# **Regularizing Extrapolation in Causal Inference**

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# **Abstract**

Many common estimators in machine learning and causal inference are linear smoothers, where the prediction is a weighted average of the training outcomes. Some estimators, such as ordinary least squares and kernel ridge regression, allow for arbitrarily negative weights, which improve feature imbalance but often at the cost of increased dependence on parametric modeling assumptions and higher variance. By contrast, estimators like importance weighting and random forests (sometimes implicitly) restrict weights to be non-negative, reducing dependence on parametric modeling and variance at the cost of worse imbalance. In this paper, we propose a unified framework that directly penalizes the level of extrapolation, replacing the current practice of a hard non-negativity constraint with a soft constraint and corresponding hyperparameter. We derive a worst-case extrapolation error bound and introduce a novel "bias-bias-variance" tradeoff, encompassing biases due to feature imbalance, model misspecification, and estimator variance; this tradeoff is especially pronounced in high dimensions, when positivity is poor. We then develop an optimization procedure that regularizes this bound while minimizing imbalance and outline how to use this approach as a sensitivity analysis for dependence on parametric modeling assumptions. We demonstrate the effectiveness of our approach through synthetic experiments and a real-world application, involving the generalization of randomized controlled trial estimates to a target population of interest.

### 1 Introduction

A core challenge in observational causal inference and domain adaptation is to adjust data distributions so that features are comparable across distinct groups, such as control and treated groups or source and target populations [Imbens and Rubin, 2015, Farahani et al., 2021]. Weighting estimators and linear smoothers, in which the predictions is a weighted average of training outcomes, are widely used for such adjustment; examples include implicit weighting estimators like ordinary least squares (OLS) and random forests and explicit weighting approaches like inverse propensity score weighting [IPW Li et al., 2013] and importance sampling [Thomas and Brunskill, 2017].

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An important divide among weighting estimators is whether weights are constrained to be non-negative, such as in traditional IPW, matching [Stuart, 2010], the synthetic control method [Abadie et al., 2010], and stable balancing weights [Zubizarreta, 2015, Ben-Michael et al., 2021a], as well as in the weighting component of popular doubly robust estimators like double machine learning [Chernozhukov et al., 2018]. This constraint limits extrapolation and dependence on parametric modeling assumptions, but typically at the cost of worse feature imbalance between re-weighted groups. This imbalance is especially pronounced in high-dimensional settings, when the curse of dimensionality means that positivity is less likely to hold, leading to further bias [D'Amour et al., 2021]. By contrast, linear smoothers like OLS and kernel ridge regression allow for arbitrarily negative weights [Robins et al., 2007], which can improve feature imbalance but at the cost of greater model dependence and higher estimator variance. Finally, augmented estimators that combine outcome modeling with explicit weighting strategies can therefore be viewed as performing controlled extrapolation, balancing model dependence against feature imbalance. Pure weighting and pure outcome modeling thus represent two extremes: no extrapolation versus uncontrolled extrapolation.

In this paper, we utilize this geometric perspective to establish a general framework for systematically controlling extrapolation. In particular, we propose a unified approach that directly penalizes the level of extrapolation, replacing the current practice of a hard non-negativity constraint with a soft constraint and corresponding hyperparameter. Unlike prior research on extrapolation in machine learning that emphasizes predictions beyond the observed covariate support, we conceptualize extrapolation through unit weights, a particularly natural framework for handling high-dimensional covariates [Ben-Michael et al., 2021b]. Specifically, our contributions are:

- Bias-bias-variance tradeoff. We propose a framework quantifying a "bias-bias-variance" tradeoff, decomposing error into bias from distributional imbalance, bias from outcome model misspecification, and estimator variance. This captures key tradeoffs encountered in common causal inference and distribution shift scenarios.
- Error bound and constrained optimization. We derive an error bound based on worst-case Hölder continuity deviations from linearity. We present an optimization approach to minimize this bound, explicitly controlling tradeoffs between biases. We also characterize the asymptotic variance properties of our estimator.
- Sensitivity analysis framework. We introduce a sensitivity analysis methodology integrated into our optimization framework, enabling systematic evaluation of distributional imbalance and outcome model misspecification impacts. We illustrate this using synthetic data and a practical application involving the transportation of causal estimates to a novel target population.

#### 1.1 Related work

Extrapolation and generalization are core topics in causal inference and machine learning. Recent surveys by Degtiar and Rose [2023] and Johansson et al. [2022] provide comprehensive overviews on generalizability and transportability methods.

**Extrapolation and the synthetic control method.** Extrapolating far from the support of the data is a longstanding concern in statistics and the social sciences especially; see King and Zeng [2006] for a seminal discussion of possible dangers of unchecked extrapolation. Methods that limit extrapolation are common; the synthetic control method [Abadie et al., 2010] is a particularly prominent example. Doudchenko and Imbens [2016] discuss the non-negativity constraint in this context, and explore possible regularization. Most relevant to our approach, Ben-Michael et al. [2021b] developed the augmented synthetic control method, which combines outcome modeling with constrained weights to reduce bias while controlling extrapolation.

**Extrapolation in machine learning.** Within machine learning, there has been substantial recent progress on approaches for addressing extrapolation. Shen and Meinshausen [2024] introduced engression, a framework that views extrapolation through the lens of distributional regression, enabling principled uncertainty quantification outside the training distribution. Kong et al. [2024] developed a causal lens for understanding extrapolation, establishing theoretical connections between causal structure and extrapolation. Netanyahu et al. [2023] proposed a transductive approach for learning to extrapolate, leveraging unlabeled test points to guide the extrapolation process. Dong and Ma [2022] provided foundational analysis toward understanding the extrapolation of nonlinear models

to unseen domains, establishing bounds on extrapolation error. Finally, Pfister and Bühlmann [2024] developed extrapolation-aware nonparametric statistical inference methods, with formal guarantees on validity beyond the support of training data.

Unlike this recent literature, we approach extrapolation from a weighting perspective, which offers particular advantages in high-dimensional settings. Rather than focusing on predictions outside the covariate support, we frame extrapolation in terms of the properties of unit weights, providing a natural parameterization for high-dimensional settings [Ben-Michael et al., 2021b]. This perspective allows us to directly quantify and regularize the degree of extrapolation without relying on complex directional derivatives or high-dimensional density estimation.

**Positivity violations and shifting the target.** Our discussion is closely related to the literature on positivity violations in causal inference. Crump et al. [2006], Li et al. [2018], and Parikh et al. [2025] all proposed to avoid issues due to positivity violations by shifting the estimand to regions with greater overlap. By contrast, our approach directly incorporates the severity of positivity violations into the weight estimation process.

Weighting representations. A growing literature highlights the connections between various causal estimators through their weighting representations [Chattopadhyay and Zubizarreta, 2023]. Knaus [2024] provided a unified framework for viewing treatment effect estimators as weighted outcomes. Bruns-Smith et al. [2023] showed that augmented balancing weights can be interpreted as a form of linear regression. Lin and Han [2022] examined regression-adjusted imputation estimators through their weighting properties. Our framework builds on these insights by explicitly parameterizing the degree of extrapolation through weight regularization, providing a continuum of estimators that navigate the bias-variance tradeoff.

## 2 Preliminaries

#### 2.1 Setup and notation

We set up our problem as an instance of prediction/estimation under general distribution shift; the causal inference problems of interest will largely be special cases of these. Consider that we observe n independent and identical draws from source population P. For each unit  $i \in \{1, \ldots, n\}$ , we observe  $(X_i, Y_i), X_i \in \mathcal{X}$  are covariates and  $Y \in \mathbb{R}$  is the outcome. We also observe  $n_q$  iid draws from target population Q, with covariates  $X \in \mathcal{X}$  but with corresponding missing outcome  $Y \in \mathbb{R}$ . Finally, define outcome model  $\mu(x) = \mathbb{E}[Y \mid X = x]$  and density ratio dQ/dP(x).

For any canonical point in the target population,  $x^* \in \mathcal{X}$ , our goal is to estimate the expected outcome:  $\mathbb{E}_Q[Y \mid X = x^*]$ . Typically,  $x^*$  is chosen to be the centroid of the target population (e.g., estimating average treatment effect on treated). The literature typically make following two key assumptions to guide estimation:

- A.1. (Conditional Ignorability)  $\mathbb{E}_P[Y \mid X] = \mathbb{E}_Q[Y \mid X]$
- A.2. (Population overlap)  $dQ/dP(x) < \infty$  for all  $x \in \mathcal{X}$

Under these restrictions, we can identify the estimand of interest via (1) the outcome function:  $\mathbb{E}_Q[\mathbb{E}_P[Y\mid X]\mid X]$ ; (2) the weighting function  $\mathbb{E}_Q[\mathbb{E}_P[dQ/dP(X)Y]\mid X]$ ; or (3) via both using the doubly robust formulation. In our setup, we consider situations when A.2. (population overlap) assumption is violated, especially at  $x=x^*$ . For regions of  $\mathcal X$  where A.2. is violated, one needs to rely on parametric assumptions (such as linearity of outcome-covariate relationship) to extrapolate, and identify and estimate the expected outcomes.

**Linear in features.** Our paper is concerned with parametric model dependence and the bias due to violation of the same. Since we are also focused on linear smoothers, we therefore focus on models that are linear in some features, which are possibly complex functions of the underlying covariates. This is an extremely large model class that ranges from *simple linear models* to the last layer embedding from a *pre-trained large language model*. For our setup, we let  $\boldsymbol{x}$  be the features in the representation implied by the parametric model, rather than simply the raw covariates.

We further assume:

**Assumption 2.1.**  $\mu$  is Hölder continuous such that  $|\mu(x) - \mu(x')| \le a \cdot ||x - x'||^{\alpha}$  where, a > 0 and  $\alpha > 0$ .

Parameterizing  $\mu$  in terms of its Hölder constants is useful for characterizing departures from *linearity* that directly affect the estimation error bound.

## 2.2 Weighting form of causal inference estimators

Our focus is on weighting estimators or linear smoothers [Buja et al., 1989] of the form:

$$\hat{\mu}(\boldsymbol{x}^*) = \sum_{i=1}^n w_{\star \leftarrow i}(\boldsymbol{x}_i) Y_i,$$

with weights  $w_{\star \leftarrow i}(x_i)$ , where  $\star \leftarrow i$  emphasizes that the weights can depend both on the source covariates  $x_i$  and the target covariates  $x^*$  [Lin and Han, 2022]. When there is no ambiguity, we suppress the dependence on the covariates  $x_i$  and the target  $x^*$ .

A broad class of estimators have this form. See Knaus [2024] for a comprehensive discussion of the weighting form for common causal inference estimators. We highlight several special cases here, with a focus on whether the implied weights are constrained to be non-negative.

**Explicit weighting estimators.** The first class of methods estimate the density ratio  $\widehat{dQ/dP}(x)$ , either directly or indirectly.

- Traditional Inverse Propensity Score Weighting. In standard IPW [Rosenbaum, 1987], researchers first estimate a propensity score,  $e(\boldsymbol{x}) = \mathbb{P}[1\{i \in P\} \mid \boldsymbol{X}_i = \boldsymbol{x}]$  via a binary classifier like logistic regression, and then plug into a known functional form for dQ/dP(x). For example, when estimating the Average Treatment Effect on the Treated,  $\hat{w}(\boldsymbol{x}) = \hat{e}(\boldsymbol{x})/(1-\hat{e}(\boldsymbol{x}))$ . Since  $\hat{e}(\boldsymbol{x}) \in (0,1)$ ,  $\hat{w}_i(\boldsymbol{x}) > 0$  for all i.
- Balancing weights, synthetic control, and matching. An alternative weighting approach instead directly estimates dQ/dP(x) via constrained optimization [Ben-Michael et al., 2021a]. For example, consider the minimum variance weights that control imbalance in x between P and Q:

$$\hat{\mathbf{w}} \in \arg\min_{\mathbf{w} \in \mathcal{W}} \left\| \sum_{i}^{n} w_{i} \mathbf{X}_{i} - \mathbf{x}^{\star} \right\|_{p}^{2} + \lambda \|\mathbf{w}\|_{2}^{2}, \tag{1}$$

where  $\|\cdot\|_p$  is the p vector norm and where  $\mathcal{W}$  are possible constraints on the weights. Stable balancing weights [Zubizarreta, 2015] and the Synthetic Control Method [Abadie et al., 2010] are special cases where  $\mathcal{W}$  is the simplex  $(w_i \geq 0, \sum w_i = 1)$  and the imbalance norm is  $p = \infty$  and p = 2, respectively. Matching is a special case where the weights are also constrained to be discrete.

• Riesz regression. A final weighting approach, also known as automatic estimation of the Riesz representer [Chernozhukov et al., 2022b] also finds weights via Problem (1), albeit without imposing the constraint that weights are non-negative. For example, minimum distance lasso Riesz regression in Chernozhukov et al. [2022b] solves Equation (1) with  $W = \mathbb{R}^n$  and  $p = \infty$ .

Linear smoothers and implicit weighting estimators. A wide range of popular outcome models are linear smoothers [Buja et al., 1989], which implicitly estimate weights w, including (kernel ridge) regression, k-nearest neighbors, random forests, xgboost, and many implementations of neural networks; see Lin and Han [2022], Curth et al. [2024]. We highlight two prominent examples with and without a non-negativity constraint.

• (Kernel) ridge regression. For features X, the implied ridge regression weights are:

$$w_{\star \leftarrow i} = \boldsymbol{x}^{\star \top} (\boldsymbol{X}^{\top} \boldsymbol{X} + \lambda \mathbb{I})^{-1} \boldsymbol{X}_{i},$$

where  $\lambda$  is a regularization parameter; ordinary least squares (OLS) as a special case when  $\lambda=0$ . Kernel ridge regression is instead based on the implied kernel features  $\phi(\boldsymbol{x})$ ; see Bruns-Smith et al. [2023], Hirshberg et al. [2019]. As Bruns-Smith et al. [2023] discuss, the ridge regression weights are equivalent to solving optimization problem (1) with the imbalance norm set to p=2 and with  $\mathcal{W}=\mathbb{R}^n$ , which does *not* include a non-negativity constraint.

 Random forests. As Athey et al. [2019] discuss in the context of causal inference, (honest) random forests is a locally adaptive linear smoother with non-negative weights:

$$\hat{w}_{\star \leftarrow i} = \frac{1}{B} \sum_{b=1}^{B} \frac{\mathbb{I}\{\boldsymbol{x}^{\star} \in L_{b}(\boldsymbol{x})\}}{|L_{b}(\boldsymbol{x})|},$$

where  $L_b$  is the set of units that share a leaf node with the target  $x^*$  and b = 1, ..., B index the trees.

**Augmented and hybrid estimators.** Finally, augmented or hybrid estimators combine initial weights  $w^0$  and outcome model  $\hat{m}$ :

$$\hat{\mu}^{dr}(\boldsymbol{x}^{\star}) = \sum_{i=1}^{N} \hat{w}_{i}^{0} Y_{i} + \left( \hat{m}(\boldsymbol{x}^{\star}) - \sum_{i=1}^{N} w_{i}^{0} \hat{m}(\boldsymbol{x}_{i}) \right) = \hat{m}(\boldsymbol{x}^{\star}) + \sum_{i=1}^{N} \hat{w}_{i}^{0} (Y_{i} - \hat{m}(\boldsymbol{x}_{i})).$$

When  $\hat{m}$  is a linear smoother, then  $\hat{\mu}^{dr}(\boldsymbol{x})$  also has a weighting representation. Let  $\hat{m}(\boldsymbol{x}^{\star}) = \sum \hat{\omega}_i(\boldsymbol{x})Y_i$  for a weighting function  $\hat{\omega} : \mathbb{R}^d \to \mathbb{R}^n$ . Following Ben-Michael et al. [2021b]:

$$\hat{\mu}^{dr}(\boldsymbol{x}^*) = \sum_{i=1}^N \left( \hat{w}_i^0 + \hat{w}_i^{\text{adj}} \right) Y_i \qquad \text{ where } \quad \hat{w}_i^{\text{adj}} \equiv \hat{\omega}_i(\boldsymbol{x}_\star) - \sum_{j=1}^n \hat{w}_j^0 \hat{\omega}_i(\boldsymbol{x}_j)$$

For example, when the outcome model is ridge regression, the implied weights for the doubly robust estimator has the following form:

$$\hat{w}_i^{dr} = \hat{w}_i^0 + (\boldsymbol{x}^* - \boldsymbol{x}' \hat{\boldsymbol{w}}^0)' (\boldsymbol{x}' \boldsymbol{x} + \lambda \mathbb{I})^{-1} \boldsymbol{x}_i.$$

Importantly, even if the initial weights  $w^0$  are constrained to be non-negative, such as in traditional IPW, the implied doubly robust weights  $w^{dr}$  could be negative. In fact, the combined weights can be negative even if both the initial weights  $w^0$  and the outcome model-implied weights  $\alpha$  are non-negative.

There are many examples of combined estimators of this form: standard Augmented IPW [Chattopadhyay and Zubizarreta, 2023], bias correction for inexact matching [Lin et al., 2021], augmented synthetic control method [Ben-Michael et al., 2021b], and regression-adjusted imputation estimators more broadly [Lin and Han, 2022]. Finally, both debiased machine learning [Chernozhukov et al., 2018] and *automatic* debiased machine learning [Chernozhukov et al., 2022a]; the former constrains the initial weights to be non-negative, the latter does not.

# 3 Regularizing Worst-Case Extrapolation Bias

Our goal is to bound the estimation error:  $|\mu(\boldsymbol{x}^*) - \sum_{i=1}^n w_i Y_i|$ . We begin by building intuition for our approach. First, note that, under linearity, a negative weight on training point  $\boldsymbol{x}_i$  is equivalent to reflecting the training point around the origin:  $-\mu(\boldsymbol{x}_i) = \mu(-\boldsymbol{x}_i)$ . We can use this to construct a "reflected" estimator, denoted by ‡, which reflects points with negative weights around the origin:

$$\hat{\mu}^{\ddagger}(\boldsymbol{x}^*) = \sum_{i=1}^{n} w_i \mathbb{1}(w_i \ge 0) \mu(\boldsymbol{X}_i) + |w_i| \mathbb{1}(w_i < 0) \mu(-\boldsymbol{X}_i)$$

$$= \sum_{i=1}^{n} |w_i| \mu(\boldsymbol{X}_i^{\ddagger}), \qquad \boldsymbol{X}_i^{\ddagger} = \begin{cases} \boldsymbol{X}_i, & w_i \ge 0 \\ -\boldsymbol{X}_i, & w_i < 0 \end{cases},$$

where  $\hat{\mu}(x^*) = \hat{\mu}^{\ddagger}(x^*)$  if  $\mu$  is an odd-function, and where  $w_i X_i = |w_i| X_i^{\ddagger}$  for all i.

Second, the difference between  $\hat{\mu}(\boldsymbol{x}^*)$  and  $\hat{\mu}^{\dagger}(\boldsymbol{x}^*)$  is a measure of nonlinearity. In particular, we can decompose  $\mu(-\boldsymbol{x}_i)$  as  $\delta(\boldsymbol{x}_i) - \mu(\boldsymbol{x}_i)$  where  $\delta(\boldsymbol{x}_i) = (\mu(-\boldsymbol{x}_i) + \mu(\boldsymbol{x}_i))$ . In general,  $\hat{\mu}(\boldsymbol{x}^*) = \hat{\mu}^{\dagger}(\boldsymbol{x}^*) + \sum_i |w_i| \mathbb{1}(w_i < 0)\delta(\boldsymbol{x}_i)$ ; again if  $\mu$  is an "odd function", e.g.,  $\mu$  is a linear function, then  $\delta(\boldsymbol{X}) = 0$  because  $\mu(-\boldsymbol{X}) = -\mu(\boldsymbol{X})$ . Thus,  $\delta(\boldsymbol{X})$  is a point-specific measure of nonlinearity in the underlying data generating process.

We use this representation to decompose the estimator  $\hat{\mu}(x^*)$ :

$$\begin{split} \hat{\mu}(\boldsymbol{x}^*) &= \sum_{i=1}^n w_i Y_i &= \sum_{i=1}^n w_i (\mu(\boldsymbol{X}_i) + \epsilon_i) \\ &= \sum_{i=1}^n w_i \mathbbm{1}(w_i \geq 0) \mu(\boldsymbol{X}_i) + |w_i| \, \mathbbm{1}(w_i < 0) \left(\mu(-\boldsymbol{X}_i) - \delta(\boldsymbol{X}_i)\right) \; + \; w_i \epsilon_i \\ &= \underbrace{\sum_{i=1}^n |w_i| \mu(\boldsymbol{X}_i^{\dagger})}_{\hat{\mu}^{\dagger}(\boldsymbol{x}^*)} + \underbrace{\sum_{i=1}^n |w_i| \mathbbm{1}(w_i < 0) \delta(\boldsymbol{X}_i)}_{\text{nonlinearity}} + \underbrace{\sum_{i=1}^n w_i \epsilon_i}_{\text{noise}}. \end{split}$$

Although  $\delta(\boldsymbol{X})$  is unknown, we can bound its magnitude using the Hölder continuity assumption:  $\|\delta(\boldsymbol{X})\| \le 2a\|\boldsymbol{X}\|^{\alpha} + 2\|\mu(\boldsymbol{X})\|$ . Further, if we assume  $\mu(0) = 0$ , then  $\|\delta(\boldsymbol{X})\| \le 2a\|\boldsymbol{X}\|^{\alpha}$ .

The resulting error bound is therefore:

$$|\mu_1(\boldsymbol{x}^{\star}) - \hat{\mu}(\boldsymbol{x}^{\star})| \leq \underbrace{\left|\sum_{i=1}^{n} |w_i| \mu(\boldsymbol{X}_i^{\ddagger}) - \mu(\boldsymbol{x}^{\star})\right|}_{\text{error in } \hat{\mu}^{\ddagger}(\boldsymbol{x}^{\star})} + \underbrace{2a \sum_{i=1}^{n} |w_i| \mathbb{1}(w_i < 0) \|\boldsymbol{X}_i\|^{\alpha}}_{\text{error due to nonlinearity}} + \underbrace{\left|\sum_{i=1}^{n} w_i \epsilon_i\right|}_{\text{noise}}.$$

The first term directly depends on the imbalance between the target point  $x^*$  and the re-weighted (reflected) training points  $|w|'X^{\ddagger}$ . The second term captures additional error due to nonlinearity, which corresponds to the  $\delta(X)$  term above. The final term is the noise term.

#### 3.1 Characterizing asymmetry-induced bias

Thus far we have presented a conservative nonparametric bound. We now provide a slightly refined characterization by noting that the extent of the bias induced by negative weights is driven by the asymmetry in  $\mu$ . We do so by considering the decomposition of the  $\mu$  into its even and odd components, i.e.,  $\mu(x) = \mu_e(x) + \mu_o(x)$ . By the definition of odd functions, we have  $-\mu_o(x) = \mu_o(-x)$ , so we can bound the risk by bounding the worst-case risk of  $\hat{w}$  using the assumed Hölder constants a and a and isolating the effect of the even component. The formal statement is given below in Proposition 3.1 the proof is given in Appendix B.

**Proposition 3.1.** Let  $\hat{\mu}(x^*) = \sum_{i=1}^n \hat{w}_i Y_i$  be the estimate of  $\mu(x^*)$  with weights estimated via Equation 5. Given  $Y_i = \mu(X_i) + \epsilon_i$  where  $\epsilon_i$  are independent random variables with  $\mathbb{E}[\epsilon_i] = 0$  and finite second moment  $\sigma^2 = \mathbb{E}[\epsilon_i^2]$ , and  $\mu$  is Hölder continuous with constants a and  $\alpha$ . If  $\epsilon_i$  are sub-Gaussian<sup>2</sup> with parameter  $\sigma$ , then with probability at least  $1 - \delta$ ,

$$|\mu(x^*) - \hat{\mu}(x^*)| \le B_{even}(x^*) + \sigma \|\hat{w}\|_2 \sqrt{2\log(2/\delta)}$$
 (3)

where

$$B_{even}(x^*) = \left| \sum_{i=1}^{n} \hat{w}_i [\mu_e(X_i) - \mu_e(x^*)] + 2 \sum_{i=1}^{n} |\hat{w}_i| \mathbf{1}(\hat{w}_i < 0) a \|X_i - x^*\|^{\alpha} \right|$$
(4)

and  $\mu_e(x) = \frac{\mu(x) + \mu(-x)}{2}$  denotes the even part of  $\mu$ .

The worst-case bound provided earlier is recovered if  $\mu$  is an even function, i.e., contains no odd component. One of the fundamental limitations of Proposition 3.1 is that it requires access to the separate even and odd functions constituting  $\mu$  which are latent in practice. In our proposed estimator and empirical application we address this by preferring the conservative form which assumes the worst case form. For completeness we all provide the following proposition that provides an empirical analog of Proposition 3.1. Intuitively, when the observations of X are symmetric, i.e., for every  $X_i$  is also in the dataset, then we can recover both the even and odd functions. In practice, because this symmetry is unlikely to hold we approximate it with a one-nearest neighbor and incorporate the induced uncertainty into the bound using the Hölder constants. The formal statement is below, the proof is deferred to Appendix B.

<sup>&</sup>lt;sup>2</sup>We assume mean zero sub-Gaussian noise, analogous results can be obtained with this assumption replaced by bounded noise.

**Proposition 3.2** (Approximate Bounds). Let  $\hat{\mu}(x^*) = \sum_{i=1}^n \hat{w}_i Y_i$  be the estimate of  $\mu(x^*)$  with weights estimated via Equation (5). Given  $Y_i = \mu(X_i) + \epsilon_i$  where  $\epsilon_i$  are independent sub-Gaussian random variables with parameter  $\sigma$ , and  $\mu$  is Hölder continuous with constants a and a. Let  $I_{paired} = \{i: -X_i \in \{X_1, \dots, X_n\}\}$ ,  $I_{nn} = \{1, \dots, n\} \setminus I_{paired}$ , and for each  $i \in I_{nn}$ , define  $j^*(i) = \arg\min_{j \neq i} \|X_j - (-X_i)\|$ . Then with probability at least  $1 - \delta$ :

$$\begin{aligned} |\mu(x^*) - \hat{\mu}(x^*)| &\leq \left| \sum_{i \in I_{paired}} \hat{w}_i \frac{Y_i + Y_{-i}}{2} + \sum_{i \in I_{nn}} \hat{w}_i \frac{Y_i + Y_{j^*(i)}}{2} - \mu_e(x^*) \sum_{i=1}^n \hat{w}_i \right| \\ &+ \sum_{i \in I_{nn}} |\hat{w}_i| a \|X_{j^*(i)} - (-X_i)\|^{\alpha} + 2 \sum_{i=1}^n |\hat{w}_i| \mathbf{1}(\hat{w}_i < 0) a \|X_i - x^*\|^{\alpha} \\ &+ \sigma \|\hat{w}\|_2 \sqrt{2 \log(6/\delta)} + \frac{\sigma}{\sqrt{2}} (\|\hat{w}_{I_{paired}}\|_2 + \|\hat{w}_{I_{nn}}\|_2) \sqrt{2 \log(6/\delta)} \end{aligned}$$

where  $\mu_e(x^*)$  is bounded using the closest observation  $j^* = \arg\min_{j=1,\dots,n} \|X_j - x^*\|$ ,

$$|\mu_e(x^*)| \le \left| \frac{Y_{j^*} + Y_{j^*(j^*)}}{2} \right| + \sigma \sqrt{2\log(6/\delta)} + a \|X_{j^*(j^*)} - (-X_{j^*})\|^{\alpha} + a \|X_{j^*} - x^*\|^{\alpha}$$

Proposition 3.2 can be used as a companion to Chattopadhyay and Zubizarreta [2023], who propose computing the effective sample size of units with negative weight,  $\frac{\sum_{i}\mathbf{1}[w_{i}<0]|w_{i}|}{\sum_{i}|w_{i}|}$ , to indicate the extent to which the estimate relies on extrapolation and parametric assumptions.

#### 3.2 Learning Estimator

We now propose a estimator to learn weights  $\boldsymbol{w}$  that directly control the error bound in Equation (2). To do so, we modify the standard balancing weights optimization problem in Equation (1) by using the Lagrangian form of the non-negative restriction, rather than the hard constraint. Thus, the combined estimator minimizes the error bound by controlling three terms: covariate imbalance, dispersion of the weights, and level of extrapolation:

$$\hat{\mathbf{w}} \in \arg\min_{\mathbf{w}} \underbrace{\|\sum_{i}^{n} w_{i} \mathbf{X}_{i} - \mathbf{x}^{\star}\|_{p}^{2}}_{(a)} + \lambda \underbrace{\|\mathbf{w}\|_{2}^{2}}_{(b)} + \gamma \underbrace{\|\mathbf{1}(w_{i} < 0)|w_{i}| (\|\mathbf{X}_{i}\|_{2}^{\alpha})\|_{p}}_{(c)}.$$
(5)

Where:

- Term (a): Enforces balance between the target point  $x^*$  and the re-weighted training points  $\{X_1,\ldots,X_n\}$ , recalling that  $w_iX_i=|w_i|X_i^{\frac{1}{i}}$  for all i. We will focus on the case where p=2, but this setup immediately generalizes to  $p=\infty$ .
- Term (b): Regularizes the dispersion of the weights w to control the variance of the overall estimator
- Term (c): Controls extrapolation, particularly through penalization of negative weights.

The standard balancing weights problem in Equation (1) only focuses on a single bias-variance tradeoff: trading off covariate imbalance in the first term — which directly introduces bias — and the norm of the weights in the second term — which directly controls the estimator variance. By contrast, the new optimization problem (5) has a more elaborate bias-bias-variance trade-off. Allowing for negative weights introduces an additional trade-off between the first two terms and term (c): when the target unit lies outside the convex hull of the training points, controlling imbalance often requires some  $w_i$  values to be negative, which also increases the norm  $\|w\|_2$ . Allowing negative weights also necessitates reliance on parametric assumptions for extrapolation.

Term (c) mitigates the risk of biased estimation by regulating the contribution of negative weights. For  $\gamma=0$ , Equation (5) recovers a standard, unconstrained balancing weights problem as in Equation (1). At the other extreme  $\gamma\to\infty$  is equivalent to a hard non-negativity constraint. Increasing  $\gamma$  constrains extrapolation, reducing bias due to possible violations of parametric assumptions and limiting  $\|\boldsymbol{w}\|_2$ , but worsening bias due to insufficient balance in term (a).

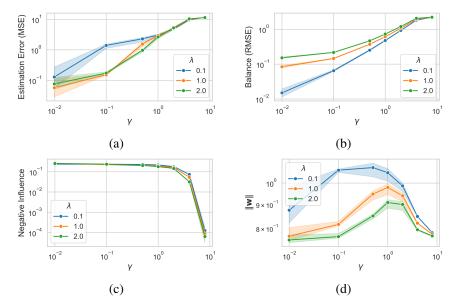


Figure 1: Results on synthetic data generated using linear DGP. (a) Estimation error measured as mean squared error, (b) balance between the weighted source and target populations, (c) extent of extrapolation measured as negative influence – contribution on units with negative weights, (d) L2 norm w capturing asymptotic variance.

# 4 Synthetic Data Study

We evaluate our approach using synthetic data with both (i) linear and (ii) nonlinear data-generating processes (DGPs) where the target point lies outside the convex hull of training points, creating a challenging extrapolation scenario with limited sample size (10 training units) (see Figure 6). We provide a brief summary in the main text and defer the full description and analysis to Appendix C.

For the linear setting where parametric assumptions hold, Figure 7(a) shows that estimation error increases as we regularize extrapolation (as expected). This is in congruence lack of balance shown in Figure 7(b). As the parametric assumption holds, relying on it for extrapolation yields optimal estimates. However, for the nonlinear DGP where parametric assumptions are violated through quadratic and interaction terms, this is not true. Figure 8 illustrates our theoretical bias-bias-variance tradeoff. Small amounts of extrapolation remain beneficial due to the linear component, but excessive extrapolation leads to high error rates due to assumption violations. Regularization reduces extrapolation bias from parametric misspecification but increases distributional imbalance bias.

# 5 Application: Generalizing Opioid Use Disorder Trial Evidence

We demonstrate our framework using data from the START trial [Saxon et al., 2013], which compared buprenorphine versus methadone for treating opioid use disorder.

**Data Description.** The Starting Treatment With Agonist Replacement Therapies (START) trial, initiated in 2006, was a multi-center study comparing buprenorphine versus methadone in treating opioid use disorder [Saxon et al., 2013, Hser et al., 2014]. The trial enrolled 1,271 participants, who were randomized in a 2:1 ratio to receive either buprenorphine or methadone. Methadone was found to have higher rates of patient retention in treatment compared to buprenorphine (though buprenorphine in this trial was given in an unusual way to mimic methadone medication administration—requiring near daily clinic visits of participants) [Hser et al., 2014]. Our analysis focuses on the outcome of relapse to regular opioid use within 24 weeks of medication assignment, defined as non-study opioid use for four consecutive weeks or daily use for seven consecutive days. Data on opioid use were collected through urine drug screens and self-reports, with relapse assessment beginning 20 days post-randomization to account for residual drug presence during stabilization.

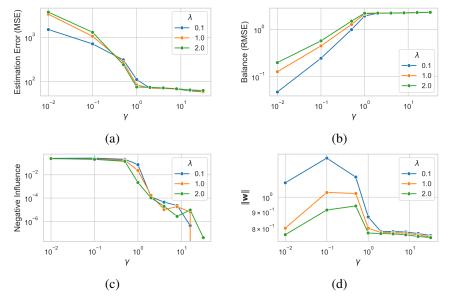


Figure 2: Results on synthetic data generated using non-linear DGP. (a) Estimation error measured as mean squared error, (b) balance between the weighted source and target populations, (c) extent of extrapolation measured as negative influence, (d) L2 norm w capturing asymptotic variance.

Parikh et al. [2025] identified that Latina women with a pre-treatment history of amphetamine and benzodiazepine use were underrepresented in the START trial relative to the target population, highlighting a practical violation of the positivity assumption. In this study, we estimate the average treatment effects (ATE) for this underrepresented subgroup using our proposed framework alongside standard linear regression and inverse probability weighting (IPW) estimators. We also evaluate the sensitivity of these estimates to parametric assumptions.

The target sample is drawn from the 2015–2017 Treatment Episode Dataset - Admissions (TEDS-A), which includes data on individuals entering publicly funded substance use treatment programs across 48 states (excluding Oregon and Georgia) and the District of Columbia. Our analysis focuses on Latina women with a pre-treatment history of amphetamine and benzodiazepine use.

**Analysis.** We code methadone as T=1 and buprenorphine as T=0, with Y=1 representing relapse. Pretreatment covariates include age, race, biological sex, and substance use history (amphetamine, benzodiazepines, cannabis, and intravenous drug use) measured at the initiation of medication for opioid use disorder (MOUD) treatment.

Using linear regression, the estimated treatment effect for our subgroup of interest is -0.278, indicating that relapse rates are approximately 28 percentage points lower under methadone compared to buprenorphine. In contrast, the IPW estimate is -0.014, suggesting that both treatments are similarly effective. However, as shown in Figure 11, the negative influence of the linear regression-based estimate is 35% and 40% for T=0 and T=1, respectively, compared to 0% for IPW. Despite this, Figure 10 demonstrates that the IPW estimator achieves worse covariate balance than linear regression. These findings reveal that while linear regression relies heavily on parametric assumptions and negative weights, it may be biased if these assumptions are violated. Conversely, the IPW estimator avoids additional parametric assumptions but introduces bias due to poor covariate balance and violations of the positivity assumption.

We apply our proposed framework to address these issues, which regularizes extrapolation to mitigate reliance on extreme weights. By varying  $\gamma$  from 0.01 to 10, we examine how treatment effect estimates shift with increasing regularization of negative weights. Without regularization, the estimates converge with those from linear regression. However, as regularization intensifies, the estimates smoothly shift towards zero and occasionally change the sign from negative to positive for smaller values of  $\lambda$ . This sensitivity underscores the influence of assumptions on the point estimates. While increasing  $\gamma$  reduces negative influence (Figure 11), it worsens covariate balance, as reflected

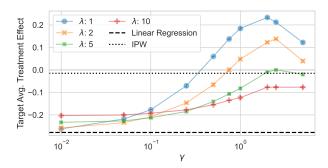


Figure 3: Average Treatment Effects for the Target Sample from TEDS-A of Hispanic Females who have a history of Amphetamize and Benzodiazepine use. Each hue corresponds to a value of  $\lambda$  and the x-axis corresponds to different values of  $\gamma$  (on log scale). The dashed line represents the estimate using linear regression and the dotted represents the estimate using inverse probability weighting (IPW).

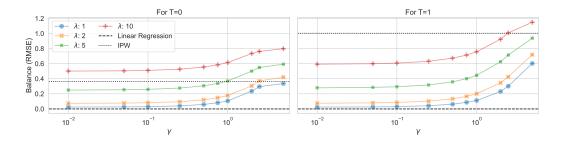


Figure 4: Balance between the trial and the target samples measured as the root mean squared error (RMSE) for different values of  $\gamma$  and  $\lambda$  along with implied linear regression weights and inverse probability weights (IPW).

in higher RMSE values (Figure 10). Thus, our framework highlights a trade-off between minimizing reliance on parametric assumptions and achieving optimal covariate balance.

These findings suggest that applied researchers should interpret treatment effect estimates among under-represented subgroups with caution, given their sensitivity to modeling assumptions. As Parikh et al. [2025] emphasized, collecting more representative trial data is critical to credibly estimate treatment effects for this underrepresented subgroup in future medication for opioid use disorder studies.

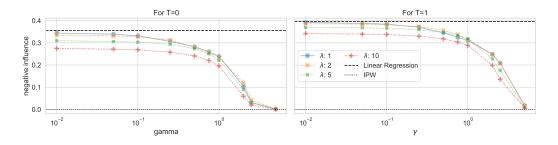


Figure 5: Negative influence, defined as the contribution of negative weights in estimation, for different values of  $\gamma$  and  $\lambda$  along with implied linear regression weights and inverse probability weights (IPW).

## 6 Conclusion

This work proposes a unified framework for regularizing extrapolation in causal inference by replacing hard non-negativity constraints with soft penalties on negative weights. Our approach reveals a fundamental "bias-bias-variance" tradeoff between distributional imbalance, model misspecification, and estimator variance, with theoretical error bounds that decompose extrapolation bias through a novel reflection perspective. Empirical studies on synthetic data and a real-world medication trial demonstrate that controlled extrapolation can outperform both fully constrained and unconstrained approaches, particularly in high-dimensional settings with poor positivity. Our approach focuses primarily on weighting-type estimators, leaving open questions about how our results extend to other estimator classes. Second, our theoretical guarantees rely on Hölder continuity assumptions for expected outcomes, which may not hold in all practical settings. Future research directions include extending the bias-bias-variance tradeoff analysis to a broader class of estimators and exploring weaker or alternative continuity assumptions that might better capture real-world outcome functions. The framework presented here represents an important step toward more nuanced approaches to positivity violations in causal inference, moving beyond binary perspectives on extrapolation toward a continuous spectrum of regularization strategies.

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# **A** Implementational Details

We implement the methods and case studies in this paper using Python 3.10. We implemented our weight estimation framework using PyTorch (version 2.7.0) for efficient automatic differentiation and optimization. The optimization is performed using Adam optimizer with defaults learning rate of 0.01 for default of 5,000 epochs. By default the weights are normalized to sum to one after each optimization step – however, user can choose otherwise. The implementation includes comprehensive visualization tools, including Love plots for covariate balance assessment and 2D scatter plots with convex hull visualization for geometric interpretation. All random operations are seeded for reproducibility, and the code supports both single and multiple outcome variables. For the MOUD case study in Section D, we scale the pre-treatment data to ensure that the maximum value for each covariate is 1 and the minimum is 0; it is important to note that most covariates in this instance are discrete binary.

#### **B** Proofs

### **B.1** Proof of Proposition 3.1

*Proof.* First taking the bound of the estimation error

$$|\mu(x^*) - \hat{\mu}(x^*)| = \left| \mu(x^*) - \sum_{i=1}^n \hat{w}_i Y_i \right|$$

$$= \left| \mu(x^*) - \sum_{i=1}^n \hat{w}_i (\mu(X_i) + \epsilon_i) \right|$$

$$\leq \left| \mu(x^*) - \sum_{i=1}^n \hat{w}_i \mu(X_i) \right| + \left| \sum_{i=1}^n \hat{w}_i \epsilon_i \right|$$

Substituting in the even-odd decomposition gives

$$\left| \mu(x^*) - \sum_{i=1}^n \hat{w}_i \mu(X_i) \right| = \left| \left[ \mu_e(x^*) + \mu_o(x^*) \right] - \sum_{i=1}^n \hat{w}_i \left[ \mu_e(X_i) + \mu_o(X_i) \right] \right|$$

$$\leq \left| \mu_e(x^*) - \sum_{i=1}^n \hat{w}_i \mu_e(X_i) \right| + \left| \mu_o(x^*) - \sum_{i=1}^n \hat{w}_i \mu_o(X_i) \right|$$

Then decomposing based on the sign of the weights gives

$$\sum_{i=1}^{n} \hat{w}_{i} \mu_{o}(X_{i}) = \sum_{i=1}^{n} \hat{w}_{i} [\mathbf{1}(\hat{w}_{i} \ge 0) + \mathbf{1}(\hat{w}_{i} < 0)] \mu_{o}(X_{i})$$

$$= \sum_{i=1}^{n} \hat{w}_{i} \mathbf{1}(\hat{w}_{i} \ge 0) \mu_{o}(X_{i}) + \sum_{i=1}^{n} \hat{w}_{i} \mathbf{1}(\hat{w}_{i} < 0) \mu_{o}(X_{i})$$

By definition  $\mu_o$  is odd, which gives  $\mu_o(-X_i) = -\mu_o(X_i)$ . The additional worst-case bias from negative weights would be:

$$\sum_{i=1}^{n} |\hat{w}_{i}| \mathbf{1}(\hat{w}_{i} < 0) [\mu_{o}(-X_{i}) - \mu_{o}(X_{i})]$$

$$= \sum_{i=1}^{n} |\hat{w}_{i}| \mathbf{1}(\hat{w}_{i} < 0) [-\mu_{o}(X_{i}) - \mu_{o}(X_{i})] = -2 \sum_{i=1}^{n} |\hat{w}_{i}| \mathbf{1}(\hat{w}_{i} < 0) \mu_{o}(X_{i})$$

By applying the definition of the odd function the bias cancels out with the original bias term giving

$$\left| \mu_o(x^*) - \sum_{i=1}^n \hat{w}_i \mu_o(X_i) \right| = \left| \sum_{i=1}^n \hat{w}_i [\mu_o(X_i) - \mu_o(x^*)] \right|$$

For the even component we have

$$\left| \mu_e(x^*) - \sum_{i=1}^n \hat{w}_i \mu_e(X_i) \right| \le \left| \sum_{i=1}^n \hat{w}_i [\mu_e(X_i) - \mu_e(x^*)] \right| + 2 \sum_{i=1}^n |\hat{w}_i| \mathbf{1}(\hat{w}_i < 0) |\mu_e(-X_i) - \mu_e(x^*)|$$

Applying Hölder continuity of  $\mu_e$  and using the worst-case bias terms gives

$$\left| \mu_e(x^*) - \sum_{i=1}^n \hat{w}_i \mu_e(X_i) \right| \le \left| \sum_{i=1}^n \hat{w}_i [\mu_e(X_i) - \mu_e(x^*)] \right| + 2 \sum_{i=1}^n |\hat{w}_i| \mathbf{1}(\hat{w}_i < 0) a \|X_i - x^*\|^{\alpha}$$

Putting the even and odd component portions together gives

$$|\mu(x^*) - \hat{\mu}(x^*)| \le B_{\text{even}}(x^*) + \left| \sum_{i=1}^n \hat{w}_i \epsilon_i \right|$$

Now turning to the noise term, we have by assumption that the sum  $\sum_{i=1}^{n} \hat{w}_i \epsilon_i$  is sub-Gaussian with parameter  $\sigma \|\hat{w}\|_2$ . Using standard sub-Gaussian concentration,

$$P\left(\left|\sum_{i=1}^{n} \hat{w}_{i} \epsilon_{i}\right| > t \mid \hat{w}\right) \leq 2 \exp\left(-\frac{t^{2}}{2\sigma^{2} \|\hat{w}\|_{2}^{2}}\right)$$

Solving for t, setting the right hand side to  $\delta$ 

$$\begin{split} 2 \exp\left(-\frac{t^2}{2\sigma^2 \|\hat{w}\|_2^2}\right) &= \delta \\ \exp\left(-\frac{t^2}{2\sigma^2 \|\hat{w}\|_2^2}\right) &= \frac{\delta}{2} \\ &-\frac{t^2}{2\sigma^2 \|\hat{w}\|_2^2} &= \log\left(\frac{\delta}{2}\right) \\ &t^2 &= -2\sigma^2 \|\hat{w}\|_2^2 \log\left(\frac{\delta}{2}\right) = 2\sigma^2 \|\hat{w}\|_2^2 \log\left(\frac{2}{\delta}\right) \end{split}$$

We then have,  $t = \sigma \|\hat{w}\|_2 \sqrt{2 \log(2/\delta)}$ , and in turn that with probability at least  $1 - \delta$  we have

$$\left| \sum_{i=1}^{n} \hat{w}_{i} \epsilon_{i} \right| \leq \sigma \|\hat{w}\|_{2} \sqrt{2 \log(2/\delta)}$$

We can then obtain our desired statement by taking the expectation over  $\hat{w}$  and combining it with the bias bound.

#### **B.2** Proof of Proposition 3.2

*Proof.* Our approach will be to modify Proposition 3.1 which requires access to the even and odd components, with empirical estimates of the even components. Recall the previous statement was

$$|\mu(x^*) - \hat{\mu}(x^*)| \le B_{even}(x^*) + \sigma ||\hat{w}||_2 \sqrt{2\log(2/\delta)}$$

where

$$B_{even}(x^*) = \left| \sum_{i=1}^n \hat{w}_i [\mu_e(X_i) - \mu_e(x^*)] \right| + 2 \sum_{i=1}^n |\hat{w}_i| \mathbf{1}(\hat{w}_i < 0) a ||X_i - x^*||^{\alpha}.$$

We first rewrite the bias as

$$\left| \sum_{i=1}^{n} \hat{w}_{i} \mu_{e}(X_{i}) - \mu_{e}(x^{*}) \sum_{i=1}^{n} \hat{w}_{i} \right|$$

and replace  $\mu_e(X_i)$  with observable approximations. For  $i \in I_{\text{paired}}$ :,

$$\mu_e(X_i) = \frac{Y_i + Y_{-i}}{2} - \frac{\epsilon_i + \epsilon_{-i}}{2}$$

. For  $i \in I_{nn}$ ,

$$\mu_e(X_i) = \frac{Y_i + Y_{j^*(i)}}{2} - \frac{\epsilon_i + \epsilon_{j^*(i)}}{2} + \frac{\mu(X_{j^*(i)}) - \mu(-X_i)}{2}$$

where  $Y_{j^*(i)}$  is the approximation of  $Y_{-i}$  using NN, and  $\left|\frac{\mu(X_{j^*(i)}) - \mu(-X_i)}{2}\right| \le a \|X_{j^*(i)} - (-X_i)\|^{\alpha}$  by Hölder continuity. Substituting those terms in gives

$$\begin{split} & \left| \sum_{i=1}^{n} \hat{w}_{i} \mu_{e}(X_{i}) - \mu_{e}(x^{*}) \sum_{i=1}^{n} \hat{w}_{i} \right| \leq \left| \sum_{i \in I_{\text{paired}}} \hat{w}_{i} \frac{Y_{i} + Y_{-i}}{2} + \sum_{i \in I_{\text{nn}}} \hat{w}_{i} \frac{Y_{i} + Y_{j^{*}(i)}}{2} - \mu_{e}(x^{*}) \sum_{i=1}^{n} \hat{w}_{i} \right| \\ & + \left| \sum_{i \in I_{\text{paired}}} \hat{w}_{i} \frac{\epsilon_{i} + \epsilon_{-i}}{2} \right| + \left| \sum_{i \in I_{\text{nn}}} \hat{w}_{i} \frac{\epsilon_{i} + \epsilon_{j^{*}(i)}}{2} \right| + \sum_{i \in I_{\text{nn}}} |\hat{w}_{i}| a \|X_{j^{*}(i)} - (-X_{i})\|^{\alpha}. \end{split}$$

To address the fact that  $\mu_e(x^*)$  is unobservable, we bound it using the closest observation  $j^* = \arg\min_j \|X_j - x^*\|$ . By Hölder continuity:

$$|\mu_e(x^*)| \le |\mu_e(X_{j^*})| + a||X_{j^*} - x^*||^{\alpha}.$$

For  $j^* \in I_{\text{paired}}$ ,

$$|\mu_e(X_{j^*})| \le \left| \frac{Y_{j^*} + Y_{-j^*}}{2} \right| + \left| \frac{\epsilon_{j^*} + \epsilon_{-j^*}}{2} \right|.$$

A similar analysis holds for  $j^* \in I_{nn}$ .

Finally for the noise terms, we apply concentration with  $\delta/4$  allocation:

$$\begin{split} \left| \sum_{i=1}^n \hat{w}_i \epsilon_i \right| &\leq \sigma \|\hat{w}\|_2 \sqrt{2 \log(6/\delta)}, \\ \left| \sum_{i \in I_{\text{paired/nn}}} \hat{w}_i \frac{\epsilon_i + \epsilon_j}{2} \right| &\leq \frac{\sigma}{\sqrt{2}} \left\| \hat{w}_{I_{\text{paired/nn}}} \right\|_2 \sqrt{2 \log(6/\delta)} \end{split}$$

since  $\frac{\epsilon_i + \epsilon_j}{2}$  is sub-Gaussian with parameter  $\frac{\sigma}{\sqrt{2}}$ ,

$$\left| \frac{\epsilon_{j^*} + \epsilon_{-j^*}}{2} \right| \le \sigma \sqrt{2 \log(6/\delta)}.$$

By union bound, all hold with probability  $1-\delta$ . The final result follows by combining each constituent term.  $\Box$ 

# C Synthetic Data Study

In this section, we study the performance of our estimator using two synthetic studies, one using a linear data generative process (DGP) and the second one using a non-linear data generative process (DGP). In this simulation study, we specifically consider a case when the target point  $x^*$  is outside the convex hull of the training points  $\{X_1,\ldots,X_n\}$ . For linear DGP, the outcome Y is a linear function of X while for nonlinear DGP, the outcome is a quadratic function of X. In particular, the DGPs are as follows:

Linear DGP:
$$\mu(\boldsymbol{X}) = \beta^T \boldsymbol{X}$$
  
Nonlinear DGP: $\mu(\boldsymbol{X}) = 2X_0^2 + X_1 + X_0 X_1 + \epsilon$ 

Here, we consider a sample of 10 training units and a target unit as shown in Figure 6. This scenario is particularly interesting because of the limited sample size compared to the problem's dimensionality.

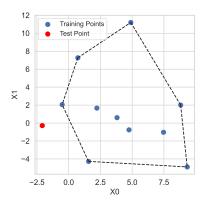


Figure 6: Convex Hull of source and target units in the simulation Study

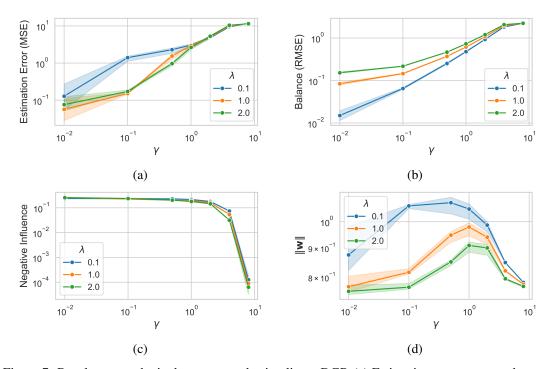


Figure 7: Results on synthetic data generated using linear DGP. (a) Estimation error measured as mean squared error, (b) balance between the weighted source and target populations, (c) extent of extrapolation measured as negative influence – contribution on units with negative weights, (d) L2 norm w capturing asymptotic variance.

For the linear data-generating process, our parametric assumption holds. We observe that increasing the regularization on extrapolation  $(\gamma)$  decreases the negative influence while increasing the balance RMSE, as shown in Figures 7(b) and (c) – consistent with theoretical expectations. As underlying DGP is linear, relying on parametric assumptions for extrapolation yields optimal estimates with the smallest estimation error corresponding to least level of regularization on extrapolation (see Figure 7(a)).

Unlike linear DGP, the outcome function in the nonlinear DGP is not an odd function and thus the parametric assumption is violated. The outcome function has a quadratic term, an interaction term, and a linear term. Intuitively, we expect that a small amount of extrapolation might be beneficial due to the linear component however large amount of extrapolation may result in a high error rate due to violation of parametric assumption. The estimation error rate shown in Figure 8(a) is in congruency

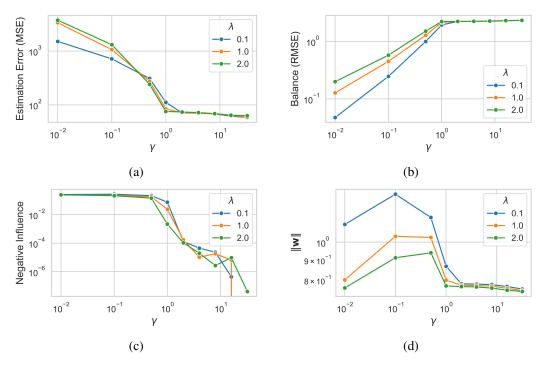


Figure 8: Results on synthetic data generated using non-linear DGP. (a) Estimation error measured as mean squared error, (b) balance between the weighted source and target populations, (c) extent of extrapolation measured as negative influence – contribution on units with negative weights, (d) L2 norm w capturing asymptotic variance.

with the above-discussed expectation – thus highlighting tradeoff between two different kinds of biases .

# D Generalizing Medication for Opioid Use Disorder Trial Evidence

**Data Description.** The Starting Treatment With Agonist Replacement Therapies (START) trial, initiated in 2006, was a multi-center study comparing buprenorphine versus methadone in treating opioid use disorder [Saxon et al., 2013, Hser et al., 2014]. The trial enrolled 1,271 participants, who were randomized in a 2:1 ratio to receive either buprenorphine or methadone. Methadone was found to have higher rates of patient retention in treatment compared to buprenorphine (though buprenorphine in this trial was given in an unusual way to mimic methadone medication administration—requiring near daily clinic visits of participants) [Hser et al., 2014]. Our analysis focuses on the outcome of relapse to regular opioid use within 24 weeks of medication assignment, defined as non-study opioid use for four consecutive weeks or daily use for seven consecutive days. Data on opioid use were collected through urine drug screens and self-reports, with relapse assessment beginning 20 days post-randomization to account for residual drug presence during stabilization.

Parikh et al. [2025] identified that Latina women with a pre-treatment history of amphetamine and benzodiazepine use were underrepresented in the START trial relative to the target population, highlighting a practical violation of the positivity assumption. In this study, we estimate the average treatment effects (ATE) for this underrepresented subgroup using our proposed framework alongside standard linear regression and inverse probability weighting (IPW) estimators. We also evaluate the sensitivity of these estimates to parametric assumptions.

The target sample is drawn from the 2015–2017 Treatment Episode Dataset - Admissions (TEDS-A), which includes data on individuals entering publicly funded substance use treatment programs across 48 states (excluding Oregon and Georgia) and the District of Columbia. Our analysis focuses on Latina women with a pre-treatment history of amphetamine and benzodiazepine use.

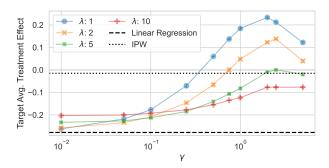


Figure 9: Average Treatment Effects for the Target Sample from TEDS-A of Hispanic Females who have a history of Amphetamize and Benzodiazepine use. Each hue corresponds to a value of  $\lambda$  and the x-axis corresponds to different values of  $\gamma$  (on log scale). The dashed line represents the estimate using linear regression and the dotted represents the estimate using inverse probability weighting (IPW).

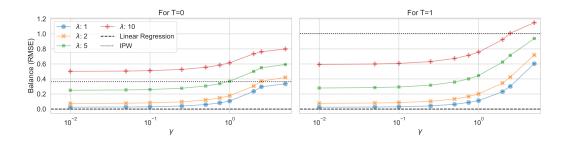


Figure 10: Balance between the trial and the target samples measured as the root mean squared error (RMSE) for different values of  $\gamma$  and  $\lambda$  along with implied linear regression weights and inverse probability weights (IPW).

**Analysis.** We code methadone as T=1 and buprenorphine as T=0, with Y=1 representing relapse. Pretreatment covariates include age, race, biological sex, and substance use history (amphetamine, benzodiazepines, cannabis, and intravenous drug use) measured at the initiation of medication for opioid use disorder (MOUD) treatment.

Using linear regression, the estimated treatment effect for our subgroup of interest is -0.278, indicating that relapse rates are approximately 28 percentage points lower under methadone compared to buprenorphine. In contrast, the IPW estimate is -0.014, suggesting that both treatments are similarly effective. However, as shown in Figure 11, the negative influence of the linear regression-based estimate is 35% and 40% for T=0 and T=1, respectively, compared to 0% for IPW. Despite this, Figure 10 demonstrates that the IPW estimator achieves worse covariate balance than linear regression. These findings reveal that while linear regression relies heavily on parametric assumptions and negative weights, it may be biased if these assumptions are violated. Conversely, the IPW estimator avoids additional parametric assumptions but introduces bias due to poor covariate balance and violations of the positivity assumption.

We apply our proposed framework to address these issues, which regularizes extrapolation to mitigate reliance on extreme weights. By varying  $\gamma$  from 0.01 to 10, we examine how treatment effect estimates shift with increasing regularization of negative weights. Without regularization, the estimates converge with those from linear regression. However, as regularization intensifies, the estimates smoothly shift towards zero and occasionally change the sign from negative to positive for smaller values of  $\lambda$ . This sensitivity underscores the influence of assumptions on the point estimates. While increasing  $\gamma$  reduces negative influence (Figure 11), it worsens covariate balance, as reflected in higher RMSE values (Figure 10). Thus, our framework highlights a trade-off between minimizing reliance on parametric assumptions and achieving optimal covariate balance.

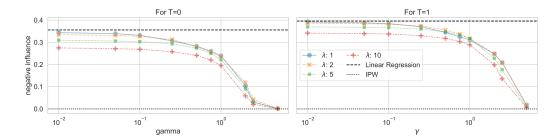


Figure 11: Negative influence, defined as the contribution of negative weights in estimation, for different values of  $\gamma$  and  $\lambda$  along with implied linear regression weights and inverse probability weights (IPW).

These findings suggest that applied researchers should interpret treatment effect estimates among under-represented subgroups with caution, given their sensitivity to modeling assumptions. As Parikh et al. [2025] emphasized, collecting more representative trial data is critical to credibly estimate treatment effects for this underrepresented subgroup in future medication for opioid use disorder studies.