## OVERLAP IN OBSERVATIONAL STUDIES WITH HIGH-DIMENSIONAL COVARIATES\* WORKING DRAFT; REVISED: NOVEMBER 4, 2017

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Causal inference in observational settings typically rests on a pair of identifying assumptions: (1) unconfoundedness and (2) covariate overlap, also known as positivity or common support. Investigators often argue that unconfoundedness is more plausible when many covariates are included in the analysis. Less discussed is the fact that covariate overlap is more difficult to satisfy in this setting. In this paper, we explore the implications of overlap in high-dimensional observational studies, arguing that this assumption is stronger than investigators typically realize. Our main innovation is to frame (strict) overlap in terms of bounds on a likelihood ratio, which allows us to leverage and expand on existing results from information theory. In particular, we show that strict overlap bounds discriminating information (e.g., Kullback-Leibler divergence) between the covariate distributions in the treated and control populations. We use these results to derive explicit bounds on the average imbalance in covariate means under strict overlap and a range of assumptions on the covariate distributions. Importantly, these bounds grow tighter as the dimension grows large, and converge to zero, in some cases. We examine how restrictions on the treatment assignment and outcome processes can weaken the implications of overlap, but at the cost of stronger requirements for unconfoundedness. Taken together, our results suggest that adjusting for high-dimensional covariates does not necessarily make causal identification more plausible.

1. Introduction. Accompanying the rapid growth in online platforms, administrative databases, and genetic studies, there has been a push to extend methods for observational studies to settings with high-dimensional covariates. These studies typically require a pair of identifying assumptions: (1) unconfoundedness—conditional on observed covariates, treatment assignment is as good as random; and (2) covariate overlap, also known as

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positivity or common support—all units have a non-zero probability of assignment to each treatment condition [29].

A key argument for high-dimensional observational studies is that unconfoundedness is more plausible when the analyst conditions on many covariates [28, 31]. There are notable counter-examples to this argument [23, 24, 25. For example, conditioning on either colliders or instruments may increase bias. Setting aside these counter-examples, the intuition is straightforward to state: the richer the set of covariates, the more likely that unmeasured confounding variables become measured confounding variables. This intuition, however, has the opposite implications for overlap: the richer the set of covariates, the more likely these covariates can perfectly predict treatment assignment for at least some subgroups. For example, online recommendation systems often use deterministic algorithms that are based on high dimensional covariates. In these cases, treatment assignment is perfectly predicted by the covariates if one observes them all. Similar problems may arise when using observational electronic medical health records if doctors make treatment decisions using a deterministic rule based on patients' medical history. Even if the decision rule varied across doctors, the overlap assumption would be violated because the observed data would perfectly explain treatment assignment.

In this paper, we explore the implications of overlap in high-dimensional causal inference, arguing that this assumption is much stronger with high-dimensional covariates than with low-dimensional covariates — and much stronger, we believe, than most investigators realize. In particular, we focus on the *strict* overlap assumption, which asserts that the propensity score is bounded away from 0 and 1 with probability 1.

Our main innovation, presented in Section 2 is to frame overlap in terms of bounds on the likelihood ratio that contrasts the covariate distributions in the treated and control populations. As we show, strict overlap imposes a bound on this likelihood ratio that remains fixed even as the dimension of the covariates grows. Building on results from the intersection of information theory and statistics, we show in Section 3 that the likelihood ratio bound imposed by strict overlap induces upper bounds on a family of information divergences that measure discrepancies between the treated and control covariate distributions. In Section 4, we use these results to derive explicit bounds on the average imbalance in covariate means under a range of assumptions on the covariate distributions. In several cases, we are able to show that, as the dimension of the covariates grows, strict overlap implies that the average imbalance in covariate means converges to zero.

Finally, in Section 5, we examine how the implications of strict overlap

align with modeling assumptions, such as sparsity in the propensity score, that are commonly made in high-dimensional causal inference. We show that, under these modeling assumptions, the strict overlap assumption has fewer unique implications, but that these assumptions also impose stronger requirements for unconfoundedness.

1.1. Literature Review. Overlap has been a central idea in formalizing causal inference in observational studies. Previous work has discussed difficulties with the overlap assumption without an explicit focus on the highdimensional covariate setting. Methods such as "trimming" (dropping observations in regions without overlap) have been proposed at least as early as Rosenbaum and Rubin [29], and are recommended in textbooks such as Rosenbaum [28] and Imbens and Rubin [19]. Recently, Petersen et al. [26] discussed strategies for detecting overlap violations in finite samples and provided advice for adjusting the target of estimation in response to overlap violations. Crump et al. [10] discussed similar strategies, with a focus on optimizing the estimand by trimming the sample to minimize the asymptotic variance of an optimal semiparametric estimator of the average treatment effect within the trimmed population. Hill and Su [17] proposed using flexible outcome modeling techniques, such as Bayesian additive regression trees (BART), to identify "common causal support" violations, or areas of the covariate space where there is lack of overlap in confounders. The Collaborative Targeted Maximum Likelihood Estimator (C-TMLE), a modification of the Targeted Maximum Likelihood Estimator (TMLE), was proposed by van der Laan and Gruber [35] to address finite sample overlap violations. More recently, Luo, Zhu and Ghosh [22] suggested that, in cases where overlap in all of the covariates is a strong assumption, a specific sufficient dimension reduction strategy could be used to identify causal parameters under a weaker overlap condition.

The results in this paper suggest that the high-dimensional setting exacerbates the concerns raised in prior work because population overlap, and not just sample overlap, becomes a concern with high-dimensional covariates. In this sense, our paper makes an argument similar to Robins and Ritov [27] in showing that the conditions for valid causal estimation in high-and low-dimensional settings can be qualitatively different. However, this paper differs from Robins and Ritov [27] in several ways. Robins and Ritov [27] were primarily concerned with how dimensionality affects the rates of convergence of certain nuisance function estimators, and showed that these issues translate to slow rates of convergence for the parameter of interest. Here, we are primarily concerned with how dimensionality affects the plau-

sibility of population assumptions that precede estimation. Nonetheless, the conclusions from these paper interact in important ways.

For example, one of the most important conclusions of Robins and Ritov [27] is that, in high-dimensional settings, semiparametric estimation that combines a model of the treatment assignment mechanism with a model of the outcome process is essential for estimating parameters like the ATE. The validity of these estimation techniques depends heavily on the strict overlap assumption. Many estimators in this class have recently been proposed or modified to operate in high-dimensional settings, including TMLE [36], Double/Debiased Machine Learning (DML) [8], and double selection methods (DS) [4, 12]. These estimators are regular in that they are  $n^{1/2}$ -consistent and asymptotically normal along any sequence of parametric models that approach the true data-generating process. Khan and Tamer [20] showed that the strict overlap assumption is a necessary condition for this desirable behavior. Thus, our results have particular implications for the application of these regular semiparametric estimators in high-dimensional settings.

Many of the information-theoretic concepts discussed in this paper, including information divergences, Fano's inequality, and the data-processing inequality are detailed in Cover and Thomas [9]. Some of our results use concepts common in high dimensional probability, including concentration inequalities and formalism from high-dimensional testing. Here, Boucheron, Lugosi and Massart [7] and Vershynin [37] are useful references.

### 2. Framework and Preliminaries.

2.1. Overlap. We focus on an observational study with a binary treatment. For each sampled unit i,  $(Y_i(0), Y_i(1))$  are potential outcomes,  $T_i$  is the treatment indicator, and  $X_i$  is a sequence of covariates. Let  $\{(Y_i(0), Y_i(1)), T_i, X_i\}_{i=1}^n$  be iid, distributed according to a superpopulation probability measure P. Because of this iid sampling, we drop the i subscript when discussing stochastic properties of these quantities. We observe triples  $(Y^{\text{obs}}, T, X)$  where  $Y^{\text{obs}} = (1 - T)Y(0) + TY(1)$ .

We would like to estimate the average treatment effect

$$\tau^{\text{ATE}} = E[Y(1) - Y(0)].$$

The standard approach in observational studies is to argue that identification is plausible conditional on a (possibly large) set of covariates [29]. Specifically, the investigator chooses a set of p covariates  $X_{1:p} \subset X$ , and

assumes the relation (1):

$$\tau^{ATE} = \mathbb{E}[\mathbb{E}[Y(1) \mid X_{1:p}] - \mathbb{E}[Y(0) \mid X_{1:p}]]$$

$$= \mathbb{E}[\mathbb{E}[Y^{\text{obs}} \mid T = 1, X_{1:p}] - \mathbb{E}[Y^{\text{obs}} \mid T = 0, X_{1:p}]].$$

The functional in (1) identifies  $\tau^{ATE}$  under the following two assumptions. First, the relation (1) holds if the following unconfoundedness assumption is satisfied.

Assumption 1 (Unconfoundedness).

(2) 
$$(Y(0), Y(1)) \perp T \mid X_{1:p}$$

This assumption is slightly stronger than is necessary for (\*) to hold, but is the most common variant because it allows similar conditioning arguments to estimate more general estimands.

Second, the conditional expectations in (1) are non-parametrically identifiable only if the following population overlap assumption is satisfied.

Assumption 2 (Population Overlap). Letting  $e(X_{1:p}) = P(T=1 \mid X_{1:p})$  be the propensity score

$$0 < e(X_{1:p}) < 1$$
 with probability (w. p.) 1.

In this paper, we explore the implications of Assumption 2 when there are many covariates. To do so, we set up an analytical framework in which the covariate sequence X is a stochastic process  $(X^{(k)})_{k>0}$ . For any single problem, the investigator selects a finite set of covariates  $X_{1:p}$  from the infinite pool of covariates  $(X^{(k)})_{k>0}$ . This framing makes explicit the investigator's role in choosing a particular subset of covariates  $X_{1:p}$  among all observable covariates  $(X^{(k)})_{k>0}$  to include in an analysis. However, it differs from the more common setup of causal inference in high dimensions, which considers a sequence of distinct problems indexed by increasing dimension p [4, 5, 12].

We also depart from the standard treatment of high-dimensional causal inference problems by treating the covariates generatively. Formally, we define control and treatment measures for covariates, for all p, for all A such that  $P(X_{1:p} \in A) > 0$ :

$$P_0(X_{1:p} \in A) := P(X_{1:p} \in A \mid T = 0),$$
  
 $P_1(X_{1:p} \in A) := P(X_{1:p} \in A \mid T = 1).$ 

In addition, define  $\alpha = P(T = 1)$  as the marginal probability that any unit is assigned to treatment. For the remainder of the paper, we will assume

that  $0 < \alpha < 1$ . With a slight abuse of notation, the relationship between the marginal probability measure on covariates, implied by the superpopulation distribution P, and the condition-specific probability measures  $P_0$  and  $P_1$  is given by the mixture

$$P = \alpha P_1 + (1 - \alpha) P_0.$$

We write the densities of  $P_1$  and  $P_0$  with respect to the dominating measure P as  $dP_1/dP$  and  $dP_0/dP$ . When discussing density ratios, we will omit the dominating measure dP. Finally, we write the marginal probability measures of finite-dimensional covariate sets  $X_{1:p}$  as  $P_0(X_{1:p})$  and  $P_1(X_{1:p})$ , and the marginal densities as  $dP_1/dP(X_{1:p})$  and  $dP_0/dP(X_{1:p})$ .

With this formalism, we restate the overlap assumption in likelihood ratio form.

Assumption 3 (Overlap, Likelihood Ratio Form).

$$0 < \frac{dP_1(X_{1:p})}{dP_0(X_{1:p})} < \infty$$
 with *P*-probability (w.p.) 1.

Assumption 3 states that the overlap assumption is a restriction on the likelihood ratio between  $P_0$  and  $P_1$ . It also hints at the fact that the probability measures  $P_0$  and  $P_1$  cannot be too distinct as p grows large; if they were, then the likelihood ratio would diverge, as it does in large-sample hypothesis testing settings.

2.2. Sample versus Population Overlap. We emphasize that, in this paper, we are concerned exclusively with population overlap, not with overlap in finite samples. Finite sample overlap does not have a unique definition, but can be heuristically defined as having a "sufficient" number of treated and control units sampled in each "neighborhood" of the covariate space. Many previous works concerning the overlap assumption are primarily concerned with finite sample overlap [e.g., 26].

This distinction is important for several reasons. First, finite sample overlap depends on many aspects of the realized sample, such as sample size. Population overlap, on the other hand, characterizes certain properties of the superpopulation distribution, so sample properties are irrelevant. For this reason, our results are stated purely in terms of the covariate dimension p, without any mention of sample sizes.

Second, and in the same vein, dimensionality has a different relationship with finite sample overlap than it does with population overlap. Finite sample overlap depends primarily on the relationship between sample size and dimensionality. For example, in cases where the covariates are discrete, the number of cells in the covariate space increases exponentially with the dimension of the covariates, so finite sample overlap will be violated unless the sample size is assumed to grow exponentially as well. On the other hand, the covariate distributions  $P_0$  and  $P_1$  may still place positive probability in each of these cells for each treatment assignment, so population overlap may hold for any p. Our results are concerned with what this sort of constraint implies about the similarity between the covariate distribution  $P_0$  and  $P_1$ .

Finally, we note that population overlap is necessary for sample overlap, but it is not sufficient. For example, in randomized trials with high-dimensional covariate information, population overlap is satisfied trivially, but for a given sample size, investigators may determine that finite sample overlap fails in a particular sample.

2.3. Strict Overlap. While investigators typically invoke the overlap assumption in Assumption 2 for identification, they instead invoke a stronger overlap assumption to characterize the behavior of ATE estimators. For the remainder of the paper, we will focus on this stronger variant of the overlap assumption that we call the *strict overlap assumption*.

ASSUMPTION 4 (Strict Overlap, Propensity Score Form). For some constant  $\eta \in (0, 0.5)$ ,

$$\eta < e(X_{1:p}) < 1 - \eta$$
 w.p. 1.

We call  $\eta$  the bound of the strict overlap assumption.

Strict overlap is a necessary condition for regular semiparametric estimators of the ATE to be  $n^{1/2}$ -consistent [20]. Specifically, all regular semiparametric estimators have asymptotic variance proportional to the following variance lower bound, known as the semiparametric efficiency bound [14, 10]:

(3) 
$$V^{\text{eff}} = \mathbb{E}\left[\frac{\text{var}(Y(1) \mid X_{1:p})}{e(X_{1:p})} + \frac{\text{var}(Y(0) \mid X_{1:p})}{1 - e(X_{1:p})} + (\tau(X_{1:p}) - \tau^{ATE})^2\right],$$

where  $\tau(X_{1:p}) := E[Y(1) - Y(0) \mid X_{1:p}]$  is the conditional average treatment effect. Since the propensity score appears in the denominator, these these fractions are only bounded if strict overlap holds. If it does not, all regular semiparametric estimators will converge to the ATE at a rate slower than  $O(n^{-1/2})$ .

The strict overlap assumption can also be represented in likelihood ratio form.

ASSUMPTION 5 (Strict Overlap, Likelihood Ratio Form). For some  $\eta \in (0, 0.5)$ , for each  $A \in \sigma(X_{1:p})$  such that  $P(X_{1:p} \in A) > 0$ ,

(4) 
$$\frac{\eta}{1-\eta} < \frac{\alpha}{1-\alpha} \frac{dP_1(X_{1:p})}{dP_0(X_{1:p})} < \frac{1-\eta}{\eta} \quad \text{w.p. 1.}$$

Assumption 5 makes clear that the strict overlap assumption is a bounded likelihood ratio assumption. This representation establishes a relationship between the strict overlap assumption and the literature on testing and estimation in contexts where the likelihood ratio is bounded [16, 32, 33]. We make use of many of these results to state implications of strict overlap.

REMARK 1. From the definition (4) we can conclude that  $\eta \leq \min\{\alpha, 1-\alpha\}$ . Otherwise, if  $\eta > \alpha$  and  $\alpha \leq \frac{1}{2}$ , then  $\frac{dP_1(X_{1:p})}{dP_0(X_{1:p})} > 1 + \frac{\eta - \alpha}{\alpha(1-\eta)}$  almost surely. But this would imply that  $\int dP_1/dP = \int \frac{dP_1}{dP_0}dP_0 > 1$ , which contradicts the fact that  $dP_1/dP$  is a probability density. An implication of this fact is that the strict overlap assumption is harder to satisfy when the control and treated groups have very different sizes.

Remark 2 (Strict Overlap and Gaussian Covariates). While we focus on the implications of strict overlap in high dimension, this assumption also has surprising implications in low dimensions. For example, if X is one-dimensional and follows a Gaussian distribution under both  $P_0$  and  $P_1$ , strict overlap implies that  $P_0 = P_1$ , or that the covariate is perfectly balanced. This is because if  $P_0 \neq P_1$ , the log-likelihood ratio diverges for values of X with large magnitude. Similar results can be derived when  $X_{1:p}$  is multi-dimensional. Thus, for Gaussianly distributed covariates, the implications of strict overlap are so strong that they are uninteresting. For this reason, we do not give any examples of the implications of the strict overlap assumption when the covariates are Gaussianly distributed. This implication can be weakened if the covariates  $X_{1:p}$  are restricted to lie on some compact subset of  $\mathbb{R}^p$ , but still have density proportional to a Gaussian distribution under both  $P_0$  and  $P_1$ . Covariates defined in this way are a special case of multivariate sub-exponential covariates, which we consider in Section 4.2.

3. Strict Overlap Bounds Discriminating Information. We now present our primary results that strict overlap bounds certain measures of discrepancy between the covariate measures  $P_0(X_{1:p})$  and  $P_1(X_{1:p})$ . We show that strict overlap imposes an upper bound on discrepancies measured by the family of f-divergences. We then give specific bounds for two f-divergences, the KL divergence and the  $\chi^2$ -divergence. Finally, we show that strict overlap

imposes a lower bound on the error of any hypothesis test that attempts to distinguish between  $P_0(X_{1:p})$  and  $P_1(X_{1:p})$ .

3.1. f-Divergence Bounds. We now show that strict overlap bounds the discriminating information between  $P_0(X_{1:p})$  and  $P_1(X_{1:p})$  as measured by f-divergences, also known as  $\phi$ -divergences [33]. f-divergences are a family of discrepancy measures between probability distributions defined in terms of a non-negative convex function f satisfying f(1) = 0 [11, 2, 21]. Formally, the f-divergence from some probability measure  $Q_0$  to another  $Q_1$  is defined as

(5) 
$$D_f(Q_1(X_{1:p})||Q_0(X_{1:p})) := \mathcal{E}_{Q_0} \left[ f\left(\frac{dQ_1(X_{1:p})}{dQ_0(X_{1:p})}\right) \right],$$

f-divergences are non-negative and achieve a minimum when  $Q_0 = Q_1$ , and are, in general, asymmetric in their arguments.

Two well-known f-divergences are the KL divergence and the  $\chi^2$ -divergence (also known as the Pearson divergence), defined as follows.

(6) 
$$KL(Q_1(X_{1:p}) || Q_0(X_{1:p})) := \mathcal{E}_{Q_1} \left[ \log \frac{dQ_1(X_{1:p})}{dQ_0(X_{1:p})} \right]$$

(7) 
$$\chi^{2}(Q_{1}(X_{1:p})||Q_{0}(X_{1:p})) := \mathbb{E}_{Q_{0}} \left[ \left( \frac{dQ_{1}(X_{1:p})}{dQ_{0}(X_{1:p})} - 1 \right)^{2} \right].$$

These divergences correspond to the convex functions  $f_{KL}(x) = x \log x$  and  $f_{\chi^2} = (x-1)^2$ .

Theorem 1 shows that strict overlap bounds any f-divergence between  $P_0(X_{1:p})$  and  $P_1(X_{1:p})$ . This bound does not depend on the dimension p. In the sections that follow, we will show that this implies the bound becomes more restrictive the larger the dimension p.

For this theorem and the following discussion, it is useful to define notation for the lower and upper bound on the likelihood ratio implied by Assumption 5:

(8) 
$$b_{\min} := \frac{1 - \alpha}{\alpha} \frac{\eta}{1 - \eta} < \frac{dP_1(X_{1:p})}{dP_0(X_{1:p})} < \frac{1 - \alpha}{\alpha} \frac{1 - \eta}{\eta} =: b_{\max}.$$

Given the constraint on the likelihood ratio in Assumption 5 and the positivity and convexity of f, it should be clear that under strict overlap, any f-divergence is upper-bounded by  $\max\{f(b_{\max}), f(b_{\min})\}$ . Rukhin [33] derived tighter bounds, which we present in Theorem 1.

THEOREM 1 (f-Divergence Bound; Adaptation of Rukhin [33] Theorem 2.1). The strict overlap assumption with bound  $\eta$  implies that for any f-divergence  $D_f$ ,

(9) 
$$D_f(P_1(X_{1:p})||P_0(X_{1:p})) < \frac{b_{\max} - 1}{b_{\max} - b_{\min}} f(b_{\min}) + \frac{1 - b_{\min}}{b_{\max} - b_{\min}} f(b_{\max})$$

PROOF. By the definition in Assumption 5, the likelihood ratio  $\frac{dP_0(X_{1:p})}{dP_1(X_{1:p})}$  is bounded by  $b_{\min}$  and  $b_{\max}$  as shown in (8). Theorem 2.1 of Rukhin [33] gives the bound in (9).

Rukhin [33] showed that the bound in (9) is tight. A similar result can be obtained for f-divergences in the opposite direction by switching the roles of  $P_0$  and  $P_1$ . This entails swapping  $(b_{\min}^{-1}, b_{\max}^{-1})$  for  $(b_{\max}, b_{\min})$ .

Using this result, we can state bounds on the KL divergence and the  $\chi^2$ -divergence, each of which gives unique insight into the strength of the strict overlap assumption as the dimensionality of  $X_{1:p}$  increases.

3.2. KL Divergence Bound. Here, we use Theorem 1 to show that strict overlap imposes an upper bound on the KL divergence between  $P_0$  and  $P_1$ . We use the chain rule that decomposes the overall KL divergence into a summation across dimensions to formally state that the strict overlap assumption becomes more restrictive as the dimension p of the covariates  $X_{1:p}$  increases. In particular, we show that when p is large, the strict overlap condition implies that, on average, each covariate  $X^{(k)}$  contains very little unique information discriminating between  $P_0$  and  $P_1$ .

Proposition 1 shows that strict overlap bounds the KL divergence between  $P_0(X_{1:p})$  and  $P_1(X_{1:p})$  in both directions.

PROPOSITION 1 (KL Divergence Bound). The strict overlap assumption with bound  $\eta$  implies the following two inequalities

(10) 
$$KL(P_1(X_{1:p})||P_0(X_{1:p}))$$
  
  $< \frac{(1-b_{\min})b_{\max}\log b_{\max} + (b_{\max}-1)b_{\min}\log b_{\min}}{b_{\max}-b_{\min}} =: B_{KL(1||0)},$ 

(11) 
$$KL(P_0(X_{1:p})||P_1(X_{1:p}))$$
  
 $< -\frac{(1-b_{\min})\log b_{\max} + (b_{\max}-1)\log b_{\min}}{b_{\max}-b_{\min}} =: B_{KL(0||1)}.$ 

For the KL-divergence, we can obtain a loose upper bound on  $B_{\mathrm{KL}(1||0)}$  and  $B_{\mathrm{KL}(0||1)}$  that is more interpretable. This bound follows almost immediately from the statement of Assumption 5.

(12) 
$$\max\left\{B_{\mathrm{KL}(1\parallel0)}, B_{\mathrm{KL}(0\parallel1)}\right\} \le \left|\log\frac{\eta}{1-\eta}\right| + \left|\log\frac{\alpha}{1-\alpha}\right|$$

The first term of this loose bound shows that the information bound approaches 0 as the strict overlap bound  $\eta$  approaches 0.5, which would imply that T is randomly assigned. The second term vanishes when treatment assignment is balanced,  $\alpha = 0.5$ . In the case of balanced treatment assignment,  $B_{\text{KL}(1||0)}$  and  $B_{\text{KL}(0||1)}$  also take a simple form that highlights the slack in the loose bound in (12):

$$B_{\mathrm{KL}(1||0)} = B_{\mathrm{KL}(0||1)} = (1 - 2\eta) \left| \log \frac{\eta}{1 - \eta} \right|.$$

Importantly, neither bound in Proposition 1 depends on p, in contrast to KL divergence, which can only grow in p. In particular, the KL divergence can be expanded into a summation of p non-negative terms [9, Theorem 2.5.3]:

$$KL(P_1(X_{1:p}) || P_0(X_{1:p})) = \sum_{k=1}^p E_{P_1} KL(P_1(X^{(k)} | X_{1:k-1}) || P_0(X^{(k)} | X_{1:k-1})).$$

Thus, the bound in Proposition 1 becomes more restrictive as p increases.

We can also use (13) to assess the discriminating information in the kth covariate,  $X^{(k)}$ , after conditioning on all previous covariates  $X_{1:k-1}$ . Specifically, each term in (13) is the expected KL divergence between the conditional distributions of the covariate  $X^{(k)}$  under  $P_0$  and  $P_1$ . Thus, Proposition 1 also bounds the average unique discriminating information contained in each covariate  $X^{(k)}$ ; this upper bound converges to zero as p grows large.

COROLLARY 1. Let  $(X^{(k)})_{k>0}$  be a sequence of covariates, and for each p, let  $X_{1:p}$  be a finite subset of  $(X^{(k)})_{k>0}$ . As p grows large, strict overlap with fixed bound  $\eta$  implies

(14) 
$$\frac{1}{p} \sum_{k=1}^{p} \mathrm{E}_{P_1} \mathrm{KL}(P_1(X^{(k)} \mid X_{1:k-1}) || P_0(X^{(k)} \mid X_{1:k-1})) = O(p^{-1}),$$

and likewise for the KL divergence evaluated in the opposite direction.

Thus, strict overlap implies that, on average, the discrepancy between conditional distributions must vanish as p grows large, implying that these conditional distributions are, on average, arbitrarily close to balance. In the special case where the covariates  $X^{(k)}$  are mutually independent under both  $P_0$  and  $P_1$ , Corollary 1 would imply that, on average, the marginal treated and control distributions for the covariates  $X^{(k)}$  are arbitrarily close to balance.

3.3.  $\chi^2$ -Divergence Bound. Here, we use Theorem 1 to show that strict overlap imposes an upper bound on the  $\chi^2$ -divergence between  $P_0(X_{1:p})$  and  $P_1(X_{1:p})$ . We can use this result to bound arbitrary discrepancies of the form:

(15) 
$$|\mathbf{E}_{P_0}[g(X_{1:p})] - \mathbf{E}_{P_1}[g(X_{1:p})]|$$

for any measurable function  $f: \mathbb{R}^p \to \mathbb{R}$  that is square-integrable under  $P_0$  and  $P_1$ . We apply this result in the following subsection to bound the mean discrepancy between  $P_0(X_{1:p})$  and  $P_1(X_{1:p})$ .

Recall the definition of the  $\chi^2$ -divergence in (7), and the definitions of  $b_{\min}$  and  $b_{\max}$  in (8). Applying Theorem 1, strict overlap imposes the following upper bounds on the  $\chi^2$ -divergences between  $P_0(X_{1:p})$  and  $P_1(X_{1:p})$ .

Proposition 2. The strict overlap assumption with bound  $\eta$  implies the following two inequalities

(16) 
$$\chi^2(P_1(X_{1:p})||P_0(X_{1:p})) < (1 - b_{\min})(b_{\max} - 1) =: B_{\chi^2(1||0)}$$

(17) 
$$\chi^2(P_0(X_{1:p})||P_1(X_{1:p})) < (1 - b_{\max}^{-1})(b_{\min}^{-1} - 1) =: B_{\chi^2(0||1)}.$$

The  $\chi^2$ -divergence is an important discrepancy measure because it appears in upper bounds on functional discrepancies of the form (15) derived by the Cauchy-Schwarz inequality. In particular, the expression in (15) has the following upper bound

(18)  

$$|\mathbf{E}_{P_{1}}g(X_{1:p}) - \mathbf{E}_{P_{0}}g(X_{1:p})| = \left|\mathbf{E}_{P_{0}}\left[\left(g(X_{1:p}) - C\right) \cdot \left(\frac{dP_{1}(X_{1:p})}{dP_{0}(X_{1:p})} - 1\right)\right]\right|$$

$$\leq \|g(X_{1:p}) - C\|_{P_{0},2} \cdot \sqrt{\chi^{2}(P_{1}(X_{1:p})\|P_{0}(X_{1:p}))},$$

for any finite constant C, and where  $||g||_{P,q} := \{E_P[|g|^q]\}^{1/q}$  denotes the q-norm of the function g under measure P. A similar bound holds with respect to the  $\chi^2$ -divergence evaluated in the opposite direction.

Combining this observation with Proposition 2, we obtain the following explicit upper bound on functional discrepancies between  $P_0$  and  $P_1$ .

Theorem 2. The strict overlap assumption with bound  $\eta$  implies

(20) 
$$|\mathcal{E}_{P_1}g(X_{1:P}) - \mathcal{E}_{P_0}g(X_{1:p})| \le \min \left\{ \sqrt{\operatorname{var}_{P_0}(g(X_{1:p}))} \cdot \sqrt{B_{\chi^2(1\parallel 0)}}, \sqrt{\operatorname{var}_{P_1}(g(X_{1:p}))} \cdot \sqrt{B_{\chi^2(0\parallel 1)}} \right\}.$$

and likewise for  $P_0$  and  $P_1$  switched.

PROOF. Let 
$$C = \mathbb{E}_{P_0} g(X_{1:p})$$
 and apply (19) and Proposition 2. Do the same for  $C = \mathbb{E}_{P_1} g(X_{1:p})$ .

Note that Theorem 2 remains valid even when  $\operatorname{var}_{P_0}(g(X_{1:p})) = \operatorname{var}_{P_1}(g(X_{1:p})) = \infty$ ; this case, inequality (20) holds automatically.

REMARK 3 (Generalization to  $\chi^{\alpha}$ -Divergences). The decomposition in (18) can be used to construct additional upper bounds on the mean discrepancy in g using Hölder's inequality in combination with  $\chi^{\alpha}$ -divergences [34]. These bounds give a tighter bound in terms of  $\eta$ , but are functions of higher-order moments of  $g(X_{1:p})$ . We give full details of these generalized results in the appendix.

3.4. Test Error Lower Bound. To close this section, we present an information bound stated in a slightly different way: we show that strict overlap implies a lower bound on the error probability of any hypothesis test of the form

(21) 
$$H_0: X_{1:p} \sim P_0; \quad H_A: X_{1:p} \sim P_1.$$

This corresponds to an intuitive interpretation of strict overlap: when strict overlap holds, one should not be able to guess with a low error rate whether any unit was assigned to treatment or control on the basis of its covariate vector  $X_{1:p}$ . This result is closely related to the information divergence results stated above although its statement is superficially different. We discuss this connection after presenting the result.

Our approach in this section is similar to approaches that appear in the high-dimensional testing literature, for example, Addario-Berry et al. [1]. Formally, let  $\phi : \mathbb{R} \mapsto \{0,1\}$  be a testing procedure of the point hypothesis  $P_0$  against the alternative  $P_1$  (or, equivalently, T=0 against T=1) based on statistic  $S(X_{1:p})$ . Let  $\phi(S(X_{1:p}))$  output 0 if it fails to reject the hypothesis

that T=0 and output 1 if it rejects the hypothesis that T=0. We upper bound the error probability of the test as the maximum of the Type I and Type II errors of the test  $\phi$ .

(22) 
$$\delta_{\phi} := \max\{P(\phi(S(X_{1:p})) = 1 \mid T = 0), P(\phi(S(X_{1:p})) = 0 \mid T = 1)\}.$$

With this formalism, we state our result.

THEOREM 3 (No test with low error probability). The strict overlap assumption with bound  $\eta$  implies that, for any p, there exists no testing procedure  $\phi$  of  $P_0(X_{1:p})$  against  $P_1(X_{1:p})$  such that  $\delta_{\phi} \leq \eta$ .

PROOF. Let  $\mathcal{E} := \{\phi(S(X_{1:p})) \neq T\}$ , or the event that the test  $\phi$  makes an error. By construction,

$$P(\mathcal{E}) = (1 - \alpha)P(\phi(S(X_{1:p})) = 1 \mid T = 0) + \alpha P(\phi(S(X_{1:p})) = 0 \mid T = 1)$$
  
  $\leq \delta_{\phi}.$ 

By Fano's inequality [9, Corollary of Theorem 2.10.1]:

(23) 
$$h(P(\mathcal{E})) \ge H(T \mid X_{1:p}),$$

where  $h(x) := -x \log x - (1-x) \log(1-x)$  and  $H(T \mid X_{1:p})$  is the conditional entropy of T given  $X_{1:p}$ , defined as

$$H(T \mid X_{1:p}) = E[-e(X_{1:p})\log(e(X_{1:p})) - (1 - e(X_{1:p}))\log(1 - e(X_{1:p}))]$$
  
=  $h(e(X_{1:p}))$ .

Note that h is concave, with a maximum at x = 0.5, and is symmetric about x = 0.5, so  $h(\eta) = h(1 - \eta)$ . Thus, by Assumption 4,

$$h(\eta) < h(e(X_{1:p})) = H(T \mid X_{1:p}) \le h(P(\mathcal{E}))$$

Finally, because  $\eta < 1/2$  by construction, this implies  $\eta \leq P(\mathcal{E}) \leq \delta_{\phi}$ .

Theorem 3 is closely related to the f-divergence bounds stated earlier in this section. In particular, the probability of error  $P(\mathcal{E})$  can itself be expressed as an f-divergence, and bounded using Theorem 1 [33, 32]. The bound in Theorem 3 derived from Fano's inequality is tighter; in particular, it is not a function of  $\alpha := P(T = 1)$ .

For additional intuition, we can also re-state Theorem 3 from the perspective of classification. For any number of features p, strict overlap implies there exists no classifier that can classify units into T=1 or T=0

with misclassification probability less than  $\eta$ . This framing immediately suggests empirical tests of whether the test bound in Theorem 3 is satisfied; we discuss this in more detail in Section 6.1.

Finally, Theorem 3 is a useful proof device for deriving concrete implications of overlap. In particular, we use this to convert any test of  $P_0$  against  $P_1$ , regardless of whether that test is optimal, into an upper bound on the discrepancy between parameters of  $P_0$  and  $P_1$  identified by the test statistic  $S(X_{1:p})$ . We can also test this error bound empirically, a topic we leave to future work, but which we describe broadly in Section 6.1.

The implications of Theorem 3 also grow more restrictive as p increases. This is because, for a fixed covariate sequence  $(X^{(k)})_{k>0}$ , the error probability of an optimal test in terms of  $\delta_{\phi}$  is non-increasing in the dimension of  $X_{1:p}$ . In particular, strict overlap implies that a test cannot be consistent in the large-p limit. We make this formal below.

DEFINITION 1. A test  $\phi(S(X_{1:p}))$  is *p-consistent* if and only if  $\delta_{\phi} \to_P 0$  as *p* grows large.

COROLLARY 2 (No Consistent Test). Let  $(X^{(k)})$  be a sequence of covariates, and for each p, let  $X_{1:p}$  a finite subset. If strict overlap with fixed bound  $\eta$  holds as p grows large, there exists no p-consistent test of  $P_0$  against  $P_1$ .

4. Application to Mean Discrepancy Bounds. We now apply the results from the previous section to show that strict overlap bounds the mean discrepancy between covariate distributions  $P_0(X_{1:p})$  and  $P_1(X_{1:p})$ . In particular, these bounds imply that when the covariates are high-dimensional, strict overlap implies that either the covariates are highly correlated in both the treated and control distributions, or the average discrepancy in means across covariates is small. In other words, strict overlap restricts covariate imbalance.

We give two bounds on mean imbalance on this section. The first is a bound that applies generally, whenever the covariance of  $X_{1:p}$  has a finite operator norm under  $P_0$  or  $P_1$ . We derive this bound by applying Theorem 2. The second is a tighter bound that applies in the case where  $X_{1:p}$  is multivariate sub-exponential under both  $P_0$  and  $P_1$ . We derive this second bound by applying Theorem 3.

Throughout this section, we use the following notation for the expecta-

tions and covariance matrices of  $X_{1:p}$  under  $P_0$  and  $P_1$ :

$$\mu_{0,1:p} := (\mu_0^{(1)}, \dots, \mu_0^{(p)}) := \mathcal{E}_{P_0}[X_{1:p}] \qquad \qquad \Sigma_{0,1:p} := \operatorname{var}_{P_0}(X_{1:p})$$

$$\mu_{1,1:p} := (\mu_1^{(1)}, \dots, \mu_1^{(p)}) := \mathcal{E}_{P_1}[X_{1:p}] \qquad \qquad \Sigma_{1,1:p} := \operatorname{var}_{P_1}(X_{1:p}).$$

We use  $\|\cdot\|$  to denote the Euclidean norm of a vector, and  $\|\cdot\|_{op}$  to denote the operator norm of a matrix.

### 4.1. General Mean Discrepancy Bound.

4.1.1. Bound. Here, we apply Theorem 2 to derive an upper bound on the mean discrepancy between  $P_0(X_{1:p})$  and  $P_1(X_{1:p})$ . Under weak distributional assumptions, this upper bound becomes more restrictive as the dimension of  $X_{1:p}$  grows.

COROLLARY 3. Strict overlap with bound  $\eta$  implies

(24) 
$$\|\mu_{0,1:p} - \mu_{1,1:p}\| \le \min \left\{ \|\Sigma_{0,1:p}\|_{op}^{1/2} \cdot \sqrt{B_{\chi^2(1\|0)}}, \|\Sigma_{1,1:p}\|_{op}^{1/2} \cdot \sqrt{B_{\chi^2(0\|1)}} \right\}.$$

PROOF. Let  $g(X_{1:p}) := a'(X_{1:p} - \mu_{0,1:p})$ , where  $a := \frac{\mu_{1,1:p} - \mu_{0,1:p}}{\|\mu_{1,1:p} - \mu_{0,1:p}\|}$  is a vector of unit length, and apply Theorem 2.  $\text{var}_{P_0}(a'(X_{1:p} - \mu_{0,1:p}))$  is upperbounded by  $\|\Sigma_{0,1:p}\|_{op}$  by definition, and the result follows.

To more easily represent the relationship between dimension and the upper bound on mean discrepancy in Corollary 3, we convert the Euclidean distance bound to an upper bound on mean absolute discrepancy between the covariate means.

COROLLARY 4. Strict overlap with bound  $\eta$  implies

(25) 
$$\frac{1}{p} \sum_{i=1}^{p} \left| \mu_0^{(k)} - \mu_1^{(k)} \right| \le p^{-1/2} \cdot \min \left\{ \| \Sigma_{0,1:p} \|_{op}^{1/2} \cdot \sqrt{B_{\chi^2(1\|0)}}, \| \Sigma_{1,1:p} \|_{op}^{1/2} \cdot \sqrt{B_{\chi^2(0\|1)}} \right\}.$$

We can characterize the conditions under which Corollary 4 becomes more restrictive as p increases. A particularly important case is the setting in which the bound converges to zero. In that case, strict overlap implies that, for large p, the mean absolute distance in covariate means converges to zero.

To explore this, let  $(X^{(k)})_{k>0}$  be a sequence of covariates such that for each  $p, X_{1:p} \subset (X^{(k)})_{k>0}$ . Then the bound in Corollary 4 behaves as

$$(26) \qquad \frac{1}{p} \sum_{i=1}^{p} \left| \mu_0^{(k)} - \mu_1^{(k)} \right| \le O\left( p^{-1/2} \cdot \min\left\{ \|\Sigma_{0,1:p}\|_{op}^{1/2}, \|\Sigma_{1,1:p}\|_{op}^{1/2} \right\} \right)$$

and converges to zero when min  $\left\{\|\Sigma_{0,1:p}\|_{op}^{1/2}, \|\Sigma_{1,1:p}\|_{op}^{1/2}\right\} = o(p^{1/2})$ . Thus, if the operator norm (i.e., largest eigenvalue) of either covariance matrix does not grow too fast, the constraint in Corollary 4 becomes more binding as p grows large.

4.1.2. Operator Norm. The behavior of the bounds in Corollaries 3 and 4 depend on the operator norm of the covariance matrix under  $P_0$  and  $P_1$ . Heuristically, this operator norm is large whenever there is high correlation between the covariates  $X_{1:p}$  under the corresponding probability measure. Thus, these bounds on mean imbalance become more restrictive as the dimension grows

First, we note the relationship between the operator norm and the orthogonality of the covariates contained in  $X_{1:p}$ . The operator norm of a covariance matrix  $\|\Sigma_{1:p}\|_{op}$  is the largest eigenvalue of the covariance matrix  $\Sigma_{1:p}$ , and is therefore equal the variance of the variance-maximizing one-dimensional linear projection of  $X_{1:p}$ . Thus, heuristically, when the covariates in  $X_{1:p}$  are mostly orthogonal, the variance-maximizing projection contains a small fraction of the total variance in  $X_{1:p}$  and the operator norm is small. On the other hand, when the covariates  $X_{1:p}$  are highly correlated, the variance-maximizing projection will contain a large fraction of the total variance. Thus, the question of how quickly the operator norm grows is closely related to how the number of non-degenerate orthogonal projections of  $X_{1:p}$  grows with p.

We now give several examples of covariance structures and the behavior of their corresponding operator norm as p grows large. In the first two examples, the operator norm is of constant order; in the third example, the growth rate of the operator norm can vary from O(1) to O(p).

EXAMPLE 1 (Independent Case). When the components of  $(X^{(k)})_{k>0}$  are independent, with component-wise variance given by  $\sigma_k^2$ ,  $\|\Sigma_{1:p}\|_{op} = \max_k \sigma_k^2$ . Thus, if the covariate-wise variances are bounded, the operator norm is O(1).

EXAMPLE 2 (Stationary Covariance Case). When  $(X^{(k)})_{k>0}$  is a stationary ergodic process with spectral density bounded by M,  $\|\Sigma_{1:p}\|_{op} \leq M$  [6].

For example, when  $(X^{(k)})_{k>0}$  is an MA(1) process with parameter  $\theta$ , it has a banded covariance matrix so that all elements on the diagonal  $\sigma_{k,k} = \sigma^2$  and all elements on the first off-diagonal  $\sigma_{k,k\pm 1} = \theta$ . In this case, the spectral density is upper bounded by  $\frac{\sigma^2}{2\pi}(1+\theta)^2$ , so the operator norm is O(1).

EXAMPLE 3 (Restricted Rank Case). If  $(X^{(k)})_{k>0}$  has component-wise variances given by  $\sigma_k^2$  and a number  $s_p \leq p$  of factors, so that  $\Sigma_{1,1:p}$  has rank  $s_p$ , then  $\|\Sigma_{1:p}\|_{op} \geq s_p^{-1} \sum_k \sigma_k^2$ , because the maximum eigenvalue of  $\Sigma_{1:p}$  must be larger than the average of its non-zero eigenvalues. Thus, if  $s_p = s$  is constant in p and the the component-wise variances are bounded away from 0 and  $\infty$ , the operator norm is O(p). In the special case where s = 1, the covariates are perfectly correlated. On the other hand, if  $s_p$  is a non-decreasing function of p, then the operator norm grows as  $O(p/s_p)$ .

Each example shows that if the covariates  $X_{1:p}$  are not too correlated, so that  $\|\Sigma_{1:p}\|_{op} = o(p)$ , strict overlap implies that the mean absolute discrepancy in (26) converges to zero, and the covariate means approach balance, on average, as p grows large.

4.2. Sub-Exponential Mean Discrepancy Bound. Here, we combine Theorem 3 with distributional assumptions about  $X_{1:p}$  to derive tighter bounds on mean discrepancy than those obtained in Corollary 3.

In particular, we consider the case where  $X_{1:p}$  is multivariate sub-exponential under both  $P_0$  and  $P_1$  [7, 18]. We say a covariate set  $X_{1:p}$  is multivariate sub-exponential if all one-dimensional projections of  $X_{1:p}$  are sub-exponential. Formally, we assume that there exist some finite constants  $\sigma_p^2$  and  $b_p$ , such that for all  $a \in \mathbb{R}^p$ ,

(27) 
$$E_{P_0} \exp(a'[X_{1:p} - \mu_{0,1:p}]) \le \exp\left(\frac{\|a\|^2 \sigma_p^2}{2}\right) \quad \text{for} \quad \|a\| \le \frac{1}{b_p},$$

and likewise for  $P_1$  and  $\mu_{1,1:p}$ . A consequence of (27) is that all one-dimensional linear projections of multivariate sub-exponential random variables have tails that can be upper bounded by Gaussian or exponential random variables. These bounds can be used to construct tight, non-asymptotic concentration inequalities that are useful for constructing statistical tests.

Examples of multivariate sub-exponential random variables include multivariate Gaussian and multivariate Laplace random variables, as well as multivariate random variables that are bounded in all dimensions. Multivariate sub-Gaussian random variables, which have been invoked in previous

discussions of covariate distributions in the high-dimensional setting [3], are a special case of multivariate sub-exponential random variables.

We apply Theorem 3 to a test based on tail bounds to obtain the following result.

THEOREM 4 (Sub-exponential Mean Distance Bound). Let  $X_{1:p}$  be multivariate sub-exponential with parameters  $(\sigma_p^2, b_p)$  under both  $P_0$  and  $P_1$ . Strict overlap with bound  $\eta$  implies that

(28) 
$$\|\mu_{0,1:p} - \mu_{1,1:p}\| \le \begin{cases} \sqrt{8\sigma_p^2 \log \frac{1}{\eta}} & \text{if } \sigma_p^2/b_p^2 > -2\log \eta \\ 4b_p \log \frac{1}{\eta} & \text{if } \sigma_p^2/b_p^2 \le -2\log \eta. \end{cases}$$

PROOF OF THEOREM 4. Let  $\Delta_p = \|\mu_{1,1:p} - \mu_{0,1:p}\|$ . Define  $a = \frac{\mu_{0,1:p} - \mu_{1,1:p}}{\|\mu_{0,1:p} - \mu_{1,1:p}\|}$  and test statistic  $S(X_{1:p}) = a'(X_{1:p} - \mu_{0,1:p})$ , or the projection  $X_{1:p} - \mu_{0,1:p}$  onto the vector  $\mu_{0,1:p} - \mu_{1,1:p}$ . Under  $P_0$  and  $P_1$ ,  $S(X_{1:p})$  is sub-exponential with parameters  $(\sigma_p^2, b_p)$ . Define a test that rejects  $P_0$  whenever  $S(X_{1:p}) > \Delta_p/2$ , i.e., when the projection of  $X_{1:p} - \mu_{0,1:p}$  is closer to  $\mu_{1,1:p}$  than it is to  $\mu_{0,1:p}$ , and accepts  $P_0$  otherwise.

The probability of rejecting under  $P_0$  is

$$\delta := P_0(S(X_{1:p}) > \Delta_p/2) \le \begin{cases} \exp\left(-\frac{\Delta_p^2}{8\sigma_p^2}\right) & \text{for } 0 \le \Delta_p < \frac{2\sigma_p^2}{b_p} \\ \exp\left(-\frac{\Delta_p}{4b_p}\right) & \text{for } \Delta_p > \frac{2\sigma_p^2}{b_p} \end{cases}$$

and likewise for accepting under  $P_1$ , so  $\delta$  is the error probability of the test. By Theorem 3, strict overlap implies  $\delta < \eta$ .

Denote by  $\Delta_{p,\eta}^*$  the value of  $\Delta_p$  that sets  $\delta=\eta$  in each case. Solving for  $\Delta_{p,\eta}^*$  gives the result. Further,  $\Delta_{p,\eta}^*<\frac{2\sigma_p^2}{b_p p^{1/2}}$  if and only if  $\sigma_p^2/b_p^2>-2\log\eta$ .

The bounds obtained in Theorem 4 have tighter scaling in  $\eta$  than those in Corollary 3; the bounds in (28) scale in  $\log^{1/2} \frac{1}{\eta}$  and  $\log \frac{1}{\eta}$ , whereas the bound in (24) scales in  $\eta^{-1/2}$ .

REMARK 4. One could obtain tighter bounds on the mean discrepancy in this case by specifying separate sub-exponential parameters  $(\sigma_p^2, b_p)$  for each of  $P_0$  and  $P_1$ . We have chosen to present the simpler, looser bound for clearer exposition.

As with Corollary 3, we can translate Theorem 4 into a bound on the absolute difference in means.

COROLLARY 5. In the same setting as Theorem 4, strict overlap with bound  $\eta$  implies that

$$(29) \qquad \frac{1}{p} \sum_{k=1}^{p} \left| \mu_0^{(k)} - \mu_1^{(k)} \right| \le \begin{cases} \sigma_p p^{-1/2} \sqrt{8 \log \frac{1}{\eta}} & \text{if } \sigma_p^2 / b_p^2 > -2 \log \eta \\ b_p p^{-1/2} 4 \log \frac{1}{\eta} & \text{if } \sigma_p^2 / b_p^2 \le -2 \log \eta. \end{cases}$$

We can analyze Corollary 5 asymptotically in the same way that we did with Corollary 4. Let  $(X^{(k)})_{k>0}$  be a sequence of covariates so that, for any p, a finite covariate set  $X_{1:p}$  is multivariate sub-exponential under  $P_0$  and  $P_1$  with parameters  $(\sigma_p^2, b_p)$ . Then the bound on mean absolute deviation in means behaves as

(30) 
$$\frac{1}{p} \sum_{k=1}^{p} \left| \mu_0^{(k)} - \mu_1^{(k)} \right| \le O(\max\{\sigma_p, b_p\} p^{-1/2})$$

and converges to zero when  $\max\{\sigma_p, b_p\} = o(p^{1/2})$ . Once again, the case where the upper bound in (30) approaches zero is of particular interest because it implies that, for large p, the covariate means are, on average, arbitrarily close to balance.

The asymptotic behavior of the bound on Corollary 5 is determined by the scaling of the sub-exponential parameters  $(\sigma_p^2, b_p)$ .  $\sigma_p^2$  and  $b_p^2$  are the variances deviations of the Gaussian and exponential random variables used to upper bound the tails of all one-dimensional linear projections of  $X_{1:p}$ ; in this way, they are analogous to the operator norm discussed in Section 4.1.2, but they are associated with the bounding distribution rather than the covariate distribution itself. As in the cases considered in Examples 1–3,  $\sigma_p^2$  and  $b_p^2$  are of constant order when the individual covariates  $X^{(k)}$  are independent, but grow when the covariates are correlated so that an increasing proportion of the total variance in  $X_{1:p}$  aligns with a particular projection. Thus, the sub-exponential bounds derived here also describe an orthogonality-imbalance trade-off.

5. Overlap and Models for Sufficiency. So far, we have shown that strict overlap imposes restrictions on the covariate distributions in a study that become more binding as the dimension of the covariates grows. In this section, we explore how these restrictions align with modeling assumptions about the treatment assignment and outcome processes in a study. We show that certain modeling assumptions already imply many of the constraints that overlap implies. In these cases, strict overlap introduces few additional implications beyond those of the model itself. However, there is a key tension

in cases where these modeling assumptions hold: while overlap may have fewer unique implications, unconfoundedness will be a stronger assumption.

We will focus specifically on the class of modeling assumptions that assert that some simple summary of the covariates is sufficient for the conditional distribution of the treatment assignment or potential outcomes. Models in this class include sparse models, latent variable models, and sufficient dimension reduction models. Under these models, identification of the ATE only requires overlap in the sufficient summary.

5.1. Overlap and Models for Balancing Scores. We now explore the case where the propensity score  $e(X_{1:p})$  is only a function of a sufficient summary of the covariates  $b(X_{1:p})$ . In this case, overlap in the summary  $b(X_{1:p})$  implies overlap in the full set of covariates  $X_{1:p}$ . We give several examples of the assumption and relate them to settings that have been invoked in the literature.

Assumption 6 (Sufficient Condition for Strict Overlap). There exists some function of the covariates  $b(X_{1:p})$  satisfying the following two conditions:

(31) 
$$X_{1:n} \perp T \mid b(X_{1:n})$$

(32) 
$$\eta < e_b(X_{1:p}) := P(T = 1 \mid b(X_{1:p})) < 1 - \eta.$$

Here, the variable  $b(X_{1:p})$  is a balancing score, introduced by Rosenbaum and Rubin [29].  $b(X_{1:p})$  is a sufficient summary of the covariates  $X_{1:p}$  for the treatment assignment T because the propensity score  $e(X_{1:p})$  can be written as a function of  $b(X_{1:p})$  alone, i.e., there exists some h such that

$$e(X_{1:p}) = h(b(X_{1:p})).$$

This is a restatement of the fact that the propensity score is the coarsest balancing score [29].

Overlap in a balancing score  $b(X_{1:p})$  is a sufficient condition for overlap in the entire covariate set  $X_{1:p}$ .

PROPOSITION 3 (Sufficient Condition Statement). Assumption 6 implies strict overlap in  $X_{1:p}$  with bound  $\eta$ .

PROOF. 
$$e(X_{1:p}) = E[P(T = 1 \mid X_{1:p}, b(X_{1:p})) \mid X_{1:p}] = E[P(T = 1 \mid b(X_{1:p})) \mid X_{1:p}] = E[e_b(X_{1:p}) \mid X_{1:p}], \text{ where } e_b(X_{1:p}) := P(T = 1 \mid b(X_{1:p})).$$
 Then  $\eta < e_b(X_{1:p}) < 1 - \eta \text{ w.p. 1 implies } \eta < E[e_b(X_{1:p}) \mid X_{1:p}] < 1 - \eta \text{ w.p. 1.}$ 

Assumption 6 has some trivial specifications, which are useful examples. At one extreme, we may specify that  $b(X_{1:p}) = e(X_{1:p})$ . In this case, Assumption 6 is vacuous: this puts no restrictions on the form of the propensity score and strict overlap with respect to  $b(X_{1:p})$  is equivalent to strict overlap. At the other extreme, we may specify  $b(X_{1:p})$  to be a constant; i.e., we assume that the data were generated from a randomized trial. In this case, the overlap condition in Assumption 6 holds automatically.

Of particular interest are restrictions on  $b(X_{1:p})$  between these two extremes, such as the sparse propensity score model in Example 4 below. Such restrictions trade off stronger modeling assumptions on the propensity score  $e(X_{1:p})$  with weaker implications of strict overlap. Importantly, these specifications exclude cases such as the deterministic treatment rules discussed in the introduction: even when the covariates are high-dimensional, the information they contain about the treatment assignment is upper bounded the information contained in  $b(X_{1:p})$ .

EXAMPLE 4 (Sparse Propensity Score). Consider a study where the propensity score is sparse in the covariate set  $X_{1:p}$ , so that for some subset of covariates  $X_{1:s} \subset X_{1:p}$ ,

$$e(X_{1:p}) = e(X_{1:s}).$$

This implies

(33) 
$$X_{1:p} \perp T \mid X_{1:s}$$
,

and  $X_{1:s}$  is a balancing score. In this case, strict overlap in the finite-dimensional  $X_{1:s}$  implies strict overlap for  $X_{1:p}$ .

Belloni, Chernozhukov and Hansen [4] and Farrell [12] propose a specification similar to this, with an "approximately sparse" specification for the propensity score. The approximately sparse specification in these papers is broader than the model defined here, but has similar implications for overlap.

Example 5 (Latent Variable Model for Propensity Score). Consider a study where the treatment assignment mechanism is only a function of some low-dimensional latent variable U, such that

$$X_{1:p} \perp \!\!\! \perp T \mid U$$
.

For example, such a structure exists in cases where treatment is assigned only as a function of a latent class or latent factor. In this case, the projection of  $e(U) := P(T = 1 \mid U)$  onto  $X_{1:p}$  is a balancing score:

$$b(X_{1:p}) = E[e(U) \mid X_{1:p}].$$

Here strict overlap in the latent variable U implies strict overlap in  $b(X_{1:p})$ , which implies strict overlap in  $X_{1:p}$  by Proposition 3.

Athey, Imbens and Wager [3] propose a specification similar to this in their simulations, in which the propensity score is dense with respect to observable covariates but can be specified simply in terms of a latent class.

5.2. Overlap and Models for Prognostic Scores. Here, we discuss the case where there exists a non-trivial sufficient summary of the covariates with respect to the outcome process. In this case, the ATE can be identified under a weaker overlap condition than Assumption 2. We make this precise in a slight modification of the setup in Hansen [15], who established that, for a given covariate set  $X_{1:p}$ , the ATE is identified under the following assumption.

Assumption 7 (Prognostic Identification).

- 1. Unconfoundedness holds with respect to  $X_{1:p}$  (Assumption 1).
- 2. There exists some function  $r(X_{1:p})$  satisfying the following two conditions

$$(34) (Y(0), Y(1)) \perp X_{1:p} \mid r(X_{1:p}).$$

(35) 
$$\eta < e_r(X_{1:p}) := P(T = 1 \mid r(X_{1:p})) < 1 - \eta$$

We modify the nomenclature of Hansen [15] slightly and call  $r(X_{1:p})$  a prognostic score.<sup>1</sup> Petersen et al. [26] and Luo, Zhu and Ghosh [22] proposed similar identification conditions. When assumption 7 holds, the ATE can be identified by the following functional

(36) 
$$\tau^{ATE} = \mathbb{E}[\mathbb{E}[Y^{\text{obs}} \mid T = 1, r(X_{1:p})] - \mathbb{E}[Y^{\text{obs}} \mid T = 0, r(X_{1:p})]].$$

If strict overlap holds with respect to  $r(X_{1:p})$ , a  $n^{1/2}$ -consistent non-regular semiparametric estimator of (36) exists. We discuss some examples of these non-regular semiparametric estimators at the end of this section.

The assumption of strict overlap in the full covariates  $X_{1:p}$  is at least as strong as the assumption of strict overlap in a prognostic score  $r(X_{1:p})$ , and is stronger whenever  $r(X_{1:p})$  is not finer than the propensity score  $e(X_{1:p})$  [22]. Thus, imposing restrictions on the outcome process can weaken the necessary

<sup>&</sup>lt;sup>1</sup> Hansen used the "prognostic score" to refer to sufficient statistics of Y(0) alone given covariates; here, we use it to refer to sufficient statistics of both Y(0) and Y(1). In Hansen's terminology, this would be the union of the prognostic score and the "effect modifier".

strict overlap condition for the existence of a  $n^{1/2}$ -consistent estimator of the ATE. Below, we give two examples of structural assumptions regarding prognostic scores that have appeared in the literature.

EXAMPLE 6 (Sparse Prognostic Score). Consider a study where some subset of covariates  $X_{1:s} \subset X_{1:p}$ , is sufficient for (Y(0), Y(1)), so that

$$(Y(0), Y(1)) \perp X_{1:p} \mid X_{1:s}$$

Then  $X_{1:s}$  is a prognostic score. In this case, strict overlap in the low-dimensional subset  $X_{1:s}$  is sufficient for identification of the ATE.

This structural assumption is implicit in practical advice given in the propensity score estimation and matching literatures, when it is recommended that only variables that are related to treatment be incorporated into propensity score models or matching objectives [28, 19]. Roy et al. [30] formalized this approach by specifying a matching procedure that selects covariates based on their ability to predict outcomes.

EXAMPLE 7 (Low-Dimensional Prognostic Subspace). Consider a study where an s-dimensional linear transformation of the covariates, encoded by an  $p \times d$  matrix  $\beta$ , is sufficient for (Y(0), Y(1)), so that

$$(Y(0), Y(1)) \perp X_{1:p} \mid X_{1:p}^{\top} \beta.$$

Then  $X_{1:p}^{\top}\beta$  is a prognostic score. In this case, overlap in the low-dimensional transformation  $X_{1:p}^{\top}$  is sufficient for identification of the ATE.

This case is treated in detail by Luo, Zhu and Ghosh [22], with accompanying sufficient dimension reduction methodology for estimating the linear subspace spanned by the columns of  $\beta$ .

Given a prognostic score, one can specify a non-regular semiparametric estimator for the ATE with respect to the prognostic score  $r(X_{1:p})$ , as opposed to the full covariates  $X_{1:p}$ . Such an estimator is subject to a semiparametric efficiency bound parameterized in terms of  $e_r(X_{1:p}) = P(T = 1 \mid r(X_{1:p}))$  instead of  $e(X_{1:p})$  [22]:

(37) 
$$V_r^{\text{eff}} = \mathrm{E}\left[\frac{\mathrm{var}(Y(1) \mid r(X_{1:p}))}{e_r(X_{1:p})} + \frac{\mathrm{var}(Y(0) \mid r(X_{1:p}))}{1 - e_r(X_{1:p})} + (\tau(r(X_{1:p})) - \tau^{ATE})^2\right],$$

where  $\tau(r(X_{1:p})) := E[Y(1) - Y(0) \mid r(X_{1:p})]$ . In cases where strict overlap holds with respect to  $r(X_{1:p})$ , but not with respect to  $X_{1:p}$ , no  $n^{1/2}$ -consistent

regular semiparametric estimator exists, and this non-regular estimator is super-efficient, meaning it has lower asymptotic variance than the semiparametric efficiency bound for regular estimators. van der Laan and Gruber [35] proposed that constructing such an estimator would be possible via the Collaborative TMLE (C-TMLE) method, while Luo, Zhu and Ghosh [22] outlined the construction of such an estimator when the structural assumptions in Example 7 are satisfied.

The caveat is that such a non-regular estimator only enjoys uniform  $n^{1/2}$ consistency guarantees within the non-parametric family of data-generating
processes where

$$E[(Y(0), Y(1)) \mid X_{1:p}] = E[(Y(0), Y(1)) \mid r(X_{1:p})].$$

In particular, the non-regular estimator can have unbounded bias if the summary  $r(X_{1:n})$  is misspecified and is not in fact a prognostic score.

We discuss a more general class of covariate reductions that may further weaken overlap conditions in Section 6.2.

5.3. Implications for Unconfoundedness. So far, we have shown that under certain model specifications for sufficiency in the treatment assignment or outcome processes, the overlap conditions necessary for identification have fewer unique implications. At the same time, these structural restrictions can complicate the unconfoundedness assumption. In particular, if unconfoundedness holds with respect to  $X_{1:p}$  and the treatment assignment mechanism or outcome process admits a non-trivial sufficient summary, then unconfoundedness must also hold with respect to the sufficient summary alone. We make this statement precise in the following proposition, which is a restatement of claims proved by Rosenbaum and Rubin [29] and Hansen [15], respectively.

Proposition 4 (Constraints on Confounding).

1. Suppose that  $b(X_{1:p})$  is a balancing score and unconfoundedness (Assumption 1) holds with respect to  $X_{1:p}$ . Then unconfoundendess holds with respect to  $b(X_{1:p})$  alone:

$$(Y(0), Y(1)) \perp T \mid b(X_{1:p}).$$

2. Suppose that  $r(X_{1:p})$  is a prognostic score and unconfoundedness (Assumption 1) holds with respect to  $X_{1:p}$ . Then unconfoundendess holds with respect to  $r(X_{1:p})$  alone:

$$(Y(0), Y(1)) \perp T \mid r(X_{1:n}).$$

Although these claims are not new, we state them here to emphasize that simultaneously assuming that unconfoundedness and imposing a model of sufficiency on the treatment assignment or outcome process indirectly imposes structure on the confounders in a study.

Proposition 4 highlights a tension between the strengths of the unconfoundedness and overlap assumptions in the presence of assumptions about the treatment assignment and outcome processes. Under minimal structure on these processes, adjusting for high-dimensional covariates allows for weaker assumptions about confounding, but the strict overlap assumption has more unique implications, which can be difficult to verify. On the other hand, with more structure on these processes, strict overlap introduces many fewer unique constraints, but unconfoundedness under these modeling assumptions is a stronger assumption.

This tension highlights the fact that adjusting for high-dimensional covariates does not necessarily make causal identification more plausible. Even in high-dimensional studies, careful justification regarding the structures of the treatment assignment and outcome process are necessary to argue that overlap and unconfoundedness hold in the same study.

6. Discussion and Future Work. The central insight underlying our results is that distributional discrepancies accumulate in dimension in the same way that information accumulates in sample size. We have shown that intuition derived from low-dimensional settings regarding the acceptable degrees of covariate imbalance in each dimension do not translate to high-dimensional settings. Our results establish that the strict overlap assumption has strong implications with high-dimensional covariates. Some type of structure must exist in the covariates in these settings: either covariate discrepancies shrink, or most of the covariates contain redundant information.

We briefly discuss two implications of our theoretical results that we propose to explore in greater detail in future work. First, we are developing tests for population overlap in finite samples. Second, we are exploring new covariate reduction methods.

6.1. Future Work on Testing for Overlap. One of the primary implications of our results is that the strict overlap assumption has significant empirical content. Unlike the unconfoundedness assumption, the strict overlap assumption can be tested. In particular, the bounds derived in Sections 3 and 4 have testable implications in finite samples, the clearest being the

mean discrepancy bounds in Corollary 3 and Theorem 4.<sup>2</sup> The test error bound in Theorem 3 can also be tested directly: the out-of-sample classification error of any classification procedure trained to classify units into "treated" and "control" is an estimate of an upper bound on the test error.

Assumptions about sufficient structure in the treatment assignment mechanism (Assumption 6) also have testable implications. In particular, when  $b(X_{1:p}) \subset \mathcal{B}$  is a balancing variable, the following equality holds for each set A where P(A) > 0:

$$P_0(X_{1:p} \in A) = \int_{\mathcal{B}} P_1(X_{1:p} \in A \mid b(X_{1:p})) P_0(db(X_{1:p})).$$

In cases where B is estimable, this hypothesis could be tested using non-parametric two-sample testing methods such as kernel MMD [13], modified to use balancing weights.

6.2. Future Work on Covariate Reduction. Our results suggest that novel covariate reduction techniques could be useful in analyzing observational studies with high-dimensional covariates. Whenever unconfoundedness holds with respect to a covariate set  $X_{1:p}$ , such techniques could be used to construct a generalization of balancing scores and prognostic scores that satisfy

(38) 
$$(Y(0), Y(1)) \perp T \mid d(X_{1:p}).$$

We call a summary  $d(X_{1:p})$  that satisfies (38) a deconfounding score. If strict overlap holds with respect to  $d(X_{1:p})$ , the ATE could be identified by the functional

(39) 
$$\tau^{ATE} = \mathbb{E}[\mathbb{E}[Y^{\text{obs}} \mid T = 1, d(X_{1:p})] - \mathbb{E}[Y^{\text{obs}} \mid T = 0, d(X_{1:p})]].$$

Hill and Su [17] referred to overlap in a deconfounding score as "common causal support."

For deconfounding scores to be useful in this context, they should be neither balancing scores nor prognostic scores. On the one hand, for overlap in a deconfounding score  $d(X_{1:p})$  to be a weaker assumption than overlap in the full covariates  $X_{1:p}$ , the summary  $d(X_{1:p})$  must shed some information about the treatment assignment T. This is only possible if  $d(X_{1:p})$  is not a sufficient statistic for treatment assignment, i.e., a balancing score. On the other hand, if  $d(X_{1:p})$  is a prognostic score, then overlap in  $d(X_{1:p})$  will be a weaker assumption, but too much information about the treatment

<sup>&</sup>lt;sup>2</sup>In the case of sub-exponential variables (Theorem 4) some additional assumptions are necessary because the sub-exponential parameters  $(\sigma_p^2, b_p)$  are not estimable in general.

assignment mechanism may be lost to efficiently estimate the ATE. In particular, an analysis on the basis of a prognostic score would be equivalent to estimating the ATE using only an outcome model. Robins and Ritov [27] showed that, in high-dimensional contexts, this can result in a too-slow rate of convergence without strong parametric assumptions.

Thus, we are particularly interested in exploring the space of *insufficient* deconfounding scores that incorporate information about both the treatment assignment mechanism and the outcome processes, but which are sufficient for neither process. This may require novel methodology because the constraint (38), which enforces that the deconfounding score retain unconfoundedness, is notably more difficult to work with than the sufficiency constraints that define balancing scores and prognostic scores.

# APPENDIX A: GENERALIZED FUNCTIONAL DISCREPANCY BOUNDS USING $\chi^{\alpha}$ DIVERGENCES

This section gives details of the claim made in Remark 3, that one can obtain additional bounds on the functional discrepancy

$$|E_{P_1}g(X_{1:p}) - E_{P_0}g(X_{1:p})|$$

by bounding the  $\chi^{\alpha}$  divergences between  $P_0$  and  $P_1$ .

Formally,  $\chi^{\alpha}$ -divergences are a class of divergences that generalize the  $\chi^2$ -divergence [34]:

(40) 
$$\chi^{\alpha}(P_0(X_{1:p})||P_1(X_{1:p})) := \mathbb{E}_{P_0} \left[ \left| \frac{dP_1(X_{1:p})}{dP_0(X_{1:p})} - 1 \right|^{\alpha} \right] \quad \text{for } \alpha \ge 1.$$

The  $\chi^{\alpha}$  divergence in the opposite direction is obtained by switching the roles of  $P_0$  and  $P_1$ .

Theorem 2.1 of Rukhin [33] implies that, under strict overlap with bound  $\eta$ ,

$$\chi^{\alpha}(P_0(X_{1:p}) \| P_1(X_{1:p})) \leq (b_{\max} - 1)(1 - b_{\min}) \frac{(1 - b_{\min})^{\alpha - 1} + (b_{\max} - 1)^{\alpha - 1}}{b_{\max} - b_{\min}}$$
$$\chi^{\alpha}(P_1(X_{1:p}) \| P_0(X_{1:p})) \leq (b_{\min}^{-1} - 1)(1 - b_{\max}^{-1}) \frac{(1 - b_{\max}^{-1})^{\alpha - 1} + (b_{\min}^{-1} - 1)^{\alpha - 1}}{b_{\min}^{-1} - b_{\max}^{-1}}.$$

We denote these bounds as  $B_{\chi^{\alpha}(0||1)}$  and  $B_{\chi^{\alpha}(1||0)}$ , respectively. Applying Hölder's inequality to (18), we obtain

$$|E_{P_1}g(X_{1:p}) - E_{P_0}g(X_{1:p})| \le \min \left\{ ||g(X_{1:p}) - C||_{P_0,q_\alpha} \cdot B_{\chi^\alpha(1||0)}^{1/\alpha}, ||g(X_{1:p}) - C||_{P_1,q_\alpha} \cdot B_{\chi^\alpha(0||1)}^{1/\alpha} \right\},$$

where  $q_{\alpha} := \frac{\alpha}{\alpha-1}$  is the Hölder conjugate of  $\alpha$ . Setting  $C = E_{P_0}g(X_{1:p})$  establishes a relationship between the  $q_{\alpha}$ th central moment of  $g(X_{1:p})$  under  $P_0$  and the functional discrepancy between  $P_0$  and  $P_1$ . This bound scales as  $\eta^{-1/\alpha}$ , whereas (20) scales as  $\eta^{-1/2}$ .

### APPENDIX B: WEAKENED MEAN-DISCREPANCY IMPLICATIONS

In the following example, the latent variable B induces strong correlation in the covariates  $X_{1:p}$  so that the mean discrepancy bound from Corollary 3 is not binding as p increases.

EXAMPLE 8 (Mixture exception to mean difference bounds). In the setting of Example 5, suppose each unit is a member of a latent class, say  $b_1$  or  $b_2$ , denoted by a categorical variable B with two levels  $\{b_1, b_2\}$ , and that

$$X_{1:p} \perp \!\!\! \perp T \mid B$$
.

Suppose that the distribution of B differs under treatment and control,

$$P_0(B = b_1) = \pi_0 \quad P_1(B = b_1) = \pi_1,$$

and the conditional distribution of covariates given latent class also differs by class membership

$$P_{b_1}(X_{1:p}) = P(X_{1:p} \mid B = b_1) \quad P_{b_2}(X_{1:p}) = P(X_{1:p} \mid B = b_2).$$

Then  $P_0(X_{1:p})$  and  $P_1(X_{1:p})$  are mixtures of  $P_{b_1}(X_{1:p})$  and  $P_{b_2}(X_{1:p})$ ,

$$P_0(X_{1:p}) = \pi_0 P_{b_1}(X_{1:p}) + (1 - \pi_0) P_{b_2}(X_{1:p})$$
  

$$P_1(X_{1:p}) = \pi_1 P_{b_1}(X_{1:p}) + (1 - \pi_1) P_{b_2}(X_{1:p}).$$

Note that strict overlap holds if and only if

$$\frac{\eta}{1-\eta} < \frac{\pi_1}{\pi_0} < \frac{1-\eta}{\eta}.$$

In this case, the difference between control and treated means  $\mu_{0,1:p}$  and  $\mu_{1,1:p}$  is a function of the difference between the class means  $\mu_{b_1,1:p}$  and  $\mu_{b_2,1:p}$ . In particular,

$$\|\mu_{0,1:p} - \mu_{1,1:p}\| = |\pi_0 - \pi_1| \cdot \|\mu_{b_1,1:p} - \mu_{b_2,1:p}\|.$$

Thus, even if the strict overlap assumption holds, if the discrepancy  $\|\mu_{b_1,1:p} - \mu_{b_2,1:p}\|$  is not bounded as p grows large, then neither is the discrepancy between  $\mu_{0,1:p}$  and  $\mu_{1,1:p}$ .

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