How Balanced Should Causal Covariates Be?

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Abstract

Covariate balancing is a popular technique for controlling confounding in observational studies. It finds weights for the treatment group which are close to uniform, but make the group's covariate means (approximately) equal to those of the entire sample. A crucial question is: how approximate should the balancing be, in order to minimize the error of the final estimate? Current guidance is derived from heuristic or asymptotic analyses, which are uninformative when the size of the sample is small compared to the number of covariates. This paper presents the first rigorous, nonasymptotic analysis of covariate balancing; specifically, we use PAC-Bayesian techniques to derive valid, finite-sample confidence intervals for the treatment effect. More generally, we prove these guarantees for a flexible form of covariate balancing where the regularization parameters weighting the trade-off between bias (imbalance) and variance (divergence from uniform) are optimized, not fixed. This gives rise to a new balancing algorithm which empirically delivers superior adaptivity. Our overall contribution is to make covariate balancing a more reliable method for causal inference.

1 INTRODUCTION

In an observational study, some unknown mechanism splits the participants between the treatment and control groups. This can lead to systematic differences between the two groups, biasing estimates of the treatment effect. A key assumption in causal inference is unconfoundedness [Rosenbaum and Rubin, 1983], which posits that biases of the selection mechanism can be wholly accounted for by the covariates $X_i \in \mathbb{R}^d$ observed for each participant i. This assumption is more plausible when the number of covariates

d is large. Under this assumption, any meaningful differences between the groups must manifest as discrepancies between their covariate statistics; eliminating such discrepancies therefore controls confounding. This motivates the the technique of covariate balancing, also referred to as balancing weights, calibration weights or minimal weights (surveyed by Ben-Michael et al. [2021], Chattopadhyay et al. [2020]). This technique is embodied by the following optimization program for weighting the treatment group; a similar program can be written for the control group.

$$\min_{W} \quad \max_{1 \le j \le d} \Big| \sum_{\text{treated } i} W_i X_{ij} - \widehat{M}_j \Big| + \tag{1}$$
$$\lambda \cdot \text{Divergence}(W \,||\, \text{Uniform})$$
$$\text{s.t.} \quad W \text{ is a distribution on the treatment group}$$

Here, $\lambda > 0$ is a regularization parameter and Divergence is an f-divergence between probability distributions. $\widehat{M} \in \mathbb{R}^d$ is the target mean vector, typically taken to be the empirical mean $\sum_{i=1}^{n} \frac{1}{n} X_{ij}$ of the entire sample, both treatment and control. An equivalent, more common formulation constrains imbalance by a tolerance parameter $\tau \ge 0$:

$$\min_{W} \quad \text{Divergence}(W \,||\, \text{Uniform}) \tag{2}$$
$$\text{s.t.} \quad W \text{ is a distribution on the treatment group}$$
$$\Big| \sum_{\text{treated } i} W_i X_{ij} - \widehat{M}_j \Big| \le \tau \quad \forall\, 1 \le j \le d$$

This program expresses an intuitive tradeoff between covariate imbalance and overfitting. The constraint ensures that each (weighted) covariate mean in the treatment group matches the target $\widehat{M}$, up to tolerance τ; in other words, the weighted treatment group looks roughly like an unbiased random sample, insofar as covariate means are concerned. However, tightly balancing the means ($\tau \approx 0$) may cause some weights to become very small, reducing the effective sample size. Furthermore, $\tau \approx 0$ is generally not feasible when $n < d$. Using the KL divergence leads to entropy balancing [Hainmueller, 2012], and using the χ^2 divergence leads to stable balancing weights [Zubizarreta, 2015].

The success of covariate balancing depends on choosing τ (or λ) well. Because covariate balancing isn't predictive — it estimates an unknown population quantity — techniques for tuning τ on held-out data (e.g. cross-validation) aren't readily adapted [Chattopadhyay et al., 2020]. Ideally, τ should be chosen to minimize the error of the estimate derived from the weights (i.e. the radius of its confidence interval). Unfortunately, no valid, nontrivial finite-sample confidence intervals have been derived for covariate balancing. Instead, practitioners rely on heuristics and asymptotic analyses. In early work studying approximate covariate balancing, Zubizarreta [2015] noted that $\tau = 0.1$ had been adopted in observational study matching with standardized covariates, but that this setting was problem-dependent. As noted by Ben-Michael et al. [2021], various asymptotic analyses [Hirshberg et al., 2019, Hirshberg and Wager, 2021] support $\tau = \Theta(1/n)$. The most complete, concrete guidance is currently given by the selection algorithm of Wang and Zubizarreta [2020], which was simplified slightly by Chattopadhyay et al. [2020]. Unfortunately, this algorithm still offers no provable guarantees. Furthermore, it (impractically) requires resolving (2), and performing d distinct bootstrap procedures, for every candidate value of τ.

Choosing τ remains a serious practical hurdle for covariate balancing. For example, in the recent benchmark comparison by Cousineau et al. [2023], entropy balancing and stable balancing weights could not be successfully applied to over 40% of the studies, due to infeasibility issues involving τ. These problems arose even with a moderate number of covariates: each study in the benchmark had $n = 4802$ participants and $d = 58$ covariates. In production-scale, observational healthcare studies which inform clinical practice [Suchard et al., 2019, Chen et al., 2021], it is common to have $n \ll d$, with d in the tens or hundreds of thousands [Tian et al., 2018, Zhang et al., 2022]. Such studies instead use propensity score methods (such as propensity score matching or inverse propensity weighting, per Hripcsak et al. [2021]), which may not achieve balance.

1.1 OUR CONTRIBUTIONS

This paper provides the missing finite-sample analysis of covariate balancing. We derive the first valid, nontrivial, finite-sample confidence intervals for the weighted estimates produced by covariate balancing. Our results hold when the observational data come from a different distribution than the target of our inference — a scenario called covariate shift or target transportation [Dahabreh et al., 2020, Josey et al., 2021a]. Furthermore, we analyze an extension of (1) where λ is optimized along with W. This leads not just to satisfying theoretical guarantees, but to a new balancing algorithm which demonstrates empirical benefits when hyperparameter settings are uncertain.

The starting point of our analysis is the simple observation that the program (1) conceptually aligns with the PAC-Bayesian paradigm of generalization (initiated by McAllester [1998] and Shawe-Taylor and Williamson [1997]; recently surveyed by Alquier et al. [2024]). This approach was developed to upper bound the expected population risk of a "posterior" distribution over hypotheses which is computed from a "prior" distribution and the data. The population risk bound is lower for posteriors (in our setting, W) which maintain low divergence from the the prior (for us, the uniform distribution) but also achieve low empirical risk (for us, empirical imbalance). There are conceptual and technical incompatibilities between covariance balancing and existing PAC-Bayesian inequalities, so we derive a fresh analysis starting from the underlying variational representation of f-divergences [Donsker and Varadhan, 1983, Ruderman et al., 2012, Ohnishi and Honorio, 2021].

Section 4 presents a generalization of covariate balancing which involves dynamically-optimized regularization parameters. We prove a nonasymptotic confidence interval for the estimates produced by this program, which (as a special case) apply to standard covariate balancing. Despite its generality, this proof is short and simple, relying on basic convex analysis. We describe how this improves upon a naive confidence interval presented earlier in Section 3.3. Section 6 presents a pair of carefully-designed simulations which demonstrate that our new algorithm breaks through an adaptivity barrier, using the data to correctly, automatically optimize regularization parameters. Finally, the experiments in Section 6.2 show these adaptivity benefits carry over to (completely) real data.

2 PREVIOUS WORK

2.1 MAIN BALANCING ALGORITHMS

The following algorithms involve solving either (1) or (2), so they are the main baselines for this paper.

Entropy balancing [Hainmueller, 2012]: this solves (2) with the KL divergence. τ is set to a constant with a default value of 1.0. The convex dual problem is unconstrained, so the Levenberg–Marquardt algorithm is used to solve it. Since this algorithm depends on a reasonably-conditioned $d \times d$ Hessian, it doesn't work when $n < d$. Though easily circumvented by using a standard gradient algorithm on the primal, this issue portends some of the practical inadequacies of covariate balancing in high dimensions.

Stable balancing weights [Zubizarreta, 2015]: this solves (2) with the χ^2 divergence. By default, τ is chosen according to the algorithm of Wang and Zubizarreta [2020] from a grid of 8 possible values between 0.0001 and 0.1.

Covariate balancing propensity score [Imai and Ratkovic, 2014] is typically described as a kind of logistic regression, with exact ($\tau = 0$) balance constraints imposed on the

fitted inverse-propensity weights. When used to estimate μ_1, the inverse-propensity weights are normalized if a constant covariate is included [Słoczyński et al., 2023]. Under this normalization, it can be formulated as (2) with a shifted KL divergence [Josey et al., 2021b]. Appendix A elucidates this connection and presents the relevant f-divergence.

2.2 OTHER BALANCING ALGORITHMS

Approximate residual balancing [Athey et al., 2018]: this approach solves a mild variant of (1). By default, $\lambda = 1$. However, the weights are not directly used to form the weighted estimate (5). Instead, an elastic net regression is fit to the observed outcomes, and the weighted sum of its residuals are added back into the treatment effect estimate.

Kernel methods replace the maximum imbalance, over the d covariates, with a maximum over smooth functions f within a reproducing kernel Hilbert space. Wong and Chan [2018] add a term which penalizes the nonsmoothness of f, which reduces the maximum over f to finding the top eigenvalue of a (W-dependent) matrix; furthermore, this eigenvalue can be differentiated with respect to W. Whereas Wong and Chan [2018] solve a variant of (1), Hazlett [2020, 2014] focuses on (2). Exact balance ($\tau = 0$) is imposed on the subspace corresponding to the top r eigenvalues of the kernel matrix, where r is chosen to minimize a proxy for estimator bias. Some of the ideas in this paper can be generalized to the kernel setting.

An alternative to minimizing a combination of imbalance and divergence, as in (1) or (2), is to minimize a covariate-aware distance between distributions. For example, Kong et al. [2023] minimize an integral probability metric, such as the Wasserstein distance. Huling and Mak [2024] minimize the energy distance. These distances are very stringent, so minimizing them ensures consistent estimates without parametric assumptions. Unfortunately, these distances are even more difficult to constrain when $n \ll d$. For example, the Wasserstein distance converges at a slow rate of $O(n^{-1/d})$.

More algorithms are discussed in Appendix B.

2.3 BALANCING ANALYSES

Most mathematical analyses of covariate balancing, and of causal inference more generally, have focused on asymptotics. The most well-studied asymptotic desideratum is $\sqrt{n}$-*consistency*, which means the error of the estimate is $O(1/\sqrt{n})$. When $d = o(n)$, the weights from (2) are consistent in this sense [Wang and Zubizarreta, 2020]. When, $d = \omega(n)$, some kind of sparsity assumption is necessary to achieve consistency. However, even under such assumptions, covariate balancing has not been generally proven $\sqrt{n}$-consistent. This motivated the work of Athey et al. [2018], which augments covariate balancing with sparse regression.

Other desirable asymptotic properties include *double robustness*, which means the estimate is consistent if at least one of the following holds: the model for the outcomes is correct (e.g. linear in the covariates), or the model for the propensity scores is correct [Fan et al., 2016, Zhao and Percival, 2017]. *Semiparametric efficiency* essentially refers to achieving the lowest possible variance among estimators making the same assumptions about either the outcomes or propensity scores [Chan et al., 2016, Zhao and Percival, 2017].

Despite the focus on asymptotics, some finite-sample guarantees have been proven for covariate balancing. To justify their algorithm for automatically selecting τ, Wang and Zubizarreta [2020] bound, up to some positive constants, the excess loss incurred by balancing too many covariates. Bruns-Smith and Feller [2022] derive the optimal weights (i.e. the optimal bias-variance tradeoff) in terms of mean squared error. However, these are phrased in terms of unknown population quantities. Su et al. [2023] prove a useful finite-sample decomposition of the inverse propensity weighting error.

It should be noted that all theoretical results for covariate balancing, including this paper's finite-sample intervals, depend upon causal assumptions which are strong and potentially unrealistic. (These will be discussed in Section 3.2). Thus, a truly "rigorous" process of causal inference must perform additional sensitivity checks [Imai et al., 2010] and/or embed itself in meta-analytic inference which does not require such assumptions [Kaul and Gordon, 2024]. In these circumstances, practitioners often disregard the nominal coverage probability of confidence intervals, and just make use of point estimates [Schuemie et al., 2020]. We stress that the theoretical guarantees developed in this paper are presented not just for their own sake, but to help design new algorithms which are easier to use, demonstrate better adaptivity, and ultimately achieve lower error.

2.4 DATA-DRIVEN REGULARIZATION

The problem of optimizing regularization parameters in a data-dependent manner is a recurring topic in the PAC-Bayesian literature [Catoni, 2007, Alquier et al., 2024]. As the latter survey notes, the subtlety of this issue has resulted in the publication of mistaken proofs. The fundamental difficulty arises from the fact that the thresholds in Markov's inequality and Hoeffding's lemma cannot be random. Recently, Rodríguez-Gálvez et al. [2024] derived a version of Catoni's classic PAC-Bayesian inequality which holds uniformly for all (potentially data-dependent) λ, with a small cost of $\log n/n$ in the confidence term. As Section 4 demonstrates, we exploit specific aspects of covariate balancing to obtain results which may not be achievable in the most general PAC-Bayesian setting.

3 PRELIMINARIES

Suppose there are n_0 participants in the control group and n_1 participants in the treatment group. Each participant i has data $(X_i, Y_i(0), Y_i(1), T_i)$. $X_i \in \mathbb{R}^d$ are covariates, possibly generated by computing features of underlying lower-dimensional covariates. $Y_i(0)$ and $Y_i(1)$ are the potential outcomes under no treatment and treatment, respectively. $T_i \in \{0, 1\}$ denotes whether the participant was actually treated. We observe only $(X_i, Y_i(T_i), T_i)$, leaving one of the potential outcomes unobserved. Our goal is to estimate the average treatment effect (ATE), which is the difference between the treatment-specific means μ_1 and μ_0:

$$\text{ATE} = \underbrace{\mathbb{E}_{\mathcal{T}} \, Y(1)}_{\mu_1} - \underbrace{\mathbb{E}_{\mathcal{T}} \, Y(0)}_{\mu_0} \qquad (3)$$

The expectation in (3) may be over a different "target" distribution $\mathcal{T}$ than the one sourcing the data $\mathcal{S}$. If $\mathcal{S} \neq \mathcal{T}$ — a phenomenon referred to as covariate shift or transportation — we don't see individual data from $\mathcal{T}$, just a target vector $\widehat{M} \in \mathbb{R}^d$ formed by averaging n samples from $\mathcal{T}$. (For example, imagine using observational data to emulate a randomized trial for which summary statistics are published, but individual patient data are unavailable). More commonly, $\mathcal{S} = \mathcal{T}$ and $\widehat{M} = \sum_{i=1}^{n} \frac{1}{n} X_i$ where $n = n_0 + n_1$. The following mean vectors — weighted, target and true — should, ideally, all be close to one another.

$$\widetilde{M} = \sum_{\text{treated } i} W_i X_i \qquad \widehat{M} \in \mathbb{R}^d \qquad M = \mathbb{E}_{\mathcal{T}} \, \widehat{M} \qquad (4)$$

As is typical in the covariate balancing literature, we focus on deriving an estimate $\hat{\mu}_1$ of μ_1. Then, an estimate $\hat{\mu}_0$ of μ_0 can be similarly produced, and the two can be combined into an estimate $\widehat{\text{ATE}}$ of ATE.

Task 3.1 (Weighted estimation of treatment-specific means). Let $\{(X_i, Y_i(T_i), T_i)\}_i$ be data from $\mathcal{S}$ and $\widehat{M}$ be an empirical target vector from $\mathcal{T}$. Use these to pick a probability distribution W over the treated $\{i : T_i = 1\}$ and estimate:

$$\hat{\mu}_1 = \sum_{\text{treated } i} W_i Y_i(1) \qquad (5)$$

Given $\alpha \in (0, \frac{1}{2})$, find ϵ such that $|\hat{\mu}_1 - \mu_1| \leq \epsilon$ with probability $1 - \alpha$ over the randomness of the participant data. That is, $\hat{\mu}_1 \pm \epsilon$ is a $1 - \alpha$ confidence interval for μ_1.

3.1 MATHEMATICAL NOTATION

Given any d-dimensional real vector $v \in \mathbb{R}^d$, these are its ℓ_1, ℓ_2, and ℓ_∞ norms:

$$||v||_1 = \sum_j |v_j| \qquad ||v||_2^2 = \sum_j v_j^2 \qquad ||v||_\infty = \max_j |v_j|$$

Let $f : [0, +\infty) \to (-\infty, +\infty]$ be a convex function such that $f(t)$ is finite for all $t > 0$, $f(1) = 0$, and $f(0) = \lim_{t \to 0^+} f(t)$. Let U (sometimes expanded as Uniform) be the uniform distribution over the treatment group. Let W be any other distribution on the treatment group. Then the f-divergence between W and U is:

$$\text{Divergence}(W \,||\, U) = \sum_{\text{treated i}} \frac{1}{n_1} f(n_1 \cdot W_i) \qquad (6)$$

Its (restricted) convex conjugate is defined for $Z \in \mathbb{R}^{n_1}$:

$$\text{Divergence}^*(Z \,||\, U) = \sup_W Z^\top W - \text{Divergence}(W \,||\, U)$$

where the supremum is taken over probability distributions W [1]. For example, the KL divergence between W and U is the difference of the Shannon entropies $H(U)$ and $H(W)$:

$$\text{KL}(W \,||\, U) = \underbrace{\log(n_1)}_{H(U)} - \underbrace{\sum_{\text{treated } i} -W_i \log W_i}_{H(W)} \qquad (7)$$

$$\text{KL}^*(Z \,||\, U) = \log \frac{1}{n_1} \sum_{\text{treated } i} \exp Z_i$$

The equality (7) shows why entropy balancing, which maximizes $H(W)$, is a special case of (2).

3.2 ASSUMPTIONS

Much like Athey et al. [2018], we assume that the outcomes are linear functions of the covariates.

Assumption 3.2 (Linear outcomes). Let $0 < k \leq d$ be some sparsity constant. There are $u_* \in \mathbb{R}^d$ and $v_* \in \mathbb{R}^d$ such that $||u_*||_1 \leq k$, $||v_*||_1 \leq k$. For all covariates $X \in \mathbb{R}^d$ and potential outcomes $(Y(0), Y(1))$ sampled from either $\mathcal{S}$ or $\mathcal{T}$, $Y(0) = u_*^\top X$ and $Y(1) = v_*^\top X$.

Note that we assume only "approximate" sparsity, with ℓ_1 norm bounds on u_* and v_*. By contrast, Athey et al. [2018] assumes an exact sparsity bound on the number of nonzero coordinates of u_* and v_*. On the other hand, our assumption does not permit noise in the outcomes. Additive zero-mean noise can be handled by standard techniques, which we omit to highlight the novelties of our approach. Note that we permit $n \ll d$, where it is typically not difficult to fit the outcomes with near-zero error.

We also assume that the empirical target $\widehat{M}$ concentrates to the true M at a typical rate. If each of the d covariates is bounded (i.e. is normalized to take values in $[-1, 1]$), and the samples are independent, then the following assumption is just a consequence of Hoeffding's inequality.

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[1] If the supremum were taken over the larger set of nonnegative vectors (i.e. measures) then Divergence^* could be tidily expressed in terms of the conjugate f^* of f. However, that leads to looser bounds [Ruderman et al., 2012, Ohnishi and Honorio, 2021].

Assumption 3.3 (Concentration of covariates). For constants $\alpha \in (0, \frac{1}{2})$ and $C > 0$, $||\widehat{M} - M||_\infty \leq \frac{C \log d}{\sqrt{n}}$ with probability $1 - \alpha$.

Our nonasymptotic confidence interval depends on only the aforementioned assumptions. When extending it to an asymptotic consistency guarantee, we will need to invoke more traditional causal assumptions, in order to ensure the existence of (correct) inverse-propensity weights. As discussed in Appendix C, the following assumption is a consequence of strong ignorability [Rosenbaum and Rubin, 1983]. When $\mathcal{S} \neq \mathcal{T}$, a condition such as positive participation probability is also needed [Dahabreh et al., 2020].

Assumption 3.4 (Inverse-propensity weights). There is a probability distribution W^* which is ratio-bounded (i.e. $\frac{\max_i W_i^*}{\min_i W_i^*} \leq R$ for some constant $R \geq 1$) and satisfies:

$$\left\| \sum_{\text{treated } i} W_i^* X_i - M \right\|_\infty = O\left(\frac{\log d}{n_1} \right)$$

We will demonstrate consistency in the same high-dimensional regime as Athey et al. [2018].

Assumption 3.5 (Asymptotics). As $n \to \infty$, $\frac{k \log d}{\sqrt{n_1}} \to 0$.

3.3 A NAIVE CONFIDENCE INTERVAL

To motivate our main results, consider the following naive attempt to construct a confidence interval. Expanding the definitions in (5) and (4), then applying Hölder's inequality in conjunction with Assumptions 3.2 and 3.3, we can upper bound $\hat{\mu}_1 - \mu_1$. Then, we can repeat the same logic on $\mu_1 - \hat{\mu}_1$ to bound $|\hat{\mu}_1 - \mu_1|$.

$$
\begin{aligned}
\hat{\mu}_1 - \mu_1 &= \sum_{\text{treated } i} W_i Y_i(1) - \mathbb{E}\, Y(1) \\
&= \sum_{\text{treated } i} W_i v_*^\top X - \mathbb{E}\, v_*^\top X \\
&= v_*^\top (\widetilde{M} - M) \qquad\qquad (8) \\
&= v_*^\top (\widetilde{M} - \widehat{M}) + v_*^\top (\widehat{M} - M) \\
&\leq ||v_*||_1 ||\widetilde{M} - \widehat{M}||_\infty + ||v_*||_1 ||\widehat{M} - M||_\infty \\
&\leq k\left(||\widetilde{M} - \widehat{M}||_\infty + \frac{C \log d}{\sqrt{n}} \right) \quad (9)
\end{aligned}
$$

Note that when $n < d$, there generally aren't weights which perfectly balance the covariates; the imbalance term will typically have to be (substantially) positive. Nonetheless, this interval blithely suggests weights which make $\widetilde{M}$ as close as possible to $\widehat{M}$; there is no benefit to choosing W with low divergence from uniform. Thus, the challenge for our analysis is: can we use the PAC-Bayesian machinery to (1) scale down the imbalance term, and (2) quantitatively explain the intuitive benefit of near-uniform weights?

4 PAC-BAYESIAN ANALYSIS

We propose the following program, which generalizes (1). We call this **flexible covariate balancing** because the regularization parameter λ is no longer fixed; it is optimized jointly with the weights W, along with a new parameter δ. The appropriate tradeoff between imbalance and divergence is determined by the data.

$$
\begin{aligned}
\min_{W, \lambda, \delta} \max_z \Big((1-\delta)k + \delta\beta_z \Big) &\max_j \Big| \sum_{\text{treated } i} W_i X_{ij} - \widehat{M}_j \Big| + \\
&(1-\delta)(Ck \log d)/\sqrt{n} + \qquad (10) \\
&\lambda\, \text{Divergence}(W \,||\, U) + \\
&\lambda\, \text{Divergence}^*\Big(\frac{\delta}{\lambda}[zY_i(1) - \widehat{Y}_i(1)]_{\text{treated } i} \,\Big|\Big|\, U \Big)
\end{aligned}
$$

$\quad$ s.t. W is a distribution on the treatment group

$$\lambda > 0 \qquad 0 \leq \delta \leq 1 \qquad z \in \{-1, 1\}$$

Here, $\widehat{Y}_i(1)$ is a sort of fulcrum for $Y_i(1)$ which is calculated from X_i and the largest-magnitude covariate of $\widehat{M}$:

$$j_* = \operatorname{argmax}_j |\widehat{M}_j| \quad s = \operatorname{sign}(\widehat{M}_{j^*}) \quad \widehat{Y}_i(1) = -s\beta_z X_{ij^*}$$

For each sign $z \in \{-1, 1\}$, $\beta_z \geq 0$ is the value of the following program, which is solved for each value $z \in \{-1, 1\}$ in preparation for (10). It can be rephrased as a linear program, as shown Appendix D.

$$
\max_{v_* \in \mathbb{R}^d, M \in \mathbb{R}^d} \quad \frac{-z}{||\widehat{M}||_\infty} v_*^\top M \qquad\qquad (11)
$$

$$\text{s.t.} \quad ||v_*||_1 \leq k \qquad ||\widehat{M} - M||_\infty \leq \frac{C \log d}{\sqrt{n}}$$

$$v_*^\top X_i = Y_i(1) \text{ for all treated } i$$

The estimate derived from (10) enjoys the following nonasymptotic guarantee on its error.

Theorem 4.1. Fix $\alpha \in (0, \frac{1}{2})$. Let ν be the objective value of (10) obtained by any feasible (W, λ). Construct $\hat{\mu}_1$ from W as in (5). Then, under Assumptions 3.2 and 3.3, $|\hat{\mu}_1 - \mu_1| \leq \nu$ with probability $1 - \alpha$.

In other words, the objective of (10) is the radius of a confidence interval solving Task 3.1. W, λ and δ are jointly optimized to shrink the confidence interval. This interval has guaranteed finite-sample coverage — not just for the global solution of the program, but every feasible iterate. So, by keeping λ and δ fixed, we obtain confidence intervals for plain covariate balancing (1) as a special case.

4.1 INTUITION WITH KL DIVERGENCE

At first glance, the program (10 is seemingly complicated and opaque, especially since it involves a precursor program (11). Let us gain some more concrete intuition for how it

improves upon plain covariate balancing (1), and how Theorem 4.1 improves upon the naive interval (9). First note that, with $\delta = 0$ and $\lambda \to 0$, the naive interval is recovered. This pessimistic, oblivious bound may be useful asymptotically, if very non-uniform weights can, and must, be taken to achieve low imbalance. Larger δ enable a more optimistic, scale-sensitive analysis which explains the benefit of near-uniform weights in smaller samples.

At the other extreme $\delta = 1$, the imbalance term is scaled by β_k rather than k. Typically $\beta_k \ll k$, so this scaling achieves the goal described in Section 3.3. To see when the β_z are small, let us examine the program (11) which define them, focusing on the common case where $\widehat{M} \approx M$. Without the equality constraints, the value of the program would be roughly k, attained by v_* in the coordinate direction $-z \cdot e_{j*}$. However, the equality constraints usually prevent this value from being attained. As the notation in this program suggests, it bounds the magnitude of $v_*^T M = \mu_1$, i.e. the average treatment outcome in the target distribution. We don't observe such outcomes, but by Assumption 3.2, we know they must be linearly consistent with the treatment outcomes we do observe. β_z will be small when we can safely conclude that outcomes in the unseen target distribution aren't much larger than those in the data. (We have therefore controlled for the possibility that, under covariate shift, the outcomes are wildly different in the target distribution).

To improve upon the naive interval, the extra divergence-related terms cannot be too large. To gain intuition for these, consider (10) in the specific case of the KL divergence (7):

$$
\min_{W,\lambda,\delta} \max_z \left((1-\delta)k + \delta\beta_z \right) \max_j \left| \sum_{\text{treated } i} W_i X_{ij} - \widehat{M}_j \right| +
$$
$$
(1-\delta)(Ck \log d)/\sqrt{n} + \tag{12}
$$
$$
\lambda \, \mathrm{KL}(W \,||\, U) +
$$
$$
\lambda \log \mathop{\mathbb{E}}_{i \sim U} \exp \left(\frac{\delta}{\lambda} (z Y_i(1) - \widehat{Y}_i(1)) \right)
$$
$$
\text{s.t. } W \text{ is a distribution on the treatment group}
$$
$$
\lambda > 0 \qquad 0 \le \delta \le 1 \qquad z \in \{-1, 1\}
$$

Recall that, as $\lambda \to 0$, the logmeanexp function approaches max. As $\lambda \to \infty$, it approaches mean. Without loss of generality, we can linearly center the treatment-group means of the outcomes $Y_i(1)$ and the covariate X_{ij*}. So, in the benign case where $W \approx U$ achieves good imbalance, we can take λ to be large, and keep both divergence terms near zero. In this way, the bound adapts to treatment groups which are empirically similar to the combined population.

In general, to keep imbalance low, we have to choose weights with nontrivial KL divergence. We can justify higher KL divergence if the data exhibit low variation around their mean. This makes intuitive sense: if the $Y_i(1)$ are all close to one another, then choosing extreme weights can't change $\sum_i W_i Y_i(1)$ as much. Whereas plain covariate balancing completely ignores the outcomes while choosing

W, flexible covariable balancing makes use of these data to help optimize all the variables. This argues against the principle, advocated by Rubin [2008], that outcome data should not affect the design of observational studies.

The bound depends on k, the ℓ_1 norm of the linear function generating the outcomes. k is usually unknown, but more standard regression techniques can be used to reason about it. For example, since the outcomes are assumed to be consistent with the linear function, a prospective value of k is too small if it leads to nonzero training error.

4.2 PROOF WITH KL DIVERGENCE

The proof of Theorem 4.1 is short and simple. The proof using the KL divergence contains all the ideas; extending it to all f-divergences, in Appendix E, requires just a bit more notation. The proof begins with the Donsker-Varadhan formula for the KL divergence, which holds for all W:

$$
\mathrm{KL}(W \,||\, U) = \sup_\phi \mathop{\mathbb{E}}_{i \sim W} \phi(i) - \log \mathop{\mathbb{E}}_{i \sim U} \exp \phi(i) \tag{13}
$$

Here, the supremum is taken over all bounded functions ϕ from the set of treated i to $\mathbb{R}$. Therefore, by restricting the supremum to any smaller set of functions, we get a lower bound on the KL divergence. We restrict to the following functions parameterized by $z \in \{-1, 1\}$, $\lambda > 0$ and $\hat{v} \in \mathbb{R}^d$. Recalling the notation for means in (4) and the definition of v_* in Assumption 3.2:

$$
\phi(i; z, \lambda, \hat{v}) = \frac{z}{\lambda} \left(v_*^\top (X_i - M) - \hat{v}^\top (X_i - \widehat{M}) \right)
$$

By linearity of expectation:

$$
\mathop{\mathbb{E}}_{i \sim W} \phi(i; z, \lambda, \hat{v}) = \frac{z}{\lambda} v_*^\top (\widetilde{M} - M) - \frac{z}{\lambda} \hat{v}^\top (\widetilde{M} - \widehat{M})
$$

Plugging these terms back into (13) obtains, for all W:

$$
\mathrm{KL}(W \,||\, U) \ge \sup_{z,\lambda,\hat{v}} \frac{z}{\lambda} v_*^\top (\widetilde{M} - M) -
$$
$$
\frac{z}{\lambda} \hat{v}^\top (\widetilde{M} - \widehat{M}) -
$$
$$
\log \mathop{\mathbb{E}}_{i \sim U} \exp \phi(i; z, \lambda, \hat{v})
$$

This inequality holds no matter the choice of z, λ and $\hat{v}$ in the supremum. Thus, following rearranged inequality holds for all (adaptively-chosen) W, z, λ and $\hat{v}$:

$$
z v_*^\top (\widetilde{M} - M) \le \lambda \, \mathrm{KL}(W \,||\, U) + \tag{14}
$$
$$
z \hat{v}^\top (\widetilde{M} - \widehat{M}) +
$$
$$
\lambda \log \mathop{\mathbb{E}}_{i \sim U} \exp \phi(i; z, \lambda, \hat{v})
$$

First, let's make sure that bounding the left-hand side leads to a bound on $|\hat{\mu}_1 - \mu_1|$. Recalling (8), we just need the bound the right-hand side for both values of z:

$$
\max_{z \in \{-1, 1\}} z \, v_*^T (\widetilde{M} - M) = |\hat{\mu}_1 - \mu_1| \tag{15}
$$

On the right-hand side of (14), we will consider the worst-possible direction of $\hat{v}$ for the second term, so that we may choose it arbitrarily to minimize the third term. By the duality of the ℓ_1 and ℓ_∞ norms, the second term is just the scaled imbalance:

$$
\begin{aligned}
z\hat{v}^\top(\widetilde{M} - \widehat{M}) &= ||\hat{v}||_1 \frac{z\hat{v}^\top}{||\hat{v}||_1}(\widetilde{M} - \widehat{M}) \\
&\leq ||\hat{v}||_1 \sup_{||v||_1 \leq 1} v^\top(\widetilde{M} - \widehat{M}) \\
&= ||\hat{v}||_1 \max_{1 \leq j \leq d} \left| \sum_{\text{treated } i} W_i X_{ij} - \widehat{M}_j \right|
\end{aligned}
$$

Let us pick $\hat{v}$ as follows:

$$\hat{v} = (1-\delta)v_* + \delta u \quad \text{where } u = -zs\beta_z e_{j^*}$$

By the triangle inequality and Assumption 3.2, we have $||\hat{v}||_1 \leq (1-\delta)k + \delta\beta_z$, so the imbalance is scaled to match (10). Now we turn to bounding the logmeanexp moment term in (14). Grouping terms in ϕ which depend on i:

$$\phi(i; z, \lambda, \hat{v}) = \frac{z}{\lambda}\left(Y_i(1) - \hat{v}^\top X_i\right) + \frac{z}{\lambda}\left(\hat{v}^\top\widehat{M} - v_*^\top M\right)$$

The terms which don't depend on i fall out of the exponent:

$$
\begin{aligned}
\lambda \log \mathbb{E}_{i \sim U} \exp \phi = z(\hat{v}^\top\widehat{M} - v_*^\top M) + \\
\lambda \log \mathbb{E}_{i \sim U} \exp \frac{z}{\lambda}\left(Y_i(1) - \hat{v}^\top X_i\right)
\end{aligned}
$$

The terms remaining in the exponent simplify as desired:

$$
\begin{aligned}
\hat{v}^\top X_i &= (1-\delta)Y_i(1) + \delta z\widehat{Y}_i(1) \\
z(Y_i(1) - \hat{v}^\top X_i) &= \delta(zY_i(1) - \widehat{Y}_i(1))
\end{aligned}
$$

In the linear terms that fell out, one part is bounded by Hölder's inequality and Assumptions 3.2 and 3.3:

$$
\begin{aligned}
z(\hat{v}^\top\widehat{M} - v_*^\top M) &= (1-\delta)zv_*^\top(\widehat{M} - M) + z\delta(\ldots) \\
&\leq (1-\delta)Ck\log(d)/\sqrt{n} + z\delta(\ldots)
\end{aligned}
$$

Finally, we show the other, elided $z\delta(\ldots)$ part is zero:

$$
\begin{aligned}
z\delta(u^\top\widehat{M} - v_*^\top M) &= -\beta_z||\widehat{M}||_\infty - zv_*^\top M \\
&\leq -\beta_z||\widehat{M}||_\infty + \beta_z||\widehat{M}||_\infty = 0
\end{aligned}
$$

The first equality holds by construction of u. The second equality holds because the value of β_z is given by (11). By Assumptions 3.2 and 3.3, that program's feasible set contains the actual v_* and M with probability $1 - \alpha$.

5 EXTENSIONS OF MAIN ANALYSIS

5.1 AVERAGE TREATMENT EFFECTS

The following standard reduction is used to estimate ATE. This estimate still has confidence $1 - \alpha$, because the concentration of Assumption 3.3 has to be invoked just once.

Theorem 5.1. *Suppose the treatment group weights W attain value ν_1 in the program (10). Let $\hat{\mu}_1$ be constructed as in (5). Analogously, suppose the control group weights V attain value ν_0 in the program (10) when it involves reweighting the control i rather than the treated i. Let $\hat{\mu}_0 = \sum_{\text{control } i} V_i Y_i(0)$ and $\widehat{ATE} = \hat{\mu}_1 - \hat{\mu}_0$. Then, under Assumptions 3.2 and 3.3, with probability $1 - \alpha$, $|\widehat{ATE} - ATE| \leq \nu_0 + \nu_1$.*

5.2 ASYMMETRIC CONFIDENCE INTERVAL

Solving (10) produces a single estimate $\hat{\mu}_1$ with a symmetric confidence interval. For an asymmetric (and potentially tighter) confidence interval, it is valid to solve (10) twice, using fixed values of $z \in \{-1, 1\}$ each time. This achieves two different objective values ν_z, and produces a pair of weights W_z with two corresponding estimates $\hat{\mu}_{1,z}$. Then $[\hat{\mu}_{1,1} - \nu_1, \hat{\mu}_{1,-1} + \nu_{-1}]$ is a $1 - \alpha$ confidence interval for μ_1. This is because, for a one-sized bound, it is not necessary to take the maximum over z in (15). There is no loss in confidence because Assumption 3.3 is invoked just once.

5.3 CONSISTENCY IN HIGH DIMENSIONS

The naive interval (9) shows that covariate balancing is consistent under Assumptions 3.2 to 3.5. Flexible covariate balancing inherits this property; see Appendix F for proof.

Theorem 5.2. *Let $\hat{\mu}_1$ be constructed as in (5) from the solution W of (10). Then, under Assumptions 3.2 to 3.5, $|\hat{\mu}_1 - \mu_1| \to 0$ as $n \to \infty$.*

6 EXPERIMENTS

In this section, we compare flexible covariate balancing (FBAL, 10) to the baseline algorithms described in Section 2.1. These competitors are abbreviated as EBAL, SBW, and nCBPS (where the n denotes weight normalization). Since these methods do not produce confidence intervals with provable coverage, we use (pointwise) estimation error as the primary evaluation metric.

6.1 SIMULATIONS

We present two purposefully-designed simulations in which algorithms driven by a fixed tolerance (or regularization) parameter will do poorly on at least one. It is not possible to simultaneously achieve good performance on both simulations without problem-specific, data-driven adaptivity.

1. The subgroup simulation. Suppose the combined population is 50% white and 50% black. The control outcomes $Y_i(0)$ are all zero. The treatment outcome is $Y_i(1) = 1$ in the white population, but is -1 in the black population, so

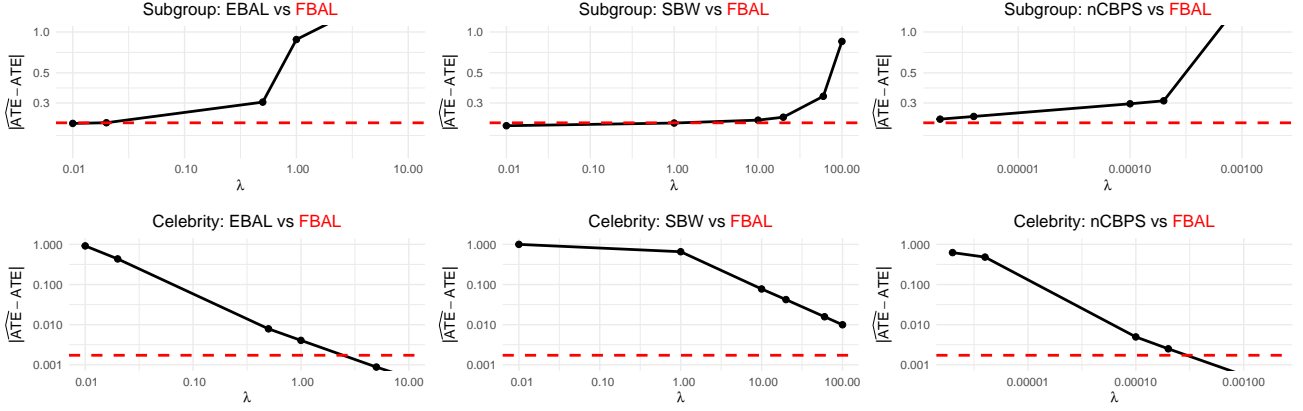Figure 1: Results of the **subgroup** simulation (above) and the **celebrity** simulation (below). Since the true ATE = 0 in both simulations, lower estimates are better. Flexible entropy balancing (FBAL) is compared to EBAL, SBW, and nCBPS in the left, middle, and right columns, respectively. For all of the competing methods, a fixed setting of λ may do well in the subgroup simulation, but then that value performs badly in the celebrity simulation — or vice versa. FBAL does not have a fixed hyperparameter, and is capable of solving both problems very well.

ATE = 0. The treatment group is (exactly) 95% white and 5% black; the control group is (exactly) 5% white and 95% black. Besides race (which is encoded as 10 for white, and -10 for black) the rest of the $d - 1$ covariates are irrelevant Uniform$(-1, 1)$. The correct approach is to heavily upweight the underrepresented black subgroup among the (mostly white) treated, and to similarly upweight the white subgroup among the (mostly black) controls. However, an algorithm with too high λ (or τ) will hesitate to place very heavy weights on just 5% of the group. As n increases, an algorithm must allow itself to diverge from uniform and perform this reweighting, balancing the covariate for race.

2. The celebrity simulation. Suppose 95% of the participants, in both the treatment and control groups, come from the general population. All d of their covariates are Uniform$(-10, 10)$, potentially exhibiting substantial individual variation. The remaining 5% are celebrities, whose covariates are all completely zero vectors, perfectly matching the true mean. It is tempting for an algorithm to achieve low imbalance from the mean by placing heavy weight on the celebrities. Unfortunately, the celebrities are very atypical in the sense that, just for them, the treatment effect is substantially positive, equaling 1. (This makes the simulation misspecified relative to Assumption 3.2). For the general population, the effect is mildly negative at $-0.05/0.95$, which renders the overall ATE null. As n increases, the general population mean converges to zero, so the benefit of emphasizing the celebrities dissipates. The most accurate algorithm will keep uniform weights over the population to obtain a null estimate. An algorithm with too low λ (or τ) will not do this as well.

So, heavily weighting the 5% is beneficial in the first simulation, and it is harmful in the second. The algorithm is not allowed to be told, implicitly via problem-specific regu-

larization parameters, which scenario is active. To be successful, it must judge different degrees of tradeoff between imbalance and divergence based upon the data. As Figure 1 illustrates, flexible covariate balancing is able to solve this challenge, because it is built from a more complete theory of how this tradeoff works.

6.2 REAL TRIAL EMULATIONS

Both of the following experiments involve using observational data to emulate a randomized controlled trial. By treating an RCT as (approximate) ground truth, we avoid generating synthetic ground truth. That practice, though widespread in causal inference benchmarking, can be controversial and potentially misleading [Curth et al., 2021].

1. Random-Fourier LaLonde. This experiment is based on the dataset of LaLonde [1986], which is a hobbyhorse in causal inference [Imbens and Xu, 2024]. The intervention in this dataset is a job training program, and the outcome is personal annual income. This dataset includes a randomized trial whose control group consists of $n = 260$ participants. By averaging their outcomes, we can reliably estimate the control response of *not* participating in a job program, and informally treat it as ground truth: $\mu_0 = 4554.80$. The dataset also includes an observational control group with $n_0 = 15,992$ participants. Both the experimental and observational participants have 9 covariates. To make this data more algorithmically involved, we expand $d = 16,000$ random Fourier features from the original 9 [Rahimi and Recht, 2008]. Then, we use different balancing algorithms to estimate μ_0 (as $\hat{\mu}_0$) by reweighting the observational control.

The results are depicted in Figure 2. As observed in previous works [Hainmueller, 2012], $\lambda \approx 0$ works well on this dataset; this setting is determined automatically by FBAL.
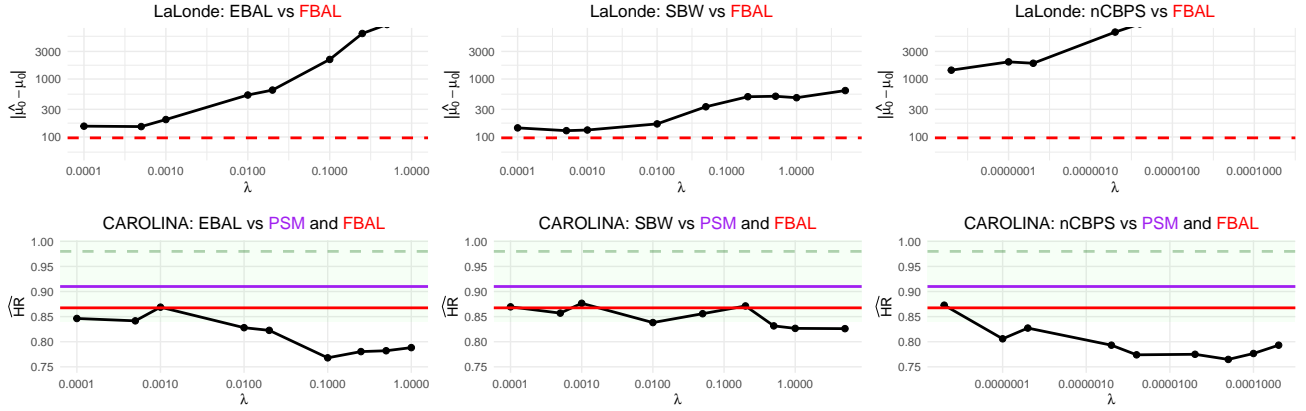
Figure 2: Results of the **LaLonde** emulation (above) and the **CAROLINA** emulation (below). In the LaLonde plot, the error of the estimate $\hat{\mu}_0$ is on the y-axis, so lower values are better. For CAROLINA, higher estimates of HR are better: the trial's observed HR of 0.98 is plotted as a dashed green line, and its confidence interval of $[0.84 - 1.14]$ is shaded in light green. FBAL performs better than, or equal to, all the other covariate balancing algorithms. Propensity score matching (PSM) performs better than FBAL; however, it was performed on a separate dataset which is an order of magnitude larger, with careful manual oversight of the matching and covariate balance [Patorno et al., 2019].

2. The CAROLINA trial. Between 2010 and 2018, Rosenstock et al. [2019] conducted a randomized controlled trial comparing linagliptin (a new drug) and glimepiride (a baseline drug) for patients with type 2 diabetes and elevated cardiovascular risk. Its primary outcome was the occurrence of a major cardiovascular event (myocardial infarction, non-fatal stroke, and/or cardiovascular death). From $n = 6033$ randomized patients, they estimated a hazard ratio (HR) of 0.98, with a 95% confidence interval $[0.84, 1.14]$. Thus, the trial reasonably concluded that linagliptin's cardiovascular safety profile is noninferior to that of glimepiride.

While this trial was ongoing, Patorno et al. [2019] attempted to predict its result using observational data and propensity score matching. Based on the initially-published protocol and baseline statistics of the trial [Marx et al., 2015], Patorno et al. [2019] propensity-score matched 24,131 patients, for a total of 48,262 participants. They predicted $\widehat{HR} = 0.91$, which fell within the confidence interval eventually reported by the trial. Our goal is to do the same using covariate balancing algorithms, upon observational data drawn from a single institution within FeederNet [You et al., 2022].

Our cohort for this emulation involves $n_0 = 3739$ patients given glimepiride and $n_1 = 488$ patients given linagliptin. There are 12,900 covariates, but most of them are very sparse; after removing covariates which are are over 50% zero, 208 covariates remain. (As shown in Figure 4 in the Appendix, keeping these sparse features led to poor results from all the covariate balancing algorithms). From these 208 covariates, we extracted $d = 5000$ random Fourier features. In order to estimate HR, the learned weights are used to fit weighted Cox models upon the time-to-event data.

Our results are displayed in Figure 2. As hoped, FBAL's estimate $\widehat{HR} = 0.867$ lies within the 95% CI of the trial. By

contrast, the other covariate balancing algorithms tended to predict outside the CI, depending on the setting of λ. However, this experiment may also indicate some limitations of covariate balancing as an algorithmic strategy. All the covariate balancing algorithms required some separate feature extraction, and they were still outperformed by propensity score matching. In covariate balancing, the maximum imbalance is fundamentally susceptible to the inclusion of irrelevant and/or corrupted features.

7 CONCLUSION

This paper initiates the PAC-Bayesian analysis of covariate balancing. It presents the first confidence interval which explains the generalization benefits of near-uniform weights in this setting. This theoretical result illuminates the tradeoff between imbalance and divergence, internalizes the complexities of covariate shift, offers an alternative proof of asymptotic consistency, and gives rise to a flexible new balancing algorithm with optimizable regularization parameters. This algorithm empirically demonstrates more adaptivity than existing methods. It would be interesting to pair our new balancing algorithm with a regression or propensity score model, much as Athey et al. [2018] pair stable balancing weights with the elastic net.

Aside from causal inference, our techniques are of possible interest to the machine learning community in general. Rigorously, simultaneously optimizing both weights and hyperparameters is an interesting topic for further research. We achieved this through a uniform distribution on exchangeable data, and many linear learning problems can be dually expressed as (unnormalized, signed) weights over such data.

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A   f-DIVERGENCE FOR CBPS

In this section, we present the f-divergence which places the covariate balancing propensity score [Imai and Ratkovic, 2014] in the form of (2).

Lemma A.1 (CBPS). *Suppose there is a constant covariate (i.e. an index j such that $X_{ij} = \widehat{M}_j$ for all i). Then CBPS, when formulated to estimate μ_1, is equivalent to (2) with $\tau = 0$ and the following f-divergence away from uniform:*

$$W \mapsto \frac{1}{n_1} \sum_{\text{treated } i} \left(\frac{1}{W_i} - 1 \right) \log \left(\frac{1}{W_i} - 1 \right) - \frac{1}{W_i} + c$$

In this divergence, the constant c is defined in (16).

CBPS fits a logistic regression to the propensity scores, but constrains the fitted scores to satisfy covariate balancing constraints. When estimating μ_1, these constraints are:

$$\sum_{\text{treated } i} \frac{1}{p_i} X_{ij} = \widehat{M}_j \quad \forall\, 1 \leq j \leq d$$

Here, $p_i \in [1, \infty)$ is the fitted propensity score given X_i. As highlighted by Słoczyński et al. [2023], if there is a constant covariate, this normalizes the inverse-propensity scores:

$$\sum_{\text{treated } i} \frac{1}{p_i} = 1$$

As described by Josey et al. [2021b], the CBPS primal objective can be rephrased to minimize over the p_i themselves, rather than the logistic regression coefficients:

$$\text{CBPS}(p) = \sum_{\text{treated } i} (p_i - 1) \log(p_i - 1) - p_i + 2$$

(Their displayed formula actually includes target weights q_i, but these are set uniformly to $q_i = 2$). Since (2) optimizes over probability weights, we perform the inversion $W_i = 1/p_i$. Note that the two aforementioned constraints on the p_i correctly translate to W being a probability distribution. In analogy to the CBPS objective, let us define the f-divergence away from the uniform distribution using the following function:

$$f(t) = \left(\frac{n_1}{t} - 1 \right) \log \left(\frac{n_1}{t} - 1 \right) - \frac{n_1}{t} + c$$

Here, the constant c is chosen to make $f(1) = 0$:

$$c = -(n_1 - 1)\log(n_1 - 1) + n_1 \qquad (16)$$

It is easy to see that the divergence (6) matches the CBPS objective, up to constants:

$$\text{Divergence}(W \parallel U) = \sum_{\text{treated } i} \frac{1}{n_1} f(n_1 \cdot W_i)$$
$$= \frac{1}{n_1} \sum_{\text{treated } i} f\left(\frac{n_1}{p_i} \right) \propto \text{CBPS}(p)$$

We simply need to show that this f satisfies the necessary conditions to define an f-divergence, per Section 3.1. As mentioned before, $f(1) = 0$. Next, note $\lim_{t \to 0^+} f(t)$ does indeed grow to $f(0) = \infty$. Finally, we need to show f is convex. When used to define a divergence away from the uniform distribution, f is evaluated only over $t \in [0, n_1]$. Thus, for Lemma A.1, f needs to be convex just over that range. Its second derivative is:

$$f''(t) = \frac{n_1}{t^3} \left(2 \log \left(\frac{n_1 - t}{t} \right) + \frac{n_1}{n_1 - t} \right)$$
$$= \frac{n_1}{t^3} \underbrace{\left(2 \log \left(\frac{1 - s}{s} \right) + \frac{1}{1 - s} \right)}_{g(s)}$$

The second line substitutes $s = t/n_1$. for $s \in [0, 1]$. To prove f is convex, we just need to show $g(s) \geq 0$ on $[0, 1]$. As $s \to 0$ or $s \to 1$, $g(s) \to +\infty$. Now we show g is nonnegative within those endpoints by finding its sole critical point, showing it is a local minimum, and that g remains nonnegative there. Taking derivatives:

$$g'(s) = \frac{-2}{s(1 - s)} + \frac{1}{(1 - s)^2}$$
$$g''(s) = \frac{2(1 - 2s)}{s^2(1 - s)^2} + \frac{2}{(1 - s)^3}$$

Solving $g'(s) = 0$, the unique critical point is at $s_{\min} = 2/3$. We find $g''(s_{\min}) > 0$ and $g(s_{\min}) > 0$. This completes the proof of convexity.

B   ADDITIONAL RELATED WORK

B.1   MODELING ALGORITHMS

Another approach to causal inference is modeling the propensity score. This is the probability $e(x) = \mathbb{P}(T = 1 \mid X = x)$ that a participant having covariates x is assigned to the treatment group. Such modeling is often performed using ℓ_1-regularized logistic regression [Tibshirani, 1996]. Though the modeling approach is superficially distinct from covariate balancing, they are mathematically intertwined [Ben-Michael et al., 2021]. The inverse propensity score produces weights $W_i^* = 1/e(X_i)$ which balance all covariate means. In fact, these are the unique weights which balance means of all bounded functions of the covariates. In terms of optimization, balancing and modeling are linked via convex duality.

Due to these close connections, some algorithms attempt to simultaneously model and balance. As previously discussed, CBPS [Imai and Ratkovic, 2014] fits a logistic regression propensity score while constraining the inverse propensity scores (i.e. the weights) to balance all covariate means. Its successor HDCBPS [Ning et al., 2020] does not attempt to balance all covariates, but focuses on balancing only
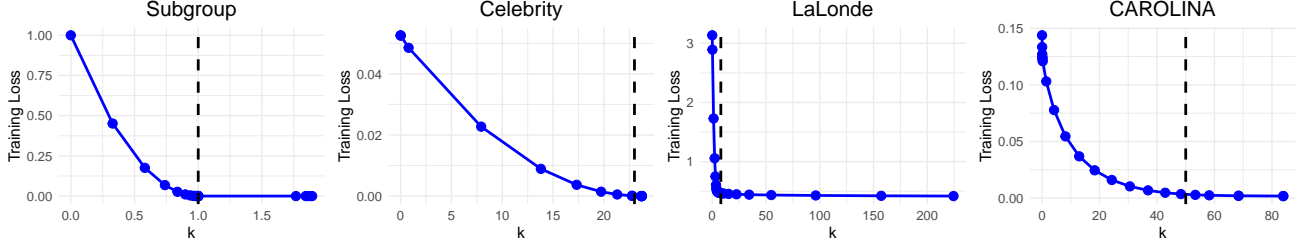
Figure 3: Residual bend analyses used to choose k in the experiments. For each experiment, the observed data (X, Y) are fit by the Lasso [Tibshirani, 1996], for different regularization values λ. k is chosen as the ℓ_1 norm where the training loss begins to depart sharply from zero. This is a somewhat imprecise heuristic, but seems to work reasonably in practice.
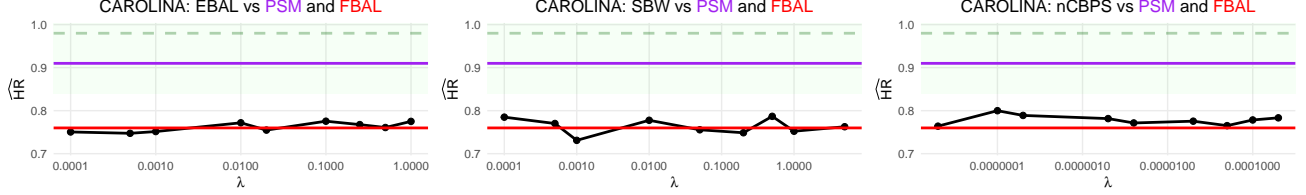

Figure 4: Worse results for the **CAROLINA** emulation (below) when sparse features are not removed. A naive, unweighted Cox model yields $\widehat{HR} = 0.793$, so all of the balancing methods have essentially trivial performance. This makes intuitive sense: covariate balancing methods must balance *all* the covariates, so including noisy or meaningless covariates greatly impacts their performance. By contrast, irrelevant features can be automatically ignored in propensity score estimation — though they are still (manually) inspected and adjudicated in matching.

covariates which are relevant to the outcomes. This is akin to how Differentiated Confounder Balancing [Kuang et al., 2017] learns which subset of covariates are confounders along with the weights W balancing that subset.

Matching [Rosenbaum and Rubin, 1983] is another way to use the propensity score. This pairs each member of the treatment group with a control who has approximately the same propensity score; otherwise, if no such control is found, the member is dropped. Because this method may not use all of the data, it can be problematic when n is relatively small. Furthermore, if the minor differences between matched pairs accumulate in the same direction, substantial bias can arise; overall covariate imbalance still needs to be separately adjudicated.

B.2 REINFORCEMENT LEARNING

The observational study setup in this paper is a special case of off-policy evaluation in reinforcement learning [Uehara et al., 2022]. More specifically, it is a special case of behavior-agnostic off-policy evaluation in contextual bandits. In our setting, the states are covariates, the two actions are assignment to either treatment or control, the historical policy is the unknown selection mechanism (i.e. the propensity score) in the observational data, and ATE is the value of the policy which chooses assignment randomly. In this more difficult and general setting, finite-sample confidence intervals [Dai et al., 2020] have been derived. How-

ever, it is unclear whether they improve the naive interval (9) when specialized to observational studies. Subsequent works on off-policy confidence sequences [Karampatziakis et al., 2021, Waudby-Smith et al., 2024] assume a known behavior policy (i.e. propensity score), which makes them inapplicable to our setting.

C EXISTENCE OF W^*

This section describes why Assumption 3.4 is a consequence of standard assumptions in causal inference. The two following assumptions are jointly known as strong ignorability [Rosenbaum and Rubin, 1983].

Assumption C.1 (Unconfoundedness). For all $i \in \{1, \ldots, n\}$, $T_i \perp Y_i(0), Y_i(1) \mid X_i$. (Given the covariates, the treatment selection is independent of both potential outcomes).

Assumption C.2 (Overlap). There is a constant $\gamma > 0$ such that, for all x, $\gamma < \mathbb{P}(T_i = 1 \mid X = x) < 1 - \gamma$. (Each participant has a positive probability of being assigned to either the treatment or the control).

For the moment, let us assume $\mathcal{S} = \mathcal{T}$ (i.e. the source and target distributions are the same). Define W^* as the true (unknown) inverse-propensity weights:

$$W_i^* \propto \frac{1}{\mathbb{P}(T_i = 1 \mid X = X_i)} \qquad \sum_{\text{treated } i} W_i^* = 1 \quad (17)$$

Under Assumptions C.1 and C.2, it is a standard result that $\sum_{\text{treated } i} W_i^* Y_i(1)$ has mean M (see e.g. Ben-Michael et al. [2021]). Thus, by the central limit theorem, its error is $O(1/\sqrt{n})$. Next, we show W^* satisfies the ratio-boundedness property of Assumption 3.4.

Lemma C.3. *Under Assumption C.2:*

$$R = \frac{\max_i W_i^*}{\min_i W_i^*} \leq \left(\frac{1-\gamma}{\gamma}\right)^2.$$

Proof. Abbreviate $W = W_*$, $n = n_1$ and $p_i = \mathbb{P}(T_i = 1 \mid X = X_i)$, so $W_i = \frac{p_i}{Z}$ where $Z = \sum_i \frac{1}{p_i}$. By Assumption C.2, each $p_i \in (\gamma, 1-\gamma)$. Thus, we have:

$$\frac{1}{1-\gamma} \leq \frac{1}{p_i} \leq \frac{1}{\gamma}.$$

Therefore, taking sums:

$$\frac{n}{1-\gamma} \leq Z \leq \frac{n}{\gamma}.$$

Hence each component of W lies within this range:

$$W_i = \frac{1}{p_i Z} \in \left[\frac{1}{\left(\frac{1}{\gamma}\right)\left(\frac{n}{\gamma}\right)}, \frac{1}{\left(\frac{1}{1-\gamma}\right)\left(\frac{n}{1-\gamma}\right)} \right]$$

$$= \left[\frac{\gamma}{n(1-\gamma)}, \frac{1-\gamma}{n\gamma} \right]$$

Dividing these by one another, we see the ratio of largest to smallest W_i is bounded. $\square$

Now let us consider the case when $\mathcal{S} \neq \mathcal{T}$. In the literature studying this case, it is common to assume a positive participation probability, i.e. that all participants in $\mathcal{T}$ have some chance of being sampled in $\mathcal{S}$. To ensure ratio-boundedness of W^*, we can make the following, somewhat stronger assumption.

Assumption C.4 (Bounded density ratio). There are constants $r_0, r_\infty > 0$ such that $r_0 \leq \frac{d\mathcal{S}(x)}{d\mathcal{T}(x)} \leq r_\infty$.

Then, W^* just needs to be adjusted by this ratio, and the standard arguments go through as before.

D LINEAR PROGRAM FOR β_z

This section shows that (11) can be reformulated as a linear program. (Strictly speaking, this linear program is an upper bound, but it will usually be exactly tight). For readability, we copy (11) here:

$$\max_{v_*, M \in \mathbb{R}^d} \quad \frac{-z}{||\widehat{M}||_\infty} v_*^\top M$$

$$\text{s.t.} \quad ||v_*||_1 \leq k \qquad ||\widehat{M} - M||_\infty \leq \frac{C \log d}{\sqrt{n}}$$

$$v_*^\top X_i = Y_i(1) \text{ for all treated } i$$

The first step is to eliminate the optimization over M. For any fixed v_*, the objective is maximized at $M = \widehat{M} - z \frac{C \log d}{\sqrt{n}} \text{sign}(v_*)$. (For example, in case $z = -1$, this perturbs $\widehat{M}$ in the direction of $\text{sign}(v_*)$. Using this optimal M, along with the the fact that $v_*^\top \text{sign}(v_*) = ||v_*||_1$, the objective becomes just a maximization over v_*:

$$\frac{1}{||\widehat{M}||_\infty} \left(-z v_*^\top \widehat{M} + \frac{C \log d}{\sqrt{n}} ||v_*||_1 \right)$$

The ℓ_1 norm is not concave, but this is not a problem. The constraint $||v_*||_1 \leq k$ is typically active (i.e. the sparsity constraint makes it more challenging to fit the data). This is trivially the case if there is an all-zero covariate. Thus, we can replace the non-concave $||v_* 1||$ by just k.

Now the ℓ_1 norm constraint is linearized in the usual fashion. Let $v_* = u - w$ with $u, w \geq 0$. Then $||v_*||_1 = \sum_{i=1}^d (u_i + w_i)$ and $v_*^\top X_i = (u-w)^\top X_i$. The final program is:

$$\max_{u, v \in \mathbb{R}^d} \quad \frac{1}{||\widehat{M}||_\infty} \left(\frac{Ck \log d}{\sqrt{n}} - z \sum_{j=1}^d \widehat{M}_j (u_j - w_j) \right)$$

$$\text{s.t.} \quad \sum_{j=1}^d u_j + w_j \leq k \qquad u_j, v_j \geq 0$$

$$(u - w)^\top X_i = Y_i(1) \text{ for all treated } i$$

The potential for $||\widehat{M}||_\infty \approx 0$ may make this program seem ominous. However, in the linear setting of Assumption 3.2, is typically the case that a constant covariate is added. It is appropriate to think of $||\widehat{M}||_\infty = 1$ in our setting.

E GENERAL f-DIVERGENCES

This section explains how to extend the proof of Section 4.2 to all f-divergences, thereby establishing Theorem 4.1 in full generality. This elaboration is very straightforward. Instead of beginning with the Donsker-Varadhan formula (13), we use the more abstract variational representation of f-divergences [Ruderman et al., 2012]:

$$\text{Divergence}(W \parallel U) = \sup_\phi \mathbb{E}_{i \sim W} \phi(i) -$$

$$\text{Divergence}^*([\phi(i)]_{\text{treated } i} \parallel U)$$

The proof remains the same until the part where terms which don't depend on i drop out of the logmeanexp. It is easy to see that the same equality holds for Divergence*. Let $z_0 \in \mathbb{R}$ be an additive term constant across all the i. Because W is a probability distribution:

$$\text{Divergence}^*(Z + \mathbf{1}z_0 \parallel U)$$

$$= \sup_W (Z + \mathbf{1}z_0)^\top W - \text{Divergence}(W \parallel U)$$

$$= \sup_W z_0 \mathbf{1}^\top W + Z^\top W - \text{Divergence}(W \parallel U)$$

$$= z_0 + \text{Divergence}^*(Z \parallel U)$$

This completes the generalization of the proof. Let us see how it can be used to derive another covariate balancing algorithm. Consider the χ^2 divergence and its conjugate [Ohnishi and Honorio, 2021]:

$$\chi^2(W \parallel U) = \sum_{\text{treated } i} \left(W_i - \frac{1}{n_1} \right)^2 \qquad (18)$$

$$\chi^{2*}(Z \parallel U) = \mathop{\mathbb{E}}_{i \sim U} Z_i - \frac{1}{4} \mathop{\text{Var}}_{i \sim U} Z_i$$

Using these in (10) yields a flexible analogue of stable balancing weights [Zubizarreta, 2015]. As discussed in Section 4.2, the data can be centered, without loss of generality, to eliminate the mean term. This instantiation of (10) makes it clear that Divergence* quantifies empirical variation of the data.

F PROOF OF CONSISTENCY

Assumptions 3.2 and 3.3 secure the finite-sample guarantee in Theorem 4.1. Take $W = W^*$, $\delta = 0$ and $\lambda \to 0$. (The actual solution to (12) may be better, but this only helps our argument). Setting $\lambda \to 0$ eliminates the divergence terms. The remaining terms are $O(k \log(d)/\sqrt{n})$ which, by Assumptions 3.4 and 3.5, goes to zero.

G EXPERIMENT DETAILS

Algorithms. In most of the experiments, FBAL is flexible entropy balancing (12). The CAROLINA experiment involves the flexible analogue of stable balancing weights, using the χ^2 divergence described in (18). k is not manually set, but is chosen from the data according to the the residual bend analysis depicted in Figure 3. To handle $n < d$, we implement EBAL, SBW, and nCBPS ourselves, minimizing the penalized formulation (1) using gradient descent.

Optimization. With fixed λ, the standard covariate balancing program (1) is convex. Flexible covariate balancing (10) is not convex, due to the product terms. We attempt to optimize (10) using gradient descent. Instead of implementing the constraints on W, λ and δ as projections, we embrace nonconvexity: we reparameterize $W = \text{softmax}(\widetilde{W})$, $\lambda = \text{softplus}(\tilde{\lambda})$ and $\delta = \text{sigmoid}(\tilde{\delta})$ using new unconstrained variables $\widetilde{W} \in \mathbb{R}^{n_1}$ and $\tilde{\lambda}, \tilde{\delta} \in \mathbb{R}$. We initialize $\widetilde{W} = 0$, $\tilde{\lambda} = 1$ and $\tilde{\delta} = 0$.

Simulations. Both the subgroup and celebrity simulations are run with $n = 1000, d = 3000$. All presented results are averaged over multiple independent runs.