use a
            root-finding method to identify it, STOP;
        else
            | One stationary point in  $[a, b]$  equal to  $p^{*1}$ , STOP;
        end
    end
end
end
end
```

We note that Algorithm **RRA** can utilize any root finding algorithm, such as the bisection method [9] that we utilize in our case study; and its time complexity is equivalent to the time complexity of the utilized root finding algorithm.

Having developed an algorithm that solves the inner problem to optimality, we next discuss the problem of determining the group size $n \in \mathbb{Z}^+$ that minimizes the maximum Regret function without resorting to an exhaustive enumeration on all possible values of the group size, which is simply infeasible if there is no upper bound on the group size. To this end, in what follows, we establish key structural properties of the maximum Regret function that guarantees global optimality.

Theorem 3. *If $a \leq \underline{p}$, then:*

- (i) $n_r^* \geq n_0(\min\{\bar{p}, b\})$, where $n_0(\cdot)$ is given by Eq. (4).
- (ii) The maximum Regret function, i.e., $\max_{p \in [a, b]} \{\text{Regret}(n|P = p)\}$, is decreasing in n for all $n \geq n_{-1}(a)$, where $n_{-1}(\cdot)$ is given by Eq. (5), with $\lim_{n \rightarrow \infty} \max_{p \in [a, b]} \{\text{Regret}(n|P = p)\} \rightarrow (Se + Sp - 1)(1 - a)^{n_d^*(a)} - 1/n_d^*(a)$.

In light of Theorem 3, when $a \leq \underline{p}$, it is sufficient to enumerate over the set $\{\lceil n_0(\min\{\bar{p}, b\}) \rceil, \lceil n_0(\min\{\bar{p}, b\}) \rceil + 1, \dots, \lceil n_{-1}(a) \rceil\}$, to determine the global optimal solution to the robust group testing problem. To this end, let $\hat{n}$ denote the group size that minimizes the maximum regret over this set.

Corollary 6. The global optimal solution to the robust group testing problem, n_r^* , is given by:

$$n_r^* = \begin{cases} \hat{n}, & \text{if } a \leq \underline{p} \text{ and } \max_{p \in [a, b]} \{\text{Regret}(\hat{n}|P = p)\} \leq (Se + Sp - 1)(1 - a)^{n_d^*(a)} - 1/n_d^*(a), \\ \infty, & \text{otherwise.} \end{cases}$$

To explain the result in Corollary 6, we note that when $a > \underline{p}$, by Corollary 5, n_r^* is infinity. On the other hand, if $a \leq \underline{p}$ and $\max_{p \in [a, b]} \{\text{Regret}(\hat{n}|P = p)\} > (Se + Sp - 1)(1 - a)^{n_d^*(a)} - 1/n_d^*(a)$, then, by Theorem 3, the optimal solution is infinity. Lastly, if $a \leq \underline{p}$ and $\max_{p \in [a, b]} \{\text{Regret}(\hat{n}|P = p)\} \leq (Se + Sp - 1)(1 - a)^{n_d^*(a)} - 1/n_d^*(a)$, then by Theorem 3, it must be true that $n_r^* = \hat{n}$. As such, while Lemmas 5–7 enable us to solve the inner problem to optimality, Theorem 3 enables us

to determine the global minimizer of the maximum Regret function by enumerating over a finite and countable domain.

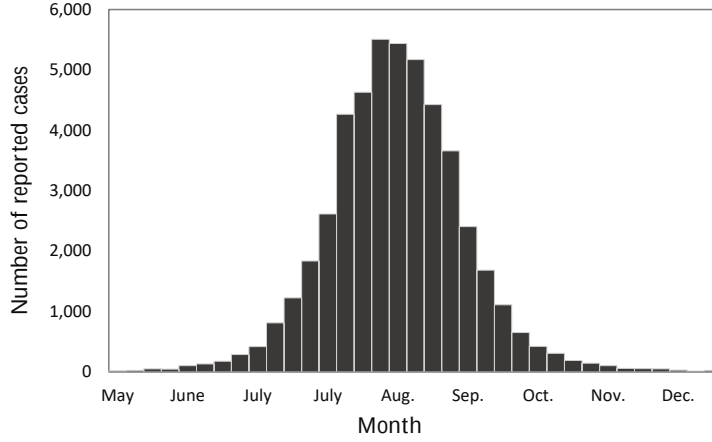
5 Case Study

In this section, we conduct a case study on disease screening under dynamically changing prevalence rates, i.e., the prevalence rate is not a constant but rather varies with time. This case study aims to demonstrate the versatility and effectiveness of robust models, and illustrate how they can be utilized in various settings that go beyond uncertainty in prevalence rates.

Diseases with dynamically changing prevalence rates are common in practice. Consider, for example, vector-borne diseases, which are diseases transmitted by the bite of arthropod vectors, such as bloodsucking insects (e.g., ticks and mosquitoes). Arthropods are exceptionally sensitive to climate variations, and in turn the rates of vector-borne diseases are highly seasonal and vary, sometimes substantially, throughout the year [20]. Vector-borne diseases account for more than 17% of all infectious diseases, and lead to more than 700,000 deaths annually [31]. As such, constructing testing schemes that take into account seasonal variations of the rate of the disease is of utmost importance. Towards this end, in our case study we consider screening for West Nile virus (WNV), the leading cause of mosquito-borne diseases in the US [17]. Currently, the American Red Cross screens all donated blood for WNV, which can be transmitted through blood transfusion [12]. However, to be able to screen a high volume of blood units (around four million blood units annually), the American Red Cross uses Dorfman testing to drastically reduce screening costs [35]. Consequently, determining optimal testing schemes for WNV, as we do in this case study, is of great relevance.

On average, around 230,000 cases of WNV infections are estimated to occur in the US each year [33], and data reveals that the number of reported cases varies substantially throughout the year, as shown in Figure 2, which plots the number of reported cases of WNV, by month, in the US from 1997 till 2017 [18]. Because of this high seasonality, estimates for the rate of WNV vary widely, e.g., [33] reports the rate of the disease to range from 8 to 1,100 cases per 100,000. As such, in this case study we set, a to 0.008% and b to 1.10%. Such a wide range makes the task of developing optimal testing schemes difficult, as the optimal group size is highly sensitive to prevalence rate variations, as shown in Section 3. For example, when $Se = Sp = 0.95$, which represent realistic test

Figure 2: Number of reported cases of WNV, by month, in the US, 1997-2017 [18]



efficacy values for WNV screening [13], the optimal group size varies from 118, when $p = a$, to 11, when $p = b$.

Our objectives in this case study are two-fold: First, we wish to study the sensitivity of the optimal robust solution to variations in the test efficacy values, i.e., Se and Sp . In reality, the testing facility may have several tests to select from, and each of these tests can potentially have different test efficacy values. Thus, a sensitivity analysis on Se and Sp will shed important light on this aspect. Second, and more importantly, we want to compare the performance of robust testing schemes to their deterministic counterparts, and quantify the trade-offs involved. Specifically, we are interested in quantifying the extent to which robust testing schemes improve the maximum regret over their deterministic counterpart, and *the price of robustness*, i.e., the relative change in the objective function value under the optimal robust solution compared to its expectation-based deterministic counterpart.

5.1 Sensitivity Analysis on Se and Sp

Towards the first objective, we conduct a two-way sensitivity analysis, and explore a wide range of values for the test efficacy values, Se and Sp , in $\{0.55, 0.60, 0.65, 0.70, 0.75, 0.80, 0.85, 0.90, 0.95, 1.00\}$. These represent realistic ranges, as several tests for the screening of WNV fall within these ranges (e.g., [6, 13, 34]). We note that for all possible pairs of (Se, Sp) considered in this case study, the condition $b \leq \underline{p}$ is satisfied. Table 1 reports the optimal robust group size, n_r^* , and maximum Regret function value (in parenthesis), $\max_{p \in [a, b]} \{Regret(n_r^* | P = p)\}$, for the different cases of Se

and Sp . Our results indicate that n_r^* is quite sensitive to the test efficacy values, with n_r^* ranging from 19 (corresponding to the most accurate test) to 73 (corresponding to the least accurate test). Interestingly, our results reveal that n_r^* is decreasing in both Se and Sp , implying that smaller group sizes ought to be used when utilizing more accurate tests. One possible explanation for this behavior is that this monotonicity property is also observed in the deterministic model (see Lemma 2), which states that for all $p \in [a, b]$, the use of more accurate tests reduces the optimal deterministic group size, n_d^* . As such, one would expect n_r^* to also reduce, as in the robust model we are attempting to find a group size that works well for all $p \in [a, b]$. Analyzing the maximum regret value, we also find that it is sensitive to variations in Se and Sp , but, interestingly, our results reveal that the maximum regret value is increasing in both Se and Sp . To explain this behavior, we note that the cross-partial derivative of $\mathbb{E}[T(n)]$, with respect to p and $Se + Sp$, is always non-negative. As such, for more accurate tests, $\mathbb{E}[T(n)]$ is more sensitive to variations in p , implying that the maximum regret value is expected to increase.

Current screening practices for WNV use group sizes of either 6 or 16 [35]. Based on our analysis in Table 1, all situations considered led to an optimal group size of 19 or greater. In fact, using $Se = Sp = 0.95$, which represent realistic test efficacy values for the screening of WNV [13], the optimal robust group size is equal to 20 (see Table 1). If a group of size 16 is used instead of 20, then the per subject expected number of tests is slightly reduced (by an average of 2.5%), but the maximum regret value is substantially increased (by 35%). This may be an undesirable outcome, especially in settings in which prevalence rates are highly variable. On the other hand, a group of size 6 significantly increases both the per subject expected number of tests and maximum regret, by an average of 27% and 333%, respectively, over the proposed robust model.

5.2 Comparison of the Robust and Deterministic Models

In this section, we compare the performance of the robust and deterministic models. To achieve this, one needs to select a prevalence rate for the deterministic model, which we denote as p_d . To gain insight, we perform this comparison for all possible values of $p_d \in [a, b]$, specifically for each p_d -value we determine the optimal deterministic group size, given by $n_d^*(p_d)$, and then evaluate the maximum regret value for this group size, i.e., $\max_{p_d \in [a, b]} \{Regret(n_d^*(p_d) | P = p_d)\}$. Of course, the

Table 1: Optimal robust group size, n_r^* , and maximum regret value (in parenthesis), $\max_{p \in [a,b]} \{Regret(n_r^* | P = p)\}$, for the robust group size problem for various test efficacy values (Se, Sp)

$Se \backslash Sp$	0.55	0.60	0.65	0.70	0.75	0.80	0.85	0.90	0.95	1.00
0.55	73 (0.0087)	56 (0.0116)	47 (0.0141)	41 (0.0163)	37 (0.0183)	34 (0.0204)	31 (0.0220)	29 (0.0236)	27 (0.0255)	26 (0.0264)
0.60	56 (0.0116)	47 (0.0141)	41 (0.0163)	37 (0.0183)	34 (0.0204)	31 (0.0220)	29 (0.0236)	27 (0.0255)	26 (0.0264)	25 (0.0277)
0.65	47 (0.0141)	41 (0.0163)	37 (0.0183)	34 (0.0204)	31 (0.0220)	29 (0.0236)	27 (0.0255)	26 (0.0264)	25 (0.0277)	24 (0.0293)
0.70	41 (0.0163)	37 (0.0183)	34 (0.0204)	31 (0.0220)	29 (0.0236)	27 (0.0255)	26 (0.0264)	25 (0.0277)	24 (0.0293)	23 (0.0304)
0.75	37 (0.0183)	34 (0.0204)	31 (0.0220)	29 (0.0236)	27 (0.0255)	26 (0.0264)	25 (0.0277)	24 (0.0293)	23 (0.0304)	22 (0.0313)
0.80	34 (0.0204)	31 (0.0220)	29 (0.0236)	27 (0.0255)	26 (0.0264)	25 (0.0277)	24 (0.0293)	23 (0.0304)	22 (0.0313)	21 (0.0330)
0.85	31 (0.0220)	29 (0.0236)	27 (0.0255)	26 (0.0264)	25 (0.0277)	24 (0.0293)	23 (0.0304)	22 (0.0313)	21 (0.0330)	20 (0.0349)
0.90	29 (0.0236)	27 (0.0255)	26 (0.0264)	25 (0.0277)	24 (0.0293)	23 (0.0304)	22 (0.0313)	21 (0.0330)	20 (0.0349)	20 (0.0347)
0.95	27 (0.0255)	26 (0.0264)	25 (0.0277)	24 (0.0293)	23 (0.0304)	22 (0.0313)	21 (0.0330)	20 (0.0349)	20 (0.0347)	19 (0.0367)
1.00	26 (0.0264)	25 (0.0277)	24 (0.0293)	23 (0.0304)	22 (0.0313)	21 (0.0330)	20 (0.0349)	20 (0.0347)	19 (0.0367)	19 (0.0375)

robust solution is not a function of p_d ; Figure 3a shows the maximum regret for the deterministic model as a function of p_d , and compares it to the maximum regret of the robust model. These results are for $(Se, Sp) = (0.95, 0.95)$, where the maximum regret of the robust model is 0.0347 (see Table 1). Figure 3b provides a histogram of the percent reduction in the maximum regret of the robust solution over the deterministic solution. The figure reveals that for 74% of p_d values, the maximum regret is reduced by at least 30%. In particular, if one sets p_d to the average yearly WNV prevalence rate (equal to 0.10% [33]), which is a reasonable and commonly used choice, the robust model reduces the maximum regret over the deterministic model by an average 71%. Such substantial reductions in the maximum regret value, which occur for a wide range of p_d -values, underscore the importance and value of robust testing schemes.

Having compared the maximum regret value, we now focus on the per subject expected number of tests, i.e., $\mathbb{E}[T(n)]$, for the robust and deterministic solutions so as to quantify the price of robustness,

Figure 3: Performance comparison of the robust and deterministic models, in terms of maximum regret value, when $(Se, Sp) = (0.95, 0.95)$. The figures demonstrate the substantial reductions observed for a wide choice of prevalence rates used in the deterministic model

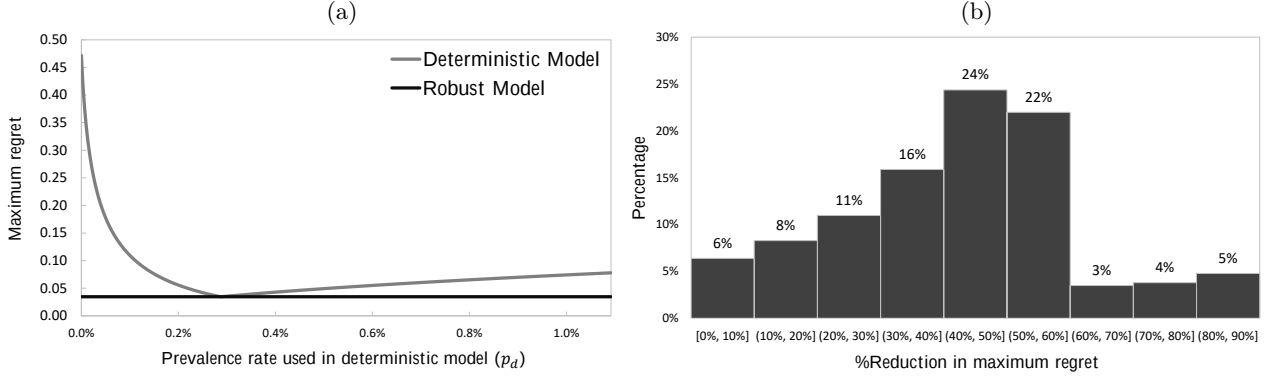
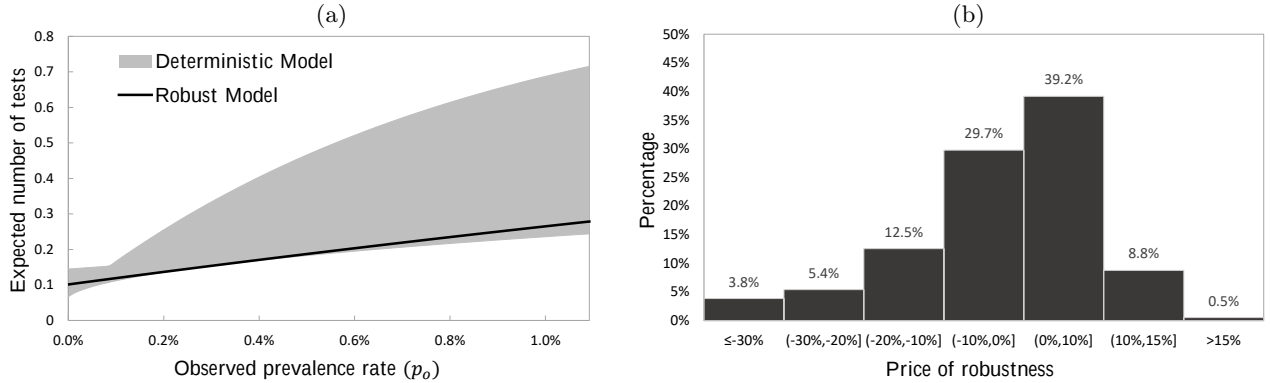


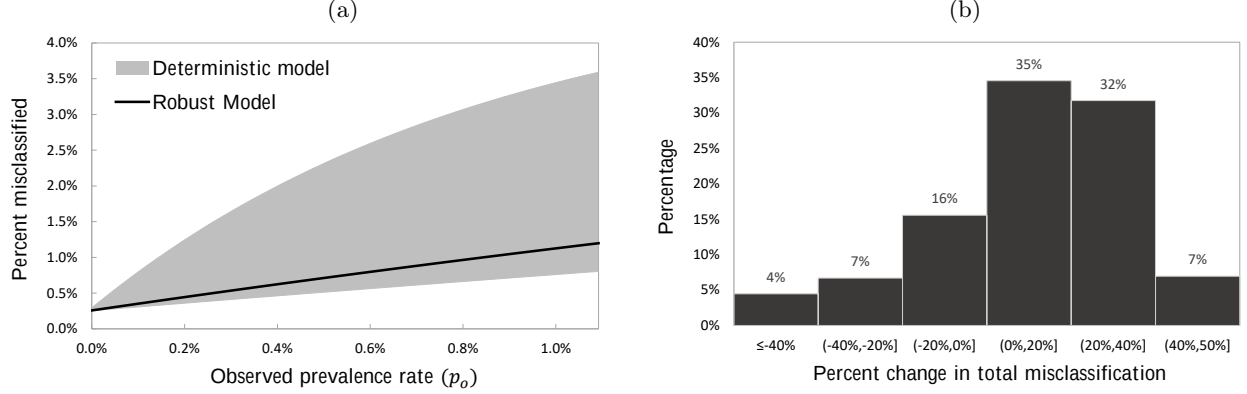
Figure 4: Performance comparison of the robust and deterministic models, in terms of $\mathbb{E}[T(n)]$, when $(Se, Sp) = (0.95, 0.95)$. The figures demonstrate that in the majority of the scenarios, i.e., a combination of p_o and p_d , the robust model outperforms the deterministic model in both the maximum regret and per subject expected number of tests



i.e., the relative change in the per subject expected number of tests under the optimal robust solution compared to its deterministic counterpart [5]. For this purpose, we evaluate $\mathbb{E}[T(n)]$ for each solution as a function of the observed prevalence rate value, denoted by p_o , i.e., the prevalence rate value that the testing facility encounters upon testing. In particular, for the robust solution, we plot $\mathbb{E}[T(n)]$ corresponding to the robust solution, n_r^* , at each observed prevalence rate value, p_o , that is, $\mathbb{E}[T(n_r^*)|P = p_o]$. The deterministic model, on the other hand, is more involved, as one needs to take into account the point estimate of the prevalence rate chosen in the deterministic model, i.e., p_d . Therefore, for each p_o , we derive $\mathbb{E}[T(n_d^*(p_d))|P = p_o]$, for all $p_d \in [a, b]$, thus leading to a *range* of objective function values, each of which represents a different point estimate (p_d) used in the deterministic model.

Figure 4a displays $\mathbb{E}[T(n)]$ for the case of $(Se, Sp) = (0.95, 0.95)$. Specifically, for the robust model, the plot represents the function $\mathbb{E}[T(n_r^* = 20)|P = p_o]$ (see Table 1, the case of $(Se, Sp) = (0.95, 0.95)$); for the deterministic model, each p_o value gives rise to a range of objective function values, each of which corresponding to a different prevalence rate used in the deterministic model (p_d). As expected, when the observed prevalence rate is perfectly aligned with the prevalence rate used in the deterministic model, i.e., $p_o = p_d$, the deterministic model outperforms the robust model in terms of $\mathbb{E}[T(n)]$, and there is a price of robustness associated with the robust solution. This can be seen in Figure 4a by the lower bound of the shaded region, as the gap between this lower bound and the black solid line of the robust model represents the price of robustness. Interestingly, however, in the majority of the cases (i.e., when the point estimate used in the deterministic model is not accurate), the robust model provides a lower per subject expected number of tests than the deterministic model. This is depicted in Figure 4a by the large gap between the upper bound of the shaded region and the black solid line of the robust model, as well as Figure 4b, which displays the histogram for the price of robustness values obtained from all scenarios: In more than 50% of the scenarios, the robust model reduces $\mathbb{E}[T(n)]$ over the deterministic model. We note that a scenario in this case is characterized by a combination of the observed prevalence rate, p_o , and the prevalence rate used in the deterministic model, p_d . While both parameters have continuous sample spaces, in our numerical experiments we uniformly discretize this space into 101 components, leading to a total of $10,201 = 101 \times 101$ (p_o, p_d) scenarios. Thus, in 50% of the scenarios, not only does the robust model substantially reduce the maximum regret value (see Figure 3a), but it also reduces $\mathbb{E}[T(n)]$ due to forecast error in the deterministic model. Figure 4b also shows that only 0.5% of the cases report a price of robustness larger than 15%. Cases with a high price of robustness correspond to scenarios in which the point estimate used in the deterministic model is close to the actual realization, i.e., $p_d \approx p_o$. While such scenarios can occur, in reality the probability of p_o being close to p_d is quite low, especially for emerging or seasonal diseases, such as the WNV considered in our study. Further, setting p_d to the average yearly WNV prevalence rate (equal to 0.10% [33]), leads to the robust model reducing the per subject expected number of tests by an average of 16% over the deterministic model.

Figure 5: Performance comparison of the robust and deterministic models, in terms of misclassification, when $(Se, Sp) = (0.95, 0.95)$. The figures demonstrate that the robust model can lead to substantial reductions in total misclassification over the deterministic model, but, on average, increase the total misclassification over the deterministic model



5.3 Comparison of Expected Misclassification

In this section, we compare the accuracy of robust testing schemes to their deterministic counterparts. While the main objective of this paper is to minimize the per subject expected number of tests, one cannot ignore the importance of classification accuracy, especially within the context of public health screening (see the end of Section 3 for a discussion). In what follows, we conduct a similar comparison to that of the per subject expected number of tests, i.e., we evaluate $\mathbb{E}[FN(n)] + \mathbb{E}[FP(n)]$ for each solution as a function of the observed prevalence rate value, p_o , with the deterministic solution leading to a *range* of values, each of which representing a different point estimate (p_d) used in the deterministic model. Figure 5a displays $\mathbb{E}[FN(n)] + \mathbb{E}[FP(n)]$ for the case of $(Se, Sp) = (0.95, 0.95)$, and it reveals that the robust model can, in some cases, offer substantial reductions in the total number of misclassifications over the deterministic model. This is depicted in Figure 5a by the large region of space between the upper bound of the shaded region and the black solid line. However, Figure 5b, which displays the histogram for the percent change in total misclassification obtained from all scenarios, reveals that the robust model leads to a lower total misclassification in only 27% of the cases. Consequently, the robust model increases the total misclassification by an average of 10% over the deterministic model. To explain this phenomenon, we note that 74% of p_d choices lead to robust group sizes that are larger than that of the deter-

ministic model³. This, in turn, leads to a higher total misclassification, as $\mathbb{E}[FP]$ is increasing in n (see the last part of Section 3). Such an increase in misclassification is an undesirable outcome, but if classification accuracy is of major concern, then the decision-maker should adopt a formulation that incorporates an accuracy metric into the framework (such as Models (9) and (10) discussed in Section 3).

Interestingly, if one sets p_d to the average yearly WNV prevalence rate equal to 0.10% [33], which is a common and sensible choice for p_d , then the robust model reduces the total misclassification by an average of 28%, the maximum regret by 71%, and the per subject expected number of tests by an average of 16%. Consequently, in such a setting, the robust model significantly outperforms the deterministic model with respect to all three measures.

In summary, this case study demonstrates the substantial benefits of robust testing schemes under uncertainty; robust testing schemes significantly reduce the maximum regret value, and, in the majority of the cases, they can also reduce testing costs. Such results underscore the importance and value of considering robust models when designing group testing schemes, especially in settings in which prevalence rate values are either uncertain or dynamically changing.

6 Conclusions

In this paper, we formulate and study a novel regret-based robust formulation of the Dorfman group size problem under prevalence rate uncertainty. By analyzing a robust version of the Dorfman group size problem, we also characterize key structural properties of the deterministic group size problem, and show that the group size that minimizes the per subject expected number of tests follows a threshold policy. These new results allow us to provide exact closed-form expressions for the optimal group size in the deterministic setting, as a function of key problem parameters. We also discuss how our analytical results unify the existing, mostly empirical, results on the deterministic Dorfman group size problem. Our results on the deterministic problem enable us to efficiently solve the robust problem to optimality, which, without the results on the deterministic setting, proves to be intractable. Our case study on the screening of diseases with dynamically changing prevalence

³Specifically, in this example, the robust model leads to larger group sizes if and only if $p_d > 0.294\%$. Because $p_d \in [0.008\%, 1.10\%]$, the proportion of p_d values that satisfy this condition is given by $(1.10\% - 0.294\%)/(1.10\% - 0.008\%) \approx 74\%$.

rates demonstrates that robust testing schemes have the potential to significantly outperform their deterministic counterparts, by not only significantly reducing the maximum regret value, but, in the majority of the cases, reducing testing costs as well, especially when the prevalence rate estimate in the deterministic model does not coincide with the true prevalence rate value. Such results underscore the importance of taking into account prevalence rate uncertainty or variation into the modeling framework.

This work can be expanded in several ways. An important research direction is to explicitly model the dilution effect of grouping. In some settings, the test sensitivity may deteriorate for larger groups (see Section 1). One approach to mitigate the effect of dilution is to set appropriate limits on group size, as discussed in Section 3. A more accurate approach, however, is to model the test sensitivity value as a function of group size, but such functional forms of test sensitivity versus group size are not readily available in the literature for most tests; further, this approach may complicate the analysis considerably. Our analysis also restricts the study to a single test; in reality, multiple tests may be available for a certain disease, with varying efficacy and cost values. Therefore, an interesting future research direction is to consider multiple tests, and let the optimization model select the optimal set of test(s) to administer. Yet another important consideration is to relax the assumption of a binary test outcome. In reality, test outcomes need not be binary, e.g., the test may measure the viral load of an infection. However, continuous test outcomes are typically converted into binary outcomes via the use of predefined testing thresholds. If the testing facility has no control over the testing threshold, then the assumption of a binary test outcome is not limiting, and the results developed in this paper would hold. However, in settings where the testing facility can modify the testing threshold, relaxing this assumption, and allowing the tester to determine both the optimal group size *and* the optimal testing threshold, would be a worthwhile extension of the models studied in this paper. The testing threshold impacts both the classification accuracy and the testing efficiency, and determining the optimal threshold becomes an important component of a screening scheme. We hope that our work drives future research in the aforementioned directions, motivates practitioners to consider implementing robust group testing schemes over their deterministic counterparts, and leads to policy changes to improve screening outcomes.

Acknowledgments: We are grateful to the Associate Editor and two Referees for excellent com-

ments and suggestions that improved the analysis and presentation of the results in the paper. This material is based upon work supported in part by the National Science Foundation under Grant No. #1761842. Any opinion, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the National Science Foundation.

References

- [1] H. Aprahamian, D. R. Bish, and E. K. Bish. Residual risk and waste in donated blood with pooled nucleic acid testing. *Statistics in Medicine*, 35(28):5283–5301, 2016.
- [2] H. Aprahamian, D. R. Bish, and E. K. Bish. Optimal risk-based group testing. *Management Science*, 2019.
- [3] T. Berger, N. Mehravari, D. Towsley, and J. Wolf. Random multiple-access communication and group testing. *IEEE Transactions on Communications*, 32(7):769–779, 1984.
- [4] D. Bertsimas, D. B. Brown, and C. Caramanis. Theory and applications of robust optimization. *SIAM Review*, 53(3):464–501, 2011.
- [5] D. Bertsimas and M. Sim. The price of robustness. *Operations Research*, 52(1):35–53, 2004.
- [6] D. R. Bish, E. K. Bish, R. S. Xie, and S. L. Stramer. Going beyond “same-for-all” testing of infectious agents in donated blood. *IIE Transactions*, 46(11):1147–1168, 2014.
- [7] M. S. Black, C. R. Bilder, and J. M. Tebbs. Group testing in heterogeneous populations by using halving algorithms. *Journal of the Royal Statistical Society: Series C (Applied Statistics)*, 61(2):277–290, 2012.
- [8] A. Blass and Y. Gurevich. The logic in computer science column pairwise testing. *Bulletin of EATCS*, 78:100–132, 2002.
- [9] R. L. Burden and J. D. Faires. 2.1 the bisection algorithm. *Numerical Analysis*, 1985.
- [10] CNN. *Rates of three STDs in US reach record high, CDC says*, accessed September, 2018. <https://www.cnn.com/2018/08/28/health/std-rates-united-states-2018-bn/index.html>.
- [11] R. M. Corless, G. H. Gonnet, D. E. Hare, D. J. Jeffrey, and D. E. Knuth. On the Lambert W function. *Advances in Computational Mathematics*, 5(1):329–359, 1996.
- [12] American Red Cross. *Details of tests performed for different infectious agents*, accessed February, 2017. <http://www.redcrossblood.org/learn-about-blood/what-happens-donated-blood/blood-testing>.
- [13] G. Dauphin and S. Zientara. West nile virus: recent trends in diagnosis and vaccine development. *Vaccine*, 25(30):5563–5576, 2007.
- [14] R. Dorfman. The detection of defective members of large populations. *The Annals of Mathematical Statistics*, 14(4):436–440, 1943.

- [15] H. El-Amine, E. K. Bish, and D. R. Bish. Robust postdonation blood screening under prevalence rate uncertainty. *Operations Research*, 66(1):1–17, 2017.
- [16] Centers for Disease Control and Prevention. *Summary of Notifiable Diseases — United States, 2012*, accessed August, 2018. <https://www.cdc.gov/mmwr/preview/mmwrhtml/mm6153a1.htm>.
- [17] Centers for Disease Control and Prevention. *West Nile virus*, accessed February, 2019. <https://www.cdc.gov/westnile/index.html>.
- [18] Centers for Disease Control and Prevention. *West Nile virus*, accessed February, 2019. <https://www.cdc.gov/westnile/statsmaps/cumMapsData.html>.
- [19] Centers for Disease Control and Prevention. *Diagnoses of HIV infection in the United States and dependent Areas, 2015*, accessed July, 2017. <https://www.cdc.gov/hiv/pdf/library/reports/surveillance/cdc-hiv-surveillance-report-2015-vol-27.pdf>.
- [20] European Centre for Disease Prevention and Control. *Vector-borne diseases*, accessed October, 2018. <https://ecdc.europa.eu/en/climate-change/climate-change-europe/vector-borne-diseases>.
- [21] L. E. Graff and R. Roeloffs. Group testing in the presence of test error; an extension of the Dorfman procedure. *Technometrics*, 14(1):113–122, 1972.
- [22] F. K. Hwang. A generalized binomial group testing problem. *Journal of the American Statistical Association*, 70(352):923–926, 1975.
- [23] D. J. Jeffrey, G. A. Kalugin, and N. Murdoch. Lagrange inversion and Lambert W. In *Symbolic and Numeric Algorithms for Scientific Computing (SYNASC), 2015 17th International Symposium*, pages 42–46. IEEE, 2015.
- [24] N. L. Johnson, S. Kotz, and X. Z. Wu. *Inspection Errors for Attributes in Quality Control*, Volume 44. CRC Press, 1991.
- [25] H. Y. Kim, M. G. Hudgens, J. M. Dreyfuss, D. J. Westreich, and C. D. Pilcher. Comparison of group testing algorithms for case identification in the presence of test error. *Biometrics*, 63(4):1152–1163, 2007.
- [26] C. T. Korves, S. J. Goldie, and M. B. Murray. Cost-effectiveness of alternative blood-screening strategies for West Nile virus in the United States. *PLOS Medicine*, 3(2):e21, 2006.
- [27] J. L. Lewis, V. M. Lockary, and S. Kobic. Cost savings and increased efficiency using a stratified specimen pooling strategy for Chlamydia trachomatis and Neisseria gonorrhoeae. *Sexually Transmitted Diseases*, 39(1):46–48, 2012.
- [28] C. S. McMahan, J. M. Tebbs, and C. R. Bilder. Informative Dorfman screening. *Biometrics*, 68(1):287–296, 2012.
- [29] K. Natarajan, D. Shi, and K. C. Toh. A probabilistic model for minmax regret in combinatorial optimization. *Operations Research*, 62(1):160–181, 2013.
- [30] North Carolina State Laboratory of Public Health. *Virology/Serology: Chlamydia/Gonorrhea*, accessed November, 2016. <http://slph.ncpublichealth.com/virology-serology/chlamydia/default.asp>.

- [31] World Health Organization. *Vector-borne diseases*, accessed September, 2018. <http://www.who.int/news-room/fact-sheets/detail/vector-borne-diseases>.
- [32] G. Perakis and G. Roels. Regret in the newsvendor model with partial information. *Operations Research*, 56(1):188–203, 2008.
- [33] L. R. Petersen, P. J. Carson, B. J. Biggerstaff, B. Custer, S. M. Borchardt, and M. P. Busch. Estimated cumulative incidence of West Nile virus infection in US adults, 1999–2010.
- [34] C. Pfliegerer, J. Blümel, M. Schmidt, W. K. Roth, M. K. Houfar, J. Eckert, M. Chudy, E. Menichetti, S. Lechner, and C. M. Nübling. West Nile virus and blood product safety in Germany. *Journal of Medical Virology*, 80(3):557–563, 2008.
- [35] M. Rios, S. Daniel, C. Chancey, I. K. Hewlett, and S. L. Stramer. West Nile virus adheres to human red blood cells in whole blood. *Clinical Infectious Diseases*, 45(2):181–186, 2007.
- [36] S. M. Samuels. The exact solution to the two-stage group-testing problem. *Technometrics*, 20(4):497–500, 1978.
- [37] B. A. Saraniti. Optimal pooled testing. *Health Care Management Science*, 9(2):143–149, 2006.
- [38] E. Shipitsyna, K. Shalepo, A. Savicheva, M. Unemo, and M. Domeika. Pooling samples: the key to sensitive, specific and cost-effective genetic diagnosis of chlamydia trachomatis in low-resource countries. *Acta Dermato-venereologica*, 87(2):140–143, 2007.
- [39] M. Sobel and P. A. Groll. Group testing to eliminate efficiently all defectives in a binomial sample. *Bell System Technical Journal*, 38(5):1179–1252, 1959.
- [40] S. L. Stramer, C. T. Fang, G. A. Foster, A. G. Wagner, J. P. Brodsky, and R. Y. Dodd. West Nile virus among blood donors in the United States, 2003 and 2004. *New England Journal of Medicine*, 353(5):451–459, 2005.
- [41] L. M. Wein and S. A. Zenios. Pooled testing for HIV screening: Capturing the dilution effect. *Operations Research*, 44(4):543–569, 1996.

Online Supplement:

Optimal Group Testing: Structural Properties and Robust Solutions, with Application to Public Health Screening

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A Mathematical Proofs

Lemma 8 (Supporting Lemma). *If $p < \bar{p}$, then: (i) $\partial \mathbb{E}[T(n)]/\partial n$ has exactly two stationary points; and (ii) $\partial \mathbb{E}[T(n)]/\partial n > 0$ for all $n \in (n_0, n_{-1})$.*

Proof of Lemma 8(i). To prove the result of the lemma, we show that when $p < \bar{p}$ the second derivative of the per subject expected number of tests has exactly two roots. The second derivative of the per subject expected number of tests is given by:

$$\frac{\partial^2 \mathbb{E}[T(n)]}{\partial n^2} = \frac{2}{n^3} - (Se + Sp - 1)[\ln(1 - p)]^2(1 - p)^n.$$

Setting the second derivative to zero, and after some algebraic manipulations, we get:

$$\frac{n \ln(1 - p)}{3} e^{\frac{n \ln(1 - p)}{3}} = \frac{1}{3} \left[\frac{2 \ln(1 - p)}{Se + Sp - 1} \right]^{\frac{1}{3}}. \quad (12)$$

According to [11], Eq. (12) has exactly two real solutions if and only if:

$$\frac{1}{3} \left[\frac{2 \ln(1 - p)}{Se + Sp - 1} \right]^{\frac{1}{3}} > -\frac{1}{e} \Leftrightarrow p < 1 - e^{-\frac{27}{2}(Se + Sp - 1)e^{-3}}.$$

Since $p < \bar{p} \leq 1 - e^{-\frac{27}{2}(Se + Sp - 1)e^{-3}}$ for all $Se + Sp - 1 \in [0, 1]$, then this condition is satisfied, hence, for all $p < \bar{p}$, $\partial \mathbb{E}[T(n)]/\partial n$ has exactly two stationary points, completing the proof. $\square$

Proof of Lemma 8(ii). We first note that $\partial \mathbb{E}[T(n)]/\partial n$ does not have any roots between n_0 and n_{-1} , hence for all $n \in (n_0, n_{-1})$, $\partial \mathbb{E}[T(n)]/\partial n$ is of a constant sign. Suppose, by contradiction, that there exists $p < \bar{p}$ such that $\partial \mathbb{E}[T(n)]/\partial n < 0$ for all $n \in (n_0, n_{-1})$. Since $\partial \mathbb{E}[T(n)]/\partial n$ is negative as n approaches zero or infinity, then $\partial \mathbb{E}[T(n)]/\partial n \leq 0$ for all $n > 0$, with zero attained twice at n_0 and n_{-1} . The following conclusions can be made:

- $\partial \mathbb{E}[T(n)]/\partial n$ must increase in n for some interval in $[0, n_0]$ in order to attain a zero at n_0 (since $\partial \mathbb{E}[T(n)]/\partial n < 0$ for all $n < n_0$ and $\mathbb{E}[T(n)]/\partial n|_{n=n_0} = 0$).
- $\partial \mathbb{E}[T(n)]/\partial n$ must decrease after n_0 (since, by contradiction assumption, $\partial \mathbb{E}[T(n)]/\partial n < 0$ for all $n \in (n_0, n_{-1})$). However, since $\partial \mathbb{E}[T(n)]/\partial n$ is zero at n_{-1} , then it must start increasing before n_{-1} to attain zero at n_{-1} .

- $\partial \mathbb{E}[T(n)]/\partial n$ must decrease after n_{-1} (since $\partial \mathbb{E}[T(n)]/\partial n < 0$ for all $n > n_{-1}$).

Based on the above observations, one can conclude that $\partial \mathbb{E}[T(n)]/\partial n$ must have at least three stationary points, which is a contraction, as we showed in Lemma 8(i) that it has exactly two stationary points. Hence, it must be true that for all $p < \bar{p}$, $\partial \mathbb{E}[T(n)]/\partial n > 0$ for all $n \in (n_0, n_{-1})$, completing the proof. $\square$

Proof of Lemma 1. Since $p < \bar{p}$, then, Eq. (13) will have two real roots, which are given by the principle and secondary Lambert W functions [11]. The two solutions, n_0 and n_{-1} , are given by:

$$\begin{aligned}\frac{n_0 \ln(1-p)}{2} &= W_0 \left(-\frac{1}{2} \left(\frac{\ln \left(\frac{1}{1-p} \right)}{Se + Sp - 1} \right)^{1/2} \right), \\ \frac{n_{-1} \ln(1-p)}{2} &= W_{-1} \left(-\frac{1}{2} \left(\frac{\ln \left(\frac{1}{1-p} \right)}{Se + Sp - 1} \right)^{1/2} \right).\end{aligned}$$

Solving for n_0 and n_{-1} leads to the expressions provided in the theorem. To show that $n_0 < n_{-1}$, we note that $W_0(x) > W_{-1}(x)$, for all $x \in (-1/e, 0)$ [11]. Since the following equivalence holds:

$$0 < p < \bar{p} \Leftrightarrow -\frac{1}{e} < -\frac{1}{2} \left(\frac{\ln \left(\frac{1}{1-p} \right)}{Se + Sp - 1} \right)^{1/2} < 0,$$

then one can conclude that $n_0 < n_{-1}$.

To show that n_0 (n_{-1}) is a local minimum (maximum), we note that $\partial \mathbb{E}[T(n)]/\partial n$ is negative as n approaches zero or infinity. Hence, for all $n \leq n_0$ and $n \geq n_{-1}$, $\mathbb{E}[T(n)]$ is decreasing in n . Moreover, for all $n \in (n_0, n_{-1})$, $\partial \mathbb{E}[T(n)]/\partial n$ is positive (see Lemma 8). As such, one can conclude that n_0 is a local minimum and n_{-1} is a local maximum. $\square$

Proof of Theorem 1(i). Taking the derivative of Eq. (1) with respect to n gives:

$$\frac{\partial \mathbb{E}[T(n)]}{\partial n} = -\frac{1}{n^2} - (Se + Sp - 1) \ln(1-p)(1-p)^n.$$

Setting the derivative to zero, i.e., $\partial \mathbb{E}[T(n)]/\partial n = 0$, and after some algebraic manipulations, we get:

$$\frac{n \ln(1-p)}{2} e^{n \ln(1-p)/2} = \pm \frac{1}{2} \left(\frac{\ln \left(\frac{1}{1-p} \right)}{Se + Sp - 1} \right)^{1/2}.$$

Since $p \in (0, 1)$, we have that:

$$\frac{n \ln(1-p)}{2} e^{n \ln(1-p)/2} \leq 0,$$

hence it is sufficient to consider the case where

$$\frac{n \ln(1-p)}{2} e^{n \ln(1-p)/2} = -\frac{1}{2} \left(\frac{\ln \left(\frac{1}{1-p} \right)}{Se + Sp - 1} \right)^{1/2}. \quad (13)$$

Case I: $p = \bar{p}$

In this case, Eq. (13) has exactly one root [11], denoted by n^* , which is given by:

$$n^* = \frac{-2}{\ln(1-p)}.$$

We note that $\partial \mathbb{E}[T(n)]/\partial n$ is negative as n approaches zero or infinity. Hence, one can conclude that $\partial \mathbb{E}[T(n)]/\partial n \leq 0$ for all $n > 0$.

Case II: $p > \bar{p}$

From [11], Eq. (13) does not have real solutions if:

$$-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se + Sp - 1} \right)^{1/2} < -\frac{1}{e} \Leftrightarrow p > \bar{p}.$$

Hence, in this case the derivative does not have real roots, implying that the sign of the derivative is of a constant sign. Noting that

$$\lim_{n \rightarrow 0} \frac{\partial \mathbb{E}[T(n)]}{\partial n} = -\infty < 0, \quad \forall p \in (0, 1),$$

we can conclude that the derivative is always negative for all $n > 0$, completing the proof. $\square$

Proof of Theorem 1(ii). Solving for $\mathbb{E}[T(n_0)] > Se$ gives:

$$\begin{aligned} \Leftrightarrow \frac{1}{n_0} + Se - (Se + Sp - 1)(1-p)^{n_0} &> Se, \\ \Leftrightarrow \frac{1}{n_0} &> (Se + Sp - 1)(1-p)^{n_0}. \end{aligned}$$

Substituting n_0 from Eq. (4) gives:

$$\begin{aligned} \Leftrightarrow \frac{\ln(1-p)}{2W_0 \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se + Sp - 1} \right)^{1/2} \right)} &> (Se + Sp - 1)(1-p)^{\frac{2}{\ln(1-p)} W_0 \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se + Sp - 1} \right)^{1/2} \right)}, \\ \Leftrightarrow \frac{\ln(1-p)}{2(Se + Sp - 1)} &< W_0 \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se + Sp - 1} \right)^{1/2} \right) e^{2W_0 \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se + Sp - 1} \right)^{1/2} \right)}. \end{aligned} \quad (14)$$

From the definition of the Lambert W function, we have that:

$$W_0(x)^2 e^{2W_0(x)} = x^2 \Leftrightarrow W_0(x) e^{2W_0(x)} = \frac{x^2}{W_0(x)}. \quad (15)$$

Substituting Eq. (15) into Eq. (14) gives:

$$W_0 \left(-\frac{1}{2} \left(\frac{\ln \left(\frac{1}{1-p} \right)}{Se + Sp - 1} \right)^{1/2} \right) < -\frac{1}{2}.$$

Since $W_0(x)$ is increasing in x for all $x \in (-1/e, 0)$ [11], then:

$$\begin{aligned} -\frac{1}{2} \left(\frac{\ln \left(\frac{1}{1-p} \right)}{Se + Sp - 1} \right)^{1/2} &< W_0^{-1} \left(-\frac{1}{2} \right) = -\frac{1}{2} e^{-1/2}, \\ \Leftrightarrow p &> 1 - e^{-(Se+Sp-1)e^{-1}} = \underline{p}. \end{aligned}$$

Also, since $4e^{-2} > e^{-1}$, then $\underline{p} \leq \bar{p}$. Hence, for all $p \in (\underline{p}, \bar{p})$, n_0 is a local minimum with $\mathbb{E}[T(n_0)] > Se$. Since n_0 is the only local minimum, and $\lim_{n \rightarrow \infty} \mathbb{E}[T(n)] = Se$, then the group size that minimizes $\mathbb{E}[T(n)]$ is ∞ , concluding the proof. $\square$

Proof of Theorem 1(iii). From the proof of Theorem 1(ii), the following equivalence holds:

$$\text{if } p \leq \underline{p} \Leftrightarrow \mathbb{E}[T(n_0)] \leq Se.$$

As such, since $\lim_{n \rightarrow 0} \mathbb{E}[T(n)] = \infty$ and $\lim_{n \rightarrow \infty} \mathbb{E}[T(n)] = Se^+$, one can conclude that the local minimum n_0 is also a global minimum, completing the proof. $\square$

Proof of Remark 2. The Taylor series expansion of $W_0(x)$ around zero is given by:

$$W_0(x) = W_0(0) + \sum_{i=1}^{\infty} \frac{W_0^{(i)}(0)x^i}{i!}.$$

We note that $W_0(0) = 0$, and from [23], we have that $W_0^{(i)}(0) = (-i)^{i-1}$, which, upon substituting in the previous equation, gives:

$$W_0(x) = \sum_{i=1}^{\infty} \frac{(-i)^{i-1}x^i}{i!}.$$

Then, the first order approximation of $n_0(p)$ around zero is given by:

$$n_0(p) \approx \frac{1}{\sqrt{[-\ln(1-p)](Se + Sp + 1)}}.$$

Noting that the first order Taylor series expansion of $\ln(1-p)$ is $-p$ provides the expression in the remark, completing the proof. $\square$

Proof of Lemma 2(i). Taking the derivative of $n_0(p)$ with respect to p gives:

$$\frac{\partial n_0(p)}{\partial p} = \frac{W_0 \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se+Sp-1} \right)^{1/2} \right) \left[1 + 2W_0 \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se+Sp-1} \right)^{1/2} \right) \right]}{(1-p)[\ln(1-p)]^2 \left[1 + W_0 \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se+Sp-1} \right)^{1/2} \right) \right]}.$$

Note that if $p < \underline{p}$, then $\partial n_0(p)/\partial p \leq 0$ (see proof of Lemma 5). On the other hand, taking the derivative of $n_0(p)$ with respect to $Se + Sp$ gives:

$$\frac{\partial n_0(p)}{\partial (Se + Sp)} = - \frac{W_0 \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se+Sp-1} \right)^{1/2} \right)}{\ln(1-p)(Se + Sp - 1) \left[1 + W_0 \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se+Sp-1} \right)^{1/2} \right) \right]}.$$

Noting that $W_0(x) \in [-1, 0]$ when $x \in [-1/e, 0]$, then $\partial n_0(p)/\partial (Se + Sp) \leq 0$ $\square$

Proof of Lemma 2(ii). For a given prevalence rate value $p \leq \underline{p}$, the per subject expected number of tests at the optimal solution, equal to $n_0(p)$ (since Theorem 1(iii)), is given by:

$$\mathbb{E}[T(n_0(p)|P = p)] = \frac{1}{n_0(p)} + Se - (Se + Sp - 1)(1 - p)^{n_0(p)}.$$

Taking the derivative with respect to p gives:

$$\frac{\partial \mathbb{E}[T(n_0(p)|P = p)]}{\partial p} = - \frac{1}{2(1-p)W_0 \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se+Sp-1} \right)^{1/2} \right)} \geq 0,$$

completing the proof. $\square$

Proof of Lemma 3. For a group size of 1, the per subject expected number of tests is equal to:

$$\mathbb{E}[T(1)] = 1 + Se - (Se + Sp - 1)(1 - p).$$

Since $Sp \leq 1$, then $Se \geq Se + Sp - 1 \geq (Se + Sp - 1)(1 - p)$, and hence $\mathbb{E}[T(1)] \geq 1$. Also, notice that:

$$\lim_{n \rightarrow \infty} \mathbb{E}[T(n)] = Se^+ < 1.$$

Since $\mathbb{E}[T(n)]$ is continuous in n (for the relaxed problem), then, by the intermediate value theorem, there must exist $n > 1$ such that $\mathbb{E}[T(n)] < 1$, completing the proof. $\square$

Proof of Lemma 4. We prove the result for each case separately.

Case I: $b \leq \underline{p}$

In this case, the optimal group size that minimizes the per subject expected number of tests is equal to n_0 , that is, $n_d^* = n_0$ (see Theorem 1(iii)). Then, by the definition of the Regret function

(see Eq. (11)), the $Regret(n, p)$ function is equal to:

$$\begin{aligned} Regret(n, p) &= \mathbb{E}[T(n)] - \mathbb{E}[T(n_d^*(p))], \\ &= \mathbb{E}[T(n)] - \mathbb{E}[T(n_0(p))]. \end{aligned}$$

Hence, the maximum Regret function is given by:

$$\max_{p \in [a, b]} \{Regret(n, p)\} = \max_{p \in [a, b]} \{\mathbb{E}[T(n)] - \mathbb{E}[T(n_0(p))]\},$$

completing the proof for this case.

Case II: $b > \underline{p}$ and $a \leq \underline{p}$

In this case, the maximum Regret function is given by:

$$\max_{p \in [a, b]} \{Regret(n, p)\} = \max \left\{ \max_{p \in [a, \underline{p}]} \{\mathbb{E}[T(n)] - \mathbb{E}[T(n_d^*(p))]\}, \max_{p \in (\underline{p}, b]} \{\mathbb{E}[T(n)] - \mathbb{E}[T(n_d^*(p))]\} \right\}.$$

When $p \in [a, \underline{p}]$, the optimal group size, n_d^* , is equal to $n_0(p)$ (see Theorem 1(iii)), and when $p \in (\underline{p}, b]$ the optimal group size, n_d^* , is equal to ∞ (see Theorems 1(ii) and 1(ii)). As such, the maximum Regret function is given by:

$$\max_{p \in [a, b]} \{Regret(n, p)\} = \max \left\{ \max_{p \in [a, \underline{p}]} \{\mathbb{E}[T(n)] - \mathbb{E}[T(n_0(p))]\}, \max_{p \in (\underline{p}, b]} \{\mathbb{E}[T(n)] - \mathbb{E}[T(\infty)]\} \right\}.$$

When $p \in (\underline{p}, b]$, the $Regret(n, p)$ function is given by:

$$\begin{aligned} Regret(n, p) &= \mathbb{E}[T(n)] - \mathbb{E}[T(\infty)] \\ &= \frac{1}{n} - (Se + Sp - 1)(1 - p)^n, \end{aligned}$$

with

$$\frac{\partial Regret(n, p)}{\partial p} = n(Se + Sp - 1)(1 - p)^{n-1}.$$

Note that, for all $(Se + Sp - 1) \in [0, 1]$, and for all $p \in (0, 1)$, $\partial Regret(n, p)/\partial p \geq 0$. Hence, for this case, the $Regret(n, p)$ function is increasing in p , and the maximum regret is attained at $p = b$, leading to:

$$\max_{p \in (\underline{p}, b]} \{\mathbb{E}[T(n)] - \mathbb{E}[T(\infty)]\} = \frac{1}{n} - (Se + Sp - 1)(1 - b)^n,$$

completing the proof for this case.

Case III: $a > \underline{p}$

In this case, the condition $p > \underline{p}$ is satisfied for all $p \in [a, b]$. Hence, by Theorems 1(i) and 1(ii), the optimal group size for all $p \in [a, b]$ is equal to infinity, and the $Regret(n, p)$ function is thus given by:

$$\begin{aligned} Regret(n, p) &= \mathbb{E}[T(n)] - \mathbb{E}[T(\infty)] \\ &= \frac{1}{n} - (Se + Sp - 1)(1 - p)^n. \end{aligned}$$

Using the results of Case II, one can conclude that :

$$\max_{p \in [\underline{p}, b]} \{\mathbb{E}[T(n)] - \mathbb{E}[T(\infty)]\} = \frac{1}{n} - (Se + Sp - 1)(1 - b)^n, \quad \text{for all } p \in [a, b],$$

completing the proof. $\square$

Proof of Lemma 5. Since, $b \leq \underline{p}$, then the condition $p \leq \underline{p}$ is satisfied for all $p \in [a, b]$. As such, by Theorem 1(iii), $n_d^*(p) = n_0(p)$, and $Regret(n, p)$ is given by:

$$Regret(n, p) = \mathbb{E}[T(n)] - \mathbb{E}[T(n_0(p))].$$

The derivative of $Regret(n, p)$ with respect to p is given by:

$$\frac{\partial Regret(n, p)}{\partial p} = n(Se + Sp - 1)(1 - p)^{n-1} + \frac{1}{2(1 - p)W_0 \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se + Sp - 1} \right)^{1/2} \right)}.$$

Setting the derivative to zero gives the following equation:

$$(1 - p)^n W_0 \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se + Sp - 1} \right)^{1/2} \right) = \frac{-1}{2n(Se + Sp - 1)}. \quad (16)$$

Note that for a given n , the right hand side of Eq. (16) is a constant. The roots of the derivative are the points in which the left hand side of Eq. (16) intersects the constant right hand side term of Eq. (16). In what follows, we show that the left hand side of Eq. (16) can have at most one stationary point, which implies that it can intersect the constant right hand side term of Eq. (16) at most twice, meaning that the derivative can have at most two roots. Towards this end, we define $f(p)$ as:

$$f(p) \equiv (1 - p)^n W_0 \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se + Sp - 1} \right)^{1/2} \right).$$

The derivative of $f(p)$ with respect to p is given by:

$$\frac{\partial f(p)}{\partial p} = (1 - p)^{n-1} W_0 \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se + Sp - 1} \right)^{1/2} \right) \left[-n - \frac{1}{2 \ln(1 - p) \left(1 + W_0 \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se + Sp - 1} \right)^{1/2} \right) \right)} \right].$$

Since $p \in (0, 1)$, then the derivative of $f(p)$ can only attain zero when $h(p) = 0$, where

$$h(p) \equiv -n - \frac{1}{2 \ln(1 - p) \left(1 + W_0 \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se + Sp - 1} \right)^{1/2} \right) \right)}.$$

$h(p) = 0$ can be equivalently written as:

$$-\ln(1-p) \left(1 + W_0 \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se + Sp - 1} \right)^{1/2} \right) \right) = \frac{1}{2n}. \quad (17)$$

Note that the right hand side of Eq. (17) is a constant, and the solutions to Eq. (17) are the intersections of the left hand side of Eq. (17) with the constant right hand side term. In what follows, we show that the left hand side of Eq. (17) is monotone in p , implying that the left hand side of Eq. (17) can intersect the constant right hand side of Eq. (17) at most once. Towards this end, we define $g(p)$ as:

$$g(p) \equiv -\ln(1-p) \left(1 + W_0 \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se + Sp - 1} \right)^{1/2} \right) \right).$$

The derivative of $g(p)$ is given by:

$$\frac{\partial g(p)}{\partial p} = \frac{1}{1-p} \left[1 + W_0(x) + \frac{W_0(x)}{2(1 + W_0(x))} \right],$$

where

$$x \equiv -\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se + Sp - 1} \right)^{1/2}.$$

Next, we show that for all $p \leq \underline{p}$, the following identity holds:

$$1 + W_0(x) + \frac{W_0(x)}{2(1 + W_0(x))} \geq 0.$$

To show this, we first solve the following equation:

$$1 + W_0(x) + \frac{W_0(x)}{2(1 + W_0(x))} = 0,$$

which can be equivalently written as a quadratic equation in $W(x)$ as follows:

$$2[W_0(x)]^2 + 5W_0(x) + 2 = 0.$$

The two solutions to this quadratic equation are given by:

$$W_0(x) = -0.5 \quad \text{and} \quad W_0(x) = -2,$$

but $W_0(x) \in [-1, 0]$ if $x \leq 0$ (which is true in our case) [11], hence we only consider the solution $W_0(x) = -0.5$. From this, we can conclude that for all $W_0(x) \geq -0.5$, the following identity holds:

$$2[W_0(x)]^2 + 5W_0(x) + 2 \geq 0,$$

which, since $1 + W_0(x) > 0$ for $x < 0$ [11], implies that:

$$1 + W_0(x) + \frac{W_0(x)}{2(1 + W_0(x))} \geq 0.$$

However, we have that:

$$W_0(x) \geq -0.5 \Leftrightarrow p \leq \underline{p},$$

which is satisfied, as it is a condition specified in the lemma. Hence, for all $p \leq \underline{p}$, $\partial f(p)/\partial p$ has at most one root.

Case I: $h(a)h(b) > 0$

In this case, $h(p)$ does not have a root in the interval $[a, b]$, hence $\partial f(p)/\partial p$ does not have a root, which means that $\partial f(p)/\partial p$ is of constant sign. As such, $f(p)$ is monotone in p and Eq. (16) can have at most one solution, which implies that $Regret(n, p)$ can have at most one stationary point with respect to p .

Case II: $h(a)h(b) \leq 0$

In this case, $h(p)$ has a single root in the interval $[a, b]$, hence $\partial f(p)/\partial p$ has exactly one root, which means that Eq. (16) can have at most two solutions, which implies that $Regret(n, p)$ can have at most two stationary points with respect to p .

Notice that if $h(p)$ has a root in the interval $[a, b]$, denoted by $\tilde{p}(n)$, then, for all $p > \tilde{p}(n)$, $h(p) > 0$, and, for all $p < \tilde{p}(n)$, $h(p) < 0$. As such, for all $p > \tilde{p}(n)$, $f(p) < 0$, while for all $p < \tilde{p}(n)$, $f(p) > 0$. Thus, $\tilde{p}(n)$ is a global minimum for $f(p)$, that is, if $b < \underline{p}$, then for all $p \in [a, b]$, $f(\tilde{p}(n)) \leq f(p)$. Moreover, if $b \leq \underline{p}$, then the global maximum of $f(p)$ is a boundary point, that is, $\max\{f(a), f(b)\} \geq f(p)$ for all $p \in [a, b]$. $\square$

Proof of Lemma 6. The result directly follows from the proof of Lemma 5. $\square$

Proof of Lemma 7(i). Assume that $\tilde{p}(n)$ exists and belongs to the interval $[a, b]$. Then, for a given group size n , the derivative of $Regret(n, p)$ with respect to p is given by:

$$\frac{\partial Regret(n, p)}{\partial p} = \frac{(1-p)^{n-1}}{2} \left[2n(Se + Sp - 1) + \frac{1}{(1-p)^n W_0 \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se + Sp - 1} \right)^{1/2} \right)} \right].$$

Let:

$$f(p) \equiv (1-p)^n W_0 \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se + Sp - 1} \right)^{1/2} \right).$$

From the proof of Lemma 5, $\tilde{p}(n)$ is a global minimum for $f(p)$, that is, for all $p \in [a, b]$ $f(\tilde{p}(n)) \leq f(p)$. Then, for all $p \in [a, b]$, we have that:

$$2n(Se + Sp - 1) + \frac{1}{f(p)} \leq 2n(Se + Sp - 1) + \frac{1}{f(\tilde{p}(n))}.$$

Now, suppose that

$$\left. \frac{\partial \text{Regret}(n, p)}{\partial p} \right|_{p=\tilde{p}(n)} < 0,$$

then, since $p \in (0, 1)$, we have that:

$$2n(Se + Sp - 1) + \frac{1}{f(\tilde{p}(n))} < 0,$$

which directly implies that for all $p \in [a, b]$

$$2n(Se + Sp - 1) + \frac{1}{f(p)} < 0,$$

multiplying the latter by $(1 - p)^{n-1}/2 > 0$, we get that, for all $p \in [a, b]$:

$$\frac{\partial \text{Regret}(n, p)}{\partial p} < 0,$$

completing the proof. □

Proof of Lemma 7(ii). The derivative of $\text{Regret}(n, p)$ with respect to p is given by:

$$\frac{\partial \text{Regret}(n, p)}{\partial p} = \frac{(1 - p)^{n-1}}{2} \left[2n(Se + Sp - 1) + \frac{1}{(1 - p)^n W_0 \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se + Sp - 1} \right)^{1/2} \right)} \right].$$

Let:

$$f(p) \equiv (1 - p)^n W_0 \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se + Sp - 1} \right)^{1/2} \right).$$

From the proof of Lemma 5, we have that $\max\{f(a), f(b)\} \geq f(p)$ for all $p \in [a, b]$. A such, the following holds:

$$2n(Se + Sp - 1) + \frac{1}{\max\{f(a), f(b)\}} \leq 2n(Se + Sp - 1) + \frac{1}{f(p)}, \quad \text{for all } p \in [a, b].$$

By the condition imposed in the lemma, the following holds:

$$\left. \frac{\partial \text{Regret}(n, p)}{\partial p} \right|_{p=a} > 0 \quad \text{and} \quad \left. \frac{\partial \text{Regret}(n, p)}{\partial p} \right|_{p=b} > 0 \implies 2n(Se + Sp - 1) + \frac{1}{\max\{f(a), f(b)\}} > 0.$$

Hence, from the previous two equations, we have:

$$2n(Se + Sp - 1) + \frac{1}{f(p)} > 0, \quad \text{for all } p \in [a, b],$$

multiplying the latter by $(1 - p)^{n-1}/2 > 0$, we get that, for all $p \in [a, b]$:

$$\frac{\partial \text{Regret}(n, p)}{\partial p} > 0,$$

completing the proof. $\square$

Proof of Theorem 2. We prove that Algorithm **RRA** identifies all the stationary points of $\text{Regret}(n, p)$ with respect to the prevalence rate, p , for a given group size, n , by investigating each case separately.

Case I: $h(a)h(b) > 0$

By Lemma 5(i), $\text{Regret}(n, p)$ has at most one stationary point. Hence, if:

$$(\partial \text{Regret}(n, p)/\partial p|_{p=a})(\partial \text{Regret}(n, p)/\partial p|_{p=b}) > 0,$$

then one can conclude that $\partial \text{Regret}(n, p)/\partial p$ has no roots in $[a, b]$, as it can have at most one root. On the other hand, if:

$$(\partial \text{Regret}(n, p)/\partial p|_{p=a})(\partial \text{Regret}(n, p)/\partial p|_{p=b}) \leq 0,$$

then, by the intermediate value theorem and Lemma 5(i), $\partial \text{Regret}(n, p)/\partial p$ must have exactly one root in $[a, b]$, which can be identified by a root-finding method.

Case II: $h(a)h(b) \leq 0$

By Lemma 5(ii), $\text{Regret}(n, p)$ has at most two stationary points. Moreover, $h(p)$ must have a root in $[a, b]$, $\tilde{p}(n)$, which is unique (see Lemma 6).

- If $\partial \text{Regret}(n, p)/\partial p|_{p=\tilde{p}(n)} < 0$, then, by Lemma 7(i), $\partial \text{Regret}(n, p)/\partial p < 0$ for all $p \in [a, b]$. Thus, $\partial \text{Regret}(n, p)/\partial p$ has no roots.
- If $\partial \text{Regret}(n, p)/\partial p|_{p=\tilde{p}(n)} = 0$, then $\tilde{p}(n)$ is a stationary point. Another stationary point may exist in either $[a, \tilde{p}(n)]$ or $(\tilde{p}(n), b]$. Check the boundary values to reach a conclusion. If second stationary point exists, then it can be identified by a root-finding method.
- If $\partial \text{Regret}(n, p)/\partial p|_{p=a} > 0$ and $\partial \text{Regret}(n, p)/\partial p|_{p=b} > 0$, then, by Lemma 7(ii), $\partial \text{Regret}(n, p)/\partial p > 0$ for all $p \in [a, b]$. Thus, $\partial \text{Regret}(n, p)/\partial p$ has no roots.
- If $\partial \text{Regret}(n, p)/\partial p|_{p=a} \leq 0$ or $\partial \text{Regret}(n, p)/\partial p|_{p=b} \leq 0$, then, by noting that $\partial \text{Regret}(n, p)/\partial p|_{p=\tilde{p}(n)} > 0$ (since otherwise the algorithm would have terminated) and that at most two stationary points are possible, using the three points a , $\tilde{p}(n)$, and b to identify all stationary points (iff any) in the interval $[a, b]$ by using a root-finding method.

Proof of Theorem 3(i). We prove the result of each case separately.

Case I: $b \leq p$

In this case, the Regret function is given by:

$$\text{Regret}(n, p) = \mathbb{E}[T(n)] - \mathbb{E}[T(n_0(p))].$$

The derivative of $\text{Regret}(n, p)$ with respect to p is given by:

$$\frac{\partial \text{Regret}(n, p)}{\partial p} = n(Se + Sp - 1)(1 - p)^{n-1} + \frac{1}{2(1 - p)W_0 \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se + Sp - 1} \right)^{1/2} \right)}.$$

Setting the derivative to be less than or equal to zero, and after some algebraic manipulations, gives the condition $n \leq n_0(p)$. If the latter condition is satisfied, then $\text{Regret}(n, p)$ is decreasing in p (note that this is an implication and not an equivalence statement). Noting that since $n_0(p)$ is decreasing in p (see Lemma 2), then $n \leq n_0(b) \implies n \leq n_0(p)$ for all $p \in [a, b]$.

We are now ready to prove the result of the theorem. Suppose, by contradiction, that $n_r^* < n_0(b)$, then there exists $\tilde{n}_r$ such that $n_r^* < \tilde{n}_r < n_0(b)$. In what follows, we show that $\tilde{n}_r$ improves the objective function value. To this end, since $n_r^*, \tilde{n}_r < n_0(b)$, then the Regret function is decreasing in p for all $p \in [a, b]$. As such, the following holds:

$$\begin{aligned} \max_{p \in [a, b]} \{\text{Regret}(\tilde{n}_r | P = p)\} - \max_{p \in [a, b]} \{\text{Regret}(n_r^* | P = p)\} &= \text{Regret}(\tilde{n}_r | P = a) - \text{Regret}(n_r^* | P = a) \\ &= \mathbb{E}[T(\tilde{n}_r) | P = a] - \mathbb{E}[T(n_r^*) | P = a]. \end{aligned}$$

Note that by Lemma 1, if $n < n_0(a)$ then $\mathbb{E}[T(n) | P = a]$ is strictly decreasing in n . Thus, since $n_r^* < \tilde{n}_r < n_0(b) \leq n_0(a)$, we have that $\mathbb{E}[T(\tilde{n}_r) | P = a] < \mathbb{E}[T(n_r^*) | P = a]$, implying that:

$$\max_{p \in [a, b]} \{\text{Regret}(\tilde{n}_r | P = p)\} - \max_{p \in [a, b]} \{\text{Regret}(n_r^* | P = p)\} < 0.$$

As a result, one can conclude that $\tilde{n}_r$ improves the objective function value, which is a contradiction, and hence completing the proof.

Case II: $p \leq b < \bar{p}$

In this case, the maximum Regret function is given by:

$$\max_{p \in [a, b]} \{\text{Regret}(n, p)\} = \max \left\{ \max_{p \in [a, \underline{p}]} \{\mathbb{E}[T(n)] - \mathbb{E}[T(n_0(p))]\}, \frac{1}{n} - (Se + Sp - 1)(1 - b)^n \right\}.$$

Suppose, by contradiction, that $n_r^* < n_0(b)$, then there exists $\tilde{n}_r$ such that $n_r^* < \tilde{n}_r < n_0(b)$. In Case I of this proof, we showed that the first term of the max, i.e., $\max_{p \in [a, \underline{p}]} \{\mathbb{E}[T(n)] - \mathbb{E}[T(n_0(p))]\}$, is decreasing in n for all $n \leq n_0(\underline{p})$. Since $n_r^* < \tilde{n}_r < n_0(b) \leq n_0(\underline{p})$, then $\tilde{n}_r$ will reduce the first term of the max over n_r^* . Next, we show that $\tilde{n}_r$ also reduces the second term of the max, i.e., $1/n - (Se + Sp - 1)(1 - b)^n$. Note that, by Lemma 1, the second term of the max is decreasing in n if $n < n_0(b)$. Since $n_r^* < \tilde{n}_r < n_0(b)$, then $\tilde{n}_r$ reduces the second term of the max over n_r^* , completing the proof.

Case III: $b \geq \bar{p}$ In this case, the maximum Regret function is given by:

$$\max_{p \in [a, b]} \{\text{Regret}(n, p)\} = \max \left\{ \max_{p \in [a, \underline{p}]} \{\mathbb{E}[T(n)] - \mathbb{E}[T(n_0(p))]\}, \frac{1}{n} - (Se + Sp - 1)(1 - b)^n \right\}.$$

Suppose, by contradiction, that $n_r^* < n_0(\bar{p})$, then there exists $\tilde{n}_r$ such that $n_r^* < \tilde{n}_r < n_0(\bar{p})$. In Case I of this proof, we showed that the first term of the max, i.e., $\max_{p \in [a, \underline{p}]} \{\mathbb{E}[T(n)] - \mathbb{E}[T(n_0(p))]\}$, is decreasing in n for all $n \leq n_0(\underline{p})$. Since $n_r^* < \tilde{n}_r < n_0(\bar{p}) \leq n_0(\underline{p})$, then $\tilde{n}_r$ will reduce the first term of the max over n_r^* . Next, we show that $\tilde{n}_r$ also reduces the second term of the max, i.e., $1/n - (Se + Sp - 1)(1 - b)^n$. Note that, since $b \geq \bar{p}$, then, by Theorem 1(i), the second term of the max is decreasing in n for all n . As such, $\tilde{n}_r$ reduces the second term of the max over n_r^* , completing the proof. $\square$

Proof of Theorem 3(ii). We prove the result of each case separately.

Case I: $b \leq \underline{p}$

In this case, the Regret function is given by:

$$\text{Regret}(n, p) = \mathbb{E}[T(n)] - \mathbb{E}[T(n_0(p))].$$

The derivative of $\text{Regret}(n, p)$ with respect to p is given by:

$$\frac{\partial \text{Regret}(n, p)}{\partial p} = n(Se + Sp - 1)(1 - p)^{n-1} + \frac{1}{2(1 - p)W_0 \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se + Sp - 1} \right)^{1/2} \right)}.$$

Setting the derivative to be less than or equal to zero, and after some algebraic manipulations, gives the following condition:

$$n \geq \frac{1}{\ln(1 - p)} W_{-1} \left(\frac{-\ln(1 - p)}{2(Se + Sp - 1)W_0 \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se + Sp - 1} \right)^{1/2} \right)} \right). \quad (18)$$

If Eq. (18) is satisfied then $\text{Regret}(n, p)$ is decreasing in p (note that this is an implication and not an equivalence statement). In what follows, we show that the right hand side of Eq. (18) is decreasing in p . Towards this end, define x as:

$$x(p) \equiv -\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-p}\right)}{Se + Sp - 1} \right)^{1/2}.$$

Hence, Eq. (18) reduces to:

$$n \leq \frac{1}{\ln(1 - p)} W_{-1} \left(\frac{2(x(p))^2}{W_0(x(p))} \right).$$

Note that since $b \leq \underline{p}$, then $p \leq \underline{p}$ for all $p \in [a, b]$. From the proof of Lemma 5, we have the that:

$$0 < p \leq \underline{p} \Leftrightarrow -\frac{1}{2} \leq W_0(x(p)) < 0.$$

Define $g(p)$ as:

$$g(p) \equiv \frac{2(x(p))^2}{W_0(x(p))},$$

then, the first derivative of $g(p)$ is given by:

$$\frac{\partial g(p)}{\partial p} = \frac{\partial g(p)}{\partial x(p)} \frac{\partial x(p)}{\partial p},$$

where

$$\frac{\partial g(p)}{\partial x(p)} = \frac{2x(p) [1 + 2W_0(x(p))]}{W_0(x(p))}.$$

Since $x(p) < 0$, $W_0(x(p)) < 0$, and $W_0(x(p)) \geq -1/2$, then one can conclude that:

$$\frac{\partial g(p)}{\partial x(p)} \geq 0, \quad \text{for all } p \in [a, b].$$

On the other hand, we have that:

$$\frac{\partial x}{\partial p} = -\frac{1}{4\sqrt{Se + Sp - 1}} \left(\ln \left(\frac{1}{1-p} \right) \right)^{-1/2} \frac{1}{1-p} \leq 0, \quad \text{for all } p \in [a, b].$$

As such, one can conclude that $g(p)$ is decreasing in p for all $p \in [a, b]$. Now, consider $p_1, p_2 \in [a, b]$: $p_1 \geq p_2$, then, by the previous result, we have that:

$$\begin{aligned} g(p_1) &\leq g(p_2), \\ \Rightarrow W_{-1}(g(p_1)) &\geq W_{-1}(g(p_2)), \text{ since } W_{-1}(x) \text{ is decreasing in } x \text{ [11]}, \\ \Rightarrow \frac{1}{\ln(1-p_1)} W_{-1}(g(p_1)) &\leq \frac{1}{\ln(1-p_2)} W_{-1}(g(p_2)), \text{ since } p_1, p_2 \in (0, 1) \text{ and } p_1 \geq p_2. \end{aligned}$$

We have just shown that the right hand side of Eq. (18) is decreasing in p . Next, we show that $n_{-1}(a)$ is greater than the right hand side of Eq. (18). To achieve this, we compare $n_{-1}(a)$ to the right hand side of Eq. (18) at $p = a$, as the the right hand side is decreasing in p . We first note the following:

$$0 < a \leq \underline{p} \Leftrightarrow -\frac{1}{2}e^{-1/2} \leq x(a) < 0.$$

Let $t(x) \equiv W_0(x)/x$, it is easy to show that $t(x)$ is decreasing in x for all $x \in (-1/2e^{-1/2}, 0)$. As such, we have that:

$$t(x) \leq t\left(-\frac{1}{2}e^{-1/2}\right) \approx 1.648 \leq 2, \quad \text{for all } x \in \left(-\frac{1}{2}e^{-1/2}, 0\right).$$

As such, for all $x \in (-1/2e^{-1/2}, 0)$, we have that:

$$\begin{aligned} t(x(a)) &\leq 2, \\ \Rightarrow \frac{W_0(x(a))}{x(a)} &\leq 2, \\ \Rightarrow 2x(a) - W_0(x(a)) &\leq 0, \\ \Rightarrow x(a)(2x(a) - W_0(x(a))) &\geq 0, \\ \Rightarrow \frac{2(x(a))^2}{W_0(x(a))} &\leq x(a), \\ \Rightarrow W_{-1}\left(\frac{2(x(a))^2}{W_0(x(a))}\right) &\geq W_{-1}(x(a)) \geq 2W_{-1}(x(a)), \\ \Rightarrow \frac{1}{\ln(1-a)} W_{-1}\left(\frac{2(x(a))^2}{W_0(x(a))}\right) &\leq \frac{2}{\ln(1-a)} W_{-1}(x(a)), \\ \Rightarrow \frac{1}{\ln(1-a)} W_{-1}\left(\frac{2(x(a))^2}{W_0(x(a))}\right) &\leq n_{-1}(a). \end{aligned}$$

Hence, for all $n \geq n_{-1}(a)$, the condition in Eq. (18) is satisfied and the Regret function is decreasing in p for all $p \in [a, b]$. As a result, the maximum Regret function is given by:

$$\max_{p \in [a, b]} \{Regret(n, p)\} = \frac{1}{n} - (Se + Sp - 1)(1 - a)^n - 1/n_0(a) + (Se + Sp - 1)(1 - a)^{n_0(a)},$$

and the first derivative of the maximum Regret function with respect to n is given by:

$$\frac{\partial}{\partial n} \max_{p \in [a, b]} \{Regret(n, p)\} = -\frac{1}{n^2} - \ln(1 - a)(Se + Sp - 1)(1 - a)^n,$$

which is decreasing in n when:

$$n \geq \frac{2}{\ln(1 - a)} W_{-1} \left(-\frac{1}{2} \left(\frac{\ln \left(\frac{1}{1 - a} \right)}{Se + Sp - 1} \right)^{1/2} \right) = n_{-1}(a).$$

Thus, when $n \geq n_{-1}(a)$, one can conclude that the maximum Regret function is decreasing in n , completing the proof for this case.

Case II: $b > \underline{p}$

In this case, the maximum Regret function is given by:

$$\max_{p \in [a, b]} \{Regret(n, p)\} = \max \left\{ \max_{p \in [a, \underline{p}]} \{\mathbb{E}[T(n)] - \mathbb{E}[T(n_0(p))]\}, \frac{1}{n} - (Se + Sp - 1)(1 - b)^n \right\}.$$

In Case I of this proof, we showed that first term of the max, i.e., $\max_{p \in [a, \underline{p}]} \{\mathbb{E}[T(n)] - \mathbb{E}[T(n_0(p))]\}$, is decreasing in n for all $n \geq n_{-1}(a)$. Next, we show that the second term of the max, i.e., $1/n - (Se + Sp - 1)(1 - b)^n$ is also decreasing in n . We note, from the proof of Theorem 1(i), that if $b \geq \bar{p}$, then $1/n - (Se + Sp - 1)(1 - b)^n$ is decreasing in n for all $n > 0$. As such, we are left with proving that $1/n - (Se + Sp - 1)(1 - b)^n$ is decreasing in n when $\underline{p} < b < \bar{p}$ for all $n \geq n_{-1}(a)$. To this end, suppose $\underline{p} < b < \bar{p}$, then $1/n - (Se + Sp - 1)(1 - b)^n$ is decreasing in n when:

$$n \geq \frac{2}{\ln(1 - b)} W_{-1} \left(-\frac{1}{2} \left(\frac{\ln \left(\frac{1}{1 - b} \right)}{Se + Sp - 1} \right)^{1/2} \right). \quad (19)$$

In what follows, we show that the right hand side of Eq. (19) is lower than n_c . We note that $a < b$, which gives:

$$\begin{aligned}
& -\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-a}\right)}{Se + Sp - 1} \right) \geq -\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-b}\right)}{Se + Sp - 1} \right)^{1/2}, \\
& \Rightarrow W_{-1} \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-a}\right)}{Se + Sp - 1} \right) \right) \leq W_{-1} \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-b}\right)}{Se + Sp - 1} \right)^{1/2} \right), \\
& \Rightarrow n_{-1}(a) = \frac{2}{\ln(1-a)} W_{-1} \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-a}\right)}{Se + Sp - 1} \right) \right) \geq \frac{2}{\ln(1-b)} W_{-1} \left(-\frac{1}{2} \left(\frac{\ln\left(\frac{1}{1-b}\right)}{Se + Sp - 1} \right)^{1/2} \right).
\end{aligned}$$

Hence, for all $n \geq n_{-1}(a)$ Eq. (19) is satisfied, implying that $1/n - (Se + Sp - 1)(1 - b)^n$ is decreasing in n . Also, since the maximum Regret function is the max of two decreasing functions in n , this means that the maximum Regret function is decreasing in n for all $n \geq n_{-1}(a)$, completing the proof. $\square$

B Details on Model Extensions to Consider Classification Accuracy

In this section, we first derive expressions for the per subject expected number of false negatives, $\mathbb{E}[FN(n)]$, and the per subject expected number of false positives, $\mathbb{E}[FP(n)]$, for a Dorfman testing scheme with group size $n \in \mathbb{Z}^+$, conditioned on a given realization of the prevalence rate, p . Then, we provide details on the analysis of Models (9) and (10). Towards this end, let $(N^+(n)|P = p) \sim \text{Binomial}(n, p)$ denote the random number of true positive subjects in a group of size n for a prevalence rate realization of p . Then, we have:

$$\begin{aligned}
\mathbb{E}[FN(n)|P = p] &= \sum_{k=1}^n \mathbb{E}[FN(n)|N^+(n) = k, P = p] P(N^+(n) = k|P = p) \\
&= \sum_{k=1}^n \left[\frac{k(1 - Se)Se + k(1 - Se)}{n} \right] P(N^+(n) = k|P = p) \\
&= (1 - Se^2)p, \quad \text{and} \\
\mathbb{E}[FP(n)|P = p] &= \sum_{k=0}^{n-1} \mathbb{E}[FP(n)|N^+(n) = k, P = p] P(N^+(n) = k|P = p) \\
&= (1 - Sp)^2 P(N^+(n) = 0|P = p) + \sum_{k=1}^{n-1} \frac{(n - k)}{n} (1 - Sp) Se P(N^+(n) = k|P = p) \\
&= Se(1 - Sp)(1 - p) - (1 - Sp)(Se + Sp - 1)(1 - p)^n.
\end{aligned}$$

A complete characterization of the optimal group size for the budget-constrained model, i.e., Model (9), is detailed in Table 2. For Model (10), the corresponding threshold values are given in

Table 2: The characterization of the optimal group size for Model (9)

		$B < \mathbb{E}[T(n_0(p))]$	$\mathbb{E}[T(n_0(p))] < B \leq Se$	$Se < B < \mathbb{E}[T(n_{-1}(p))]$	$B > \mathbb{E}[T(n_{-1}(p))]$
$p \leq \underline{p}$	Infeasible		$\mathbb{E}[T(n)] = B$ has exactly two solutions ($n_1 < n_2$), with $[n_1, n_2]$ representing the feasible region, and n_1 representing the optimal solution.	$\mathbb{E}[T(n)] = B$ has exactly three solutions ($n_1 < n_2 < n_3$), with $[n_1, n_2] \cup [n_3, \infty]$ representing the feasible region, and n_1 representing the optimal solution.	$\mathbb{E}[T(n)] = B$ has exactly one solution (n_1), with $[n_1, \infty]$ representing the feasible region, and n_1 representing the optimal solution.
		$B \leq Se$	$Se < B < \mathbb{E}[T(n_0(p))]$	$\mathbb{E}[T(n_0(p))] < B < \mathbb{E}[T(n_{-1}(p))]$	$B > \mathbb{E}[T(n_{-1}(p))]$
$\underline{p} < p \leq \bar{p}$	Infeasible		$\mathbb{E}[T(n)] = B$ has exactly one solution (n_1), with $[n_1, \infty]$ representing the feasible region, and n_1 representing the optimal solution.	$\mathbb{E}[T(n)] = B$ has exactly three solutions ($n_1 < n_2 < n_3$), with $[n_1, n_2] \cup [n_3, \infty]$ representing the feasible region, and n_1 representing the optimal solution.	$\mathbb{E}[T(n)] = B$ has exactly one solution (n_1), with $[n_1, \infty]$ representing the feasible region, and n_1 representing the optimal solution.
		$B \leq Se$		$B > Se$	
$p > \bar{p}$	Infeasible			$\mathbb{E}[T(n)] = B$ has exactly one solution (n_1), with $[n_1, \infty]$ representing the feasible region, and n_1 representing the optimal solution.	

Eq.s (20) and (21):

$$\underline{p} \equiv 1 - e^{-\frac{(1-w_{FP}Sp)(Se+Sp-1)}{1-w_{FP}}} e^{-1}, \quad \text{and} \quad (20)$$

$$\bar{p} \equiv 1 - e^{-4\frac{(1-w_{FP}Sp)(Se+Sp-1)}{1-w_{FP}}} e^{-2}. \quad (21)$$

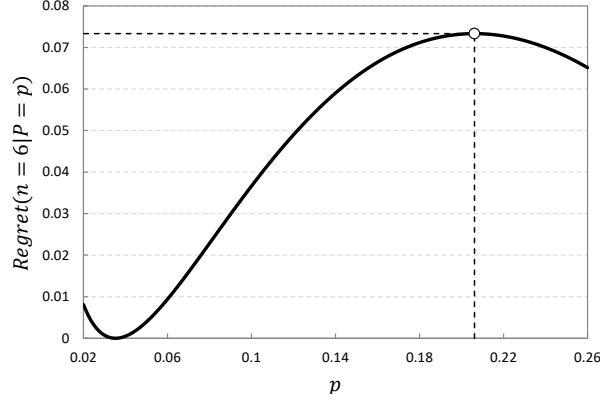
Specifically, if $p \geq \underline{p}$ then the objective function of Model (10) is non-increasing in n ; and if $p < \underline{p}$, then its objective function has exactly two stationary points, given by Eq.s (22) and (23).

$$n_0 \equiv \frac{2}{\ln(1-p)} W_0 \left(-\frac{1}{2} \left(\frac{(1-w_{FP}) \ln \left(\frac{1}{1-p} \right)}{(1-w_{FP}Sp)(Se+Sp-1)} \right)^{1/2} \right), \quad (22)$$

$$n_{-1} \equiv \frac{2}{\ln(1-p)} W_{-1} \left(-\frac{1}{2} \left(\frac{(1-w_{FP}) \ln \left(\frac{1}{1-p} \right)}{(1-w_{FP}Sp)(Se+Sp-1)} \right)^{1/2} \right), \quad (23)$$

which are derived by adopting steps similar to that of the proof of Theorem 1(i).

Figure 6: $Regret(n, p)$ as a function of p in the interval $[a, b]$, when $Se = 0.967$, $Sp = 0.993$, $a = 0.02$, $b = 0.26$, and $n = 6$



C Maximum Regret: Non-boundary Point Example

In this section, we provide an example that shows that the maximum value of the inner problem, i.e., $\max_{p \in [a, b]} \{Regret(n, p)\}$, is not necessarily attained at a boundary point. Consider the following problem instance, with $Se = 0.967$, $Sp = 0.993$, $a = 0.02$, $b = 0.26$, and $n = 6$. Figure 6 plots the $Regret(n, p)$ function as a function of the prevalence rate, p , for this problem instance. As can be seen, the prevalence rate that maximizes the $Regret(n, p)$ function is not at a boundary point, and is equal to 0.206.

References

- [1] H. Aprahamian, D. R. Bish, and E. K. Bish. Residual risk and waste in donated blood with pooled nucleic acid testing. *Statistics in Medicine*, 35(28):5283–5301, 2016.
- [2] H. Aprahamian, D. R. Bish, and E. K. Bish. Optimal risk-based group testing. *Management Science*, 2019.
- [3] T. Berger, N. Mehravari, D. Towsley, and J. Wolf. Random multiple-access communication and group testing. *IEEE Transactions on Communications*, 32(7):769–779, 1984.
- [4] D. Bertsimas, D. B. Brown, and C. Caramanis. Theory and applications of robust optimization. *SIAM Review*, 53(3):464–501, 2011.
- [5] D. Bertsimas and M. Sim. The price of robustness. *Operations Research*, 52(1):35–53, 2004.
- [6] D. R. Bish, E. K. Bish, R. S. Xie, and S. L. Stramer. Going beyond “same-for-all” testing of infectious agents in donated blood. *IIE Transactions*, 46(11):1147–1168, 2014.
- [7] M. S. Black, C. R. Bilder, and J. M. Tebbs. Group testing in heterogeneous populations by using halving algorithms. *Journal of the Royal Statistical Society: Series C (Applied Statistics)*, 61(2):277–290, 2012.
- [8] A. Blass and Y. Gurevich. The logic in computer science column pairwise testing. *Bulletin of EATCS*, 78:100–132, 2002.

- [9] R. L. Burden and J. D. Faires. 2.1 the bisection algorithm. *Numerical Analysis*, 1985.
- [10] CNN. *Rates of three STDs in US reach record high, CDC says*, accessed September, 2018. <https://www.cnn.com/2018/08/28/health/std-rates-united-states-2018-bn/index.html>.
- [11] R. M. Corless, G. H. Gonnet, D. E. Hare, D. J. Jeffrey, and D. E. Knuth. On the Lambert W function. *Advances in Computational Mathematics*, 5(1):329–359, 1996.
- [12] American Red Cross. *Details of tests performed for different infectious agents*, accessed February, 2017. <http://www.redcrossblood.org/learn-about-blood/what-happens-donated-blood/blood-testing>.
- [13] G. Dauphin and S. Zientara. West nile virus: recent trends in diagnosis and vaccine development. *Vaccine*, 25(30):5563–5576, 2007.
- [14] R. Dorfman. The detection of defective members of large populations. *The Annals of Mathematical Statistics*, 14(4):436–440, 1943.
- [15] H. El-Amine, E. K. Bish, and D. R. Bish. Robust postdonation blood screening under prevalence rate uncertainty. *Operations Research*, 66(1):1–17, 2017.
- [16] Centers for Disease Control and Prevention. *Summary of Notifiable Diseases — United States, 2012*, accessed August, 2018. <https://www.cdc.gov/mmwr/preview/mmwrhtml/mm6153a1.htm>.
- [17] Centers for Disease Control and Prevention. *West Nile virus*, accessed February, 2019. <https://www.cdc.gov/westnile/index.html>.
- [18] Centers for Disease Control and Prevention. *West Nile virus*, accessed February, 2019. <https://www.cdc.gov/westnile/statsmaps/cumMapsData.html>.
- [19] Centers for Disease Control and Prevention. *Diagnoses of HIV infection in the United States and dependent Areas, 2015*, accessed July, 2017. <https://www.cdc.gov/hiv/pdf/library/reports/surveillance/cdc-hiv-surveillance-report-2015-vol-27.pdf>.
- [20] European Centre for Disease Prevention and Control. *Vector-borne diseases*, accessed October, 2018. <https://ecdc.europa.eu/en/climate-change/climate-change-europe/vector-borne-diseases>.
- [21] L. E. Graff and R. Roeloffs. Group testing in the presence of test error; an extension of the Dorfman procedure. *Technometrics*, 14(1):113–122, 1972.
- [22] F. K. Hwang. A generalized binomial group testing problem. *Journal of the American Statistical Association*, 70(352):923–926, 1975.
- [23] D. J. Jeffrey, G. A. Kalugin, and N. Murdoch. Lagrange inversion and Lambert W. In *Symbolic and Numeric Algorithms for Scientific Computing (SYNASC), 2015 17th International Symposium*, pages 42–46. IEEE, 2015.
- [24] N. L. Johnson, S. Kotz, and X. Z. Wu. *Inspection Errors for Attributes in Quality Control*, Volume 44. CRC Press, 1991.

- [25] H. Y. Kim, M. G. Hudgens, J. M. Dreyfuss, D. J. Westreich, and C. D. Pilcher. Comparison of group testing algorithms for case identification in the presence of test error. *Biometrics*, 63(4):1152–1163, 2007.
- [26] C. T. Korves, S. J. Goldie, and M. B. Murray. Cost-effectiveness of alternative blood-screening strategies for West Nile virus in the United States. *PLOS Medicine*, 3(2):e21, 2006.
- [27] J. L. Lewis, V. M. Lockary, and S. Kobic. Cost savings and increased efficiency using a stratified specimen pooling strategy for Chlamydia trachomatis and Neisseria gonorrhoeae. *Sexually Transmitted Diseases*, 39(1):46–48, 2012.
- [28] C. S. McMahan, J. M. Tebbs, and C. R. Bilder. Informative Dorfman screening. *Biometrics*, 68(1):287–296, 2012.
- [29] K. Natarajan, D. Shi, and K. C. Toh. A probabilistic model for minmax regret in combinatorial optimization. *Operations Research*, 62(1):160–181, 2013.
- [30] North Carolina State Laboratory of Public Health. *Virology/Serology: Chlamydia/Gonorrhea*, accessed November, 2016. <http://slph.ncpublichealth.com/virology-serology/chlamydia/default.asp>.
- [31] World Health Organization. *Vector-borne diseases*, accessed September, 2018. <http://www.who.int/news-room/fact-sheets/detail/vector-borne-diseases>.
- [32] G. Perakis and G. Roels. Regret in the newsvendor model with partial information. *Operations Research*, 56(1):188–203, 2008.
- [33] L. R. Petersen, P. J. Carson, B. J. Biggerstaff, B. Custer, S. M. Borchardt, and M. P. Busch. Estimated cumulative incidence of West Nile virus infection in US adults, 1999–2010.
- [34] C. Pfleiderer, J. Blümel, M. Schmidt, W. K. Roth, M. K. Houfar, J. Eckert, M. Chudy, E. Menichetti, S. Lechner, and C. M. Nübling. West Nile virus and blood product safety in Germany. *Journal of Medical Virology*, 80(3):557–563, 2008.
- [35] M. Rios, S. Daniel, C. Chancey, I. K. Hewlett, and S. L. Stramer. West Nile virus adheres to human red blood cells in whole blood. *Clinical Infectious Diseases*, 45(2):181–186, 2007.
- [36] S. M. Samuels. The exact solution to the two-stage group-testing problem. *Technometrics*, 20(4):497–500, 1978.
- [37] B. A. Saraniti. Optimal pooled testing. *Health Care Management Science*, 9(2):143–149, 2006.
- [38] E. Shipitsyna, K. Shalepo, A. Savicheva, M. Unemo, and M. Domeika. Pooling samples: the key to sensitive, specific and cost-effective genetic diagnosis of chlamydia trachomatis in low-resource countries. *Acta Dermato-venereologica*, 87(2):140–143, 2007.
- [39] M. Sobel and P. A. Groll. Group testing to eliminate efficiently all defectives in a binomial sample. *Bell System Technical Journal*, 38(5):1179–1252, 1959.
- [40] S. L. Stramer, C. T. Fang, G. A. Foster, A. G. Wagner, J. P. Brodsky, and R. Y. Dodd. West Nile virus among blood donors in the United States, 2003 and 2004. *New England Journal of Medicine*, 353(5):451–459, 2005.
- [41] L. M. Wein and S. A. Zenios. Pooled testing for HIV screening: Capturing the dilution effect. *Operations Research*, 44(4):543–569, 1996.