

# Two-Stage Stochastic and Robust Optimization for Non-Adaptive Group Testing

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## Abstract

We consider the problem of detecting defective items amongst a large collection, by conducting tests of individual or groups of items. Group testing offers improvements over the naïve individual testing scheme by potentially certifying multiple individual items as non-defective with a single test. The *group testing problem* aims to design a group testing plan to detect the defective items using as few tests as possible. We propose novel two-stage stochastic and robust optimization formulations for the design of group testing plans in the noiseless non-adaptive setting. Our formulations enable us to certify optimality for existing group testing schemes, as well as model complex grouping constraints, a feature that is not discussed in the existing literature.

## 1 Introduction

In this paper, we consider the goal of detecting defective items amongst a large collection, by conducting tests of individual or groups of items. A test of a group of items will detect the presence of a defective item within that group, but will not indicate *which* item is defective, thus further testing is required. On the other hand, if no defective item is detected, all items in the group can be certified non-defective. Thus, group testing offers improvements over the naïve individual testing scheme by potentially certifying multiple individuals with a single test. The *group testing problem* aims to design a group testing plan to detect the defective items using as few tests as possible.

Originally introduced by Dorfman [16] in the context of medical diagnosis, group testing has proven useful in numerous other applications, including quality control in manufacturing [34], experimental design [25], high-speed communication networks [7], multi-access communication protocols [39], image compression [21] and drug discovery [23]. Amidst the SARS-CoV-2 pandemic, group testing is a promising algorithmic tool to alleviate test shortages and significantly speed up testing rates [32].

There are several dichotomies in group testing: deterministic versus stochastic; adaptive versus non-adaptive; and noisy versus noiseless.

Deterministic group testing [4, 15, 18, 37] considers the case when a fixed number of defective items are known to be present in the population. On the other hand, stochastic group testing is when each item is randomly defective with some known probability [3, 15, 24, 26, 34, 39]. The main difference between deterministic and stochastic group testing are the type of guarantees one obtains for a given plan. In the deterministic problem, guarantees are on the worst-case number of tests needed when a certain number of items are defective, whereas in the stochastic problem, the guarantee is on the expected number of items. However, testing plans designed for the deterministic problem can easily be used for the stochastic problem, and vice versa. For example, De Bonis et al. [15] provide a scheme for the deterministic problem, but then show expectation bounds for the stochastic problem.

Adaptive group testing algorithms [17, 33, 37, 38] allow testing to occur over multiple rounds, thus allowing the possibility to exploit current test results to design more efficient tests for later

stages. On the other hand, non-adaptive testing [14, 29] requires that testing be complete in one or two rounds. Ungar [36] showed that grouping is suboptimal for adaptive tests when the proportion of defective items is  $\geq (3 - \sqrt{5})/2$ , whereas Aldridge [2] showed that in the one-round regime, if the proportion of defective items remains constant as the number of items grows, then grouping is suboptimal. Adaptive testing is more efficient than non-adaptive testing in terms of the number of tests. However, non-adaptive testing can be parallelized, thus remains relevant in many applications.

Noiseless testing, the most common regime, is when test results are accurate, so if a group contains a defective item, the test will certainly indicate this. Noisy testing [11, 12, 33] relaxes this assumption: when a group contains a defective item, there is a non-zero probability that the test will not detect its presence. This is, expectedly, much more involved than the noiseless counterpart.

In this paper, we will consider the non-adaptive noiseless group testing problem. Aldridge et al. [5] provides a comprehensive survey of non-adaptive testing (in both noiseless and noisy regimes). The majority of the existing work approaches group testing from the perspective of information or coding theory and combinatorics. For example, groups may be formed by randomly placing an item in a group with some probability (Bernoulli designs), or draw upon binary codes with special properties (e.g., superimposed codes or generalizations thereof). Then, the properties of these designs are exploited to prove performance guarantees under certain parameter regimes (e.g., under different prevalence rates for defective items). To the best of our knowledge, we have not seen ideas from mathematical optimization applied to the problem of designing a group testing plan. Having said that, Aldridge [1], Aldridge et al. [4], Chan et al. [13], Malioutov and Malyutov [28] propose linear programming models to select the defective items from test results of a given group test design (e.g., a Bernoulli design). However, this is different to using mathematical optimization to *design* the group test plan.

## 1.1 Contributions and Outline

We propose a novel two-stage optimization formulation for the design of group testing plans in the noiseless non-adaptive setting. We consider both deterministic and stochastic problems, and design the objective appropriately for each case. For the deterministic problem, our objective aims to minimize the worst-case number of tests required over all possible true defective states in a given set. Thus, this formulation is exactly a robust optimization model [8, 20, 31].

For the stochastic problem, the objective is the expected number of tests. However, the distribution of the true states, while possessing finite support, can be exponentially large, so enumerating scenarios to describe the expected number of tests is intractable. Instead, we propose two alternatives. First, following Bertsimas et al. [9], we construct a confidence set of scenarios based on the distribution, and formulate a robust objective, for which the solutions enjoy confidence bounds on the performance. Second, following Subramanyam et al. [35], we propose a distributionally robust objective: we take a tractable number of samples from the true distribution, then aim to minimize the worst-case expected number of tests over all distributions within a certain Wasserstein distance of the empirical distribution. To our knowledge, this was first used by Subramanyam et al. [35] for two-stage problems with a similar combinatorial uncertainty structure to the group testing problem. Due to existing results on confidence bounds for the Wasserstein distance [19, 30], this approach also admits confidence bounds for the solution.

We present a unified Benders' decomposition approach for solving our formulation with both robust and distributionally robust objectives. We show that both master and subproblems in this approach can tractably be solved. To do this, we show that the second stage cost, originally formulated as an integer program, can actually be solved as a *linear* program, which enables an easier derivation of feasibility cuts. Bansal et al. [6] also examine Benders' decomposition in the context of two-stage distributionally robust integer programs, for both linear and integer second stages. Our analysis of the second stage costs allows us to use the simpler version of their algorithms.

Our setup, described fully in Section 2, is most similar to the so-called *conservative two-stage group testing* introduced by Aldridge [3]. However, Aldridge [3] does not use mathematical programming to design group testing plans, but instead takes existing designs and prove lower bounds on their performance for the conservative group testing setting. Note that an optimization-based approach will

obviously be less scalable than specific designs, and current discrete optimization technology, while having progressed greatly over the last few decades, limits the application to medium-sized collections of items. However, medium-sized collections appear in many applications, for example SARS-CoV-2 testing, thus we believe such an approach still maintains relevance. From a more theoretical perspective, we believe an optimization-based formulation for group testing is of interest to the community for two additional reasons:

- The current ad hoc design of testing plans cannot incorporate more complex constraints beyond limits on the number of items in a group, and the number of tests per items. However, an optimization-based framework can easily incorporate such constraints. For example, an optimization model can prevent two items being tested in the same group if needed, or it can ensure that groups correspond to connected components in a graph (where vertices correspond to items).
- In existing literature, when a design is claimed ‘optimal’ this means that the asymptotic rate of testing matches the information-theoretic lower bound for *particular parameter regimes*. For example, for the stochastic problem, De Bonis et al. [15, Section 4] show that their design based on  $(k, m, n)$ -selectors achieves the asymptotically optimal rate, assuming that the probability of an item being defective depends on the number of items in some specific way. Furthermore, in the existing literature, optimality is only guaranteed ‘up to a constant’.

In contrast, group testing plans computed from optimization models are certified optimal under whichever parameter regime that the objective was built around. Furthermore, it can also find optimal designs for non-traditional parameter regimes not analysed in existing literature, for example, a distribution over all collections with at most  $k$  defective items, a distribution where each item has a different defective probability, or a distribution over connected components in a graph (where vertices correspond to items). Relatedly, an optimization-based approach can also be used to certify that existing designs are indeed optimal.

Thus, we believe that an optimization-based framework provides a valuable new perspective for the group testing problem.

In Section 2 we formally describe our problem and present our new two-stage optimization formulation. In Section 3 we describe the algorithmic framework, then show that the second stage cost can be computed via a linear program, and use this to show that the master and subproblems can be tractably solved. In Section 4 we construct uncertainty sets based on different parameter regimes, and provide their corresponding performance guarantees for the stochastic problem.

## 2 Two-Stage Formulations

In this section, we present our new two-stage formulation for group testing. The ultimate goal is to identify defective items in as few tests as possible. We first define what a group test is.

**Definition 2.1.** Given a set of items  $[n]$ , a *group test* takes a subset  $S \subseteq [n]$  and tests for the presence of a defective item in  $S$ . The outcome of the test is +1 if there exists at least one defective item in  $S$ , and 0 if there are no items in  $S$ . Note that when the outcome is +1, the test provides no information on which specific items in  $S$  are defective, or on how many items are defective.

We assume tests are noiseless, that is, the outcome of a group test on  $S$  is provided to us accurately. We assume the following testing procedure.

- In the first stage, groups  $S_1, \dots, S_T \subseteq [n]$  will be formed and tested, and outcomes  $y_1, \dots, y_T \in \{0, 1\}$  will be observed.
- In the second stage, individual tests are conducted on items which are not certified defective or non-defective by the first-stage tests.

Thus, the problem is how to formulate the optimal first-stage groups. We introduce some parameters:

- $n$  := the total number of items
- $T$  := a limit on the number of group tests (can set to  $n$ )
- $G$  := a limit on the group size
- $r$  := a limit on the number of group tests that each item can be part of
- $D$  := the set of possible defective states for each item, a subset of  $\{0, 1\}^n$ .
- $d$  := a binary vector in  $D \subseteq \{0, 1\}^n$  that denotes the true defective state of each item.  
(If  $d_i = 1$ , then item  $i \in [n]$  is defective.)

We introduce the notation  $D$  explicitly because we will later consider restrictions on the possible states of the form

$$D^m := \left\{ d \in \{0, 1\}^n : \sum_{i \in [n]} d_i \leq m \right\}. \quad (1)$$

We define decision variables

$$X = \text{a binary matrix in } \{0, 1\}^{T \times n} \text{ describing which items are part of which tests.} \quad (2)$$

Each row  $t \in [T]$  of  $X$  denotes a group, and each  $x_{ti} \in \{0, 1\}$  indicates whether item  $i$  will be part of test  $t$  or not. Given  $X$  and the true states  $d$ , the outcomes of the tests  $y_t$  are

$$y_t(X, d) := \max_{i \in [n]} d_i x_{ti}, \quad y(X, d) := \{y_t(X, d)\}_{t \in [T]} \in \{0, 1\}^T. \quad (3)$$

In order to choose the optimal first-stage groups, we next characterize how many tests are needed in the second stage.

## 2.1 An integer program to certify items

The second-stage cost of  $X$  is defined to be the number of uncertified items after observing the outcomes  $y(X, d)$  of the group tests  $X$  on the true state  $d$ . This is because each uncertified item must be tested individually in the second stage. Throughout this section, for convenience we will simply write  $y$  and  $y_t$  in place of  $y(X, d)$  and  $y_t(X, d)$ , since we are taking  $X$  and  $d$  as given. We first define what we mean by certifying an item defective or non-defective.

**Definition 2.2.** Suppose that outcome vector  $y \in \{0, 1\}^T$  has been observed from group tests  $X \in \{0, 1\}^{T \times n}$ . Let  $[T]_0(y) := \{t \in [T] : y_t = 0\}$  and  $[T]_1(y) := \{t \in [T] : y_t = 1\}$ . We define the *set of consistent states with group tests  $X$  and outcomes  $y$*  as

$$D(X, y) := \left\{ d \in D : \begin{array}{l} \sum_{i \in [n]} d_i x_{ti} = 0 \quad \forall t \in [T]_0(y) \\ \sum_{i \in [n]} d_i x_{ti} \geq 1 \quad \forall t \in [T]_1(y) \end{array} \right\}.$$

An item  $i \in [n]$  is *certified defective* if there exists no  $d \in D(X, y)$  such that  $d_i = 0$ . Similarly,  $i \in [n]$  is *certified non-defective* if there exists no  $d \in D(X, y)$  such that  $d_i = 1$ .

Given Definition 2.2, a naïve way to test whether an item  $i$  is certified is to solve two feasibility problems:

$$\text{find } d \in D(X, y) \text{ s.t. } d_i = 0 \text{ (or } 1).$$

We now show that there is a much more efficient way to do this.

**Proposition 2.1.** *Let  $D = \{0, 1\}^n$ . Define*

$$\begin{aligned} [n]_0(X, y) &:= \{i \in [n] : \exists t \in [T] \text{ s.t. } x_{ti} = 1, y_t = 0\} \\ [n]_1(X, y) &:= \{i \in [n] : \exists t \in [T] \text{ s.t. } x_{ti} = 1, y_t = 1, x_{tj} = 0 \forall j \in [n] \setminus ([n]_0(X, y) \cup \{i\})\}. \end{aligned}$$

*Then the certified defective items are  $[n]_1(X, y)$ , and the certified non-defective items are  $[n]_0(X, y)$ .*

*Proof.* If  $d_i = 1$ , then for any  $t \in [T]$  with  $x_{ti} = 1$ , we will have  $\sum_{i' \in [n]} d_{i'} x_{ti'} \geq 1$ , so  $i \notin [n]_0(X, d)$ . Thus  $[n]_0(X, y)$  consists of only certified non-defective items. Furthermore, if  $i \notin [n]_0(X, y)$ , then  $x_{ti} = 1$  only when  $y_t = 1$ . Thus, we can set  $d_i = 1$  without violating the constraints  $\sum_{i' \in [n]} d_{i'} x_{ti'} \geq 1$  on  $D(X, y)$ . Thus,  $i$  consists exactly of the certified non-defective items.

Similarly, if  $d_i = 0$ , then for any  $t \in [T]$  with  $x_{ti} = 1$  and  $y_t = 1$ , there must be at least one  $j \neq i$  such that  $d_j x_{tj} = 1$ , so  $d_j = x_{tj} = 1$ . In particular,  $j \notin [n]_0(X, y)$  by the previous argument. But this means that  $\max_{j \in [n] \setminus ([n]_0(X, y) \cup \{i\})} x_{tj} = 1$ , so  $i \notin [n]_1(X, y)$ . Thus,  $[n]_1(X, y)$  consists of only certified non-defective items.

We now show that no item outside of  $[n]_1(X, y)$  can be certified defective. Consider  $i \in [n]$  that is not in  $[n]_0(X, y)$  or  $[n]_1(X, y)$ . For each  $t$  where  $x_{ti} = 1$ , we know that

$$d_i x_{ti} + \sum_{j \in [n] \setminus ([n]_0(X, y) \cup \{i\})} d_j x_{tj} \geq 1.$$

The sum is non-empty because  $i \notin [n]_1(X, y)$ , so setting  $d_i = 0$  and every other  $d_j = 1$  for  $j \notin [n]_0(X, y) \cup \{i\}$  creates a state vector that satisfies the inequalities.  $\square$

*Remark 2.1.* When  $D \subsetneq \{0, 1\}^n$ , then the sets of certified defective and non-defective items may be larger than  $[n]_1(X, y), [n]_0(X, y)$ . For example, if  $D = D^m$  with  $m < n$ , and we have found that  $|[n]_1(X, y)| = m$ , then the certified non-defective items are  $[n] \setminus [n]_1(X, y) \supseteq [n]_0(X, y)$ . However, if  $|[n]_1(X, y)| < m$ , describing exactly the set of certified items is much more difficult than Proposition 2.1 for  $D = \{0, 1\}^n$ . In any case, if  $D \subsetneq \{0, 1\}^n$ , then  $[n]_0(X, y) \cup [n]_1(X, y)$  can still be used as proxies for the set of certified items, but we must recognise that our resulting formulation is an approximation.  $\blacksquare$

Characterizing which items are in  $[n]_0(X, y) \cup [n]_1(X, y)$  can be done via an integer program. To this end, we define the following variables:

$$\begin{aligned} z_i^0 &:= \text{indicates whether } i \in [n]_0(X, y) \text{ or not} \\ z_i^1 &:= \text{indicates whether } i \in [n]_1(X, y) \text{ or not} \\ u_{ti} &:= \text{indicates whether test } t \in [T] \text{ can be used to certify } i \in [n]_0(X, y) \text{ or not} \\ v_{ti} &:= \text{indicates whether test } t \in [T] \text{ can be used to certify } i \in [n]_1(X, y) \text{ or not.} \end{aligned}$$

**Theorem 2.2.** *When  $D = \{0, 1\}^n$ , the number of certified items can be computed via the following 0-1 program:*

$$Q(X, d) := \max_{z^0, z^1, u, v} \sum_{i \in [n]} (z_i^0 + z_i^1) \tag{4a}$$

$$\text{s.t. } z^0, z^1 \in \{0, 1\}^n, u, v \in \{0, 1\}^{T \times n}, \tag{4b}$$

$$u_{ti} \leq x_{ti}, u_{ti} \leq 1 - d_j x_{tj}, \quad \forall t \in [T], i, j \in [n] \tag{4c}$$

$$z_i^0 \leq \sum_{t \in [T]} u_{ti}, \quad \forall i \in [n] \tag{4d}$$

$$v_{ti} \leq x_{ti}, v_{ti} \leq \sum_{i' \in [n]} d_{i'} x_{ti'}, v_{ti} \leq 1 - x_{tj} + z_j^0, \quad \forall t \in [T], i, j \in [n] \tag{4e}$$

$$z_i^1 \leq \sum_{t \in [T]} v_{ti}, \quad \forall i \in [n]. \quad (4f)$$

Furthermore, for an optimal solution  $(z^0, z^1, u, v)$  of  $Q(X, d)$ ,  $z^0$  and  $z^1$  are characteristic vectors for the sets  $[n]_0(X, y)$  and  $[n]_1(X, y)$  respectively.

*Proof.* There are two situations to consider:

- Our aim is to enforce that when item  $i \notin [n]_0(X, y)$ , then  $z_i^0 = 0$ . The maximizing objective will then ensure that when  $i \in [n]_0(X, y)$ , we have  $z_i^0 = 1$  at optimality. Recall that  $u_{ti}$  indicates whether test  $t$  can be used to certify that  $i \in [n]_0(X, y)$  or not. This means that if  $x_{ti} = 0$  or  $y_t = 1$ , then  $u_{ti} = 0$  must be enforced. We need the constraints  $u_{ti} \leq x_{ti}$ ,  $u_{ti} \leq 1 - y_t$ . Recalling the definition of  $y_t$ , we can equivalently write this as

$$u_{ti} \leq x_{ti}, \quad u_{ti} \leq 1 - d_j x_{tj} \quad \forall t \in [T], i, j \in [n].$$

The constraint on  $z_i^0$  will be

$$z_i^0 \leq \sum_{t \in [T]} u_{ti}, \quad \forall i \in [n].$$

This means that if for all  $t \in [T]$ , we have  $u_{ti} = 0$  (i.e., we cannot certify that  $i \in [n]_0(X, y)$ ), then we enforce  $z_i^0 = 0$ . This justifies constraints (4c)–(4d).

- Our aim is to enforce that whenever  $i \notin [n]_1(X, y)$ , then  $z_i^1 = 0$ . The maximization objective will then ensure that when  $i \in [n]_1(X, y)$ , we have  $z_i^1 = 1$  at optimality. Recall that  $v_{ti}$  indicates whether test  $t$  can be used to certify that  $i \in [n]_1(X, y)$ . This means that if  $x_{ti} = 0$  or  $y_t = 0$  or  $\sum_{j \in [n] \setminus \{i\}} x_{tj}(1 - z_j^0) \geq 1$ , then  $v_{ti} = 1$  must be enforced. We do this via the following constraints

$$v_{ti} \leq x_{ti}, \quad v_{ti} \leq \sum_{i' \in [n]} d_{i'} x_{ti'}, \quad w_{ti} \leq 1 - x_{tj} + z_j^0, \quad \forall t \in [T], j \in [n] \setminus \{i\}, i \in [n].$$

The rationale for the second set of constraints is because  $v_{ti} \leq y_t$  and the definition of  $y_t = \max_{i' \in [n]} d_{i'} x_{ti'}$ . The rationale for the third set of constraints is the following. We want the constraints  $\sum_{j \in [n] \setminus \{i\}} x_{tj}(1 - z_j^0) \geq 1 \implies v_{ti} = 0$ , which is equivalent to  $v_{ti} \leq 1 - x_{tj}(1 - z_j^0)$  for all  $j \in [n] \setminus \{i\}$ . It is now easy to check that  $v_{ti} \leq 1 - x_{tj}(1 - z_j^0) \iff v_{ti} \leq 1 - x_{tj} + z_j^0$ . Finally we enforce constraints

$$z_i^1 \leq \sum_{t \in [T]} w_{ti}, \quad \forall i \in [n].$$

This justifies constraints (4e)–(4f). □

*Remark 2.2.* Observe that  $Q(X, d)$  depends on knowledge of the true state  $d$  rather than the outcome vector  $y$ . In some sense, this is unavoidable since  $y$  itself depends on both  $X$  and  $d$ , thus changing  $X$  will change how the random outcomes  $y$  are distributed. Thus, in any optimization model for  $X$ , knowledge of  $d$  *must* be used to describe the outcome vector  $y$ . Despite not knowing the *true*  $d$ , the fact that (4) requires knowledge of  $d$  does not create issues when we try to solve for the optimal grouping  $X$ , which we provide algorithms for in Section 3. These algorithms (in a rough sense) use ‘guesses’ of what the true  $d$  is, then refines  $X$  based on these guesses. Thus, it is reasonable to have  $Q(X, d)$  depending on  $d$  for the purposes of optimizing  $X$ . ■

We now verify that if we certify  $i \in [n]_0(X, y)$  then we cannot certify  $i \in [n]_1(X, y)$ , and vice versa. That is, the constraints  $z_i^0 + z_i^1 \leq 1$  are implied by these constraints.

**Lemma 2.3.** *Let  $(z^0, z^1, u, v)$  satisfy constraints (4c)–(4f). If  $z_i^0 > 0$ , then  $v_{ti} \leq 0$  for any  $t \in [T]$ . If  $z_i^1 > 0$ , then  $u_{ti} \leq 0$  for any  $t \in [T]$ . Consequently, when we additionally have  $0 \leq z^0, z^1 \leq 1$ , then we deduce that  $z_i^0 + z_i^1 \leq 1$  for all  $i \in [n]$ .*

*Proof.* Suppose that  $z_i^0 > 0$ . Then we necessarily have  $\sum_{t' \in [T]} u_{t'i} > 0$ , and hence there exists at least one  $t' \in [T]$  such that  $u_{t'i} > 0$ . Consequently, for this  $t'$ , we must have  $x_{t'i} = 1$  and  $\sum_{i' \in [n]} d_{i'} x_{t'i'} = 0$ , thus  $d_i = 0$ . Now suppose for contradiction that  $v_{ti} > 0$ . This is only possible if  $x_{ti} = 1$ ,  $\sum_{i' \in [n] \setminus \{i\}} d_{i'} x_{ti'} \geq 1$  (we exclude  $i$  since we know  $d_i = 0$ ), and  $1 - x_{tj} + z_j^0 > 0$  for all  $j \neq \{i\}$ . Since  $\sum_{i' \in [n] \setminus \{i\}} d_{i'} x_{ti'} \geq 1$  there must exist some  $j \neq i$  such that  $x_{tj} = 1 = d_j$ . However, if  $d_j = 1$ , then for any constraint  $t'$  with  $x_{t'j} = 1$ , we have  $u_{t'j} \leq 1 - d_j x_{t'j} = 0$ , hence  $z_j^0 \leq \sum_{t' \in [T]} u_{t'j} \leq 0$ . This contradicts  $1 - x_{tj} + z_j^0 > 0$ , therefore  $v_{ti} = 0$ .

Suppose that  $z_i^1 > 0$ . Then there will exist some  $t'$  such that  $v_{t'i} > 0$ , so  $x_{t'i} = 1$ ,  $\sum_{i' \in [n]} d_{i'} x_{t'i'} \geq 1$  and  $1 - x_{t'j} + z_j^0 > 0$  for all  $j \neq i$ . Now for  $j \neq i$ , if  $x_{t'j} = 1$ , then  $z_j^0 > 0$ , thus by the above arguments we have  $d_j = 0$ . We deduce that  $\sum_{i' \in [n]} d_{i'} x_{t'i'} \geq d_i x_{t'i} = d_i \geq 1$ . But then this means that for any  $t \in [T]$ , if  $x_{ti} = 1$ , then  $\sum_{i' \in [n]} d_{i'} x_{ti'} \geq d_i x_{ti} \geq 1$ , hence  $u_{ti} = 1 - d_i x_{ti} \leq 0$ .  $\square$

## 2.2 Choosing optimal groups via two-stage integer programming

Now we turn our attention to the problem of choosing an optimal grouping  $X$ . Our objective is to choose  $X$  so that we minimize the total number of tests, which is the sum of the number of group tests performed in the grouping  $X$ , plus the number of subsequent individual tests performed on items not in  $[n]_0(X, y) \cup [n]_1(X, y)$ , which is  $n - Q(X, d)$ . Note that  $Q(X, y)$  depends on  $X$  and  $d$  (see also Remark 2.2). However, the true state  $d$  is unknown to us, thus we have an *optimization under uncertainty* problem. This motivates us to consider *stochastic* and *robust* objectives for optimizing  $X$ , based on knowledge of  $d$  and  $D$ .

Before addressing the objective, we describe the constraints on  $X$ . The group size limit  $G$  and the group test limit  $r$  for each item imposes the following constraints on the matrix  $X$ :

$$\begin{aligned} \sum_{i \in [n]} x_{ti} &\leq G, \quad \forall t \in [T], \\ \sum_{t \in [T]} x_{ti} &\leq r, \quad \forall i \in [n]. \end{aligned}$$

Other operational constraints can be imposed on  $X$  if needed.

We now describe how to build the objective. If there exists a group  $t \in [T]$  for which  $\sum_{i \in [n]} x_{ti} = 0$ , then since there will not be any individuals in group  $t$ , no test will be expended for group  $t$ . To capture this, we introduce binary variables  $b_t \in \{0, 1\}$  and replace the group size limit constraints with

$$\sum_{i \in [n]} x_{ti} \leq G b_t, \quad \forall t \in [T].$$

Thus, variables  $b_t$  indicates whether there are any items assigned to test  $t$  or not, and hence these can be used in the objective to minimize the number of tests. Henceforth, we will denote the domain of our decision variables as

$$\mathcal{X} := \left\{ (X, b) \in \{0, 1\}^{T \times n} \times \{0, 1\}^T : \begin{cases} \sum_{i \in [n]} x_{ti} \leq G b_t, & \forall t \in [T], \\ \sum_{t \in [T]} x_{ti} \leq r, & \forall i \in [n] \end{cases} \right\}. \quad (5)$$

As previously mentioned, the number of subsequent individual tests needed after group tests  $X$ , given that the true state is  $d$ , is  $n - Q(X, d)$ . Without loss of generality, we ignore the constant  $n$ . For the rest of the paper, we will use the following notation.

**Definition 2.3.** Write  $D = \{d^k : k \in [K]\} \subseteq \{0, 1\}^n$  and let  $\{p^k\}_{k \in [K]} \in \Delta_K$  be weights from the  $K$ -simplex. Let  $P$  be a distribution over  $D$  such that

$$\mathbb{P}_{d \sim P} [d = d^k] = p^k, \quad k \in [K].$$

Since we do not know  $d$  in advance, we look at three alternate objectives which optimize  $X$  based only on knowledge of  $D$  and  $P$ .

- If the true state vector  $d$  is randomly drawn from distribution  $P$ , then we wish to minimize the expected number of tests. We thus solve the *two-stage stochastic optimization problem*

$$\min_{b, X} \left\{ \sum_{t \in [T]} b_t - \mathbb{E}_{d \sim P} [Q(X, d)] : (X, b) \in \mathcal{X} \right\}. \quad (6)$$

- If we only know that  $d \in D$ , then we wish to optimize the worst-case cost over any  $d \in D$ . We thus solve the *two-stage robust optimization problem*

$$\min_{b, X} \left\{ \sum_{t \in [T]} b_t - \min_{d \in D} Q(X, d) : (X, b) \in \mathcal{X} \right\}. \quad (7)$$

- To interpolate between the stochastic and robust objectives, we can solve the *two-stage distributionally robust optimization problem*

$$\min_{b, X} \left\{ \sum_{t \in [T]} b_t - \min_{\tilde{P} \in \mathcal{F}_\epsilon(P)} \mathbb{E}_{d \sim \tilde{P}} [Q(X, d)] : (X, b) \in \mathcal{X} \right\}, \quad (8)$$

where  $\mathcal{F}_\epsilon(P)$  is an ambiguity set of distributions (supported on  $D$ ) built around some nominal distribution  $P$ , with size governed by  $\epsilon$ . For reasons that we explain later (see Section 4.2), in this paper we consider Wasserstein-based ambiguity sets (although others are possible):

$$\mathcal{F}_\epsilon(P) := \left\{ \tilde{P} : \exists y \geq 0 \text{ s.t. } \begin{cases} \sum_{k, k' \in [K]} \|d^k - d^{k'}\| y_{kk'} \leq \epsilon \\ \sum_{k' \in [K]} y_{kk'} = p^k, \quad k \in [K] \\ \sum_{k \in [K]} y_{kk'} = \tilde{p}^{k'}, \quad k' \in [K] \end{cases} \right\}. \quad (9)$$

Since  $Q(X, d)$  is itself the result of an optimization problem, both (6) and (7) are *two-stage optimization* problems, with fixed recourse with random technology matrices. In the next section, we conduct a closer analysis of  $Q(X, d)$ , and use this to describe some algorithms to solve (6) and (7).

### 3 Algorithms

In this section, we discuss algorithms for solving (6)–(8). Since  $D \subseteq \{0, 1\}^n$  is a finite set, a deterministic equivalent for (6)–(7) exists, as well as for (8) for the Wasserstein ambiguity sets  $\mathcal{F}_\epsilon(P)$ . Then (6)–(8) can respectively be reformulated as

$$\min_{(X, b) \in \mathcal{X}} \left\{ \sum_{t \in [T]} b_t - \sum_{k \in [K]} p^k Q(X, d^k) \right\} \quad (10a)$$



$$\min_{(X,b) \in \mathcal{X}} \left\{ \sum_{t \in [T]} b_t - \min_{k \in [K]} Q(X, d^k) \right\} \quad (10b)$$

$$\min_{(X,b) \in \mathcal{X}, \alpha \geq 0} \left\{ \sum_{t \in [T]} b_t + \alpha \epsilon - \sum_{k \in [K]} p^k \min_{d \in D} \{Q(X, d) + \alpha \|d - d^k\|\} \right\}. \quad (10c)$$

Note that (10a)–(10b) follow trivially from (6)–(7) and the notation in Definition 2.3, and (10c) follows from applying linear programming duality to the worst-case expectation over the Wasserstein ball (9). For completeness, we provide the proof of (10c) below, but we note that a more general result was proven by Blanchet and Murthy [10, Theorem 1, Remark 1] when the support of  $P$  is possibly infinite.

**Lemma 3.1.** *For  $\mathcal{F}_\epsilon(P)$  defined in (9), we have*

$$\min_{\tilde{P} \in \mathcal{F}_\epsilon(P)} \mathbb{E}_{d \sim \tilde{P}} [Q(X, d)] = - \min_{\alpha \geq 0} \left\{ \alpha \epsilon - \sum_{k \in [K]} p^k \min_{d \in D} \{Q(X, d) + \alpha \|d - d^k\|\} \right\}$$

*Proof.* Note that

$$\min_{\tilde{P} \in \mathcal{F}_\epsilon(P)} \mathbb{E}_{d \sim \tilde{P}} [Q(X, d)] = \min_{\tilde{p}, y} \left\{ \sum_{k \in [K]} \tilde{p}^k Q(X, d^k) : \begin{array}{l} \tilde{p} \geq 0, y \geq 0 \\ \sum_{k, k' \in [K]} \|d^k - d^{k'}\| y_{kk'} \leq \epsilon \\ \sum_{k' \in [K]} y_{kk'} = p^k, \quad k \in [K] \\ \sum_{k \in [K]} y_{kk'} = \tilde{p}^{k'}, \quad k' \in [K] \end{array} \right\}.$$

A standard computation shows that the dual of this is

$$\begin{aligned} & \max_{\alpha \geq 0, \gamma, \eta} \left\{ \sum_{k \in [K]} p^k \gamma^k - \alpha \epsilon : \begin{array}{l} \gamma^k + \eta^{k'} - \alpha \|d^k - d^{k'}\| \leq 0, \quad \forall k, k' \in [K] \\ -\eta^{k'} \leq Q(X, d^{k'}), \quad \forall k \in [K] \end{array} \right\} \\ &= \max_{\alpha \geq 0, \gamma} \left\{ \sum_{k \in [K]} p^k \gamma^k - \alpha \epsilon : \gamma^k \leq Q(X, d^{k'}) + \alpha \|d^k - d^{k'}\|, \quad \forall k, k' \in [K] \right\} \\ &= - \min_{\alpha \geq 0} \left\{ \alpha \epsilon - \sum_{k \in [K]} p^k \min_{k' \in [K]} \{Q(X, d^{k'}) + \alpha \|d^k - d^{k'}\|\} \right\}. \end{aligned}$$

□

Deterministic equivalents for (10a)–(10b) can be built by replicating the variables used to define  $Q(X, d)$  in (4) for each  $k \in [K]$ , adding in an epigraphical variable  $\beta^k \leq Q(X, d^k)$  and lifting appropriately. A deterministic equivalent for (10c) can be built in a similar manner, except now  $K^2$  replications of variables defining  $Q$  must be built. When  $K, T$  or  $n$  are large, this is highly inefficient. Instead of solving the deterministic equivalents, we use a Benders' decomposition approach from large-scale optimization.

Note that if  $\epsilon = 0$ , then  $\mathcal{F}_\epsilon(P) = \{P\}$ , and (8) is equivalent to (6). This is also seen in the reformulation, since we can make the variable  $\alpha$  arbitrarily large in (10c). On the other hand, if  $\epsilon$  is large, then  $\alpha$  should be set small, so that the inner minimization in (10c) essentially just ignores the

norm term, so (10c) becomes equivalent to (10b), i.e., (8) is equivalent to (7) when  $\epsilon$  is large. Due to these relationships, all three problems in (10) are instances of a more general problem:

$$\min_{x \in \mathcal{X}} \left\{ f(x) - \sum_{k \in [K]} p^k g_k(x) \right\}, \quad (11)$$

where  $f(x)$  is a convex function and each  $g_k(x)$  is a concave function. In (10),  $f$  is  $\sum_{t \in [T]} b_t$  and  $g_k$  is  $\min_{d \in D} \{Q(X, d) + \alpha \|d - d^k\|\}$ . (It is not yet clear that this is concave in  $X$ ; this will be shown in Section 3.2.) We now describe a general Benders' decomposition approach for (11).

### 3.1 Benders' decomposition

The idea is to replace the 'hard' part of the objective with piecewise linear approximations, and then iteratively refine these. For the general problem (11), the 'hard' part that we will build an approximation for is  $\sum_{k \in [K]} p^k g_k(x)$ . The basic template of the Benders' decomposition algorithm is described in Algorithm 1.

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**Algorithm 1:** Benders' decomposition for (11).

---

**Data:** Initial concave approximations  $\hat{g}_k^s(x)$  of  $g_k(x)$ ,  $k \in [K]$ . Iteration limit  $S$ , tolerance threshold  $\delta \geq 0$ .

**Result:** Final point  $\bar{x} \in \mathcal{X}$ , approximation quality  $\bar{\delta}$ .

**for**  $s \in S$  **do**

    Solve the master problem

$$\min_{x \in \mathcal{X}} \left\{ f(x) - \sum_{k \in [K]} p^k \hat{g}_k^{s-1}(x) \right\}. \quad (12)$$

    Let  $x^s$  be the solution to (12);

**for**  $k \in [K]$  **do**

        Solve the subproblem:

$$\text{compute } \nabla g_k(x^s), \text{ a supergradient of } g_k \text{ at } x^s. \quad (13)$$

        Update  $\hat{g}_k^{s-1}$  with a first-order approximation of  $g_k$  at  $x^s$ :

$$\hat{g}_k^s(x) := \min \{ \hat{g}_k^{s-1}(x), g_k(x^{s-1}) + \langle \nabla g_k(x^{s-1}), x - x^{s-1} \rangle \} \quad \forall x \in \mathcal{X}. \quad (14)$$

        Compute  $\delta_k^s := \hat{g}_k^{s-1}(x^s) - \hat{g}_k^s(x^s)$ ;

**end**

**if**  $\sum_{k \in [K]} \delta_k^s \leq \delta$  **then**

**return**  $\bar{x} = x^s \in \mathcal{X}$ ,  $\bar{\delta} = \sum_{k \in [K]} p^k \delta_k^s$ ;

**end**

**end**

**return**  $\bar{x} = x^S \in \mathcal{X}$ ,  $\bar{\delta} = \sum_{k \in [K]} p^k \delta_k^S$ ;

---

*Remark 3.1.* Note that

$$\hat{g}_k^s = \min \left\{ \hat{g}_k^0(x), \min_{\tau \in [s]} \{ g_k(x^{\tau-1}) + \langle \nabla g_k(x^{\tau-1}), x - x^{\tau-1} \rangle \} \right\},$$

so if  $\hat{g}_k^0$  is piecewise linear concave (i.e., a minimum over finitely many linear functions), then so is  $\hat{g}_k^s$ . Finite convergence of Algorithm 1 is guaranteed when  $g_k$  is itself a piecewise linear concave function. In fact, convergence can be guaranteed in more general settings, but for the purposes of this paper, we shall show in the next section that the  $g_k$  functions of interest to us are indeed piecewise linear concave. ■

The two key steps of Algorithm 1 are solving the master problem (12) and solving the subproblem (13) (i.e., computing the supergradient). As mentioned in Remark 3.1, since  $\hat{g}_k^s$  can be made to be piecewise linear concave, when  $f(x)$  is linear, solving (12) can be solved as a linear optimization problem. In the group testing problem,  $\mathcal{X}$  is an integer linear set, so (12) can be solved via integer programming. In Section 3.2 we show that when  $g_k(X, \alpha) = \min_{d \in D} \{Q(X, d) + \alpha \|d - d^k\|\}$ , it is indeed concave in  $(X, \alpha)$ , and computing the supergradient  $\nabla g_k(X, \alpha)$  can also be done via integer programming. The key step is to show that (4) can actually be solved *without* the integer constraints, i.e., it can be solved as a linear program. Strong duality then holds, so we can write  $Q(X, d)$  as a minimum of bilinear functions in  $X$  and  $d$ , and we can linearize any bilinear terms involving  $X$  and  $d$ .

### 3.2 Second stage analysis

If we remove the 0-1 constraints on  $z^0, z^1, u, v$  in (4) and replace them with  $0 \leq z^0, z^1 \leq 1$  and  $u, v \geq 0$ , it becomes a linear program, for which the dual is

$$\min_{\lambda, \gamma, \xi, \eta, \delta, \kappa, \zeta, \mu^0, \mu^1} \sum_{t \in [T], i \in [n]} \left( x_{ti}(\lambda_{ti} + \eta_{ti}) + \left( \sum_{i' \in [n]} d_{i'} x_{ti'} \right) \delta_{ti} \right) + \sum_{t \in [T], i, i' \in [n]} (1 - d_{i'} x_{ti'}) \gamma_{tii'} \quad (15a)$$

$$+ \sum_{t \in [T], j \in [n] \setminus \{i\}, i \in [n]} (1 - x_{tj}) \kappa_{tj} + \sum_{i \in [n]} (\mu_i^0 + \mu_i^1) \quad (15b)$$

$$\text{s.t. } \lambda, \gamma, \xi, \eta, \delta, \kappa, \zeta, \mu^0, \mu^1 \geq 0 \quad (15b)$$

$$1 \leq \mu_i^0 - \sum_{t \in [T], j \in [n] \setminus \{i\}} \kappa_{tj} + \xi_i, \quad \forall i \in [n] \quad (z_i^0) \quad (15c)$$

$$1 \leq \mu_i^1 + \zeta_i, \quad \forall i \in [n] \quad (z_i^1) \quad (15d)$$

$$0 \leq \lambda_{ti} + \sum_{i' \in [n]} \gamma_{tii'} - \xi_i, \quad \forall t \in [T], i \in [n] \quad (u_{ti}) \quad (15e)$$

$$0 \leq \eta_{ti} + \delta_{ti} + \sum_{j \in [n] \setminus \{i\}} \kappa_{tj} - \zeta_i, \quad \forall t \in [T], i \in [n] \quad (v_{ti}) \quad (15f)$$

We now show that the optimal solution of the linear relaxation is integral by exhibiting a primal-dual pair with the same objective value.

**Theorem 3.2.** *The value of the dual linear program (15) is exactly  $Q(X, d)$ .*

*Proof.* The primal solution will be (note that by construction it satisfies all constraints of (4)):

- For each  $t \in [T], i \in [n]$ ,  $u_{ti} = 1$  if  $x_{ti} = 1$  and  $\sum_{i' \in [n]} d_{i'} x_{ti'} = 0$ , otherwise  $u_{ti} = 0$ .
- For each  $i \in [n]$ ,  $z_i^0 = \max_{t \in [T]} u_{ti}$ .
- For each  $t \in [T], i \in [n]$ ,  $v_{ti} = 1$  if  $x_{ti} = 1$ ,  $\sum_{i' \in [n]} d_{i'} x_{ti'} \geq 1$  and  $\sum_{j \in [n] \setminus \{i\}} x_{tj} (1 - z_j^0) = 0$ . (Note that if  $x_{tj} (1 - z_j^0) = 0$  for all  $j \in [n] \setminus \{i\}$ , then  $1 \leq 1 - x_{tj} + z_j^0$  hence  $v_{ti} \leq 1 \leq 1 - x_{tj} + z_j^0$  is satisfied.)
- For each  $i \in [n]$ ,  $z_i^1 = \max_{t \in [T]} v_{ti}$ .

We construct the dual solution as follows. For each  $i \in [n]$ , we set  $\mu_i^0 = z_i^0$ ,  $\mu_i^1 = z_i^1$ ,  $\zeta_i = 1 - (z_i^0 + z_i^1)$  (this is non-negative by Lemma 2.3),  $\xi_i = \min_{t \in [T]} \left\{ \lambda_{ti} + \sum_{i' \in [n]} \gamma_{tii'} \right\}$ . Fixing  $i \in [n]$ , the system of constraints (15c)–(15f) now becomes

$$1 - z_i^0 \leq \lambda_{ti} + \sum_{i' \in [n]} \gamma_{tii'} - \sum_{t' \in [T], j \in [n] \setminus \{i\}} \kappa_{t'ji}, \quad \forall t \in [T] \quad (z_i^0) \quad (16a)$$

$$1 - z_i^1 \leq \eta_{ti} + \delta_{ti} + \sum_{j \in [n] \setminus \{i\}} \kappa_{tij}, \quad \forall t \in [T]. \quad (z_i^1) \quad (16b)$$

We now pick  $\lambda, \gamma, \eta, \delta, \kappa$  so that these are satisfied. Fix an arbitrary  $t \in [T]$ .

- For  $i, j \in [n]$ ,  $i \neq j$ , we set  $\kappa_{tij} = 1$  if  $x_{tj} = 1$  and  $v_{ti} = 1 - x_{tj} + z_j^0$ , and  $\kappa_{tii} = 0$ . This ensures that  $\sum_{t \in [T], j \in [n] \setminus \{i\}, i \in [n]} (1 - x_{tj}) \kappa_{tij} = 0$ .
- If  $x_{ti} = 0$  or there exists some  $i'$  such that  $1 - d_{i'} x_{ti'} = 0$ , then we can make the corresponding  $\lambda_{ti}$  or  $\gamma_{tii'}$  as large as we want without affecting the objective, so we can always guarantee that (16a) is satisfied. Now consider the case when  $x_{ti} = 1$  and  $1 - d_{i'} x_{ti'} = 1$  for all  $i' \in [n]$ . Then by construction of the primal solution we will have  $u_{ti} = z_i^0 = 1$ . Now considering  $\kappa_{t'ji}$ , by Lemma 2.3 we have  $v_{t'j} = 0 < z_j^0 = 1$ . Thus, according to our choice above, we have  $\kappa_{t'ji} = 0$  for all  $t' \in [T]$ ,  $j \neq i$ . In this case we set  $\lambda_{ti} = \gamma_{tii'} = 0$ , so (16a) will be satisfied.
- We now check (16b). If  $z_i^1 = 1$ , then we can pick  $\eta_{ti} = \delta_{ti} = 0$ , and (16b) will be satisfied because the left hand side is 0. Now consider the case when  $z_i^1 = 0$ . We know that  $v_{ti} = 0$  since otherwise by construction of the primal solution  $z_i^1 = 1$ . Thus, at least one of  $x_{ti} = 0$ ,  $\sum_{i' \in [n]} d_{i'} x_{ti'} = 0$  or there exists some  $j \neq i$  such that  $1 - x_{tj} + z_j^0 = 0$ . In the first two cases, we can set  $\eta_{ti} = 1$  or  $\delta_{ti} = 1$  without changing the objective to satisfy the constraints. Now consider the case when  $x_{ti} = 1$  and  $\sum_{i' \in [n]} d_{i'} x_{ti'} \geq 1$ ; we set  $\eta_{ti} = \delta_{ti} = 0$ . We show that there is at least one  $j \neq i$  such that we have  $\kappa_{tij} = 1$  (according to our choice above). By construction, this will be true if there exists some  $j \neq i$  with  $x_{tj} = 1$  and  $z_j^0 = 0$  (thus  $1 - x_{tj} + z_j^0 = 0$ ). If this is not the case, i.e., for every  $j \neq i$ , we have  $x_{tj} = 0$  or  $z_j^0 = 1$ , then since  $x_{ti} = 1 \leq \sum_{i' \in [n]} d_{i'} x_{ti'}$ , by definition of the primal solution we must have  $v_{ti} = 1$  and hence  $z_i^1 = 1$ . This contradicts our initial assumption. □

Now, the concavity of  $g_k(X, \alpha) = \min_{d \in D} \{Q(X, d) + \alpha \|d - d^k\|\}$  in  $(X, \alpha)$  is now readily apparent, since it is a minimum of linear functions of  $(X, \alpha)$ , and  $X$  only appears in the objective (15a) of (15), thus  $Q(X, d)$  is a minimum of linear functions of  $X$ .

The supergradient of  $g_k(X, \alpha)$  can be computed from the linear function that gives the minimum at the point  $(X, \alpha)$ . Notice that (15a) is bilinear in  $d \in D$  and the dual variables. Since  $d \in \{0, 1\}^n$ , the standard linearization technique can be used on the bilinear terms, so we can jointly minimize over  $d \in D$  and the dual variables, provided we have bounds on the relevant dual variables. These bounds come from proof of Theorem 3.2, where a specific solution was constructed. Next, to facilitate the easy minimization of the norm term  $\|d - d^k\|$ , it makes sense to choose a polyhedral norm, such as the  $\ell_1$ -norm. In this case, we have

$$\alpha \|d - d^k\|_1 = \alpha \sum_{i \in [n]} ((1 - d_i^k) d_i + d_i^k (1 - d_i)).$$

Thus,  $\min_{d \in D} \{Q(X, d) + \alpha \|d - d^k\|_1\}$  can be modelled as the following integer program (variables

$\xi, \zeta$  can be eliminated from (15)):

$$\begin{aligned} & \sum_{t \in [T], i \in [n]} \left( x_{ti}(\lambda_{ti} + \eta_{ti}) + \sum_{i' \in [n]} x_{ti'} \bar{\delta}_{tii'} \right) \\ & + \sum_{t \in [T], i, i' \in [n]} (\gamma_{tii'} - x_{ti'} \bar{\gamma}_{tii'}) \\ \min_{\lambda, \gamma, \eta, \delta, \kappa, \mu^0, \mu^1, \bar{\gamma}, \bar{\delta}, d} & + \sum_{t \in [T], j \in [n] \setminus \{i\}, i \in [n]} (1 - x_{tj}) \kappa_{tij} + \sum_{i \in [n]} (\mu_i^0 + \mu_i^1) \\ & + \alpha \sum_{i \in [n]} ((1 - d_i^k) d_i + d_i^k (1 - d_i)) \end{aligned} \quad (17a)$$

$$\text{s.t. } \lambda, \gamma, \eta, \delta, \kappa, \mu^0, \mu^1 \geq 0, \bar{\gamma}, \bar{\delta} \geq 0, d \in D \subseteq \{0, 1\}^n \quad (17b)$$

$$1 \leq \mu_i^0 - \sum_{t \in [T], j \in [n] \setminus \{i\}} \kappa_{tji} + \lambda_{ti} + \sum_{i' \in [n]} \gamma_{tii'}, \quad \forall t \in [T], i \in [n] \quad (17c)$$

$$1 \leq \mu_i^1 + \eta_{ti} + \delta_{ti} + \sum_{j \in [n] \setminus \{i\}} \kappa_{tij}, \quad \forall t \in [T], i \in [n]. \quad (17d)$$

$$0 \leq \bar{\delta}_{tii'} \leq d_{i'}, \quad -(1 - d_{i'}) \leq \bar{\delta}_{tii'} - \delta_{ti} \leq 1 - d_{i'}, \quad \forall t \in [T], i, i' \in [n] \quad (17e)$$

$$0 \leq \bar{\gamma}_{tii'} \leq d_{i'}, \quad -nT(1 - d_{i'}) \leq \bar{\gamma}_{tii'} - \gamma_{tii'} \leq nT(1 - d_{i'}), \quad \forall t \in [T], i, i' \in [n]. \quad (17f)$$

Given  $\bar{X}, \bar{\alpha}$ , let  $\lambda, \gamma, \eta, \delta, \kappa, \mu^0, \mu^1, \bar{\gamma}, \bar{\delta}, d$  be an optimal solution to (17). Then the linear approximation  $g_k(\bar{X}, \bar{\alpha}) + \langle \nabla g_k(\bar{X}, \bar{\alpha}), (X, \alpha) - (\bar{X}, \bar{\alpha}) \rangle$  of  $g_k(X, \alpha) = \min_{d \in D} \{Q(X, d) + \alpha \|d - d^k\|\}$  is simply the objective:

$$\begin{aligned} & \sum_{t \in [T], i \in [n]} \left( x_{ti}(\lambda_{ti} + \eta_{ti}) + \sum_{i' \in [n]} x_{ti'} \bar{\delta}_{tii'} \right) + \sum_{t \in [T], i, i' \in [n]} (\gamma_{tii'} - x_{ti'} \bar{\gamma}_{tii'}) \\ & + \sum_{t \in [T], j \in [n] \setminus \{i\}, i \in [n]} (1 - x_{tj}) \kappa_{tij} + \sum_{i \in [n]} (\mu_i^0 + \mu_i^1) + \alpha \sum_{i \in [n]} ((1 - d_i^k) d_i + d_i^k (1 - d_i)). \end{aligned} \quad (18)$$

## 4 Construction of Uncertainty Sets

In Section 2 we have described out two-stage optimization formulation for non-adaptive group testing, and in Section 3 we have described a general Benders' decomposition algorithmic framework for optimizing any objective of the form (10). However, we have not yet specified two key components: the support set  $D \subseteq \{0, 1\}^n$  and which exact objective in (10) we wish to optimize. Choosing these depends very much on the known prior information we have on the true defective state  $d$ . Existing literature mostly considers two types of regimes:

- In a so-called *combinatorial prior*, we know that  $d$  contains  $m$  defectives, but we do not know which ones. Thus  $D := \{d \in \{0, 1\}^n : \sum_{i \in [n]} d_i = m\}$ .
- In a so-called *independent and identically distributed (i.i.d.) prior*, each item  $i \in [n]$  is defective with probability  $\rho$ , where  $\rho$  is known. That is,  $d$  is a random vector where each entry  $d_i \sim \text{Bernoulli}(\rho)$ .

Besides these regimes, it is not difficult to imagine others. We provide three reasonable ones:

- The *non-i.i.d. prior* is when  $d$  is a random vector where each entry  $d_i \sim \text{Bernoulli}(\rho_i)$ , and  $\rho_1, \dots, \rho_n$  are known. This was also studied by Kealy et al. [24], Li et al. [26].
- The *deterministic graph prior* is when we are given a graph  $\mathcal{G} = (\mathcal{V} = [n], \mathcal{E})$ , and we know that  $d$  is the characteristic vector of a neighbourhood of some vertex  $i \in [n]$ , i.e.,  $d_i = 1$  and  $d_j = 1$  if and only if  $\{i, j\} \in \mathcal{E}$ .
- The *probabilistic graph prior* is similar to the deterministic graph prior, but now we have a probability distribution over which vertex is selected, i.e., vertex  $i \in [n]$  is selected with probability  $p^i$  and when it is selected,  $d$  is the characteristic vector of the neighbourhood of  $i$  in  $\mathcal{G}$ .

In these regimes, the prior information that we know is one of two types: (1) we know that  $d$  belongs to some set  $D$  but we have no information on which point in  $D$  it will be; or (2) we know that  $d \sim P^*$  where  $P^*$  is a distribution with support  $D^*$ . In the former case, it is most natural to minimize the robust objective (10b). In the latter case, it is most natural to minimize the stochastic objective (10a), unless the size of  $D^*$  is too large to do so tractably.

For the rest of this section, we address the setting when  $d \sim P^*$  but the support  $D^*$  is indeed too large to solve (10a) (which is the case for the i.i.d. and non-i.i.d. priors). We propose two options: (1) construct a set  $D$  for which  $\mathbb{P}_{d \sim P^*}[d \in D]$  is sufficiently high, then solve (10b); and (2) estimate  $P^*$  with a tractable distribution  $P$ , and estimate the Wasserstein distance  $\epsilon$  between  $P^*$  and  $P$ , then solve the distributionally robust problem (10c).

#### 4.1 Robust approach

If  $d \sim P^*$  and we have some confidence set  $D$ , then we have the following out-of-sample disappointment guarantee.

**Lemma 4.1.** *Suppose we solve the robust problem (7). Let  $X^D, b^D$  be the optimal solution. Then*

$$\mathbb{P}_{d \sim P^*} \left[ \sum_{t \in [T]} b_t^D - Q(X^D, d) \leq \sum_{t \in [T]} b_t^D - \min_{d' \in D} Q(X^D, d') \right] \geq \mathbb{P}_{d \sim P^*}[d \in D].$$

Let us now construct confidence sets for the non-i.i.d. prior, which can also be applied to the i.i.d. prior. Henceforth we denote  $a = (a_1, \dots, a_n)$  and  $\varrho = (\rho_1, \dots, \rho_n)$ . We consider concentration bounds on the random quantity  $\langle a, d \rangle$ , for which  $\mathbb{E}_{d \sim P^*}[\langle a, d \rangle] = \langle a, \varrho \rangle$ . Lu and Chung [27, Theorems 2.8, 2.9] show that

$$\mathbb{P}_{d \sim P^*} [\langle a, \varrho \rangle - \lambda \leq \langle a, d \rangle \leq \langle a, \varrho \rangle + \lambda] \geq 1 - 2 \exp \left( - \frac{\lambda^2}{2 \left( \sum_{i \in [n]} a_i^2 \rho_i + \lambda \max_{i \in [n]} |a_i| / 3 \right)} \right). \quad (19)$$

Observe that by Cauchy-Schwarz, we have

$$\left( \sum_{i \in [n]} a_i \right)^2 = \left( \sum_{i \in [n]} a_i \sqrt{\rho_i} \frac{1}{\sqrt{\rho_i}} \right)^2 \leq \left( \sum_{i \in [n]} a_i^2 \rho_i \right) \left( \sum_{i \in [n]} \frac{1}{\rho_i} \right) \implies \sum_{i \in [n]} a_i^2 \rho_i \geq \left( \sum_{i \in [n]} \frac{1}{\rho_i} \right)^{-1} \left( \sum_{i \in [n]} a_i \right)^2.$$

To make this equality, for  $c > 0$  we choose

$$a_i = \frac{c}{\rho_i}, \quad \forall i \in [n] \implies \sum_{i \in [n]} a_i^2 \rho_i = c^2 \sum_{i \in [n]} \frac{1}{\rho_i}.$$

Now we choose  $\lambda = \delta \langle a, \varrho \rangle = \delta cn$  so that we have

$$\begin{aligned} \mathbb{P}_{d \sim P^*} \left[ 1 - \delta \leq \frac{1}{n} \sum_{i \in [n]} \frac{d_i}{\rho_i} \leq 1 + \delta \right] &\geq 1 - 2 \exp \left( - \frac{\delta^2 c^2 n^2}{2 \left( c^2 \sum_{i \in [n]} \frac{1}{\rho_i} + (\delta/3) cn \max_{i \in [n]} \frac{1}{\rho_i} \right)} \right) \\ &= 1 - 2 \exp \left( - \frac{\delta^2 n}{2 \left( \frac{1}{n} \sum_{i \in [n]} \frac{1}{\rho_i} + (\delta/3) \max_{i \in [n]} \frac{1}{c \rho_i} \right)} \right) \\ \implies \mathbb{P}_{d \sim P^*} \left[ 1 - \delta \leq \frac{1}{n} \sum_{i \in [n]} \frac{d_i}{\rho_i} \leq 1 + \delta \right] &\geq 1 - 2 \exp \left( - \frac{\delta^2 n}{\frac{2}{n} \sum_{i \in [n]} \frac{1}{\rho_i}} \right), \end{aligned}$$

where the last implication follows since we can take  $c$  arbitrarily large. This suggests the following uncertainty set for the non-i.i.d. prior:

$$D_\delta := \left\{ d \in \{0, 1\}^n : 1 - \delta \leq \frac{1}{n} \sum_{i \in [n]} \frac{d_i}{\rho_i} \leq 1 + \delta \right\}.$$

## 4.2 Distributionally robust approach

Suppose that  $P^*$  is supported on  $\{0, 1\}^n$ , which we enumerate as  $\{d^1, \dots, d^N\}$ , where  $\mathbb{P}_{d \sim P^*}[d = d^i] = p^{i^*}$ . We also assume that  $P$  is supported on  $\{d^1, \dots, d^K\} \subseteq \{0, 1\}^n$ , where  $\mathbb{P}_{d \sim P}[d = d^k] = p^k$ . In this section, we will denote the Wasserstein distance as

$$W(P, P^*) := \min_z \left\{ \sum_{k \in [K]} \sum_{i \in [N]} \|d^i - d^k\| z_{ik} : \begin{array}{l} z \geq 0 \\ \sum_{k \in [K]} z_{ik} = p^{i^*}, \quad \forall i \in [N] \\ \sum_{i \in [N]} z_{ik} = p^k, \quad \forall k \in [K] \end{array} \right\}.$$

Suppose that  $P$  approximates the true distribution  $P^*$  well, in the sense that the Wasserstein distance between  $P$  and  $P^*$  is small, say  $\epsilon > 0$ . Then solving (8) to get solution  $X^{P, \epsilon}, b^{P, \epsilon}$  gives the following out-of-sample disappointment guarantee:

$$\sum_{t \in [T]} b_t^{P, \epsilon} - \mathbb{E}_{d \sim P^*} [Q(X^{P, \epsilon}, d)] \leq \sum_{t \in [T]} b_t^{P, \epsilon} - \min_{\bar{P} \in \mathcal{F}_\epsilon(P)} \mathbb{E}_{d \sim \bar{P}} [Q(X^{P, \epsilon}, d)].$$

In general, it is not possible to compute the Wasserstein distance exactly, since we do not know  $P^*$ . Even for the probabilistic priors outlined above where we do know the true  $P^*$ , it is difficult to compute the Wasserstein distance to a generic  $P$ . This is because  $P^*$  is supported on  $\{0, 1\}^n$ , so computing the Wasserstein distance involves solving a linear program with  $K \cdot 2^n$  variables.

The work-around to computing  $\epsilon$  exactly (suggested by Mohajerin Esfahani and Kuhn [30]) is to sample  $K$  i.i.d. points  $d^1, \dots, d^K$  from  $P^*$  to build  $P^K := \frac{1}{K} \sum_{k \in [K]} \delta_{d^k}$ , then use concentration results that provide an upper bound on  $\epsilon$ . The concentration result is typically of the form

$$\mathbb{P}_{d^1, \dots, d^K \sim P^*} [W(P^K, P^*) \leq \epsilon_K(\beta)] \geq 1 - \beta.$$

Then, if we set  $\epsilon := \epsilon_K(\beta)$  in (8), we have the following out-of-sample disappointment guarantee:

**Lemma 4.2** (Mohajerin Esfahani and Kuhn [30, Theorem 3.5]). *Suppose we solve the DRO problem (8) with  $P := P^K$ , an empirical distribution on samples  $d^1, \dots, d^K$  drawn from  $P^*$ , and  $\epsilon := \epsilon_K(\beta)$ . Let  $X^{K, \epsilon}, b^{K, \epsilon}$  be the optimal solution. Then*

$$\mathbb{P}_{d^1, \dots, d^K \sim P^*} \left[ \sum_{t \in [T]} b_t^{K, \epsilon} - \mathbb{E}_{d \sim P^*} [Q(X^{K, \epsilon}, d)] \leq \sum_{t \in [T]} b_t^{K, \epsilon} - \min_{\bar{P} \in \mathcal{F}_\epsilon(P)} \mathbb{E}_{d \sim \bar{P}} [Q(X^{K, \epsilon}, d)] \right] \geq 1 - \beta.$$

A general form of  $\epsilon_K(\beta)$  is  $O\left(\left(\frac{1}{K} \log\left(\frac{1}{\beta}\right)\right)^{1/n}\right)$  [30, Theorem 3.4]. This has an unfavourable dependence on the dimension  $n$ . However, since  $P^*$  is supported on  $\{0, 1\}^n$ , which is a compact set, we appeal to an improved result of Ji and Lejeune [22, Theorem 2], which states that we have

$$\epsilon_K(\beta) = \left(n + \frac{3}{4}\right) \left(\frac{1}{K} \log\left(\frac{1}{\beta}\right) + 2\sqrt{\frac{1}{K} \log\left(\frac{1}{\beta}\right)}\right).$$

Use of this choice of radius in the context of two-stage DRO with 0-1 uncertainty was first suggested by Subramanyam et al. [35] in the context of rare-event decision-making.

We also suggest an alternative to the so-called ‘data-driven’ approach of sampling to build  $P^K$ , which has potential to work well when  $\mathbb{E}_{d \sim P^*}[\|d\|] \ll 1$ . In this case, we suggest simply taking  $P$  to be the distribution with singleton support on the zero vector:  $\mathbb{P}_{d \sim P}[d = 0] = 1$ . It is then easy to verify that  $W(P, P^*) = \mathbb{E}_{d \sim P^*}[\|d\|]$ , thus we can take this to be our radius. Intuitively, this can work well because when  $\mathbb{E}_{d \sim P^*}[\|d\|] \ll 1$ , we expect  $\mathbb{P}_{d \sim P^*}[d = 0]$  to be quite high, so  $P$  is a good approximation for  $P^*$ .

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