Adaptive Hyper-box Matching for Interpretable Individualized Treatment Effect Estimation

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Abstract

We propose a matching method for observational data that matches units with others in unit-specific, hyper-box-shaped regions of the covariate space. These regions are large enough that many matches are created for each unit and small enough that the treatment effect is roughly constant throughout. The regions are found as either the solution to a mixed integer program, or using a (fast) approximation algorithm. The result is an interpretable and tailored estimate of the causal effect for each unit.

1 INTRODUCTION

Interpretability is paramount in causal inference settings: high-stakes decisions involving medical treatments, public policies, or business strategies, are increasingly made on the basis of causal estimates from pre-existing data. Decision-makers in such settings must often be able to justify their choices for purposes of accountability, and must also be able to take advantage of all existing information in their decisions, rather than complex summaries of it – interpretability plays a critical role to fulfill these needs. *Matching methods* in causal inference, which match treated and control units with the same or similar covariate values, are commonly used for interpretability and mitigating bias. However, they can suffer from problems when human analysts manually choose the distance metric for matching: humans are notoriously poor at manually constructing high dimensional functions.

For matching, units with similar values of the confounding covariates should be matched together, so as to replicate the random assignment of treatment provided by a randomized experiment within each matched group (Rubin 1974; Pearl 2009). Ideally, matching should be *exact*, where a treated unit is matched with one or more identical control units in a matched group. However, when covariates are high-dimensional, it is generally impossible to find units with identical values of all covariates. Because of this, matching methods typically use a notion of closeness between units (e.g., a distance metric), that allows matches to be made approximately rather than exactly. The question then becomes how to construct a good distance metric.

The choice of a distance metric for matching largely drives the interpretability and accuracy of the method. Coarsened exact matching (Iacus et al. 2011; Iacus et al. 2012), for example, can require a user-defined coarsening of a high dimensional covariate space, which can be error-prone. Other matching methods, such as propensity score matching (Rosenbaum and Rubin 1983) or prognostic score matching (Hansen 2008) are more automated in that they only require the user to select a model class, and may yield better estimates of average treatment effects. However, these techniques suffer from lack of interpretability: e.g., when one projects data onto the propensity score, the matched units may be distant from each other in covariate space, only having in common that they are equally likely to receive the treatment. Even in techniques like optimal matching (Rosenbaum 1989), the distance metric between units is an input parameter or a user-defined constraint, which is again problematic as the human analyst manually defines high dimensional distance metrics between units.

Our Contribution We propose a method for matching that provides both interpretability and accuracy without requiring humans to design the distance metric for matching. In particular, the approach *learns an optimal adaptive coarsening* of the covariate space from a model trained on a separate training dataset, leading to accurate estimates of the treatment effect and interpretable matches. The matched group for a unit consists

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of all units within a *learned* unit-specific high dimensional hyper-box. These hyper-boxes are constructed so that they 1. contain enough units for reliable treatment effect estimates, and also so that 2. units within each box have similar potential outcomes, which lowers the bias of the estimated treatment effect. This allows us to avoid black-box summaries (propensity or prognostic scores) and ad-hoc pre-specified metrics given by the users. Our estimates are interpretable. First, they are case-based: each individual's estimate can be explained in terms of the units they are matched with. Second, the choice of cases is itself interpretable: if two units are matched together, it is because they fall in the same easily-described hyper-box.

We formulate the problem of learning optimal partitions for matching as an optimization problem, to which we propose two solutions. Broadly, the optimization problem solves the following minimization:

$$\min_{\text{box}} \left[\begin{array}{l} \text{variability(predictions in box)+} \\ \quad \text{error(estimates of counterfactuals within box)} \end{array} \right]$$

subject to the constraint that the box contains at least m control units when estimating causal effects for a single treatment unit (the choice of m depends on the application).

By training hyper-boxes in a way that leverages a model trained on a training set, we are able to create boxes that adapt to the covariate space. There is a tradeoff in the construction of the hyper-boxes between including a large number of points within the hyper-box and keeping variance low for the predictions within the hyper-box; both goals can help preserve the quality of treatment effect estimation. As a result of these goals, hyper-boxes can be arbitrarily large along covariates that are *irrelevant* for treatment effect estimation, whereas box-widths can be small in regions where the outcome changes rapidly. Figure 1 shows an example of these adaptively-learned hyper-boxes for a two-dimensional dataset. By looking at the shapes of these boxes, one can observe where the outcome changes rapidly (regions with the smaller boxes) and where it changes slowly (regions with larger boxes).

We provide two optimization methods for the boxes. First, we formulate the problem as a *mixed integer program* (MIP) and are thereby able to solve it exactly using state-of-the-art MIP solvers, which are fairly efficient for this problem. Second, we propose a faster and more scalable approximation algorithm.

In Section 2, we present motivation, discuss issues with existing approaches to coarsening, formulate our method as a MIP, and introduce a fast approximation. In Section 3, we compare to other matching methods in a simulation study. In Section 4, we apply our method to a study of the effect of a work training program on future earnings. We conclude with a discussion in Section 5. Our method is called "*Adaptive Hyper-Box*" (*AHB*) matching.

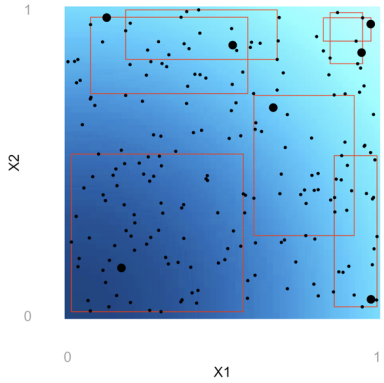

Figure 1: A toy two-dimensional dataset with covariates $X1, X2$, with a few of the matched groups shown as boxes. Each unit has its own matched group, which can overlap with others. The background indicates the true outcome values, with darker regions representing lower outcomes. The boxes are small where outcomes change rapidly, and large in regions of near-constant outcome.

1.1 RELATED WORK

There is a large literature on estimating treatment effects in observational studies (Stuart 2010), and in particular, on matching methods (e.g., Zubizarreta 2012; Pimentel et al. 2018; Keele and Pimentel 2019; Angeles Resa and Zubizarreta 2016; Rosenbaum 2017).

One formulation of our approach relies on solving a mixed integer program (MIP). MIPs have previously been used for causal inference in order to accomodate linear balance constraints on the covariates (Zubizarreta 2012; Zubizarreta et al. 2014; Morucci et al. 2018). Our goals are entirely different from those of other MIP-based causal problems.

There are also machine learning methods for estimating treatment effects with continuous confounders (e.g., double machine learning, Chernozhukov et al. 2017), that are not interpretable. The black box methods with the best current performance have been demonstrated to be variants of Bayesian Additive Regression Trees (BART) (J. L. Hill 2011; Hahn et al. 2020; J. Hill et al. 2020). Our method leverages a black box machine learning model (in our case, a BART model) loosely to help define hyper-boxes, using the help of the training set.

Our work is closely related to several threads in the literature: 1. prognostic scores (Hansen 2008; Stuart et

al. 2013), as we leverage predictions to create matches; 2. methods within the almost-exact-matching (AEM) framework (FLAME, DAME, and MALTS) (Wang, Morucci, et al. 2017; Dieng et al. 2019; Parikh et al. 2018) that leverage a training set for matching, and 3. the causal forest (CF) framework (Wager and Athey 2018), because they use a training set for assisting with "soft" matching on a test set. Matching on the prognostic score attempts to find a low dimensional summary to match on, which our approach avoids. Our method differs from FLAME and DAME (which handle only discrete covariates and use learned Hamming distances), differs from MALTS (which uses learned Mahalanobis distances on continuous covariates), and differs from CF (because it aims to specifically generate interpretable matched groups). Adaptive Hyper-Boxes handles both continuous and discrete variables in the same framework, and needs only to pinpoint hyper-box edges. We do not use nearest neighbors, we do not parameterize a distance metric; we use all points within the learned interpretable hyper-box.

Hyperboxes have been used extensively for regression (e.g., Peters 2011), classification (e.g., Xu and Papageorgiou 2009) and prediction (e.g., Goh and Rudin 2014) but notably, not for causal inference (Khuat et al. 2019). These methods (and others, such as bump hunting, Friedman and Fisher 1999) aim to find adaptive boxes around individual units and some use MIPs to find boxes, as we do. Some other works aim to create global rule-based classifiers for causal inference (Wang and Rudin 2017), whereas our method provides local rules.

2 METHODOLOGY

Throughout, we consider n units and p covariates. The units are indexed by $i = 1, \ldots, n$, and the covariates of unit i are denoted by a p-dimensional random variable $\mathbf{X}_i$, taking values $\mathbf{x}_i = (x_{i1}, x_{i2}, \ldots, x_{ip})' \in \mathbb{R}^p$. A unit's potential outcomes are given by $(Y_i(0), Y_i(1))$, which are also random variables in our setting. We use the following model for the potential outcomes: $Y_i(t) = f_t(\mathbf{X}_i) + \nu_i$, where $\mathbb{E}[\nu_i] = 0$, and, for any two units i and k, ν_i and ν_k are independent. We require f to be nonparametrically estimable from the data. We denote treatment by the random variable $T_i \in \{0, 1\}$; we refer to units with $T_i = 1$ as treated units, and to units with $T_i = 0$ as control units. We denote observed outcomes with the random variable $Y_i = Y_i(1)T_i + Y_i(0)(1 - T_i)$. Our quantity of interest is the Individual Treatment Effect (ITE) for each treated unit, defined as $\tau_i = \mathbb{E}[Y_i(1) - Y_i(0)|\mathbf{X}_i = \mathbf{x}_i]$. By definition of Y_i, we never have access to $Y_i(0)$ for treated units, and control units must be employed to construct an estimate of this missing potential outcome for treated units. To do this we make the following canonical assumptions of observational inference:

(A1) Overlap. For all values of $\mathbf{x}$ and units i, we have $0 < \Pr(T_i = 1|\mathbf{X}_i = \mathbf{x}) < 1$.

(A2) SUTVA. A unit's potential outcomes depend only on the treatment administered to that unit, i.e., if $Y_i(t_1, \ldots, t_n)$ denotes unit i's potential outcome as a function of all n units' treatment status, under SUTVA we have: $Y_i(t_1, \ldots, t_n) = Y_i(t_i)$.

(A3) Conditional ignorability. For all units i and any $t \in \{0, 1\}$, treatment is administered independently of outcomes conditionally on the observed covariates, i.e., $T_i \perp\!\!\!\perp (Y_i(1), Y_i(0))|\mathbf{X}_i = \mathbf{x}_i$. This directly implies that $\mathbb{E}[Y_i|T = t, \mathbf{X}_i = \mathbf{x}_i] = \mathbb{E}[Y_i(t)|\mathbf{X}_i = \mathbf{x}_i]$, which enables us to estimate treatment effects on observed data.

Under these assumptions, if for a treated unit i there existed a control unit k such that $\mathbf{x}_i = \mathbf{x}_k$, then we would have $\mathbb{E}[Y_i(0)|\mathbf{X} = \mathbf{x}_i] = f_0(\mathbf{x}_i) = f_0(\mathbf{x}_k) = \mathbb{E}[Y_k(0)|\mathbf{X} = \mathbf{x}_k]$, and the estimator $Y_i - Y_k$ would be unbiased for τ_i. Unfortunately, this is almost never the case in practice: since $\mathbf{x}$ is high-dimensional, it is unlikely that most units would have a match with the same exact covariate values. To remedy this issue, we match treatment units to control units with similar values of $\mathbf{x}$.

2.1 PRINCIPLES OF APPROXIMATE MATCHING VIA HYPER-BOXES

We focus without loss of generality on creating hyper-boxes for treatment units; any control unit within treatment unit i's box will be considered to be matched to i. Each hyper-box is p-dimensional. Hyper-boxes for control units can be constructed analogously.

Hyper-boxes are specified by lower and upper bounds for all covariates $\mathbf{a}_i = (a_{i1}, a_{i2}, \ldots, a_{ip})'$ and $\mathbf{b}_i = (b_{i1}, b_{i2}, \ldots, b_{ip})'$. For convenience, we define the function $H(\mathbf{a}, \mathbf{b}) = [a_1, b_1] \times \cdots \times [a_p, b_p]$ and also denote unit i's p-dimensional hyper-box as $\mathbf{H}_i = H(\mathbf{a}_i, \mathbf{b}_i)$. Necessarily, $\mathbf{x}_i \in \mathbf{H}_i$; i.e., unit i is contained in its own box. Similarly, we say that a unit k is contained in i's box if $\mathbf{x}_k \in \mathbf{H}_i$ and we define the *main matched group* for treated unit i to be the set of all units contained in i's box: $\texttt{MMG}(\mathbf{H}_i) = \{k \in 1, \ldots, n : \mathbf{x}_k \in \mathbf{H}_i\}$. We also use $n^t_{\mathbf{H}_i} = \sum_{k \in \texttt{MMG}(\mathbf{H}_i)} T_k$ and $n^c_{\mathbf{H}_i} = \sum_{k \in \texttt{MMG}(\mathbf{H}_i)} 1 - T_k$ to denote the number of treated and control units in unit i's box respectively, as well as $n_{\mathbf{H}_i} = n^t_{\mathbf{H}_i} + n^c_{\mathbf{H}_i}$.

We use the following estimators for outcomes of unit i. We emphasize that both quantities are estimated from a single box associated with unit i; the first from control

units and the second from treatment units.

$$\widehat{Y_i(0)} = \frac{1}{n^c_{\mathbf{H}_i}} \sum_{k \in \texttt{MMG}(\mathbf{H}_i)} Y_k(1 - T_k). \quad (1)$$

$$\widehat{Y_i(1)} = \frac{1}{n^t_{\mathbf{H}_i}} \sum_{k \in \texttt{MMG}(\mathbf{H}_i)} Y_k(T_k). \quad (2)$$

There are then two options to estimate τ_i: $\hat{\tau}_a = \widehat{Y_i(1)} - \widehat{Y_i(0)}$, and $\hat{\tau}_b = Y_i(1) - \widehat{Y_i(0)}$. The first option is better when wanting to extend the estimated effects to a super-population of interest, as it can lower the population variance of the estimated response function, while the second option is better in finite-sample inference settings. It is clear by definition of our quantity of interest, τ_i, that our objective should be constructing hyper-boxes for unit i such that $\widehat{Y_i(0)} \approx Y_i(0)$, and $\widehat{Y_i(1)} \approx Y_i(1)$.

We thus follow three principles in creating hyper-boxes: 1. *Bias Minimization:* Matches should yield high quality estimates of the treatment effect. To this end, we create large boxes with low variance in their estimates. 2. *Interpretability:* Matches must be interpretable to permit case-based reasoning. 3. *Honesty:* No test outcomes may be used to construct hyper-boxes. This helps lower bias, and is a general principle of causal inference (Rubin 2005; Wager and Athey 2018). We may use covariates and outcomes of a separate training set, and covariates for the (test) units to be matched.

Issues with existing fixed-width coarsening methods. Common matching methods based on pre-specified fixed-width bins (Iacus et al. 2011; Iacus et al. 2012), will take as input a desired box size for each covariate, $\boldsymbol{\epsilon} = (\epsilon_1, \ldots, \epsilon_p)$, and then construct boxes of size exactly $\|\boldsymbol{\epsilon}\|_1$. This approach suffers from two issues:
Issue 1: $\|\mathbf{x}_i - \mathbf{x}_k\|_1 \geq \|\boldsymbol{\epsilon}\|_1$, but $|f_t(\mathbf{x}_i) - f_t(\mathbf{x}_k)|$ is small. In this case we have two units that are further away on the space of $\mathbf{x}$ than the pre-specified tolerance, but it is entirely possible that these units could have similar values of the outcome function. In this case, the units would not be matched, leading to few (or no) matches for i and therefore a poor (or nonexistent) ITE estimate.
Issue 2: $\|\mathbf{x}_i - \mathbf{x}_k\|_1 \leq \|\boldsymbol{\epsilon}\|_1$, but $|f_t(\mathbf{x}_i) - f_t(\mathbf{x}_k)|$ is large. This could happen in the case in which $\boldsymbol{\epsilon}$ is pre-specified without taking variation in the response function into account. If the slope of the response function is large, then even units that have close values of $\mathbf{x}$ will have significantly different values of $y(0)$. Matching i to k in this case would lead to a bad estimate of i's ITE.

Several rules have been developed to choose fixed-width bins based on the data (e.g., Scott 1979; Freedman and Diaconis 1981; Wand 1997). These rules do not take into account relationships between covariates and outcome, and are thus vulnerable to the two issues above.

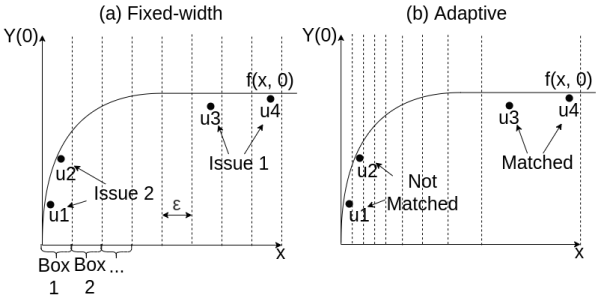

Figure 2: Issues from matching with fixed-width boxes are demonstrated in Panel a. The solid line represents the outcome function, black dots are units to be matched, and vertical dashed lines represent fixed-width boxes. Issue 1 arises when u3 and u4 are not matched together because they are in different boxes, despite having almost constant values of Y within the full range between them. Issue 2 is present because u1 and u2, matched together (as they are in the same box), have different values of Y. These issues are absent when boxes are made adaptively to the outcome function, as demonstrated in Panel b.

2.2 THE ADAPTIVE HYPER-BOX FRAMEWORK

Our proposed framework aims at creating bins for interpretable adaptive matching, avoiding the issues discussed above. Instead of starting from a pre-specified value of box size, ϵ, we learn unit-specific boxes from the data itself, by directly minimizing quantities related to the principles outlined previously. We aim for hyper-boxes that solve the following optimization problem:

$$\min_{\mathbf{H}_1, \ldots, \mathbf{H}_n} \sum_{i=1}^{n} \mathrm{Err}(\mathbf{H}_i) + \mathrm{Var}(\mathbf{H}_i)$$
$$\text{Subject to: } n_{\mathbf{H}_i} \geq m \; \forall \, i,$$

where Err and Var are as in Eqs. (3)-(4). In words, we would like to minimize bias and variability of each box, while making sure that at least m units are contained in each hyper-box. To minimize bias, we would like boxes that contain units whose observed outcomes are strongly predictive of the missing control outcome of interest. This can be achieved by defining error as follows:

$$\mathrm{Err}(\mathbf{H}_i) = \left| f_0(\mathbf{x}_i) - \frac{1}{n_{\mathbf{H}_i}} \sum_{k \in \texttt{MMG}(\mathbf{H}_i)} f_0(\mathbf{x}_k) \right| + \left| f_1(\mathbf{x}_i) - \frac{1}{n_{\mathbf{H}_i}} \sum_{k \in \texttt{MMG}(\mathbf{H}_i)} f_1(\mathbf{x}_k) \right|. \quad (3)$$

For reliable estimates, we encourage boxes to contain (1) a large number of units, and (2) to minimize variability of predicted outcomes on the control units it contains:

$$\begin{aligned}&\mathrm{Var}(\mathbf{H}_i) = \\ &\frac{1}{n_{\mathbf{H}_i}} \sum_{k \in \texttt{MMG}(\mathbf{H}_i)} \left(f_0(\mathbf{x}_k) - \frac{1}{n_{\mathbf{H}_i}} \sum_{k \in \texttt{MMG}(\mathbf{H}_i)} f_0(\mathbf{x}_k) \right)^2 \\ &+ \frac{1}{n_{\mathbf{H}_i}} \sum_{k \in \texttt{MMG}(\mathbf{H}_i)} \left(f_1(\mathbf{x}_k) - \frac{1}{n_{\mathbf{H}_i}} \sum_{k \in \texttt{MMG}(\mathbf{H}_i)} f_1(\mathbf{x}_k) \right)^2 .\end{aligned} \tag{4}$$

Minimizing $\mathrm{Err}(\mathbf{H})$ and $\mathrm{Var}(\mathbf{H})$ directly avoids Issues 1 and 2 outlined above. In the case of Issue 1, both $\mathrm{Err}(\mathbf{H})$ and $\mathrm{Var}(\mathbf{H})$ will be small even if units are far apart in terms of $\mathbf{x}$, telling us that we can make boxes larger in that part of the space. In the case of Issue 2 the opposite will be true; even if units are close in terms of $\mathbf{x}$, $\mathrm{Err}(\mathbf{H})$ and $\mathrm{Var}(\mathbf{H})$ will be large, suggesting that boxes should be smaller in that part of the space.

Our loss will be reliable if we have good estimates $f_t(\mathbf{x})$ at many points within each bin, including all points $\mathbf{x}_1, \ldots, \mathbf{x}_n$ at a minimum. We preserve honesty in such estimates by dividing the data into a training and a test set, denoted by $D^{tr} = \{(\mathbf{x}_i^{tr}, Y_i^{tr}, T_i^{tr})\}_{i=1}^n$ and $D^{ts} = \{(\mathbf{x}_i^{ts}, Y_i^{ts}, T_i^{ts})\}_{i=1}^n$ respectively, and assumed to each be of size n for notational simplicity. Lastly, under these conditions, the hyper-boxes are designed to provide balance on relevant covariates and thus lead to high quality treatment effect estimates (Stuart et al. 2013). The test set will contain the observations to be matched, while the training set will be used to estimate $f_t(\mathbf{x})$ for each $\mathbf{x}$ of interest. We will denote this estimate by $\hat{f}_t(\mathbf{x})$: any machine learning method can be used to estimate f_t, as predicted values of f_t are only going to inform loss calculations and not actual treatment effect estimates.

Adaptive Hyper-box MIP formulation. Here, we use the triangle inequality to upper-bound the error term. We consider treatment point i and points $k \in \texttt{MMG}(\mathbf{H}_i)$ for an arbitrary treatment value, t and hyper-box $\mathbf{H}_i$:

$$\begin{aligned}\mathrm{Err}(\mathbf{H}_i) &= \left| \frac{1}{n_{\mathbf{H}_i}} \sum_{k \in \texttt{MMG}(\mathbf{H}_i)} f_t(\mathbf{x}_i) - f_t(\mathbf{x}_k) \right| \\ &\leq \frac{1}{n_{\mathbf{H}_i}} \sum_{k \in \texttt{MMG}(\mathbf{H}_i)} \left| f_t(\mathbf{x}_i) - f_t(\mathbf{x}_k) \right|. \end{aligned} \tag{5}$$

We minimize the bound instead of the error term, for both treatment and control groups. We use a similar upper bound for variability. For any value of $\mathbf{H}_i$ we have:

$$\begin{aligned}&\mathrm{Var}(\mathbf{H}_i) \\ &= \frac{1}{n_{\mathbf{H}_i}} \sum_{k \in \texttt{MMG}(\mathbf{H}_i)} \left(f_t(\mathbf{x}_k) - \frac{1}{n_{\mathbf{H}_i}} \sum_{l \in \texttt{MMG}(\mathbf{H}_i)} f_t(\mathbf{x}_l) \right)^2 \\ &\leq \frac{1}{n_{\mathbf{H}_i}} \sum_{k \in \texttt{MMG}(\mathbf{H}_i)} C \left| \frac{1}{n_{\mathbf{H}_i}} \sum_{l \in \texttt{MMG}(\mathbf{H}_i)} (f_t(\mathbf{x}_k) - f_t(\mathbf{x}_l)) \right|,\end{aligned}$$

where the last line follows by setting $C = \max_{\mathbf{H}_i} \left| \frac{1}{n_{\mathbf{H}_i}} \sum_{l \in \texttt{MMG}(\mathbf{H}_i)} (f_t(\mathbf{x}_k) - f_t(\mathbf{x}_l)) \right|$ and using Hölder's Inequality. Here C is a constant, and is not affected by any optimization we will perform to obtain $\mathbf{H}_i$. We can now apply the triangle inequality twice:

$$\begin{aligned}&\mathrm{Var}(\mathbf{H}_i) \\ &\leq \frac{1}{n_{\mathbf{H}_i}} \sum_{k \in \texttt{MMG}(\mathbf{H}_i)} \frac{C}{n_{\mathbf{H}_i}} \sum_{l \in \texttt{MMG}(\mathbf{H}_i)} |f_t(\mathbf{x}_k) - f_t(\mathbf{x}_i)| \\ &\qquad + |f_t(\mathbf{x}_l) - f_t(\mathbf{x}_i)| \\ &= \frac{2C}{n_{\mathbf{H}_i}} \sum_{k \in \texttt{MMG}(\mathbf{H}_i)} |f_t(\mathbf{x}_k) - f_t(\mathbf{x}_i)|. \end{aligned} \tag{6}$$

Inequalities (5) and (6) show that minimizing $\sum_{k \in \texttt{MMG}(\mathbf{H}_i)} |f_t(\mathbf{x}_i) - f_t(\mathbf{x}_k)|$ will lower both $\mathrm{Err}(\mathbf{H}_i)$ and $\mathrm{Var}(\mathbf{H}_i)$ through the upper bounds just introduced, for fixed $n_{\mathbf{H}_i}$. Minimizing this term also ensures that treatment and control outcomes stay relatively constant within each hyper-box.

In order to ensure that the denominator of the variance (i.e., $n_{\mathbf{H}_i}$) stays large, we subtract it from the loss function. Hence, the loss now encourages larger matched groups, while maintaining linearity of the objective:

$$\min_{\mathbf{H}_i} \sum_{k \in \texttt{MMG}(\mathbf{H}_i)} |f_t(\mathbf{x}_k) - f_t(\mathbf{x}_i)| + \beta n_{\mathbf{H}_i},$$

where β trades off between the terms.

These steps give rise to the following global MIP for our entire sample. Here, decision variable $\mathbf{H}_i$ defines the box for treatment unit i, and decision variable w_{ik} is an indicator for whether k is in i's box:

$$\begin{aligned}\min_{\mathbf{H}_1, \ldots, \mathbf{H}_n} \sum_{i=1}^n \Bigg\{ &\gamma_1 \sum_{k=1}^n w_{ik} \left| \hat{f}_1(\mathbf{x}_i^{ts}) - \hat{f}_1(\mathbf{x}_k^{ts}) \right| \\ &+ \gamma_0 \sum_{k=1}^n w_{ik} \left| \hat{f}_0(\mathbf{x}_i^{ts}) - \hat{f}_0(\mathbf{x}_k^{ts}) \right| - \beta \sum_{k=1}^n w_{ik} \Bigg\}\end{aligned} \tag{7}$$

$$\text{subject to: } \mathbf{H}_i \in \mathbb{R}^{p\times p}, w_{ik} \in \{0,1\} \qquad \forall\, k$$

$$x_i^{ts} \in \mathbf{H}_i \qquad \forall\, i \qquad (8)$$

$$w_{ik} = \mathbb{I}_{[x_k^{ts} \in \mathbf{H}_i]} \qquad \forall\, i \qquad (9)$$

$$\sum_{k=1}^{n} w_{ik}(1 - T_k) \geq m \qquad \forall\, i. \qquad (10)$$

Constraint (8) forces unit i to be within its own box; (9) defines an indicator w_{ik} for whether unit k falls into the box for test unit i; (10) forces boxes to include at least m control units. We require a minimum number of control, but not treatment, units to be matched, because treatment unit i is within $\texttt{MMG}(\mathbf{H}_i)$, and thus there is always at least one treated unit in each box. This makes computing the first term in the loss always possible, and excludes trivial solutions with empty boxes. The loss in Eq. (7) is made up of three terms: the first is the upper bound on the estimation error and variability terms of our framework derived in inequalities (5) and (6) for treated outcomes. The second is the same bound, but for control outcomes. We want these terms to be small to ensure the outcome function does not vary much within a box. The third term counts units in the box, encouraging more matches. The supplement details an explicitly linear formulation of the above problem. The hyperparameters γ_1, γ_0, and β weight the three components of the loss. They can be cross-validated, set to 1, or chosen intuitively by normalizing them to the same scale as discussed in the supplement.

The form of the MIP presented above directly suggests that the optimization problem is separable in the $1 \ldots, n$ units. We take advantage of this property and solve one MIP for each of the n units to be matched separately.

Adaptive Hyper-box Fast Approximation We now describe a fast algorithm to approximate the MIP solution. For a unit i, we initialize its box to be a single point at its covariate values. We then expand the box according to the principles previously outlined: 1. we expand the box along a single covariate at a time, so that the resulting box is always axis-aligned and interpretable; 2. we expand along the covariate that extends the box into the region with least outcome variation – ensuring high quality matches – and stop expanding the box once this variation increases too much, avoiding low quality matches; and 3. we estimate the variation in the outcome via $\hat{f}_0, \hat{f}_1$ learned on a separate, training set, as for the MIP.

Algorithm 1 in the supplement provides pseudocode. The main crux of the algorithm is to determine whether a new, proposed box $\mathbf{P}$ is good. To do so, we examine the outcome function in $\mathbf{P}\backslash\mathbf{H}_i$ (the region we propose to add to our existing hyper-box). If the outcome in the new region is relatively constant, we do not expect to incur much bias from including units that lie inside. Therefore, we look at how much $\hat{f}_0, \hat{f}_1$ vary on a grid in $\mathbf{P}\backslash\mathbf{H}_i$ and choose to expand along the covariate yielding the lowest variation. Further details are in the supplement.

Scalability and Parallelization Both MIP AHB and Fast AHB create a box tailored to a specific unit i, independently from boxes of other units. Both methods are, therefore, embarassingly parallelizable. The supplement shows runtime results for the methods: Fast AHB scales well, especially in n, and can be applied to large datasets on most machines, while MIP AHB is less suited for large datasets due to its exponential nature. Discussion of the methods' computational complexity, and suggestions for speeding them up, is included in the supplement.

Matching with Non-Continuous Covariates Our method also handles non-continuous covariates, including categorical and cardinal covariates. Categorical covariates that take on k discrete values can be binarized into $k-1$ indicator variables, after which MIP and Fast can be run without modification to form matches. MIP and Fast can also be run out of the box on cardinal variables without loss in performance. We demonstrate this by matching on year-valued variables in our application.

Empirically, when we run MIP AHB and Fast AHB on categorical data, they learn identical importance weights for the covariates (see Section 3.2). That is, they either construct boxes that exactly match units with identical covariate values or prioritize matches on covariates contributing more to the outcome. This is similar to the characteristics of the FLAME and DAME algorithms described by Wang, Morucci, et al. 2017 and Dieng et al. 2019, though AHB has the added benefit of adaptively handling continuous covariates. It would not be possible to extend FLAME and DAME to this case because they rely on Hamming distance. Since AHB chooses only box edges, it avoids having to use a parameterized distance metric, allowing it to handle continuous covariates in the *same way* that it handles discrete covariates.

3 EXPERIMENTS

We generate data independently for all units, with data for unit i generated according to the following process:
1. Generate covariates: $x_{ij} \overset{ind}{\sim} F_x, j = 1, \ldots, p$
2. Generate a propensity score: $e_i = \text{expit}(\boldsymbol{\gamma}\mathbf{x}_i)$
3. Assign treatment: $Z_i \sim \text{Bernoulli}(e_i)$
4. Generate the outcome: $y_i = g(\mathbf{x}_i) + h(\mathbf{x}_i)Z_i + \epsilon_i$.

Here, $\boldsymbol{\gamma}$ is fixed. We consider various choices of confounding functions g and heterogeneous treatment func-

tions h, seen in Table 1, subject to which we evaluate estimation of the ITE of treated units. All results are averages across 10 simulations, each with $n = 600$ units. The supplement contains additional simulations studying higher dimensional settings, correlated covariates, and coverage of ITE confidence intervals.

We compare the following estimators: **BART** - Bayesian Additive Regression Trees (Chipman et al. 2010; J. L. Hill 2011) estimates ITE_i as $\hat{f}_1(\mathbf{x}_i) - \hat{f}_0(\mathbf{x}_i)$, **Best CF** - $1:k$ matching of a treated unit i to the k control units with outcomes closest to i's true counterfactual (this is cheating: one does not have this extra information in practice), **GenMatch** - Genetic Matching of a treated unit to at most k control units (Diamond and Sekhon 2013), **CEM** - Coarsened exact matching (Iacus et al. 2011; Iacus et al. 2012), **Propensity Matching** - $1:k$ propensity score matching, **Prognostic Matching** - $1:k$ prognostic score matching, **Full Matching** - Full matching (Hansen and Klopfer 2006), **Mahal** - $1:k$ matching on the Mahalanobis distance between covariates, **Fast** - Our proposed approximate algorithm for AHB, **MIP** - Our proposed MIP for AHB.

For all $1:k$ matching estimators, we consider $k \in \{1, 3, 5, 7, 10\}$ and report the best results attained. All nearest neighbor matching is performed with replacement. BART, Prognostic Matching, Fast, and MIP first split the data and fit BART on the training set to estimate an outcome model. For AHB, boxes are then constructed from the outcome model to be used on the test units. In addition to using BART to power Prognostic, MIP, and Fast, we include the BART estimator to directly predict counterfactuals for units in the test set. In this way, we compare our approach to the limits of predictive performance attainable using a highly flexible – and highly uninterpretable – method. Similarly, we include the Best CF estimator to compare to performance attainable when using counterfactual data that is unobserved in practice. We defer details of implementations to the supplement.

3.1 CONTINUOUS COVARIATES

First, we assess our method's performance in settings where different functions of continuous covariates confound the outcome and modulate the treatment effect. We simulate $x_{ij} \overset{ind}{\sim} U(0,1)$ and choose g (confounding function) and h (heterogeneity function) as specified in the first six rows of Table 2. Below, we label simulation settings as "Confounding function / Treatment function". MIP or Fast perform better than all other methods in all but the None / Const and Linear / Const setups, where BART outperforms us. This is reasonable given its highly flexible (yet uninterpretable) nature.

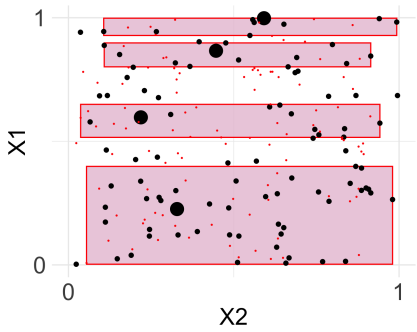

Figure 3: The boxes formed by Adaptive Hyper-Boxes for four example points (enlarged). The box widths span most of the horizontal axis, associated with an irrelevant covariate. The height of the boxes decreases moving upwards, as confounding increases. Black and red points denote treatment and control units, respectively.

MIP and Fast perform well even when there is a heterogeneous treatment effect in addition to confounding (row 6 of Table 2). Actually, MIP and Fast tend to outperform competing ones by greater margins when heterogeneous treatment is introduced on top of confounding, as can be seen by comparing the Box / Const and Box / Box setups.

When there are irrelevant covariates (e.g. row 5 of Table 2), CEM fails to make even a single match due to the high dimensionality of the space. On the other hand, AHB adapts to the irrelevant covariates; we can visualize this by examining in Figure 3 some of the boxes it learns for setup Quad / Const. The vertical axis represents the one covariate relevant to the outcome and the horizontal axis an arbitrary irrelevant covariate. We see that AHB learns which covariate is important: it makes the boxes skinny along one dimension – as they should be sensitive to the changes in outcome along that axis – and expand fully throughout the range of the other irrelevant dimension. The height of the boxes also decreases along the vertical axis, because the effect of confounding on unit i is given by x_{i1}^2. Variation in x_{i1} therefore has greater impact on the outcome near 1 than near 0 and the boxes reflect this.

3.2 DISCRETE AND MIXED COVARIATES

Here, we evaluate the performance of our method on discrete and mixed (discrete and continuous) data. Abusing notation slightly, we will use x to refer to continuous covariates, of which there will be p_c, and we use w to refer to discrete covariates, of which there will be p_d. We consider binary covariates, because we can binarize any k-level discrete covariate into $k-1$ indicator variables, allowing us to match on any subset of the k levels. Binary covariates are simulated $w_{ij} \overset{ind}{\sim}$ Bernoulli(0.5).

Choices of g and h and associated results are specified in the last three rows of Table 2. We see that CEM and AHB both perform exceedingly well when all covariates are binary. Further analysis reveals: 1. that MIP and Fast yield identical boxes and ITEs in this scenario, 2. that the ITEs are the same as those generated via exact matching *on the one, true covariate*, and 3. that CEM's ITEs are the same as those generated via exact matching *on all covariates*. Thus, while both methods yield unbiased ITE estimates in this setting, CEM's are of higher variance because it constructs more granular boxes than necessary due to its inability to adapt to irrelevant covariates. Indeed, supplemental results show that as the number of irrelevant covariates increases, CEM's performance deteriorates drastically, while AHB's stay the same. In the simulation with mixed covariates, MIP AHB outperforms all competitors but BART, and Fast AHB falls only behind BART, Best CF, and Prognostic.

Similarity Between MIP AHB and Fast AHB To compare MIP AHB and Fast AHB, we compare the overlap in units assigned to matched groups by MIP AHB and Fast AHB, denoted by $\texttt{MMG}(\mathbf{H}_i)^{\text{MIP}}$ and $\texttt{MMG}(\mathbf{H}_i)^{\text{Fast}}$. We define a 'mutual membership rate' as the maximum of the proportion of units in $\texttt{MMG}(\mathbf{H}_i)^{\text{MIP}}$ that are in $\texttt{MMG}(\mathbf{H}_i)^{\text{Fast}}$ and vice versa. Across all units, we find median mutual membership rates around 80% in our experiments. Visual comparisons of the boxes output by both methods also confirm they adapt similarly to variability in the outcome function, extending boxes where the outcome is near-constant and shrinking them where it changes rapidly. For experiments conducted entirely with discrete data, MIP AHB and Fast AHB constructed identical boxes. Lastly, ITE comparisons between the methods show little to no difference in most simulations.

4 APPLICATION

We apply our methodology to replicating a study of the effect of work training programs on future earnings originally conducted by (LaLonde 1986; R. H. Dehejia and Wahba 1999; R. Dehejia and Wahba 2002). This dataset includes an experimental sample (from the 1975-76 National Supported Work (NSW) program where treatment units received a work training program), and two observational samples (constructed by combining samples from the Panel Study of Income Dynamics (PSID) and from the Current Population Survey (CPS)). Further details about the datasets are in the Supplement. Matching methods can be evaluated on how well they can reconstruct the unbiased ATT estimate from the experimental sample, by matching treated units from the experiment to control units from the observational samples. Matching covariates include income before the training program, race, years of schooling, marital status, and age. We focus on the task of estimating the in-sample ATT, and therefore match each treated unit i to at least one control unit from each dataset, and no other treated unit. The resulting ITE estimates are then averaged to compute an ATT estimate. We employ MIP AHB, as the data is small enough to do so. Since we do not match any other treated units to each unit i, we set $\gamma_1 = 0$, and focus on finding control matches.

We compare Adaptive Hyper-Boxes to other matching methods estimating the ATT from the observational samples, shown in Table 3. *The ATT estimates that AHB produces using both observational datasets are comparable to the estimate from the experimental sample.* Most other methods fail to produce estimates of the same quality as AHB on either dataset. Figure 4 displays sample boxes constructed by MIP AHB on one of the matching covariates, together with a smoothed version of the estimated ITE and predicted outcome. Our method behaves as expected, making many small and close boxes where the predicted outcome function grows rapidly, and wider boxes where it does not.

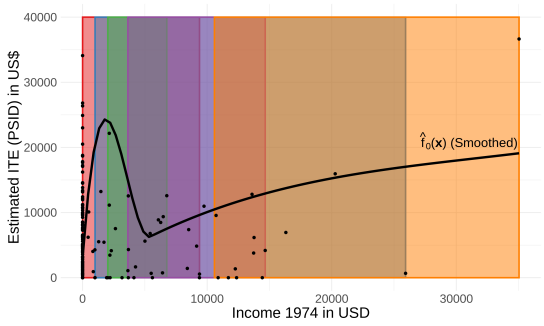

Figure 4: Relationship between pre-treatment income and estimated ITE. The solid black line is a smoothed estimate of the control response as a function of pre-treatment income. The colored boxes are five sample boxes created by Adaptive Hyper-Boxes.

Table 8 in the supplement also presents treatment effect estimates at different values of pre-treatment years of schooling. We see that years of schooling does indeed moderate the treatment effect, as individuals with fewer years of schooling are estimated to either benefit less than individuals with more years of schooling, or even lose income, after the work training program. Lastly, Table 9 shows sample matched groups produced by AHB.

5 DISCUSSION

Adaptive Hyper-Boxes Matching is a useful alternative to other matching methods. It learns

Table 1: Functions (up to a constant) used for treatment and confounding in experiments. Continuous covariates are denoted by x and discrete covariates by w. There are p_c continuous covariates and p_d discrete covariates.

	None	Const	Box	Linear	Quad	Binary	Mixed
$g(\mathbf{x}_i)$ or $h(\mathbf{x}_i)$	0	1	$\sum_j \mathbb{I}\{0.5 < x_{ij}\}$	$\sum_j x_{ij}$	$\sum_j x_{ij}^2$	w_{ij}	$\sum_j (x_{ij} + w_{ij})$
(p_c, p_d)	(0, 0)	(0, 0)	(2, 0)	(2, 0)	(2, 0)	(0, 1)	(1, 1)

Table 2: Mean absolute error as proportion of ATT for estimating ITE of treated units under different confounding regimes. The first column denotes the number of (confounding, treatment, irrelevant) covariates. The second column denotes the confounding and treatment functions, g and h respectively. Either MIP or Fast performs best in almost all simulation types. NA denotes inability to make any matches; bold denotes lowest error attained in that setting.

		AHB		Black Box	Benchmark	Matching					
p	Method / g / h	MIP	Fast	BART	Best CF	CEM	Full Matching	GenMatch	Mahal	Nearest Neighbor	Prognostic
(0, 0, 2)	None / Const	0.09	0.05	**0.04**	0.25	1.01	0.32	0.36	0.34	0.37	0.25
(2, 0, 0)	Box / Const	**0.11**	0.16	0.24	0.24	0.24	3.03	0.66	0.62	3.05	0.29
(2, 0, 0)	Linear / Const	0.17	0.22	**0.14**	0.26	0.23	0.82	0.38	0.36	0.91	0.28
(2, 0, 0)	Quad / Const	0.10	**0.04**	0.08	0.25	0.22	0.42	0.38	0.37	0.45	0.27
(2, 0, 4)	Quad / Const	**0.02**	**0.02**	**0.02**	0.16	NA	0.21	0.12	0.11	0.24	0.04
(1, 1, 0)	Box / Box	**0.30**	0.45	0.65	0.73	0.58	2.59	2.37	1.02	2.30	0.94
(1, 0, 1)	Binary / Const	**0.02**	**0.02**	**0.02**	0.09	**0.02**	0.12	0.49	0.10	0.10	0.09
(1, 1, 6)	Binary / Binary	**0.06**	**0.06**	0.09	0.17	0.20	0.71	0.97	0.27	0.61	0.18
(2, 0, 0)	Mixed / Const	0.07	0.12	**0.06**	0.09	0.12	0.48	0.15	0.15	0.55	0.10

Table 3: US $ estimates of the effect of a training program on future earnings from two observational control samples. Methods estimate the ATT by matching treated experimental units to observational control units. The unbiased experimental ATT estimate is $1794. Estimates closer to this value are better. Error in parentheses.

Method \ Dataset	CPS	PSID
Adaptive Hyper-box	**1720 (-75)**	**1762 (-32)**
Naive	-7729 (-9523)	-14797 (-16591)
Full Matching	708 (-1087)	816 (-978)
Prognostic	1319 (-475)	2224 (429)
CEM	3744 (1950)	-2293 (-4087)
Mahalanobis	1181 (-614)	-804 (-2598)
Nearest Neighbor	1576 (-219)	2144 (350)

matched groups adaptively, works for mixed categorical and continuous datasets, and produces low-variance matched groups that can be described with interpretable rules. Code implementing AHB is available at `github.com/almost-matching-exactly/Adaptive-Binning`. Hyper-boxes have a long history of successful usage in regression and classification problems. They can produce interpretable predictions which we have now leveraged to produce interpretable matches in the context of causal inference.

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