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# Neural Score Matching for High-Dimensional Causal Inference

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## Abstract

Traditional methods for matching in causal inference are impractical for high-dimensional datasets. They suffer from the curse of dimensionality: exact matching and coarsened exact matching find exponentially fewer matches as the input dimension grows, and propensity score matching may match highly unrelated units together. To overcome this problem, we develop theoretical results which motivate the use of neural networks to obtain non-trivial, multivariate balancing scores of a chosen level of coarseness, in contrast to the classical, scalar propensity score. We leverage these balancing scores to perform matching for high-dimensional causal inference and call this procedure *neural score matching*. We show that our method is competitive against other matching approaches on semi-synthetic high-dimensional datasets, both in terms of treatment effect estimation and reducing imbalance.

## 1 INTRODUCTION

Estimating the causal effect of a treatment or a policy is the fundamental task of causal inference. For binary treatments, the quantity of interest is the difference between the outcome of a subject receiving a treatment (a *treated* subject) and the outcome of that subject in the absence of treatment (a *control* subject). The main difficulty in estimating a causal effect from observational data is that one cannot observe the outcome of both the true and the alternative scenario for the same subject – also called the factual and counterfactual outcomes. For instance, to evaluate the effect of

a lockdown on reducing infection case numbers in a given country, one cannot create an exact copy of that country to study the consequences of its absence.

One possible solution would be to find a country that is very similar to the country under study, yet which did not experience a lockdown. This is the general idea behind *matching* whereby each treated subject in the sample data is assigned to one or more subjects from the control group (Stuart, 2010). Matching is among the dominant techniques used in medicine and other domains to estimate the effect of a treatment from observational data (Su et al., 2019; Farzadfar et al., 2012; Razonable et al., 2021; Webb et al., 2020). Besides estimating the treatment effect, matching can serve additional objectives. For example, matching can reduce imbalance, i.e. distributional differences between the treated and control groups that indicate confounding and consequently make treatment effect estimation more difficult. Matching can also help to decrease costs by reducing the number of control samples required when the collection of data (e.g. subjects’ outcome) is expensive (Stuart, 2010). Matching methods, however, generally suffer from the *curse of dimensionality* (Abadie and Imbens, 2006a; Roberts et al., 2020), rendering them impractical for many modern high-dimensional datasets, such as electronic health records or clinical images.

In this work, we address the curse of dimensionality by first compressing the input covariates into a lower-dimensional matching space with a neural network and then matching in this space. Our contributions are as follows: (a) We develop novel theoretical results that bound the imbalance in the original covariate space via imbalance in a lower-dimensional balancing score space. We also extend these results to functions of covariates that violate the balancing score condition and which we refer to as “non-balancing scores”. (b) These theoretical results motivate *neural score matching*, a procedure to match on low-dimensional balancing scores obtained from the intermediate layers of a neural network modelling the propensity score. This yields a simple method for estimating average or group-based

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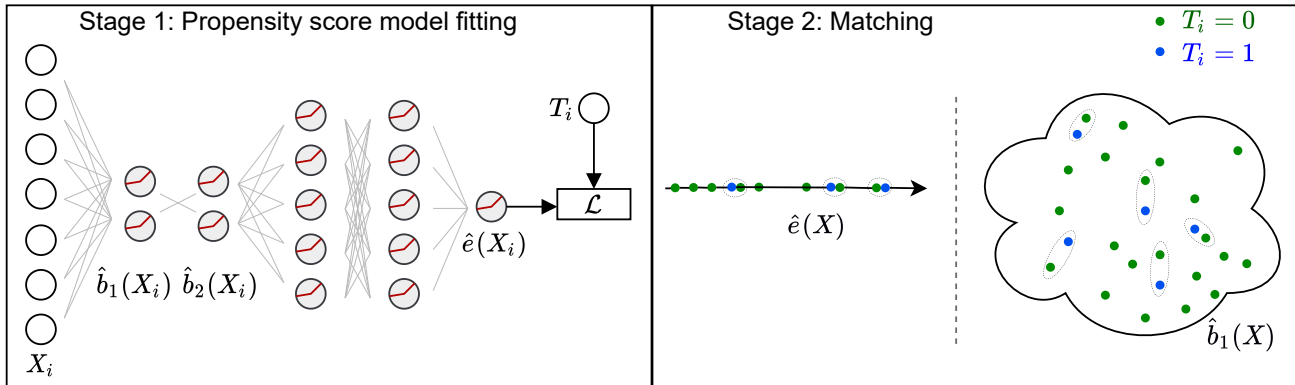


Figure 1: An illustration of neural score matching. In the first stage, a propensity score model is fitted to obtain low-dimensional balancing scores. In the second stage, samples are matched (to one neighbour) in the balancing score space based on a given distance metric. Matched samples are subsequently used to estimate the ATT.

treatment effects in the presence of high-dimensional covariates without regressing on outcomes. The intuition of neural score matching is illustrated in Fig. 1. (c) We show that neural score matching is competitive against other matching methods on two causal inference benchmarks in terms of calibration error, treatment effect estimation and balance.

## 2 MATCHING IN CAUSAL INFERENCE

### 2.1 Problem Setup

Let  $(X_i, T_i, Y_i) \sim P$  be a dataset where  $X_i$  denotes (pre-treatment) covariates,  $T_i$  is the binary variable indicating whether the treatment under scrutiny has been applied to the subject or not, and  $Y_i$  is the observed outcome after the treatment or absence of treatment, all corresponding to subject  $i$ . In the potential outcomes framework (Rubin, 2005),  $Y_i(1)$  is the outcome which would have happened (is “potential”) if  $T_i = 1$ , and  $Y_i(0)$  is the analogous outcome for when  $T_i = 0$ . Then,  $Y_i = T_i Y_i(1) + (1 - T_i) Y_i(0)$ . We denote  $N_t$  as the number of treated units in the dataset, and  $N_c$  the number of control units. Our task is to estimate the *average treatment effect on the treated (ATT)*, defined as

$$\text{ATT} = \mathbb{E}[Y(1) - Y(0) \mid T = 1].$$

This quantity measures the treatment effect for patients under treatment, and is typically the primary interest of medical applications (Ho et al., 2007). Here, covariates, such as age or BMI that are related to a treatment are of particular interest (Greifer and Stuart, 2021). The ATT can be approximated by the *sample average*

*treatment effect on the treated (SATT)*, defined as

$$\text{SATT} = \frac{1}{N_t} \sum_{i:T_i=1} Y_i(1) - Y_i(0).$$

We make the following standard assumptions :

- Consistency:  $\forall t, T_i = t \implies Y_i(t) = Y_i$ .
- Ignorability:  $Y_i(1), Y_i(0) \perp\!\!\!\perp T_i \mid X_i$ .
- Overlap:  $\forall \mathbf{x}, 0 < P(T_i = 1 \mid X_i = \mathbf{x}) < 1$ .

Consistency ensures that  $Y_i(1)$  is the observed outcome  $Y_i$  when  $T_i = 1$ . However,  $Y_i(0)$  is not observed and must be estimated, for instance through matching. In addition, the ATT can also be expressed using *conditional average treatment effects* as

$$\text{ATT} = \mathbb{E}_X \left[ \mathbb{E}[Y \mid T = 1, X] - \mathbb{E}[Y \mid T = 0, X] \mid T = 1 \right], \quad (1)$$

which can be approximated by taking the sample mean over units as

$$\text{ATT} \approx \frac{1}{N_t} \sum_{i:T_i=1} \mathbb{E}[Y_i \mid T_i = 1, X_i] - \mathbb{E}[Y_i \mid T_i = 0, X_i]. \quad (2)$$

While we focus on the potential outcomes framework in this work, we note that an alternative is Pearl’s framework of directed acyclic graphs (DAGs) and structural causal models (SCMs) (Pearl, 2009).

### 2.2 Key Concepts

In general, a matching procedure generates weights  $w_{ij}$  denoting the assignment of one or many control units  $j$  to a treated unit  $i$  (Morgan and Winship,

2014, Chapter 5). Typically, matching only assigns few control units, i.e. for a treated unit  $i$ , there is a small number of control units  $j$  such that  $w_{ij} > 0$ , and  $w_{ij} = 0$ , otherwise. This yields a new, weighted dataset  $(w_i, X_i, T_i, Y_i) \sim P'$ , where  $w_i = 1$  for all treated units  $i$  and  $w_j = \sum_i (w_{ij} / \sum_j w_{ij})$  for control units  $j$ . The matching procedure serves two main goals. One is to estimate the ATT through the following estimator of the potential outcome  $Y_i(0)$ :

$$\hat{Y}_i(0) = \frac{1}{\sum_{j:T_j=0} w_{ij}} \sum_{j:T_j=0} w_{ij} Y_j.$$

Another is to obtain *balance* or, when it is not possible, reduce *imbalance* in  $P'$  compared to the original distribution  $P$ . Balance occurs when the distributions of covariates  $X$  given  $T = 0$  on the one hand and  $T = 1$  on the other hand are equal. Perfect balance thus corresponds to zero imbalance, and is desirable because it eliminates confounding. In this ideal setting, the treatment effect can then be estimated as the difference between averaged outcomes in both distributions. In this sense, the two goals of treatment effect estimation and balance are related. However, there is also a bias-variance trade-off at stake, as selecting fewer matching units will reduce imbalance and thus the expected treatment estimation error or “bias”, at the cost of increased variance.

Formally, for a random variable  $A$ , we refer to the statement

$$P(A|T = 1) = P(A|T = 0)$$

as “balance in  $A$ ”, and, for a function  $D$  of two probability distributions, we refer to the quantity

$$D(P(A|T = 1), P(A|T = 0))$$

as “ $D$ -imbalance in  $A$ ”. When  $D$  is a probability distance, e.g. total variation or Wasserstein distance, then a zero  $D$ -imbalance in  $A$  implies balance in  $A$ . This is not true when  $D$  is *not* a probability distance, e.g. linear MMD. Note to distinguish  $D$  from the notation for a distance metric  $d$  in Section 3. We omit the mention of  $D$  or  $A$  when obvious from the context.

There are different ways to measure imbalance, such as a (standardised) difference in means (Austin, 2011), integral probability metrics such as the Wasserstein distance, the maximum mean discrepancy (MMD) and the total variation (TV) (Sriperumbudur et al., 2012; Kallus, 2020a), or histogram-based  $L_1$  distances (Iacus et al., 2012). Balance and imbalance can also apply to other variables than covariates, such as transformations of covariates (Johansson et al., 2016; Shalit et al., 2017; Iacus et al., 2011).

### 3 RELATED WORK

We now discuss existing work on matching and alternative approaches in causal inference that aim to reduce imbalance or estimate the ATT. Most commonly, choosing matched control units  $j$  is done through a nearest neighbours search among all control units  $j$  according to some distance metric  $d(\cdot, \cdot)$  (Stuart, 2010). Nearest neighbour search can be performed with or without replacement, and additionally, one may enforce a caliper, i.e. a maximal distance between matches. Alternatively, one might consider all matches simultaneously through an optimisation programme (optimal matching) (Rosenbaum, 1989). The choice of the distance metric  $d$  differs between common matching techniques:

- Exact matching (Rosenbaum and Rubin, 1985):  $d(X_i, X_j) = \infty$ , if  $X_i \neq X_j$ , and  $d(X_i, X_j) = 0$ , otherwise.
- Coarsened exact matching (Iacus et al., 2012): for a function  $f$ ,  $d(X_i, X_j) = \infty$ , if  $f(X_i) \neq f(X_j)$ , and  $d(X_i, X_j) = 0$ , otherwise.  $f$  is typically an element-wise function, mapping to some (aggregated) value.
- Mahalanobis distance matching (Stuart, 2010):  $d(X_i, X_j) = (X_i - X_j)^T \Sigma^{-1} (X_i - X_j)$ , where  $\Sigma$  is the estimated covariance matrix of the control dataset in the case of ATT estimation.
- Propensity score matching (Austin, 2011):  $d(X_i, X_j) = |\hat{e}(X_j) - \hat{e}(X_i)|$  where  $\hat{e}(\mathbf{x})$  is an estimate of the propensity score  $e(\mathbf{x}) := P(T = 1|X = \mathbf{x})$ . This method is based on the property that  $X \perp\!\!\!\perp T | e(X)$ . We provide more details on implications of this property in Section 4.1.

Other than coarsened exact matching for which the weights have a different formulation, these methods set  $w_{ij} = 1$  for matched units  $i$  and  $j$ , and  $w_{ij} = 0$ , otherwise.

All the above matching methods suffer from the *curse of dimensionality*, rendering them impractical in high-dimensional datasets. In general, theoretical results on nearest neighbour matching, to which the above techniques belong, show that the bias of the resulting ATT estimator grows with the data dimension  $D$  at a rate  $\mathcal{O}(N^{-r/D})$ , where  $N$  is the sample size and  $r \geq 1$  is a constant (Abadie and Imbens, 2006b). More precisely, exact matching and coarsened exact matching remove more and more control items as the number of covariates increases. Further, matching based on the Mahalanobis distance performs poorly in high dimensions, likely because all covariate interactions are assumed to be equally important (Stuart, 2010).

In the literature, the preferred method for high dimensions is propensity score matching. However, compression into a single dimension can lead to matches with

very different characteristics in the original covariate space, as for a fixed compression, there is no other information used to choose matches: matching is then done at random. This applies to all compressions of covariates, however as the propensity score  $p(T = 1|X)$  is the coarsest compression which can be used for matching (see Section 4.1), with the least information from  $X$ , it is most prone to actually matching at random. This can increase imbalance and consequently bias (King and Nielsen, 2019). Other than propensity score methods, approaches for matching in high dimensions include penalised regression techniques such as LASSO to perform variable selection before matching (Schneeweiss et al., 2009; Belloni et al., 2013; Farrell, 2015), sufficient dimension reduction (Luo and Zhu, 2020; Cheng et al., 2020), and distance metric learning (Li et al., 2016; Wang et al., 2021).

An alternative to matching is *weighting*, where weights  $w_j$  in the weighted dataset are directly estimated, generalising the problem formulation of matching (Kallus, 2020b). Examples include leveraging the estimated propensity score for inverse probability weighting (Horvitz and Thompson, 1952) or learning weights directly (Kallus, 2020a). A second alternative to matching is *outcome regression*. These methods estimate the quantity  $\mathbb{E}[Y|T = t, X = \mathbf{x}]$  through a regressor  $Q(t, \mathbf{x})$  that can be fitted through various methods related to linear regression (Imbens and Rubin, 2015), tree models (Athey et al., 2019), or neural networks (Shi et al., 2019; Shalit et al., 2017). Combining weighting through the propensity score estimate and outcome regression leads to the popular doubly robust methods, such as the augmented inverse probability weighted (AIPW) method (Robins et al., 1994). Recent efforts have been made to recategorise and benchmark outcome regression and doubly robust methods (Curth and Schaar, 2021).

## 4 NEURAL SCORE MATCHING

In this section, we present theoretical results that motivate the use of neural networks to obtain non-trivial, multivariate balancing scores. This approach aims to address the curse of dimensionality problem, as outlined in the previous section. In addition, some of these results have wider applicability to other models than neural networks.

### 4.1 Balancing Scores

We start by defining and analysing the use of *balancing scores*. This notion also motivated propensity score matching (Rosenbaum and Rubin, 1983).

**Definition 1.** A balancing score is a function  $b$  of  $X$  such that  $X \perp\!\!\!\perp T \mid b(X)$ .

As a consequence, for a fixed value  $\beta$  of  $b(X)$ , it holds that

$$P(X \mid b(X) = \beta, T = 1) = P(X \mid b(X) = \beta, T = 0),$$

i.e. the treatment and control distributions in the covariate space are equal for any fixed realisation of  $b(X)$ . Notably, it is possible to show that average treatment effects can be estimated by conditioning on  $b(X)$  instead of  $X$  in Equation (1) (Rosenbaum and Rubin, 1983).

We can further connect (im)balance in  $b(X)$  to (im)balance in  $X$ . The following Proposition shows that  $TV$ -imbalance in  $X$  is equal to  $TV$ -imbalance in  $b(X)$ , where  $TV$  is the total variation distance.

**Proposition 1.** Let  $b$  be a function such that  $b(X)$  is a balancing score. Then,

$$\begin{aligned} TV(P(X \mid T = 1), P(X \mid T = 0)) \\ = TV(P(b(X) \mid T = 1), P(b(X) \mid T = 0)). \end{aligned}$$

*Proof:* See Appendix A.1.  $\square$

This allows us to potentially use lower-dimensional balancing scores  $b(X)$  instead of high-dimensional covariates to achieve balance in  $X$ , as the following corollary shows that balance in  $b(X)$  ensures balance in  $X$ :

**Corollary 1.1.** Under the same conditions as Proposition 1,

$$\begin{aligned} P(b(X) \mid T = 1) = P(b(X) \mid T = 0) \\ \implies P(X \mid T = 1) = P(X \mid T = 0). \end{aligned}$$

*Proof:* See Appendix A.1.  $\square$

Matching on a given balancing score  $b(X)$  is commonly used to reduce imbalance in  $b(X)$ , with the aim of consequently reducing imbalance in  $X$ . Proposition 1 shows that a lower  $TV$ -imbalance in  $b(X)$  will also mean a lower  $TV$ -imbalance in  $X$ , but only if  $b(X)$  remains a balancing score in the post-matching distribution  $P'$ . Thankfully, the following Proposition shows that  $b(X)$  remains a balancing score after matching.

**Proposition 2.** Let  $b$  be a function such that  $b(X)$  is a balancing score,  $P'$  be a distribution obtained from matching every treated unit with control units using  $b(X)$  only. Then  $b(X)$  is also a balancing score in  $P'$ .

*Proof:* See Appendix A.1.  $\square$

Thus, all further theoretical results involving balancing scores in the original distribution will also be valid in the matched distribution. An important question left open at this point is how to find such a function  $b$  such that  $b(X)$  is a balancing score.

Leveraging theoretical results in (Rosenbaum and Rubin, 1983), balancing scores can be linked to the propensity score  $e(X) = P(T = 1 \mid X)$ .

**Proposition 3.** *A function  $b(X)$  is a balancing score, if and only if  $b(X)$  can be mapped deterministically to the propensity score  $e(X)$  through a function  $f$ , i.e.*

$$e(X) = f(b(X)).$$

*Proof:* See (Rosenbaum and Rubin, 1983, Thm. 2).  $\square$

It follows from Proposition 3 that  $e(X)$  is itself a balancing score for the identity map. When this identity does not hold,  $b(X)$  is said to be “finer” than  $e(X)$ , and conversely,  $e(X)$  is “coarser” than  $b(X)$ . As noted in (Rosenbaum and Rubin, 1983),  $X$  is the finest balancing score, containing the most information;  $e(X)$  is the coarsest balancing score, containing the least information; and any other  $b(X)$  such that  $e(X) = f(b(X))$  lies between the two. Choosing the degree of coarseness via multi-dimensional balancing scores to achieve optimal matching results rather than assuming a one-dimensional balancing score (i.e. the propensity score) is what we exploit in our method which we introduce in the following.

## 4.2 Introducing Neural Score Matching

Previous work has largely focused on the use of the propensity score  $e(X)$  as a balancing score, and relatively little attention has been paid to non-trivial balancing scores that are neither  $X$  nor  $e(X)$ . Neural networks provide a natural mechanism by which to construct such balancing scores: fundamentally, a multi-layer neural network is a composition of functions  $f_1, f_2, \dots, f_L$ . Let us for a moment assume this network (perfectly) estimates the propensity score, i.e.  $\hat{e}(X) = f_L \circ f_{L-1} \circ \dots \circ f_1(X) = e(X)$ . Then, by Proposition 3, this provides us with  $L + 1$  balancing scores ( $X$ , the  $L - 1$  intermediate hidden representations and the estimated propensity score) that are coarser and coarser with increasing “depth” of the composition. We note that instead of neural networks parameterising  $f_1, f_2, \dots, f_L$ , one may consider other hierarchical models. We formalise this general principle, which we call *neural score matching*, in the following Proposition:

**Proposition 4.** *Assume that  $e(X) = f_L \circ f_{L-1} \circ \dots \circ f_1(X)$  for some functions  $f_1, \dots, f_L$ . Define  $b_0(X) := X$  and  $b_l(X) = f_l \circ f_{l-1} \circ \dots \circ f_1(X)$  for  $l = 1, \dots, L$ . Then, every  $b_l(X)$  is a balancing score, and for any  $l < L$ ,  $b_{l+1}(X)$  is coarser than  $b_l(X)$ .*

*Proof:* See Appendix A.2.  $\square$

Using this Proposition, we can now connect these balancing scores to our goal of achieving balance in  $X$ :

**Corollary 4.1.** *Under the same conditions and notation as Proposition 4, for any  $l, l' = 0, \dots, L$ ,*

$$TV(P(b_l(X) | T = 1), P(b_l(X) | T = 0))$$

$$= TV(P(b_{l'}(X) | T = 1), P(b_{l'}(X) | T = 0)),$$

and balance in  $b_{l'}(X)$  is equivalent to balance in  $b_l(X)$ .

*Proof:* See Appendix A.2.  $\square$

This Proposition gives us a choice of balancing scores with varying degree of coarseness which we can use for matching. Note that achieving balance in *any* of the scores will yield balance in *all* of them, and particularly in  $X = b_0(X)$ . On the other hand, perfect balance is difficult to attain, but we can still aim to achieve the lowest imbalance possible. Importantly, although imbalance is identical for two given balancing scores in the same hierarchical propensity score model *when the distribution is fixed*, matching on these two balancing scores will in general result in different distributions and consequently different imbalances.

Thus, if we can compute  $TV$ -imbalances, the Proposition ensures that selecting the balancing score and matching procedure with the lowest resulting  $TV$ -imbalance will also reach the lowest  $TV$ -imbalance in covariate distributions  $X$  among the candidate balancing scores and matching procedures.

It is important to note that Proposition 4, Corollary 4.1 and the following theoretical results all assume that  $\hat{e}(X) = e(X)$ , i.e. a well-calibrated propensity score model, or at least that the obtained scores are indeed balancing scores. In Section 4.4, we will relax this assumption and provide theoretical bounds when scores violate the balancing score assumption from Definition 1.

In practice, however, the total variation distance is not suitable for this purpose of balancing score comparison due to the difficulties with estimating it in finite samples (Kallus, 2020a). We provide results with alternative metrics which overcome this issue in Section 4.3

## 4.3 Bounds With Estimable Integral Probability Metrics

To start, we consider a *linear* balancing score  $b(X)$ , meaning that  $b$  is a linear function. For example, this can be realised by considering the first layer of a neural network before applying an activation function. In this simple case, we can leverage popular integral probability metrics which *can* be estimated with finite samples, in contrast to the total variation distance.

**Proposition 5.** *Let  $b$  be a function such that  $\forall \mathbf{x}, b(\mathbf{x}) = W\mathbf{x}$  for some matrix  $W$  and  $b(X)$  is a balancing score. Let  $\|\cdot\|$  be the Euclidean norm on any vector space, and  $\|\cdot\|$  be a norm<sup>1</sup> on any matrix space*

<sup>1</sup>Examples include the operator or Euclidean norms.

such that  $\forall \mathbf{x}, A, \|A\mathbf{x}\| \leq \|A\| \cdot \|\mathbf{x}\|$ . Further, let  $W^+$  be the Moore-Penrose pseudo-inverse of  $W$ ,  $W_{\text{ass}}$  be the Wasserstein distance,  $MMD$  be the linear MMD. Then<sup>2</sup>,

$$\begin{aligned} & \frac{1}{\|W\|} \cdot W_{\text{ass}}(P(b(X) | T = 1), P(b(X) | T = 0)) \\ & \leq W_{\text{ass}}(P(X | T = 1), P(X | T = 0)) \\ & \leq \|W^+\| \cdot W_{\text{ass}}(P(b(X) | T = 1), P(b(X) | T = 0)) \end{aligned}$$

and

$$\begin{aligned} & \frac{1}{\|W\|} \cdot MMD(P(b(X) | T = 1), P(b(X) | T = 0)) \\ & \leq MMD(P(X | T = 1), P(X | T = 0)) \\ & \leq \|W^+\| \cdot MMD(P(b(X) | T = 1), P(b(X) | T = 0)) \end{aligned}$$

*Proof:* See Appendix A.3.  $\square$

This Proposition provides lower- and upper-bounds (in contrast to Proposition 1) for the Wasserstein- or linear MMD-imbalance in  $X$  which depend linearly on the corresponding imbalance in  $b(X)$ . Thus, as in Corollary 4.1, we expect to reduce the imbalance in  $X$  when reducing the imbalance in  $b(X)$ , justifying matching on  $b(X)$  as an alternative to matching on  $X$ .

One could exploit these bounds by computing them for different balancing scores and choose the one with the lowest (lower or upper) bounds of the interval, or the narrowest bounds. One might also perform a type of optimal matching minimising the Wasserstein or linear MMD imbalance in  $b(X)$ . However, it is important to point out that these bounds may be wide depending on the singular values of  $W$ . When using the operator norm and denoting  $\sigma_{\min}(W)$  and  $\sigma_{\max}(W)$  as the minimal and maximal non-zero singular values of  $W$ <sup>3</sup>, respectively, we have  $\frac{1}{\|W\|} = \frac{1}{\sigma_{\max}(W)}$  and  $\|W^+\| = \frac{1}{\sigma_{\min}(W)}$ . As a consequence, values within the bounds can vary by a factor of  $\frac{\sigma_{\max}(W)}{\sigma_{\min}(W)}$ .

However, the imbalance in  $b(X)$  can also help to speed up computations. In Appendix B, we show how the computational complexity of the estimators of the linear MMD and of the Wasserstein distance can be reduced on a lower-dimensional space.

In order to satisfy the assumptions of Proposition 5, we only use the first layer of a neural network for the purpose of matching; the other layers serve to achieve a better fit of the propensity score model. Next, we present theoretical results which allow us to use *any* layer for matching by extending the bounds of the Wasserstein imbalance as follows:

<sup>2</sup>Note that these theoretical results also hold when  $b(X)$  has a bias term. Notably, the Wasserstein distance is invariant to translations (Panaretos and Zemel, 2019).

<sup>3</sup>This assumes  $W \neq 0$ , i.e. we do not have balance in  $X$ .

**Proposition 6.** Let  $h^{(l)}$  ( $l = 1, \dots, L$ ) be a bi-Lipschitz function, i.e. an invertible multivariate function such that for any  $b, b'$  in the input space of  $h^{(l)}$  and appropriate real-valued constants  $m^{(l)}$  and  $M^{(l)}$ :

$$m^{(l)} \|b - b'\| \leq \|h^{(l)}(b) - h^{(l)}(b')\| \leq M^{(l)} \|b - b'\|$$

Let  $(b^{(l)})$  be a sequence of functions of the  $\mathcal{X}$ -space such that every  $b^{(l)}(X)$  is a balancing score, and for any  $x \in \mathcal{X}$ ,

$$\begin{aligned} b^{(0)}(x) &:= x, \\ b^{(l)}(x) &:= W^{(l)} h^{(l)}(b^{(l-1)}(x)). \quad \forall l \geq 1. \end{aligned}$$

Let  $\|\cdot\|$  be the Euclidean norm on any vector space,  $\|\cdot\|$  be a norm on any matrix space such that  $\forall \mathbf{x}, A, \|A\mathbf{x}\| \leq \|A\| \cdot \|\mathbf{x}\|$ ,  $A^+$  be the Moore-Penrose pseudo-inverse of  $A$ , and  $W_{\text{ass}}$  be the Wasserstein distance. Then,

$$\begin{aligned} & \alpha_L \cdot W_{\text{ass}}(P(b^{(L)}(X) | T = 1), P(b^{(L)}(X) | T = 0)) \\ & \leq W_{\text{ass}}(P(X | T = 1), P(X | T = 0)) \\ & \leq \beta_L \cdot W_{\text{ass}}(P(b^{(L)}(X) | T = 1), P(b^{(L)}(X) | T = 0)) \end{aligned}$$

with

$$\alpha_L = \frac{1}{\prod_{l=1}^L \|W^{(l)}\| \cdot \prod_{l=1}^L M^{(l)}} \quad \text{and} \quad \beta_L = \frac{\prod_{l=1}^L \|W^{(l)+}\|}{\prod_{l=1}^L m^{(l)}}.$$

*Proof:* See Appendix A.3.  $\square$

In this formulation of balancing scores, we are taking the outputs of neural network layers *before the activation function*, so balancing scores are real-valued. Consequently,  $h^{(1)}$  will typically be the identity function, with  $m^{(1)} = M^{(1)} = 1$ , so if  $L = 1$  then Proposition 6 will generally reduce to the bounds with Wasserstein distances in Proposition 5. Unfortunately, for common (invertible) activation functions  $h^{(l)}$  such as sigmoid, tanh or ELU, we will have  $m^{(l)} = 0$  as their derivatives converge to 0 when their inputs go to  $\pm\infty$ , rendering the Proposition vacuous in its upper bound. An alternative is to assume that the input of these functions is bounded, ensuring that the derivative is bounded below by a positive constant and thus allowing a positive  $m^{(l)}$ . Indeed, if the derivative of  $h^{(l)}$  is continuous and non-zero at any point (but can vanish on  $\pm\infty$ ) and the input space of  $h^{(l)}$  is bounded by  $B$ , then  $m^{(l)} = \min_{|b| < B} |h^{(l)'}(b)| > 0$ .

In addition, the leaky ReLU activation ( $h^{(l)} = \epsilon x$ , if  $x < 0$  for some  $\epsilon > 0$ , and  $h^{(l)} = x$ , if  $x \geq 0$ ) satisfies the conditions of the Proposition with  $m^{(l)} = \epsilon$ ,  $M^{(l)} = 1$ . However, the upper bound in Proposition 6 will diverge to  $+\infty$  at an exponential rate with the layer index  $l$ . As a consequence, it will become vacuous in deeper layers.

This shows that one should still use one of the first few layers as the balancing score for matching when

using leaky ReLU. Yet, this can also be justified in the general case. Assuming we are interested in  $b^{(L)}(X)$ , values within the bounds of the Proposition can vary up to a factor  $\frac{\beta_L}{\alpha_L} = \prod_{l=1}^L \frac{\sigma_{\max}(W^{(l)})M^{(l)}}{\sigma_{\min}(W^{(l)})m^{(l)}}$ : the interval becomes wider as  $L$  increases. Similarly, in Appendix B, we show that the computational complexities of the linear MMD and the Wasserstein distance increase with the number of layers.

#### 4.4 Bounds For Non-Balancing Scores

As mentioned above, a requirement for applying the above Propositions within the context of hidden representations of a neural network is that either the estimated propensity score of said network equals the true propensity score, or more generally, every learned function  $b$  is indeed a balancing score. When this is not the case, as the next Proposition shows, we can still bound the imbalance in  $X$  in terms of the imbalance in  $b(X)$  and some quantification of “how much” the assumption  $X \perp\!\!\!\perp T|b(X)$  is violated.

**Proposition 7.** *Let*

$$\mathcal{E}_{t,b}^D(\beta) := D\left(P(X|b(X) = \beta, T = t), P(X|b(X) = \beta)\right)$$

where  $D$  is a probability discrepancy measure,  $b$  is a function of  $X$ ,  $t \in \{0, 1\}$  is a realisation of  $T$ ,  $\beta$  is a realisation of  $b(X)$ . For any function  $b$ ,

$$\begin{aligned} & TV\left(P(b(X)|T = 1), P(b(X)|T = 0)\right) \\ & \leq TV\left(P(X|T = 1), P(X|T = 0)\right) \\ & \leq TV\left(P(b(X)|T = 1), P(b(X)|T = 0)\right) \\ & \quad + \mathbb{E}\left[\mathcal{E}_{1,b}^{TV}(b(X))|T = 1\right] + \mathbb{E}\left[\mathcal{E}_{0,b}^{TV}(b(X))|T = 0\right] \end{aligned}$$

For a linear function  $b(x) = Wx$ ,

$$\begin{aligned} & \frac{1}{\|W\|} \cdot W_{\text{ass}}\left(P(b(X)|T = 1), P(b(X)|T = 0)\right) \\ & \leq W_{\text{ass}}\left(P(X|T = 1), P(X|T = 0)\right) \\ & \leq \|W^+\| \cdot W_{\text{ass}}\left(P(b(X)|T = 1), P(b(X)|T = 0)\right) \\ & \quad + \mathbb{E}\left[\mathcal{E}_{1,b}^{W_{\text{ass}}}(b(X))|T = 1\right] + \mathbb{E}\left[\mathcal{E}_{0,b}^{W_{\text{ass}}}(b(X))|T = 0\right] \end{aligned}$$

and

$$\begin{aligned} & \frac{1}{\|W\|} \cdot MMD\left(P(b(X)|T = 1), P(b(X)|T = 0)\right) \\ & \leq MMD\left(P(X|T = 1), P(X|T = 0)\right) \\ & \leq \|W^+\| \cdot MMD\left(P(b(X)|T = 1), P(b(X)|T = 0)\right) \\ & \quad + \mathbb{E}\left[\mathcal{E}_{1,b}^{MMD}(b(X))|T = 1\right] + \mathbb{E}\left[\mathcal{E}_{0,b}^{MMD}(b(X))|T = 0\right] \end{aligned}$$

For a function  $b^{(L)}$  as in Proposition 6,

$$\begin{aligned} & \alpha_L \cdot W_{\text{ass}}\left(P(b^{(L)}(X) | T = 1), P(b^{(L)}(X) | T = 0)\right) \\ & \leq W_{\text{ass}}\left(P(X | T = 1), P(X | T = 0)\right) \\ & \leq \beta_L \cdot W_{\text{ass}}\left(P(b^{(L)}(X) | T = 1), P(b^{(L)}(X) | T = 0)\right) \\ & \quad + \mathbb{E}\left[\mathcal{E}_{1,b^{(L)}}^{W_{\text{ass}}}(b^{(L)}(X))|T = 1\right] \\ & \quad + \mathbb{E}\left[\mathcal{E}_{0,b^{(L)}}^{W_{\text{ass}}}(b^{(L)}(X))|T = 0\right] \end{aligned}$$

*Proof:* See Appendix A.4.  $\square$

Unlike the calibration error, i.e. the mean difference between true and predicted propensity scores, the extra balancing error term in the Proposition does not rely on access to the true propensity score. Therefore, it can be computed and used to obtain an upper bound of covariate imbalance in any dataset. In practice, however, it might be challenging to estimate as it relies on conditional expectations for which few samples may be available.

## 5 EXPERIMENTS

We now evaluate neural score matching on two semi-synthetic datasets and benchmark it against other matching methods. We provide code to implement neural score matching and reproduce the main results at <https://github.com/oscarclivio/neuralscorematching>.

### 5.1 Experimental Setup

Our general procedure for matching and in particular neural score matching follows two stages: in the first stage, we learn a model to obtain some representation or score  $s$  from datapoints. In the second stage, we perform matching on these scores using the Euclidean distance<sup>4</sup>  $d(s_i, s_j) = \|s_i - s_j\|_2$ . We use nearest neighbour matching with replacement using one neighbour.

To perform neural score matching, we train a neural network predicting treatment assignment from covariates, with the final one-dimensional layer being an estimator of the propensity score. Training is performed using a standard binary cross-entropy loss. The neural network has the following architecture: one low-dimensional layer with 5 hidden units, two layers with 100 units and one final 1-dimensional layer. We use the leaky ReLU activation function in all layers except the last one where we use the sigmoid function. When using the hidden representation in the first layer before applying the activation function as a score, we refer to the resulting method as NN Layer 1. Notably, if

<sup>4</sup>We use the Euclidean distance as the Mahalanobis distance was prohibitively slow to compute in high-dimensional and large sample settings.

it is indeed a balancing score, it meets the assumptions of Proposition 5. Even if other layers before the propensity score also meet the assumptions of Proposition 6, we choose to focus on one single multivariate layer for matching, and dedicate other layers to model fitting (with corresponding high dimensions as given above). The final activation of the network estimates the propensity score and is also used for matching as a balancing score. We refer to it as **NN PS**.

We benchmark these scores obtained by the neural network against other scores, namely  $X$  (**X**) and a five-dimensional PCA reduction of  $X$  (**PCA**). We also benchmark against a logistic regression estimating the propensity score given  $X$  or PCA features, which we refer to as **LogReg PS** and **PCA + LogReg PS**, respectively. In addition, we consider matching uniformly at random (**Random matching**) and leaving the treatment and control datasets unchanged w.r.t. balance by not matching at all (**No Matching**). All methods were evaluated using 10 different training random seeds.

We use variants of two standard datasets for treatment effect estimation: *ACIC 2016* and *News*. Both datasets have a large number of covariates (82 and 3477, respectively), rendering them challenging for standard matching techniques. They are both semi-synthetic: the covariates come from real-world studies, while the treatments and outcomes were generated through a data generating process. For every dataset, we will average results over different draws of the data generating process (100 for ACIC 2016 and 50 for News). Early stopping was used on News. Results on a third dataset, IHDP, are presented in Appendix D.

To evaluate the methods, we report three metrics: *calibration error*, defined as the mean absolute difference between the estimated and true propensity score, *ATT error*, defined as the absolute difference between the ATT estimated by the method and a ground-truth ATT, and *sample imbalance  $\hat{I}$* , defined as the squared Euclidean distance between sample means of covariates of treated and control groups from the dataset  $\mathcal{D}'$  obtained from the original dataset  $\mathcal{D}$  after matching. To reliably assess the performance of the methods under investigation, we average and present standard deviations over the repeated draws of the data generating processes and additionally over the different random seeds for model fitting/training.

We refer to Appendix C for further details about implementation and experimental setup.

## 5.2 Experimental Results

In this section, we present our experimental results as Tables (and refer to Appendix E for their visualisation as boxplots).

### 5.2.1 ACIC 2016

Results for the different matching methods under consideration are presented in Table 1. Propensity score models for the two dimensionality reduction methods (**NN Layer 1** and **PCA**) have better calibration than the standard logistic-regression propensity score (**LogReg PS**), with a slight advantage for **NN PS**. The relevance of using a multivariate score is demonstrated: on ATT errors and imbalances, **NN Layer 1** most often outperforms **NN PS**, and all other methods except:

- Logistic regression propensity score (**LogReg PS**) on in-sample metrics. It is possible that the dimensionality remains sufficiently low for this method to handle (unlike News, see next section). However, the method might also overfit, as shown by the hold-out performance.
- **No Matching** and **PCA** on hold-out imbalances. Neural scores might need better generalisation as they increase imbalance compared to the original dataset, unlike **PCA**. Other methods also increase imbalance, as expected.

Table 1: Results on the ACIC2016 dataset.

Calibration errors	In-Sample	Hold-Out
<b>NN PS (ours)</b>	0.055±0.000	0.055±0.000
<b>LogReg PS</b>	0.067±0.000	0.069±0.000
<b>PCA + LogReg PS</b>	0.058±0.001	0.058±0.001
ATT errors	In-Sample	Hold-Out
<b>NN Layer 1 (ours)</b>	0.707±0.012	0.918±0.018
<b>NN PS (ours)</b>	0.735±0.012	1.008±0.019
<b>X</b>	0.848±0.018	0.990±0.019
<b>Random matching</b>	1.209±0.019	1.301±0.023
<b>LogReg PS</b>	0.678±0.012	1.036±0.018
<b>PCA</b>	0.927±0.016	1.007±0.020
<b>PCA + LogReg PS</b>	0.962±0.016	1.097±0.021
Sample imbalance	In-Sample	Hold-Out
<b>NN Layer 1 (ours)</b>	0.107±0.001	0.422±0.003
<b>NN PS (ours)</b>	0.105±0.001	0.498±0.004
<b>X</b>	0.438±0.002	0.739±0.004
<b>Random matching</b>	0.232±0.003	0.558±0.006
<b>LogReg PS</b>	0.056±0.001	0.511±0.004
<b>PCA</b>	0.117±0.001	0.342±0.003
<b>PCA + LogReg PS</b>	0.134±0.001	0.488±0.004
<b>No Matching</b>	0.192±0.003	0.396±0.006

### 5.2.2 News

Results for the News dataset are presented in Table 2. Multivariate dimensionality-reduced scores (**NN**



Layer 1 and PCA) generally outperform their respective propensity scores (except NN Layer 1 and NN PS having similar performance on ATT errors), as well as Random matching, X and LogReg PS. The two latter have particularly high ATT errors and imbalances, even compared to Random matching. This shows that multivariate, but lower-dimensional scores can improve matching on high-dimensional datasets. The performance is more balanced between PCA and NN Layer 1: PCA is better on imbalances, NN Layer 1 on in-sample ATT errors, and their hold-out ATT errors are not significantly different according to standard errors.

Table 2: Results on the News dataset.

ATT errors	In-Sample	Hold-Out
NN Layer 1 (ours)	0.071±0.002	0.106±0.004
NN PS (ours)	0.073±0.002	0.105±0.004
X	0.510±0.015	0.765±0.024
Random matching	0.100±0.003	0.114±0.004
LogReg PS	1.460±0.052	0.505±0.020
PCA	0.080±0.002	0.103±0.003
PCA + LogReg PS	0.095±0.003	0.100±0.003
Sample imbalance	In-Sample	Hold-Out
NN Layer 1 (ours)	1.518±0.022	3.886±0.045
NN PS (ours)	2.104±0.035	5.105±0.079
X	12.531±0.032	18.178±0.052
Random matching	2.121±0.041	4.581±0.043
LogReg PS	371.070±36.672	131.192±4.682
PCA	1.097±0.013	3.608±0.030
PCA + LogReg PS	1.444±0.017	4.600±0.046
No Matching	1.844±0.040	3.432±0.038

## 6 DISCUSSION AND CONCLUSION

In this work, we have provided novel theoretical results motivating neural score matching: using neural networks to obtain balancing scores which can be readily used for matching. In contrast to lower-dimensional representations obtained from classical dimensionality reduction techniques (e.g. PCA), our method estimates lower-dimensional balancing scores as defined in Proposition 3, which can be mapped back to the propensity score, “for free” due to the inherent compositionality of neural networks, allowing more flexibility in choosing the degree of coarseness. This applies only if the model is correctly specified, however. Proposition 7 paves the way to rigorous analysis of situations when the constraint is violated. We found that in popular semi-synthetic datasets, neural score matching is competitive against other matching methods. In addition, our results indicate the general utility of dimensionality

reduction techniques for matching in causal inference. This leads the way towards learning suitable representations for matching which might be useful for downstream tasks to gain scientific insight, notably in areas where the use of neural networks is ubiquitous, such as medical imaging (Zhou et al., 2021), text classification (Minaee et al., 2021) and audio processing (Purwins et al., 2019).

Our work has the following two limitations: 1) It is difficult to properly specify and train neural networks for the task of matching. In particular, there is a trade-off between finding low-dimensional balancing scores, which implies low-dimensional hidden layers, and fitting the propensity score model, which implies wide hidden layers not suitable for matching. We also did not find hyperparameters that performed consistently better than others across all datasets, nor a correlation between matching performance and hold-out loss. More complex architectures than our experimental setup and a deeper understanding of the hyperparameter space should be explored. 2) Most of our theoretical results assume the propensity score model is correct, or, more generally speaking, that the hidden activations obtained are indeed balancing scores. Most often, neither is true. Proposition 7 is a first step towards theoretical guarantees for scores that are not perfectly balancing.

Future work will investigate the following ideas: 1) As outlined earlier, our propensity score model might be miscalibrated and the balancing scores might not perfectly balance covariates. Empirically measuring calibration error and the violation of the balancing score property via Proposition 7, we aim at using this to inform model training and hence improve performance. 2) We plan to extend the relatively simple setup of neural score matching as presented here to, for instance, using multiple intermediate balancing scores. This entails further questions, such as how to choose the degree of coarseness of the balancing scores, which might be assessed via empirical out-of-sample evaluation, and where to best place layers with few hidden units that are suited for matching. 3) We aim to develop a form of optimal matching which uses the bounds of Wass- or MMD-imbalance in  $b(X)$  in Proposition 5 directly in a loss function, which in turn should reduce imbalance in  $X$ . 4) Our obtained balancing scores might enable the use of coarsened exact matching (CEM), offering the possibility to pre-specify the desired level of imbalance before matching (Iacus et al., 2012). 5) We aim to explore more in depth how intermediate balancing scores compare to propensity scores, e.g. by visualising how their spaces capture features of the covariate space. We also expect these intermediate balancing scores to be preferable to propensity scores for CATE estimation as they provide less coarse representations of covariates.

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# Neural Score Matching for High-Dimensional Causal Inference: Appendices

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## A PROOFS OF THEORETICAL RESULTS

### A.1 Balance on $b(X)$ and $X$

**Proposition 1.** *Let  $b$  be a function such that  $b(X)$  is a balancing score. Then,*

$$\begin{aligned} TV(P(X|T=1), P(X|T=0)) \\ = TV(P(b(X)|T=1), P(b(X)|T=0)). \end{aligned}$$

*Proof:*

- First, let us note that for any random variable  $V$ , and by definition of the total variation distance:

$$TV(P(V|T=1), P(V|T=0)) = \sup_{\|f\|_{L^\infty} \leq 1} |\mathbb{E}[f(V)|T=1] - \mathbb{E}[f(V)|T=0]|,$$

where  $\|\cdot\|_{L^\infty}$  is the uniform norm, and  $f$  is a function.

- For any function  $f$  on the  $\mathcal{B}$  space (i.e. the image space of  $b(X)$ ) such that  $\|f\|_{L^\infty} < 1$ :

$$\begin{aligned} |\mathbb{E}[f(b(X))|T=1] - \mathbb{E}[f(b(X))|T=0]| &= |\mathbb{E}[(f \circ b)(X)|T=1] - \mathbb{E}[(f \circ b)(X)|T=0]| \\ &\leq TV(P(X|T=1), P(X|T=0)), \end{aligned}$$

where  $(f \circ b)$  is a function on the  $\mathcal{X}$  space with  $\|f\|_{L^\infty} < 1$ . Thus,

$$TV(P(X|T=1), P(X|T=0)) \geq TV(P(b(X)|T=1), P(b(X)|T=0)).$$

- As  $b(X)$  is a balancing score, we have  $T \perp\!\!\!\perp X|b(X)$  and for any measurable function  $f$ :

$$\mathbb{E}[f(X)|b(X), T] = \mathbb{E}[f(X)|b(X)] \tag{S3}$$

Then, if  $f$  is a function on the  $\mathcal{X}$  space such that  $\|f\|_{L^\infty} < 1$ ,

$$\begin{aligned} \mathbb{E}[f(X)|T=t] &= \mathbb{E}[\mathbb{E}[f(X)|b(X), T=t] \mid T=t] \text{ due to the law of total expectation} \\ &= \mathbb{E}[\mathbb{E}[f(X)|b(X)] \mid T=t] \text{ due to Equation (S3)} \\ &= \mathbb{E}[g(b(X)) \mid T=t], \end{aligned}$$

where  $g(\beta) := \mathbb{E}[f(X)|b(X) = \beta]$  is a function on the  $\mathcal{B}$  space with  $\|g\|_{L^\infty} < 1$ , and

$$\begin{aligned} \forall \beta, |g(\beta)| &= |\mathbb{E}[f(X) \mid b(X) = \beta]| \\ &\leq \mathbb{E}[|f(X)| \mid b(X) = \beta] \text{ from Jensen's inequality} \\ &\leq \mathbb{E}[1 \mid b(X) = \beta] \text{ as } \|f\|_{L^\infty} < 1 \\ &= 1 \end{aligned}$$

Thus, for any function  $f$  of  $\mathbf{x}$  s.t.  $\|f\|_{L^\infty} \leq 1$ ,

$$\begin{aligned} |\mathbb{E}[f(X)|T=1] - \mathbb{E}[f(X)|T=0]| &= |\mathbb{E}[g(b(X))|T=1] - \mathbb{E}[g(b(X))|T=0]| \\ &\quad \text{for some function } g \text{ on the } \mathcal{B} \text{ space s.t. } \|g\|_{L^\infty} \leq 1 \\ &\leq TV(P(b(X)|T=1), P(b(X)|T=0)) \end{aligned}$$

Therefore,  $TV(P(X|T=1), P(X|T=0)) \leq TV(P(b(X)|T=1), P(b(X)|T=0))$ .

- Consequently, together with the result above, it follows that

$$TV(P(X|T=1), P(X|T=0)) = TV(P(b(X)|T=1), P(b(X)|T=0)).$$

□

**Corollary 1.1.** *Under the same conditions as Proposition 1,*

$$\begin{aligned} P(b(X) | T = 1) &= P(b(X) | T = 0) \\ \implies P(X | T = 1) &= P(X | T = 0). \end{aligned}$$

*Proof:* One should note that  $P(b(X) | T = 1) = P(b(X) | T = 0)$  implies  $TV(P(b(X)|T=1), P(b(X)|T=0)) = 0$ . As a consequence,  $TV(P(X|T=1), P(X|T=0)) = 0$  from Proposition 1. As total variation TV is a distance, we obtain that  $P(X|T=1) = P(X|T=0)$ . □

**Proposition 2.** *Let  $b$  be a function such that  $b(X)$  is a balancing score,  $P'$  be a distribution obtained from matching every treated unit with control units using  $b(X)$  only. Then  $b(X)$  is also a balancing score in  $P'$ .*

*Proof:* Let  $\beta$  be a value of  $b(X)$ . Any matching method using  $b(X)$  only to match units does not change the conditional distribution of  $X$  given  $b(X) = \beta$  in the control group (Rosenbaum and Rubin, 1983). Then,

$$P'(X|b(X) = \beta, T = 0) = P(X|b(X) = \beta, T = 0). \quad (\text{S4})$$

The conditional distribution of  $X$  given  $b(X) = \beta$  in the treated group is likewise left unchanged as the matching method does not change the treated distribution in any way. Thus,

$$P'(X|b(X) = \beta, T = 1) = P(X|b(X) = \beta, T = 1). \quad (\text{S5})$$

Also, as  $b(X)$  is a balancing score in  $P$ ,  $P(X|b(X) = \beta, T = 0) = P(X|b(X) = \beta, T = 1)$ . Tying it all together, we have

$$\begin{aligned} P'(X|b(X) = \beta, T = 0) &= P(X|b(X) = \beta, T = 0) \quad \text{from Equation S4} \\ &= P(X|b(X) = \beta, T = 1) \quad \text{as } b(X) \text{ is a balancing score.} \\ &= P'(X|b(X) = \beta, T = 1) \quad \text{from Equation S5} \end{aligned}$$

so  $b(X)$  is a balancing score in  $P'$ . □

## A.2 Further Balancing Scores

**Proposition 4.** *Assume that  $e(X) = f_L \circ f_{L-1} \circ \dots \circ f_1(X)$  for some functions  $f_1, \dots, f_L$ . Define  $b_0(X) := X$  and  $b_l(X) = f_l \circ f_{l-1} \circ \dots \circ f_1(X)$  for  $l = 1, \dots, L$ . Then, every  $b_l(X)$  is a balancing score, and for any  $l < L$ ,  $b_{l+1}(X)$  is coarser than  $b_l(X)$ .*

*Proof:* According to Proposition 3,  $b_l(X)$  where  $l < L$  is a balancing score as

$$e(X) = f_L \circ f_{L-1} \circ \dots \circ f_{l+1}(b_l(X)),$$

and  $e(X)$  is the propensity score with the property  $X \perp\!\!\!\perp T | e(X)$ . Also for any  $l < L$ ,  $b_{l+1}(X)$  is coarser than  $b_l(X)$  as  $b_{l+1}(X) = f_{l+1}(b_l(X))$ .

**Corollary 4.1.** *Under the same conditions and notation as Proposition 4, for any  $l, l' = 0, \dots, L$ ,*

$$\begin{aligned} & TV(P(b_l(X) | T = 1), P(b_l(X) | T = 0)) \\ &= TV(P(b_{l'}(X) | T = 1), P(b_{l'}(X) | T = 0)), \end{aligned}$$

and balance in  $b_{l'}(X)$  is equivalent to balance in  $b_l(X)$ .

*Proof:* First, for any  $l < L$ , as  $b_{l+1}(X)$  is a balancing score w.r.t.  $b_l(X)$  from Proposition 4, we note that Proposition 1 can also be applied to  $b_l(X)$  and  $b_{l+1}(X)$  instead of  $X$  and  $b(X)$ , respectively. . Thus, it follows from Proposition 1 that

$$TV(P(b_{l+1}(X)|T = 1), P(b_{l+1}(X)|T = 0)) = TV(P(b_l(X)|T = 1), P(b_l(X)|T = 0)).$$

Consequently, it follows by induction that for any  $l, l' = 0, \dots, L$ ,

$$TV(P(b_l(X)|T = 1), P(b_l(X)|T = 0)) = TV(P(b_{l'}(X)|T = 1), P(b_{l'}(X)|T = 0)).$$

Then, the proof that balance in  $b_{l'}(X)$  is equivalent to balance in  $b_l(X)$  is analogous to Corollary 1.1.  $\square$

### A.3 Other Integral Probability Metrics

**Proposition 5.** *Let  $b$  be a function such that  $\forall \mathbf{x}$ ,  $b(\mathbf{x}) = W\mathbf{x}$  for some matrix  $W$  and  $b(X)$  is a balancing score. Let  $\|\cdot\|$  be the Euclidean norm on any vector space, and  $\|\cdot\|$  be a norm<sup>5</sup> on any matrix space such that  $\forall \mathbf{x}, A, \|A\mathbf{x}\| \leq \|A\| \cdot \|\mathbf{x}\|$ . Further, let  $W^+$  be the Moore-Penrose pseudo-inverse of  $W$ ,  $W_{\text{ass}}$  be the Wasserstein distance,  $MMD$  be the linear MMD. Then<sup>6</sup>,*

$$\begin{aligned} & \frac{1}{\|W\|} \cdot W_{\text{ass}}(P(b(X) | T = 1), P(b(X) | T = 0)) \\ & \leq W_{\text{ass}}(P(X | T = 1), P(X | T = 0)) \\ & \leq \|W^+\| \cdot W_{\text{ass}}(P(b(X) | T = 1), P(b(X) | T = 0)) \end{aligned}$$

and

$$\begin{aligned} & \frac{1}{\|W\|} \cdot MMD(P(b(X) | T = 1), P(b(X) | T = 0)) \\ & \leq MMD(P(X | T = 1), P(X | T = 0)) \\ & \leq \|W^+\| \cdot MMD(P(b(X) | T = 1), P(b(X) | T = 0)) \end{aligned}$$

*Proof.* We prove separately the bounds on the Wass distance and on the MMD.

- First, note that for any random variable  $V$ ,

$$W_{\text{ass}}(P(V|T = 1), P(V|T = 0)) = \sup_{f: \mathcal{V} \rightarrow \mathbb{R}, f \text{ 1-Lipschitz}} |\mathbb{E}[f(V)|T = 1] - \mathbb{E}[f(V)|T = 0]|.$$

- Let  $f$  be a 1-Lipschitz function  $f$  on the  $\mathcal{B}$  space of  $b(X)$ , and define  $g(x) = \frac{1}{\|W\|} f(Wx)$ . The function  $g$  is also 1-Lipschitz, since for any  $x, x'$ ,

$$\begin{aligned} |g(x) - g(x')| &= \frac{1}{\|W\|} |f(Wx) - f(Wx')| \\ &\leq \frac{1}{\|W\|} \|Wx - Wx'\| \quad \text{by 1-Lipschitzness of } f \\ &= \frac{1}{\|W\|} \|W(x - x')\| \end{aligned}$$

<sup>5</sup>Examples include the operator norm or the Euclidean norm.

<sup>6</sup>Note that these theoretical results also hold when  $b(X)$  has a bias term.

$$\begin{aligned} &\leq \frac{1}{\|W\|} \cdot \|W\| \cdot \|x - x'\| \\ &= \|x - x'\|. \end{aligned}$$

Thus,

$$\begin{aligned} |\mathbb{E}[f(b(X))|T = 1] - \mathbb{E}[f(b(X))|T = 0]| &= \|W\| \cdot |\mathbb{E}[g(X)|T = 1] - \mathbb{E}[g(X)|T = 0]| \\ &\leq \|W\| \cdot \text{Wass}(P(X|T = 1), P(X|T = 0)). \end{aligned}$$

It follows that

$$\text{Wass}(P(b(X)|T = 1), P(b(X)|T = 0)) \leq \|W\| \cdot \text{Wass}(P(X|T = 1), P(X|T = 0)).$$

- Now, let  $f$  is a 1-Lipschitz real-valued function on  $\mathcal{X}$ . then

$$\begin{aligned}\mathbb{E}[f(X)|T=t] &= \mathbb{E}[\mathbb{E}[f(X)|b(X), T=t] \mid T=t] \text{ due to the law of total expectation} \\ &= \mathbb{E}[\mathbb{E}[f(X)|b(X)] \mid T=t] \text{ due to Equation (S3)} \\ &= \|\|W^+\|\| \cdot \mathbb{E}[g(b(X)) \mid T=t],\end{aligned}$$

where  $g(\beta) := \frac{1}{\|\|W^+\|\|} \mathbb{E}[f(X)|b(X) = \beta]$  is a real-valued 1-Lipschitz function of the  $\mathcal{B}$  space. Then, for any  $\beta, \beta'$ ,

$$\begin{aligned}|g(\beta) - g(\beta')| &= \frac{1}{\|\|W^+\|\|} \cdot \left| \mathbb{E}[f(X) \mid WX = \beta] - \mathbb{E}[f(X) \mid WX = \beta'] \right| \\ &= \frac{1}{\|\|W^+\|\|} \cdot \left| \mathbb{E}[f(W^+\beta + U) \mid WU = \mathbf{0}] - \mathbb{E}[f(W^+\beta' + U) \mid WU = \mathbf{0}] \right| \\ &= \frac{1}{\|\|W^+\|\|} \cdot \left| \mathbb{E}[f(W^+\beta + U) - f(W^+\beta' + U) \mid WU = \mathbf{0}] \right| \\ &\leq \frac{1}{\|\|W^+\|\|} \cdot \mathbb{E}\left[|f(W^+\beta + U) - f(W^+\beta' + U)| \mid WU = \mathbf{0}\right] \text{ Jensen's inequality} \\ &\leq \frac{1}{\|\|W^+\|\|} \cdot \mathbb{E}\left[\|(W^+\beta + U) - (W^+\beta' + U)\| \mid WU = \mathbf{0}\right] \text{ by 1-Lipschitzness of } f \\ &= \frac{1}{\|\|W^+\|\|} \cdot \mathbb{E}\left[\|W^+(\beta - \beta')\| \mid WU = \mathbf{0}\right] \\ &= \frac{1}{\|\|W^+\|\|} \cdot \|W^+(\beta - \beta')\| \\ &\leq \frac{1}{\|\|W^+\|\|} \cdot \|\|W^+\|\| \cdot \|\beta - \beta'\| \\ &= \|\beta - \beta'\|,\end{aligned}$$

where the second equality follows from the fact that  $Wx = \beta$  iff there exists  $u$  such that  $Wu = \mathbf{0}$  and  $x = W^+\beta + u$ . Thus, for any 1-Lipschitz real-valued function  $f$  of  $\mathbf{x}$ ,

$$\begin{aligned}|\mathbb{E}[f(X)|T=1] - \mathbb{E}[f(X)|T=0]| &= \|\|W^+\|\| \cdot \left| \mathbb{E}[g(b(X))|T=1] - \mathbb{E}[g(b(X))|T=0] \right| \\ &\leq \|\|W^+\|\| \cdot \text{Wass}(P(b(X)|T=1), P(b(X)|T=0)).\end{aligned}$$

Therefore,

$$\text{Wass}(P(X|T=1), P(X|T=0)) \leq \|\|W^+\|\| \cdot \text{Wass}(P(b(X)|T=1), P(b(X)|T=0)).$$

- For MMD, note that for any random variable  $V$  :

$$\begin{aligned}\text{MMD}(P(V|T=1), P(V|T=0)) &= \sup_{\alpha \in \mathbb{R}^{\dim(V)}, \|\alpha\| \leq 1} \left| \mathbb{E}[a^T V | T=1] - \mathbb{E}[a^T V | T=0] \right| \\ &= \|\mathbb{E}[V|T=1] - \mathbb{E}[V|T=0]\| \end{aligned}$$

- We note that

$$\begin{aligned}\text{MMD}(P(b(X) \mid T=1), P(b(X) \mid T=0)) &= \|\mathbb{E}[b(X)|T=1] - \mathbb{E}[b(X)|T=0]\| \\ &= \|\mathbb{E}[WX|T=1] - \mathbb{E}[WX|T=0]\| \\ &= \|\mathbb{E}[W(\mathbb{E}[X|T=1] - \mathbb{E}[X|T=0])]\| \\ &\leq \|\|W\|\| \cdot \|\mathbb{E}[X|T=1] - \mathbb{E}[X|T=0]\| \\ &= \|\|W\|\| \cdot \text{MMD}(P(X \mid T=1), P(X \mid T=0))\end{aligned}$$



- We have

$$\begin{aligned}\mathbb{E}[X|T=t] &= \mathbb{E}[\mathbb{E}[X|b(X), T=t] \mid T=t] \text{ due to the law of total expectation} \\ &= \mathbb{E}[\mathbb{E}[X|b(X)] \mid T=t] \text{ due to Equation (S3)} \\ &= \mathbb{E}[g(b(X)) \mid T=t],\end{aligned}$$

where  $g(\beta) := \mathbb{E}[X|b(X) = \beta]$  is such that

$$\begin{aligned}g(\beta) &= \mathbb{E}[X|WX = \beta] \\ &= \mathbb{E}[W^+\beta + U|WU = \mathbf{0}] \text{ as } \forall W, x, \beta, \quad Wx = \beta \iff \exists u, Wu = \mathbf{0}, x = W^+\beta + u \\ &= W^+\beta + \mathbb{E}[U|WU = \mathbf{0}].\end{aligned}$$

Thus,

$$\begin{aligned}\mathbb{E}[X|T=t] &= \mathbb{E}[g(b(X)) \mid T=t] \\ &= \mathbb{E}[W^+b(X) + \mathbb{E}[U|WU = \mathbf{0}] \mid T=t] \\ &= W^+\mathbb{E}[b(X) \mid T=t] + \mathbb{E}[U|WU = \mathbf{0}].\end{aligned}$$

Then,

$$\begin{aligned}\text{MMD}(P(X \mid T=1), P(X \mid T=0)) &= \|\mathbb{E}[X|T=1] - \mathbb{E}[X|T=0]\| \\ &= \|(W^+\mathbb{E}[b(X) \mid T=1] + \mathbb{E}[U|WU = \mathbf{0}]) - (W^+\mathbb{E}[b(X) \mid T=0] + \mathbb{E}[U|WU = \mathbf{0}])\| \\ &= \|W^+(\mathbb{E}[b(X) \mid T=1] - \mathbb{E}[b(X) \mid T=0])\| \\ &\leq \| \|W^+\| \cdot \|\mathbb{E}[b(X)|T=1] - \mathbb{E}[b(X)|T=0]\| \\ &= \| \|W^+\| \cdot \text{MMD}(P(b(X) \mid T=1), P(b(X) \mid T=0))\|.\end{aligned}$$

□

**Proposition 6.** Let  $h^{(l)}$  ( $l = 1, \dots, L$ ) be a bi-Lipschitz function, i.e. an invertible multivariate function such that for any  $b, b'$  in the input space of  $h^{(l)}$  and appropriate real-valued constants  $m^{(l)}$  and  $M^{(l)}$ :

$$m^{(l)}\|b - b'\| \leq \|h^{(l)}(b) - h^{(l)}(b')\| \leq M^{(l)}\|b - b'\|$$

Let  $(b^{(l)})$  be a sequence of functions of the  $\mathcal{X}$ -space such that every  $b^{(l)}(X)$  is a balancing score, and for any  $x \in \mathcal{X}$ ,

$$\begin{aligned}b^{(0)}(x) &:= x, \\ b^{(l)}(x) &:= W^{(l)}h^{(l)}(b^{(l-1)}(x)). \quad \forall l \geq 1.\end{aligned}$$

Let  $\|\cdot\|$  be the Euclidean norm on any vector space,  $\|\|\cdot\|\|$  be a norm on any matrix space such that  $\forall \mathbf{x}, A, \|A\mathbf{x}\| \leq \|\|A\|\| \cdot \|\mathbf{x}\|$ ,  $A^+$  be the Moore-Penrose pseudo-inverse of  $A$ , and  $W_{\text{ass}}$  be the Wasserstein distance. Then,

$$\begin{aligned}\alpha_L \cdot W_{\text{ass}}(P(b^{(L)}(X) \mid T=1), P(b^{(L)}(X) \mid T=0)) \\ \leq W_{\text{ass}}(P(X \mid T=1), P(X \mid T=0)) \\ \leq \beta_L \cdot W_{\text{ass}}(P(b^{(L)}(X) \mid T=1), P(b^{(L)}(X) \mid T=0))\end{aligned}$$

with

$$\alpha_L = \frac{1}{\prod_{l=1}^L \|\|W^{(l)}\|\| \cdot \prod_{l=1}^L M^{(l)}} \text{ and } \beta_L = \frac{\prod_{l=1}^L \|\|W^{(l)+}\|\|}{\prod_{l=1}^L m^{(l)}}.$$

*Proof.* We prove the Proposition by induction:

- $L = 0$  is trivial, following from the equality of Wass ( $P(X | T = 1), P(X | T = 0)$ ) with itself.
- For any real-valued 1-Lipschitz function  $f$  on the  $\mathcal{B}^{(L+1)}$  space of  $b^{(L+1)}(X)$  such that  $\|f\|_{L^\infty} < 1$ :

$$\begin{aligned} & |\mathbb{E}[f(b^{(L+1)}(X))|T=1] - \mathbb{E}[f(b^{(L+1)}(X))|T=0]| \\ &= \|\|W^{(L+1)}\|\| \cdot M^{(L+1)} \cdot |\mathbb{E}[g(b^{(L)}(X))|T=1] - \mathbb{E}[g(b^{(L)}(X))|T=0]| \\ &\leq \|\|W^{(L+1)}\|\| \cdot M^{(L+1)} \cdot \text{Wass}(P(g(b^{(L)}(X))|T=1), P(g(b^{(L)}(X))|T=0)), \end{aligned}$$

where  $g(b) = \frac{1}{\|\|W^{(L+1)}\|\| \cdot M^{(L+1)}} f(W^{(L+1)}h^{(L+1)}(b))$  is a 1-Lipschitz real-valued function on the  $\mathcal{B}^{(L)}$ -space. For any  $b, b'$ ,

$$\begin{aligned} & |g(b) - g(b')| \\ &= \frac{1}{\|\|W^{(L+1)}\|\| \cdot M^{(L+1)}} \left| f(W^{(L+1)}h^{(L+1)}(b)) - f(W^{(L+1)}h^{(L+1)}(b')) \right| \\ &\leq \frac{1}{\|\|W^{(L+1)}\|\| \cdot M^{(L+1)}} \left\| W^{(L+1)}h^{(L+1)}(b) - W^{(L+1)}h^{(L+1)}(b') \right\| \quad \text{by 1-Lipschitzness of } f \\ &= \frac{1}{\|\|W^{(L+1)}\|\| \cdot M^{(L+1)}} \left\| W^{(L+1)}(h^{(L+1)}(b) - h^{(L+1)}(b')) \right\| \\ &\leq \frac{1}{\|\|W^{(L+1)}\|\| \cdot M^{(L+1)}} \cdot \|\|W^{(L+1)}\|\| \cdot \|h^{(L+1)}(b) - h^{(L+1)}(b')\| \\ &= \frac{1}{M^{(L+1)}} \cdot \|h^{(L+1)}(b) - h^{(L+1)}(b')\| \\ &\leq \frac{1}{M^{(L+1)}} \cdot M^{(L+1)} \cdot \|b - b'\| \quad \text{by } M^{(L+1)}\text{-Lipschitzness of } h^{(L+1)}. \\ &= \|b - b'\|. \end{aligned}$$

This leads to

$$\begin{aligned} & \text{Wass}(P(b^{(L+1)}(X)|T=1), P(b^{(L+1)}(X)|T=0)) \\ &\leq \|\|W^{(L+1)}\|\| \cdot M^{(L+1)} \cdot \text{Wass}(P(b^{(L)}(X)|T=1), P(b^{(L)}(X)|T=0)) \\ &= \|\|W^{(L+1)}\|\| \cdot M^{(L+1)} \cdot \prod_{l=1}^L \|\|W^{(l)}\|\| \cdot \prod_{l=1}^L M^{(l)} \cdot \text{Wass}(P(X | T=1), P(X | T=0)) \\ &\quad \text{as the theorem is true for } L \\ &= \prod_{l=1}^{L+1} \|\|W^{(l)}\|\| \cdot \prod_{l=1}^{L+1} M^{(l)} \cdot \text{Wass}(P(X | T=1), P(X | T=0)). \end{aligned}$$

- We note that  $b^{(L+1)}(X)$  is a balancing score of  $b^{(L)}(X)$ , i.e.

$$T \perp\!\!\!\perp b^{(L)}(X) | b^{(L+1)}(X),$$

which ensures that for any measurable function  $f$  :

$$\mathbb{E}[f(b^{(L)}(X))|b^{(L+1)}(X), T] = \mathbb{E}[f(b^{(L)}(X))|b^{(L+1)}(X)] \quad (\text{S6})$$

Then, if  $h$  is a 1-Lipschitz real-valued function on the  $\mathcal{B}^{(L)}$  space then

$$\begin{aligned} \mathbb{E}[f(b^{(L)}(X))|T=t] &= \mathbb{E}[\mathbb{E}[f(b^{(L)}(X))|b^{(L+1)}(X), T=t] \mid T=t] \quad \text{due to the law of total expectation} \\ &= \mathbb{E}[\mathbb{E}[f(b^{(L)}(X))|b^{(L+1)}(X)] \mid T=t] \quad \text{due to Equation (S6)} \\ &= \frac{\|\|W^{(L+1)}\|\|}{m^{(L+1)}} \cdot \mathbb{E}[g(b^{(L)}(X)) \mid T=t], \end{aligned}$$

where  $g(\beta) := \frac{m^{(L+1)}}{\|\|W^{(L+1)}\|\|} \mathbb{E}[g(b^{(L)}(X))|b^{(L+1)}(X) = \beta]$  is a real-valued 1-Lipschitz function of the  $\mathcal{B}^{(L+1)}$  space. Indeed, for any  $\beta, \beta'$ ,

$$|g(\beta) - g(\beta')|$$

$$\begin{aligned}
 &= \frac{m^{(L+1)}}{\|W^{(L+1)+}\|} \cdot \left| \mathbb{E}[f(b^{(L)}(X)) \mid W^{(L+1)}h^{(L+1)}(b^{(L)}(X)) = \beta] \right. \\
 &\quad \left. - \mathbb{E}[f(b^{(L)}(X)) \mid W^{(L+1)}h^{(L+1)}(b^{(L)}(X)) = \beta'] \right| \\
 &= \frac{m^{(L+1)}}{\|W^{(L+1)+}\|} \cdot \left| \mathbb{E}[f(b^{(L)}(X)) \mid h^{(L+1)}(b^{(L)}(X)) = W^{(L+1)+}\beta + U, \quad W^{(L+1)}U = \mathbf{0}] \right. \\
 &\quad \left. - \mathbb{E}[f(b^{(L)}(X)) \mid h^{(L+1)}(b^{(L)}(X)) = W^{(L+1)+}\beta' + U, \quad W^{(L+1)}U = \mathbf{0}] \right| \\
 &\quad \text{as } \forall W, y, \beta, \quad Wy = \beta \iff \exists u, Wu = \mathbf{0}, y = W^+\beta + u \\
 &= \frac{m^{(L+1)}}{\|W^{(L+1)+}\|} \cdot \left| \mathbb{E}[f(b^{(L)}(X)) \mid b^{(L)}(X) = h^{(L+1),-1}(W^{(L+1)+}\beta + U), \quad W^{(L+1)}U = \mathbf{0}] \right. \\
 &\quad \left. - \mathbb{E}[f(b^{(L)}(X)) \mid b^{(L)}(X) = h^{(L+1),-1}(W^{(L+1)+}\beta' + U), \quad W^{(L+1)}U = \mathbf{0}] \right| \\
 &\quad \text{as } h^{(L+1)} \text{ is invertible, with inverse } h^{(L+1),-1} \\
 &= \frac{m^{(L+1)}}{\|W^{(L+1)+}\|} \cdot \left| \mathbb{E}[f(h^{(L+1),-1}(W^{(L+1)+}\beta + U)) \mid W^{(L+1)}U = \mathbf{0}] \right. \\
 &\quad \left. - \mathbb{E}[f(h^{(L+1),-1}(W^{(L+1)+}\beta' + U)) \mid W^{(L+1)}U = \mathbf{0}] \right| \\
 &= \frac{m^{(L+1)}}{\|W^{(L+1)+}\|} \cdot \left| \mathbb{E}[f(h^{(L+1),-1}(W^{(L+1)+}\beta + U)) - f(h^{(L+1),-1}(W^{(L+1)+}\beta' + U)) \mid W^{(L+1)}U = \mathbf{0}] \right| \\
 &= \frac{m^{(L+1)}}{\|W^{(L+1)+}\|} \cdot \mathbb{E}[|f(h^{(L+1),-1}(W^{(L+1)+}\beta + U)) - f(h^{(L+1),-1}(W^{(L+1)+}\beta' + U))| \mid W^{(L+1)}U = \mathbf{0}] \\
 &\quad \text{according to Jensen's inequality} \\
 &= \frac{m^{(L+1)}}{\|W^{(L+1)+}\|} \cdot \mathbb{E}[\|h^{(L+1),-1}(W^{(L+1)+}\beta + U) - h^{(L+1),-1}(W^{(L+1)+}\beta' + U)\| \mid W^{(L+1)}U = \mathbf{0}] \\
 &\quad \text{by 1-Lipschitzness of } h^{(L+1),-1} \\
 &= \frac{m^{(L+1)}}{\|W^{(L+1)+}\|} \cdot \frac{1}{m^{(L+1)}} \cdot \mathbb{E}[\|W^{(L+1)+}\beta + U - W^{(L+1)+}\beta' + U\| \mid W^{(L+1)}U = \mathbf{0}] \\
 &\quad \text{by } \frac{1}{m^{(L+1)}}\text{-Lipschitzness of } f \\
 &= \frac{1}{\|W^{(L+1)+}\|} \cdot \mathbb{E}[\|W^{(L+1)+}(\beta - \beta')\| \mid WU = \mathbf{0}] \\
 &= \frac{1}{\|W^{(L+1)+}\|} \cdot \|W^{(L+1)+}(\beta - \beta')\| \\
 &\leq \frac{1}{\|W^{(L+1)+}\|} \cdot \|W^{(L+1)+}\| \cdot \|\beta - \beta'\| \\
 &= \|\beta - \beta'\|
 \end{aligned}$$

Thus, for any 1-Lipschitz real-valued function  $f$  of the  $\mathcal{B}^{(L)}$ -space,

$$\begin{aligned}
 &|\mathbb{E}[f(b^{(L)}(X))|T = 1] - \mathbb{E}[f(b^{(L)}(X))|T = 0]| \\
 &= \frac{\|W^{(L+1)+}\|}{m^{(L+1)}} \cdot |\mathbb{E}[g(b^{(L+1)}(X))|T = 1] - \mathbb{E}[g(b^{(L+1)}(X))|T = 0]| \\
 &\quad \text{for some 1-Lipschitz real-valued function } g \text{ on the } \mathcal{B}^{(L+1)} \text{ space} \\
 &\leq \frac{\|W^{(L+1)+}\|}{m^{(L+1)}} \cdot \text{Wass}(P(b^{(L+1)}(X)|T = 1), P(b^{(L+1)}(X)|T = 0)).
 \end{aligned}$$

Therefore,

$$\text{Wass}(P(b^{(L)}(X)|T = 1), P(b^{(L)}(X)|T = 0))$$

$$\leq \frac{\|W^{(L+1)+}\|}{m^{(L+1)}} \cdot \text{Wass}(P(b^{(L+1)}(X)|T=1), P(b^{(L+1)}(X)|T=0)),$$

which leads to

$$\begin{aligned} & \text{Wass}(P(b^{(L+1)}(X)|T=1), P(b^{(L+1)}(X)|T=0)) \\ & \geq \frac{m^{(L+1)}}{\|W^{(L+1)+}\|} \cdot \text{Wass}(P(b^{(L)}(X)|T=1), P(b^{(L)}(X)|T=0)) \\ & \geq \frac{m^{(L+1)}}{\|W^{(L+1)+}\|} \cdot \frac{\prod_{l=1}^L m^{(l)}}{\prod_{l=1}^L \|W^{(l)+}\|} \cdot \text{Wass}(P(X|T=1), P(X|T=0)) \quad \text{as the theorem is true for } L \\ & = \frac{\prod_{l=1}^{L+1} m^{(l)}}{\prod_{l=1}^{L+1} \|W^{(l)+}\|} \cdot \text{Wass}(P(X|T=1), P(X|T=0)). \end{aligned}$$

- Concluding, we showed that the Theorem is true for  $L=0$ , and if the theorem is true for  $L$ , it is true for  $L+1$ . This proves the theorem by induction for any  $L$ .

□

#### A.4 Bounds For Non-Balancing Scores

**Proposition 7.** *Let*

$$\mathcal{E}_{t,b}^D(\beta) := D(P(X|b(X)=\beta, T=t), P(X|b(X)=\beta))$$

where  $D$  is a probability discrepancy measure,  $b$  is a function of  $X$ ,  $t \in \{0, 1\}$  is a realisation of  $T$ ,  $\beta$  is a realisation of  $b(X)$ . For any function  $b$ ,

$$\begin{aligned} & TV(P(b(X)|T=1), P(b(X)|T=0)) \\ & \leq TV(P(X|T=1), P(X|T=0)) \\ & \leq TV(P(b(X)|T=1), P(b(X)|T=0)) \\ & \quad + \mathbb{E}[\mathcal{E}_{1,b}^{TV}(b(X))|T=1] + \mathbb{E}[\mathcal{E}_{0,b}^{TV}(b(X))|T=0] \end{aligned}$$

For a linear function  $b(x) = Wx$ ,

$$\begin{aligned} & \frac{1}{\|W\|} \cdot \text{Wass}(P(b(X)|T=1), P(b(X)|T=0)) \\ & \leq \text{Wass}(P(X|T=1), P(X|T=0)) \\ & \leq \|W^+\| \cdot \text{Wass}(P(b(X)|T=1), P(b(X)|T=0)) \\ & \quad + \mathbb{E}[\mathcal{E}_{1,b}^{\text{Wass}}(b(X))|T=1] + \mathbb{E}[\mathcal{E}_{0,b}^{\text{Wass}}(b(X))|T=0] \end{aligned}$$

and

$$\begin{aligned} & \frac{1}{\|W\|} \cdot \text{MMD}(P(b(X)|T=1), P(b(X)|T=0)) \\ & \leq \text{MMD}(P(X|T=1), P(X|T=0)) \\ & \leq \|W^+\| \cdot \text{MMD}(P(b(X)|T=1), P(b(X)|T=0)) \\ & \quad + \mathbb{E}[\mathcal{E}_{1,b}^{\text{MMD}}(b(X))|T=1] + \mathbb{E}[\mathcal{E}_{0,b}^{\text{MMD}}(b(X))|T=0] \end{aligned}$$

For a function  $b^{(L)}$  as in Proposition 6,

$$\alpha_L \cdot \text{Wass}(P(b^{(L)}(X)|T=1), P(b^{(L)}(X)|T=0))$$

$$\begin{aligned}
 &\leq W_{\text{ass}}(P(X | T = 1), P(X | T = 0)) \\
 &\leq \beta_L \cdot W_{\text{ass}}(P(b^{(L)}(X) | T = 1), P(b^{(L)}(X) | T = 0)) \\
 &\quad + \mathbb{E}[\mathcal{E}_{1, b^{(L)}}^{\text{Wass}}(b^{(L)}(X)) | T = 1] \\
 &\quad + \mathbb{E}[\mathcal{E}_{0, b^{(L)}}^{\text{Wass}}(b^{(L)}(X)) | T = 0]
 \end{aligned}$$

*Proof.* The lower bounds were established in the previous Proposition, while the upper bounds follow as a corollary of the following two Propositions.  $\square$

**Proposition 8.** *Let  $b$  a function of  $X$ ,  $\mathcal{F}$  a class of functions of  $X$ ,  $IPM_{\mathcal{F}}$  the associated integral probability metric. Assume that for some constant  $C_b$  depending on  $b$ :*

$$\forall f \in \mathcal{F}, \left| \mathbb{E}[\mathbb{E}[f(X)|b(X)] | T = 1] - \mathbb{E}[\mathbb{E}[f(X)|b(X)] | T = 0] \right| \leq C_b \cdot IPM_{\mathcal{F}}(P(b(X)|T = 1), P(b(X)|T = 0)) \quad (\text{S7})$$

Then, letting  $\mathcal{E}_{t,b}^D(\beta) = D(P(X|b(X) = \beta, T = t), P(X|b(X) = \beta))$  where  $D$  is a probability distance, we have

$$\begin{aligned}
 IPM_{\mathcal{F}}(P(X|T = 1), P(X|T = 0)) &\leq C_b \cdot IPM_{\mathcal{F}}(P(b(X)|T = 1), P(b(X)|T = 0)) \\
 &\quad + \mathbb{E}[\mathcal{E}_{1,b}^{IPM_{\mathcal{F}}}(b(X)) | T = 1] + \mathbb{E}[\mathcal{E}_{0,b}^{IPM_{\mathcal{F}}}(b(X)) | T = 0]
 \end{aligned}$$

*Proof.* Denote  $\Delta_t(\beta; f) := \mathbb{E}[f(X)|b(X) = \beta, T = t] - \mathbb{E}[f(X)|b(X) = \beta]$ , so that  $\mathcal{E}_{t,b}^{IPM_{\mathcal{F}}}(\beta) = \sup_{f \in \mathcal{F}} |\Delta_t(\beta; f)|$ .

We fix  $f \in \mathcal{F}$ , noting that

$$\begin{aligned}
 \mathbb{E}[f(X)|T = t] &= \mathbb{E}[\mathbb{E}[f(X)|b(X), T = t] | T = t] \text{ due to the law of total expectation} \\
 &= \mathbb{E}[\Delta_t(b(X); f) + \mathbb{E}[f(X)|b(X)] | T = t] \\
 &= \mathbb{E}[\Delta_t(b(X); f) | T = t] + \mathbb{E}[\mathbb{E}[f(X)|b(X)] | T = t].
 \end{aligned}$$

As a consequence,

$$\begin{aligned}
 &\left| \mathbb{E}[f(X)|T = 1] - \mathbb{E}[f(X)|T = 0] \right| \\
 &= \left| \mathbb{E}[\mathbb{E}[f(X)|b(X)] | T = 1] - \mathbb{E}[\mathbb{E}[f(X)|b(X)] | T = 0] + \mathbb{E}[\Delta_1(b(X); f) | T = 1] \right. \\
 &\quad \left. - \mathbb{E}[\Delta_0(b(X); f) | T = 0] \right| \\
 &\leq \left| \mathbb{E}[\mathbb{E}[f(X)|b(X)] | T = 1] - \mathbb{E}[\mathbb{E}[f(X)|b(X)] | T = 0] \right| + \left| \mathbb{E}[\Delta_1(b(X); f) | T = 1] \right| \\
 &\quad + \left| \mathbb{E}[\Delta_0(b(X); f) | T = 0] \right|,
 \end{aligned}$$

where

$$\left| \mathbb{E}[\mathbb{E}[f(X)|b(X)] | T = 1] - \mathbb{E}[\mathbb{E}[f(X)|b(X)] | T = 0] \right| \leq C_b \cdot IPM_{\mathcal{F}}(P(b(X)|T = 1), P(b(X)|T = 0))$$

by assumption

and, for  $t \in \{0, 1\}$ ,

$$\begin{aligned}
 \left| \mathbb{E}[\Delta_t(b(X); f) | T = t] \right| &\leq \mathbb{E}[|\Delta_t(b(X); f)| | T = t] \\
 &\leq \mathbb{E}[\sup_{f \in \mathcal{F}} |\Delta_t(b(X); f)| | T = t] \\
 &= \mathbb{E}[\mathcal{E}_{t,b}^{IPM_{\mathcal{F}}}(b(X)) | T = t].
 \end{aligned}$$

Thereby, for any  $f \in \mathcal{F}$ ,

$$\left| \mathbb{E}[f(X)|T = 1] - \mathbb{E}[f(X)|T = 0] \right| \leq C_b \cdot IPM_{\mathcal{F}}(P(b(X)|T = 1), P(b(X)|T = 0))$$

$$+ \mathbb{E}[\mathcal{E}_{1,b}^{IPM\mathcal{F}}(b(X))|T=1] + \mathbb{E}[\mathcal{E}_{0,b}^{IPM\mathcal{F}}(b(X))|T=0].$$

Taking the supremum over  $f \in \mathcal{F}$  yields the desired result.  $\square$

Then, Proposition 7 follows as the proofs of Propositions 1 and 5 directly show that Equation (S7) follows for their respective classes of functions and balancing scores. One case is not trivial: generalising Proposition 6 to Equation (S7). To prove that Equation (S7) also is verified in this case, we prove the following Proposition that also can be used as an alternative proof for Proposition 6.

**Proposition 9.** *Let  $h^{(l)}$  ( $l \geq 1$ ) be a bi-Lipschitz function, i.e. an invertible multivariate function such that for any  $b, b'$  in the input space of  $h^{(l)}$  :*

$$m^{(l)}\|b - b'\| \leq \|h^{(l)}(b) - h^{(l)}(b')\| \leq M^{(l)}\|b - b'\|$$

Let  $(b^{(l)})$  a sequence of functions of the  $\mathcal{X}$ -space such that every  $b^{(l)}(X)$  is a balancing score w.r.t.  $T$  and for any  $x$ ,

$$\begin{aligned} b^{(0)}(x) &:= x, \\ b^{(l)}(x) &:= W^{(l)}h^{(l)}(b^{(l-1)}(x)). \quad \forall l \geq 1 \end{aligned}$$

Let  $\|\cdot\|$  be the Euclidean norm on any vector space,  $\|\cdot\|$  be a norm on any matrix space such that  $\forall x, A, \|Ax\| \leq \|A\| \cdot \|x\|$ ,  $A^+$  be the Moore-Penrose pseudo-inverse of  $A$ ,  $W$  be the Wasserstein distance.

Then for any  $L \geq 0$ , if a function  $f$  of  $X$  is 1-Lipschitz then,  $g_h^{(L)}(\beta) := \mathbb{E}[f(X)|b^{(L)}(X) = \beta]$  is Lipschitz with constant  $\frac{\prod_{l=1}^L \|W^{(l)+}\|}{\prod_{l=1}^L m^{(l)}}$ .

*Proof.* We prove this Proposition by induction:

- It is true for  $L = 0$  as  $g_h^{(0)}(\beta) := \mathbb{E}[f(X)|X = \beta] = f(\beta)$  and  $f$  is 1-Lipschitz by assumption.
- We prove it is true for  $L + 1$  if true for  $L$  :

$$\begin{aligned} g_h^{(L+1)}(\beta) &= \mathbb{E}[f(X)|b^{(L+1)}(X)] \\ &= \mathbb{E}[\mathbb{E}[f(X)|b^{(L)}(X), b^{(L+1)}(X) = \beta] \mid b^{(L+1)}(X) = \beta] \text{ by the law of total expectation} \\ &= \mathbb{E}[\mathbb{E}[f(X)|b^{(L)}(X)] \mid b^{(L+1)}(X) = \beta] \text{ as } X \perp\!\!\!\perp b^{(L+1)}(X) \mid b^{(L)}(X) \\ &= \mathbb{E}[g_h^{(L)}(b^{(L)}(X)) \mid W^{(L+1)}h^{(L+1)}(b^{(L)}(X)) = \beta] \\ &= \mathbb{E}[g_h^{(L)}(b^{(L)}(X)) \mid h^{(L+1)}(b^{(L)}(X)) = W^{(L+1)+}\beta + U, \quad W^{(L+1)}U = \mathbf{0}] \\ &\quad \text{as } \forall W, y, \beta, \quad Wy = \beta \iff \exists u, Wu = \mathbf{0}, y = W^+\beta + u \\ &= \mathbb{E}[g_h^{(L)}(b^{(L)}(X)) \mid b^{(L)}(X) = h^{(L+1),-1}(W^{(L+1)+}\beta + U), \quad W^{(L+1)}U = \mathbf{0}] \\ &\quad \text{as } h^{(L+1)} \text{ is invertible, with inverse } h^{(L+1),-1} \\ &= \mathbb{E}[g_h^{(L)}(h^{(L+1),-1}(W^{(L+1)+}\beta + U)) \mid W^{(L+1)}U = \mathbf{0}]. \end{aligned}$$

Thereby, for any  $\beta, \beta'$ ,

$$\begin{aligned} |g_h^{(L+1)}(\beta) - g_h^{(L+1)}(\beta')| &= \left| \mathbb{E}[g_h^{(L)}(h^{(L+1),-1}(W^{(L+1)+}\beta + U)) - g_h^{(L)}(h^{(L+1),-1}(W^{(L+1)+}\beta' + U)) \mid W^{(L+1)}U = \mathbf{0}] \right| \\ &\leq \mathbb{E} \left[ \left| g_h^{(L)}(h^{(L+1),-1}(W^{(L+1)+}\beta + U)) - g_h^{(L)}(h^{(L+1),-1}(W^{(L+1)+}\beta' + U)) \right| \mid W^{(L+1)}U = \mathbf{0} \right] \\ &\quad \text{thanks to Jensen's inequality} \end{aligned}$$

$$\begin{aligned}
 &\leq \frac{\prod_{l=1}^L \|W^{(l)+}\|}{\prod_{l=1}^L m^{(l)}} \cdot \mathbb{E} \left[ \left\| h^{(L+1),-1}(W^{(L+1)+}\beta + U) \right. \right. \\
 &\quad \left. \left. - h^{(L+1),-1}(W^{(L+1)+}\beta' + U) \right\| \mid W^{(L+1)U} = \mathbf{0} \right] \\
 &\quad \text{as } g_h^{(L)} \text{ is } \frac{\prod_{l=1}^L \|W^{(l)+}\|}{\prod_{l=1}^L m^{(l)}} \text{-Lipschitz by assumption} \\
 &\leq \frac{\prod_{l=1}^L \|W^{(l)+}\|}{\prod_{l=1}^L m^{(l)}} \cdot \frac{1}{m^{(L+1)}} \cdot \mathbb{E} \left[ \left\| (W^{(L+1)+}\beta + U) - (W^{(L+1)+}\beta' + U) \right\| \mid W^{(L+1)U} = \mathbf{0} \right] \\
 &\quad \text{as } h^{(L+1),-1} \text{ is } \frac{1}{m^{(L+1)}} \text{-Lipschitz by assumption} \\
 &= \frac{\prod_{l=1}^L \|W^{(l)+}\|}{\prod_{l=1}^L m^{(l)}} \cdot \frac{1}{m^{(L+1)}} \cdot \mathbb{E} \left[ \left\| W^{(L+1)+}(\beta - \beta') \right\| \mid W^{(L+1)U} = \mathbf{0} \right] \\
 &= \frac{\prod_{l=1}^L \|W^{(l)+}\|}{\prod_{l=1}^L m^{(l)}} \cdot \frac{1}{m^{(L+1)}} \cdot \left\| W^{(L+1)+}(\beta - \beta') \right\| \\
 &\leq \frac{\prod_{l=1}^L \|W^{(l)+}\|}{\prod_{l=1}^L m^{(l)}} \cdot \frac{\|W^{(L+1)+}\|}{m^{(L+1)}} \cdot \|\beta - \beta'\| \quad \text{by sub-multiplicativity of the matrix norm} \\
 &= \frac{\prod_{l=1}^{L+1} \|W^{(l)+}\|}{\prod_{l=1}^{L+1} m^{(l)}} \cdot \|\beta - \beta'\|,
 \end{aligned}$$

which proves the Proposition for  $L + 1$ , completing the proof (of Proposition 9).

To prove Proposition 7 from this result, Equation (S7) is true for  $b^{(L)}(X)$  with  $C_b = \frac{\prod_{l=1}^L \|W^{(l)+}\|}{\prod_{l=1}^L m^{(l)}}$ . □

## B A FEW NOTES ABOUT COMPUTATIONAL COMPLEXITIES OF BOUNDS

**Computational complexity of bounds in Proposition 5** Denoting  $N := \max\{N_t, N_c\}$ , the computational complexity of the linear MMD estimator is in  $\mathcal{O}(ND)$ , and the computational complexity of the the Wasserstein distance estimator is in  $\mathcal{O}(N^2D + N^3 \log N + N^3 \log D)$  when using the auction algorithm (Peyré and Cuturi, 2020; Bertsekas, 1998). As a result, assuming the balancing score is of dimension  $d \ll D$  and that we have already computed to the ground-truth balancing scores, these complexities can be decreased to  $\mathcal{O}(Nd + Dd^2)$  and  $\mathcal{O}(N^2d + N^3 \log N + N^3 \log d + Dd^2)$ , respectively, as the computation of the singular value decomposition has a complexity  $\mathcal{O}(Dd^2)$  (Vasudevan and Ramakrishna, 2017). If we must further compute the balancing scores, we increase computational complexity by a term  $\mathcal{O}(NDd)$  due to the additional matrix multiplication operations. When  $D \sim N$ , this does not change the usefulness of dimensionality reduction for computational complexity. These results assume that covariates and balancing scores are bounded in expectation. We refer to the following paragraph for a more general discussion about the computational complexity of the Wasserstein distance.

**Computational complexity of Wasserstein distance** More precisely, the computational complexity of the Wasserstein distance is  $\mathcal{O}(N^2D + \min\{N^3 \log C_{\infty, X}, N^2 C_{\infty, X}^2 \log N\})$ , where the first term corresponds to computing the  $L_1$  distance matrix wrt  $X$ , and the second term corresponds to the minimum of the computational complexities of the auction algorithm (Peyré and Cuturi, 2020; Bertsekas, 1998) and Sinkhorn’s algorithm (Dvurechensky et al., 2018), assuming we choose the algorithm with the lowest complexity.  $C_{\infty, X}$  is an upper bound of the maximal value of the distance matrix wrt  $X$  and can further depend on  $N$  and  $D$ . If we assume covariates are bounded in expectation, then  $\mathbb{E}[C_{\infty, X}] = \mathcal{O}(ND)$ . Indeed, noting  $X_i$  covariates of treated units,  $X'_j$  those of control units,  $k$  the dimension index, we assume that covariates are bounded in expectation, meaning that  $\forall i, k, \mathbb{E}[|X_i^k|] < M$  and  $\forall j, k, \mathbb{E}[|X'_j{}^k|] < M$ . Then

$$\mathbb{E}[C_{\infty, X}] = \mathbb{E}[\max_{i,j} \|X_i - X'_j\|]$$

$$\begin{aligned}
 &= \mathbb{E}[\max_{i,j} \sum_{d=1}^D |X_i^k - X_j'^k|] \\
 &\leq \mathbb{E}[\sum_{d=1}^D \max_{i,j} |X_i^k - X_j'^k|] \\
 &\leq \mathbb{E}[\sum_{d=1}^D \max_{i,j} (|X_i^k| + |X_j'^k|)] \quad \text{by the triangle inequality} \\
 &= \mathbb{E}[\sum_{d=1}^D (\max_i |X_i^k| + \max_j |X_j'^k|)] \\
 &= \sum_{d=1}^D \mathbb{E}[\max_i |X_i^k| + \max_j |X_j'^k|] \\
 &\leq \sum_{d=1}^D \mathbb{E}[\sum_i |X_i^k| + \sum_j |X_j'^k|] \\
 &= \sum_{d=1}^D (\sum_i \mathbb{E}[|X_i^k|] + \sum_j \mathbb{E}[|X_j'^k|]) \\
 &\leq D \cdot (N_t + N_c) \cdot M
 \end{aligned}$$

which gives a  $\mathcal{O}(ND)$  bound. Substituting this into the computational complexities above, the auction algorithm might be preferable with a complexity of  $\mathcal{O}(N^3 \log N + N^3 \log D)$ , when  $D < N$ .

It is yet unclear whether the  $\mathcal{O}(ND)$  bound on  $C_{\infty, X}$  is tight. It might be tight in cases where covariate distributions are thick-tailed. We give a simple case where it is not tight wrt  $N$  but it is wrt  $D$ . Also this case shows that one might choose different algorithms depending on relationships between  $D$  (small or large) and  $N$ . We assume that  $\forall i, k, X_i^k \sim \mathcal{N}(0, 1)$  and  $\forall j, k, X_j'^k \sim \mathcal{N}(0, 1)$ .

$$\begin{aligned}
 \mathbb{E}[\max_{i,j} \|X_i - X_j'\|] &\geq \max_{i,j} \mathbb{E}[\|X_i - X_j'\|] \quad \text{by Jensen's inequality} \\
 &= \max_{i,j} \mathbb{E}[\sum_{d=1}^D |X_i^k - X_j'^k|] \\
 &= \max_{i,j} \sum_{d=1}^D \mathbb{E}[|X_i^k - X_j'^k|] \quad \text{where } X_i^k - X_j'^k \sim \mathcal{N}(0, 2) \\
 &= \max_{i,j} \sum_{d=1}^D \frac{2}{\sqrt{\pi}} \\
 &= D \cdot \frac{2}{\pi}.
 \end{aligned}$$

Remember that for any set of  $N'$  identically-distributed Gaussian r.v.s  $Y_i \sim \mathcal{N}(0, \sigma^2)$ ,  $i = 1, \dots, N'$ ,

$$\mathbb{E}[\max_i |Y_i|] \leq \sigma \sqrt{2 \log N'}$$

As a consequence,

$$\begin{aligned}
 \mathbb{E}[\max_{i,j} \|X_i - X_j'\|] &\leq \sum_{d=1}^D \mathbb{E}[\max_i |X_i^k| + \max_j |X_j'^k|] \quad \text{as before} \\
 &\leq \mathbb{E}[\sum_{d=1}^D (\sqrt{2 \log N_t} + \sqrt{2 \log N_c})] \quad \text{from the result above} \\
 &= D \cdot (\sqrt{2 \log N_t} + \sqrt{2 \log N_c})
 \end{aligned}$$



All of this shows that  $\mathbb{E}[C_{\infty, X}] = \Theta(D)$  if we ignore terms in  $N$ , and  $\mathbb{E}[C_{\infty, X}] = \mathcal{O}(D \cdot \sqrt{\log N})$  if we do not. Then it turns out that the complexity of the auction algorithm is in  $\mathcal{O}(N^3 \log D + N^3 \log \log N)$  and that of Sinkhorn’s algorithm is  $\mathcal{O}(N^2 D^2 \log^2 N)$ . In this case, the former is better when  $D \sim N$ , but the latter is preferable when  $D \ll N$ .

**Computational complexities of bounds in Proposition 6** When the balancing score takes the form  $b^{(L)}(X)$  of Proposition 6, the computational complexities of bounds increase with the number of layers  $L$ . Indeed, assuming every layer is of size  $D'$  with the exception of layer  $L$  which is of size  $d$ , we define the function  $c$  such that  $c(1) = Dd^2$  and

$$c(l) = \min(D'D^2, DD'^2) + (l-2)D'^3 + D'd^2$$

for  $l \geq 2$ , and the function  $c'$  such that  $c'(1) = Dd$  and

$$c'(l) = DD' + (l-2)D'^2 + D'd$$

for  $l \geq 2$ .  $c(L)$  represents the total computational complexity of all SVD operations, and  $c'(L)$  the total computational complexity of all matrix multiplications at a given example. Using similar arguments as before, the computational complexity of the MMD-imbalance of  $b^{(L)}(X)$  is in  $\mathcal{O}(Nd + c(L))$  the computational complexity of the Wass-imbalance of  $b^{(L)}(X)$  is in

$$\mathcal{O}(N^2 d + N^3 \log N + N^3 \log d + c(L)),$$

without computing balancing scores. If we do compute the balancing scores, this adds an extra  $\mathcal{O}(Nc'(L))$  term. Clearly, complexities of both measures increase with layer position  $L$ , especially if hidden layer size  $D'$  is large.

## C IMPLEMENTATION DETAILS

**ACIC 2016 Dataset.** This dataset is taken from the ACIC competition of 2016 (Dorie et al., 2017). Covariates were obtained from a study about developmental disorders, measuring data from pregnant women and their children. Treatment assignments and outcomes were synthetically generated from transformed versions of covariates using different data generating processes. Importantly, as treatments are synthetically generated, ground-truth propensity scores are made readily available, allowing us to compute calibration errors. We chose the provided data generating process setting number 4, which has polynomial treatment assignment, an exponential outcome model, 35% of treated units, full overlap, and high treatment heterogeneity. To preprocess the data, categorical covariates with  $F$  factors were converted to  $F - 1$  binary covariates, where the  $f$ -th binary covariate encodes factor  $f + 1$ . Due to high heterogeneity between subjects, we also centered and scaled continuous covariates to improve performance of all models. Binary covariates were left unprocessed. 4802 subjects were present in the dataset. The subjects have 82 covariates after preprocessing (23 continuous and 59 binary). In our experiments, we considered 100 versions of this dataset, each corresponding to a different random seed for the data generating process.

**News Dataset.** This dataset contains 5000 documents extracted from the NYT Corpus, where each of the 3477 covariates represents counts of a word in news articles. The treatment indicator  $T$  represents the use of a desktop ( $T = 0$ ) or a mobile device ( $T = 1$ ). The real-valued outcome  $Y$  measures the opinion of the reader about the news article. Both treatments and outcomes are generated using a data generating process. Here, 50 random seeds from the data generating process are considered. In contrast to ACIC 2016, we did not choose these random seeds ourselves as they were already provided by the original authors<sup>7</sup> (Johansson et al., 2016).

**IHDP Dataset.** For this dataset, covariates and treatment assignments are used from 747 subjects in real-world data of the Infant Health Development Program. Outcomes, however, are synthetically generated. We further apply the same scaling of outcomes as in Curth and Schaar (2021), as the absence of scaling led to a few outliers causing very high ATT errors in all methods, making comparisons very challenging. Here, 50 seeds from the data generating process are considered, directly used from the implementation of Dragonnet (Shi et al., 2019). 25 covariates are present (9 are continuous, 16 are binary). Experimental results on this dataset are presented in Appendix D.

<sup>7</sup>See “News” link in the “Software and Data” section here: <https://www.fredjo.com/>

**Evaluation Metrics.** To evaluate and compare experimental results, we use the following metrics:

- The *calibration error*, defined as the mean absolute difference between the estimated and true propensity score. This metric can only be computed when the true propensity score is assumed to be known in the dataset. The smaller the calibration error, the more suitable the estimated propensity score and estimated balancing scores obtained from a model are for matching, as we will be closer to the assumption that the propensity score is correctly estimated. Connecting the calibration error to the balancing error term in Proposition 7 is left for future work.
- The *ATT error*, defined as the absolute difference between the ATT estimated by the method and a ground-truth ATT. For every dataset, we compute the ground-truth ATT as the approximation from Equation (2), as we have access to the conditional expectations of  $Y$ .
- We empirically quantify *sample imbalance*  $\hat{I}$ , defined as the squared Euclidean distance between sample means of covariates of treated and control groups from the dataset  $\mathcal{D}'$ , which is obtained from the original dataset  $\mathcal{D}$  via matching, or formally,

$$\hat{I} = \left\| \frac{1}{N_t} \sum_{i \in \mathcal{D}: T_i=1} X_i - \frac{\sum_{j \in \mathcal{D}: T_j=0} w_j X_j}{\sum_{j \in \mathcal{D}: T_j=0} w_j} \right\|_2^2,$$

where  $N_t$  is the number of treated samples, and  $w_j$  is the total weight of control sample  $j$  after matching. As we can see from this equation, only the sample means of covariates from the control group may change due to matching; the sample means of covariates from the treated group remain unchanged. We note that this measure of imbalance is proportional to the squared linear MMD (Sriperumbudur et al., 2012).

**Data Splits.** The neural networks were trained using a 60/20/20 training/validation/testing split. The benchmarks logistic regression-based propensity score estimate and PCA were trained using the combined training and validation sets. In-sample metrics were also computed on the combined training and validation datasets, and hold-out metrics were evaluated using the testing set. Alternatively, one might also use controls from the in-sample set when computing hold-out metrics. However, for simplicity of the definition of the hold-out imbalance, we preferred to just use controls from the testing set.

**Neural Architecture.** The architecture of the neural networks used for matching is as follows : a low-dimensional layer corresponding to the multivariate balancing score (which we also call the "balancing score layer"), then wide hidden layers which are not used as balancing scores, and finally the propensity score head. This architecture is designed to focus on a linear balancing score as in Proposition 5 while keeping flexibility in the rest of the architecture to fit the propensity score model.

**Hyperparameters.** To choose hyperparameters, we ran a grid search over the following hyperparameter values, minimising validation error on the first dataset version of ACIC 2016 (setting 4, as discussed above).

- Number of hidden layers in addition to the balancing score (hidden) layer: 1, 2.
- Number of hidden units per hidden layer (besides the balancing score layer): 100, 200, 300.
- Learning rate:  $10^{-2}$ ,  $10^{-3}$ ,  $10^{-4}$ .
- Weight decay: 0, 0.001, 0.01.

Other hyperparameters which we did not tune include a batch size of 100, and stochastic gradient descent with fixed learning rate as the optimiser. The chosen values by the hyperparameter search were 2 hidden layers besides the balancing score layer, 100 hidden units per hidden layer other than the balancing score layer, a learning rate of  $10^{-2}$ , weight decay with 0.01, and leaky ReLU as an activation. Additionally, on News datasets, the chosen hyperparameters caused the validation loss to diverge after a period of decrease, causing the training to fail. Thus, for this dataset, we used early stopping as a remedy.

**Code.** We provide our code to implement neural score matching and reproduce our main results at <https://github.com/oscarclivio/neuralscorematching>.

**Resources and Assets.** Experiments were run on a laptop with a GeForce GTX 1070 GPU with Max-Q Design for training models with neural networks, and on 12 CPU cores for other tasks. For all datasets, we used our own implementation of them in NumPy and PyTorch (after downloading the data in the case of ACIC 2016 and IHDP, as discussed above), and used our own PyTorch implementation for neural network training.

## D IHDP

In addition to the experimental results in the main paper, we also provide results for the IHDP dataset (Hill, 2011) in Table 3. Boxplots are presented in Section E.

On IHDP, our method is not outperforming other methods. Plain covariates  $X$  consistently rank as the best or second best method for each metric and setting (in-sample or hold-out). This might indicate that IHDP, which is a rather low-dimensional dataset with only 25 covariates, is not suited for dimensionality reduction methods, but further work should investigate these results. We also note that matching in the raw covariate space is probably facilitated by the fact that 16 of covariates are binary.

Table 3: Results on the IHDP dataset.

ATT errors	In-Sample	Hold-Out
NN Layer 1 (ours)	0.156±0.005	0.311±0.011
NN PS (ours)	0.190±0.006	0.330±0.011
$X$	0.144±0.005	0.295±0.011
Random matching	0.216±0.007	0.342±0.012
LogReg PS	0.164±0.005	0.294±0.009
PCA	0.159±0.005	0.307±0.011
PCA + LogReg PS	0.146±0.005	0.372±0.011
Imbalances	In-Sample	Hold-Out
NN Layer 1 (ours)	0.159±0.005	0.442±0.009
NN PS (ours)	0.335±0.006	0.511±0.008
$X$	0.07±0.000	0.223±0.000
Random matching	0.592±0.006	0.658±0.012
LogReg PS	0.033±0.000	0.318±0.000
PCA	0.129±0.000	0.407±0.000
PCA + LogReg PS	0.137±0.001	0.909±0.003
No Matching	0.492±0.000	0.421±0.000

## E BOXPLOTS OF ATT ERRORS AND IMBALANCES

We show boxplots corresponding to Tables 1 to 3 in Figures S2 to S8. We provide boxplots with and without outliers. Outliers are defined as values above  $Q3 + 1.5 \cdot IQ$  and below  $Q1 - 1.5 \cdot IQ$  where  $Q1, Q3, IQ$  are the lower quartile, the upper quartile and the interquartile range of the underlying data, respectively.

## F SOCIETAL IMPACT

Possible positive societal impacts of our method include improving decision-making for various real-world applications in politics, economics or medicine. Possible negative societal impacts include the misuse of individualised treatment effect estimation to discriminate against individuals or groups, and of matching to identify protected characteristics of individuals or groups. To mitigate such impacts, we emphasise the importance of continued oversight and evaluation in the deployment of AI tools in society as well as the protection of data confidentiality via rigorous anonymisation, particularly with regards to protected characteristics.

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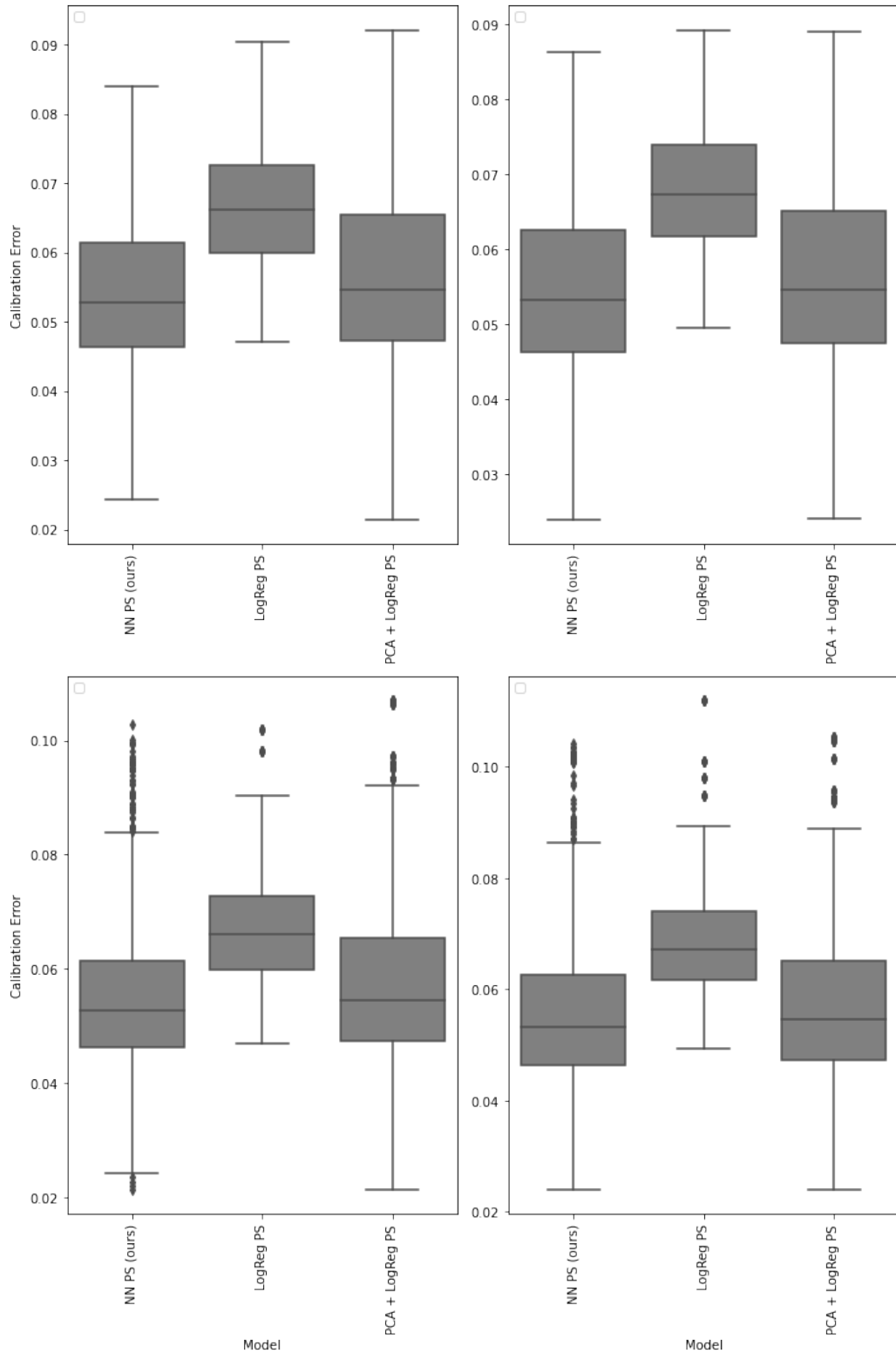


Figure S2: Calibration error boxplots on the ACIC2016 dataset: in-sample (left) and hold-out (right), without (up) and with (bottom) outliers. The data points underlying this figure refer to the average calibration error across a dataset version, corresponding to a single draw of the random seed, and a training seed.

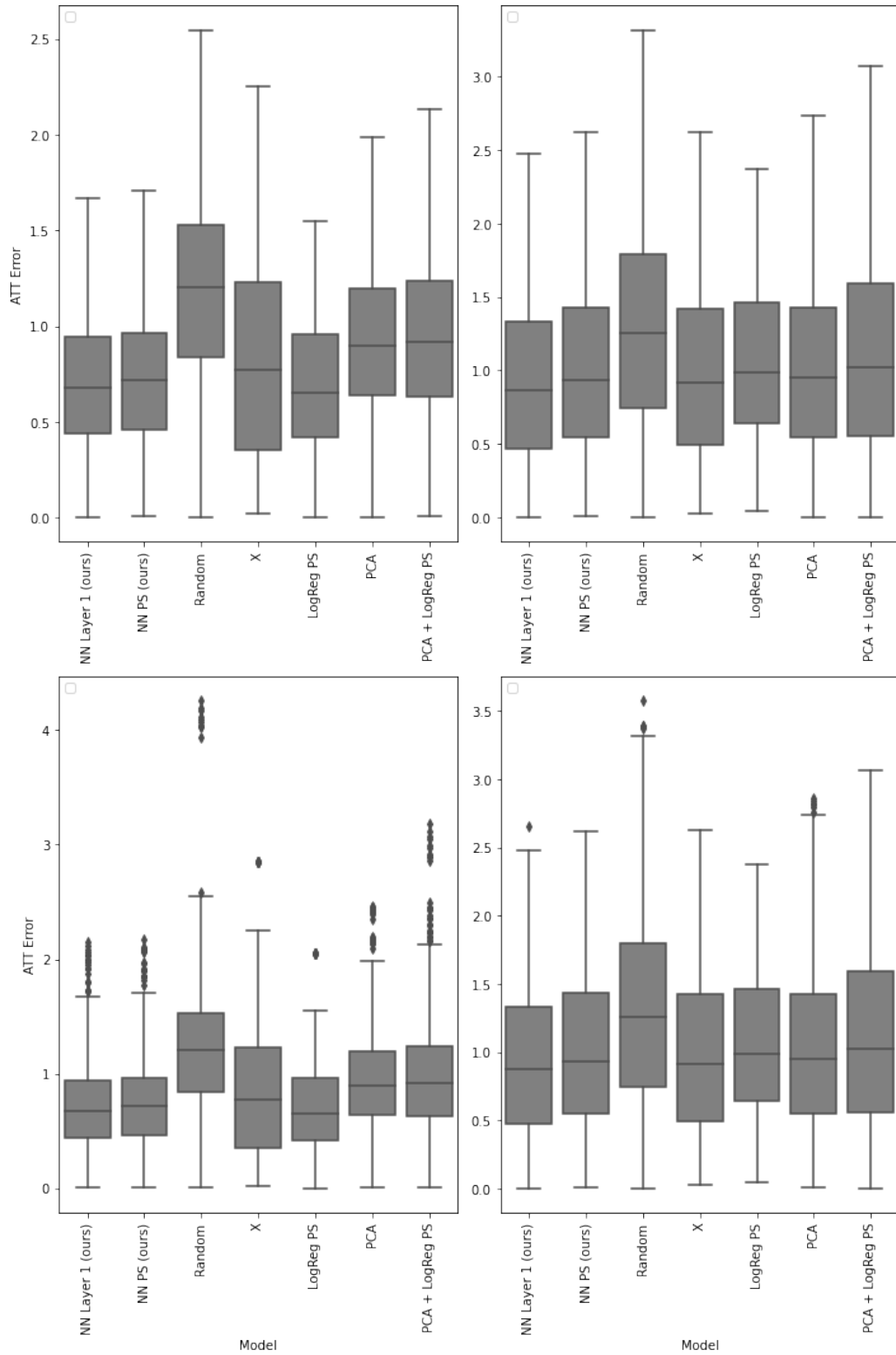


Figure S3: ATT error boxplots on the ACIC2016 dataset: in-sample (left) and hold-out (right), without (up) and with (bottom) outliers. The data points underlying this figure refer to the ATT computed on a dataset version, corresponding to a single draw of the random seed, and a training seed.

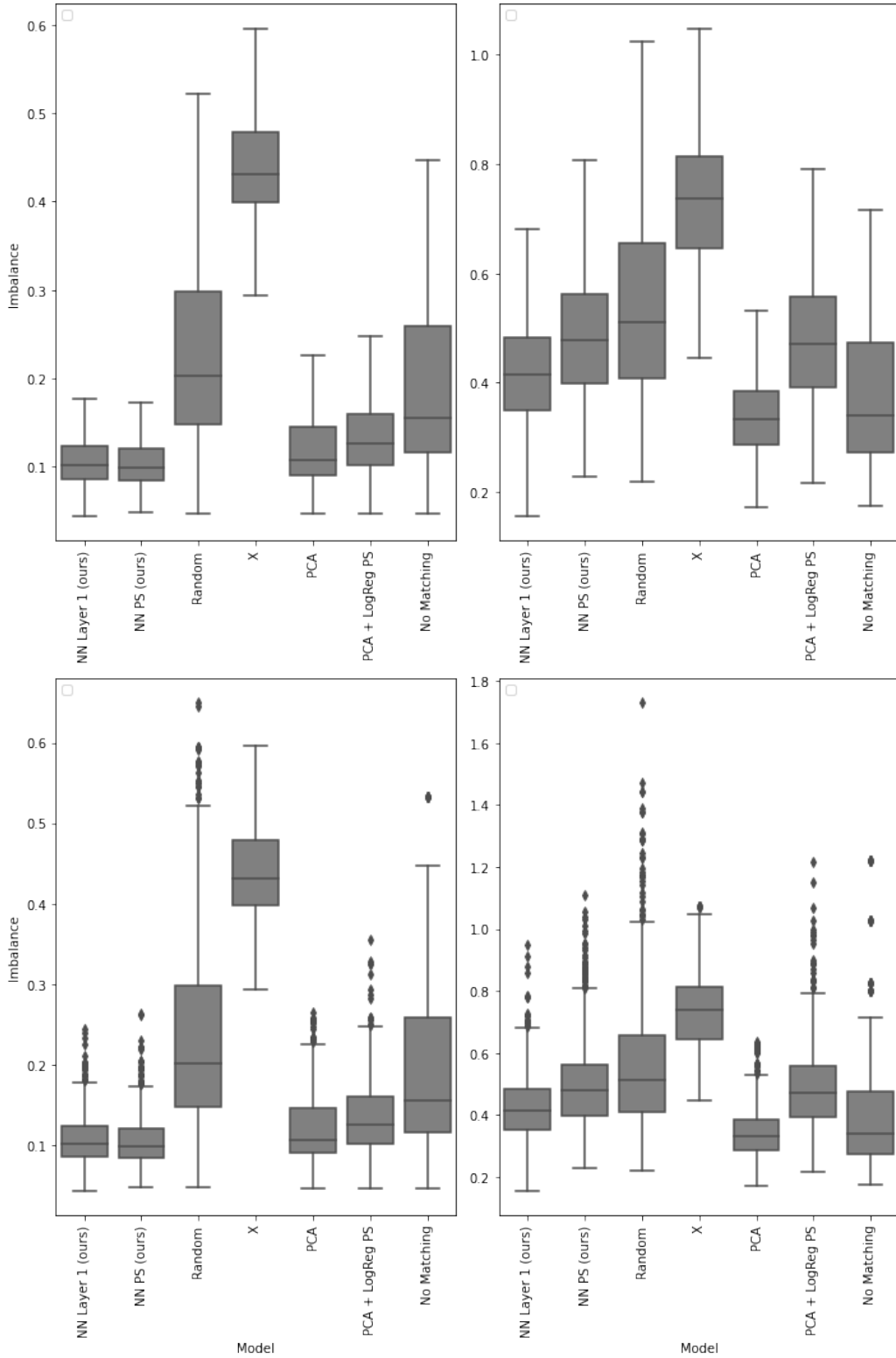


Figure S4: Sample imbalance boxplots on the ACIC2016 dataset: in-sample (left) and hold-out (right), without (up) and with (bottom) outliers. The data points underlying this figure refer to sample imbalance computed on a dataset version, corresponding to a single draw of the random seed, and a training seed.

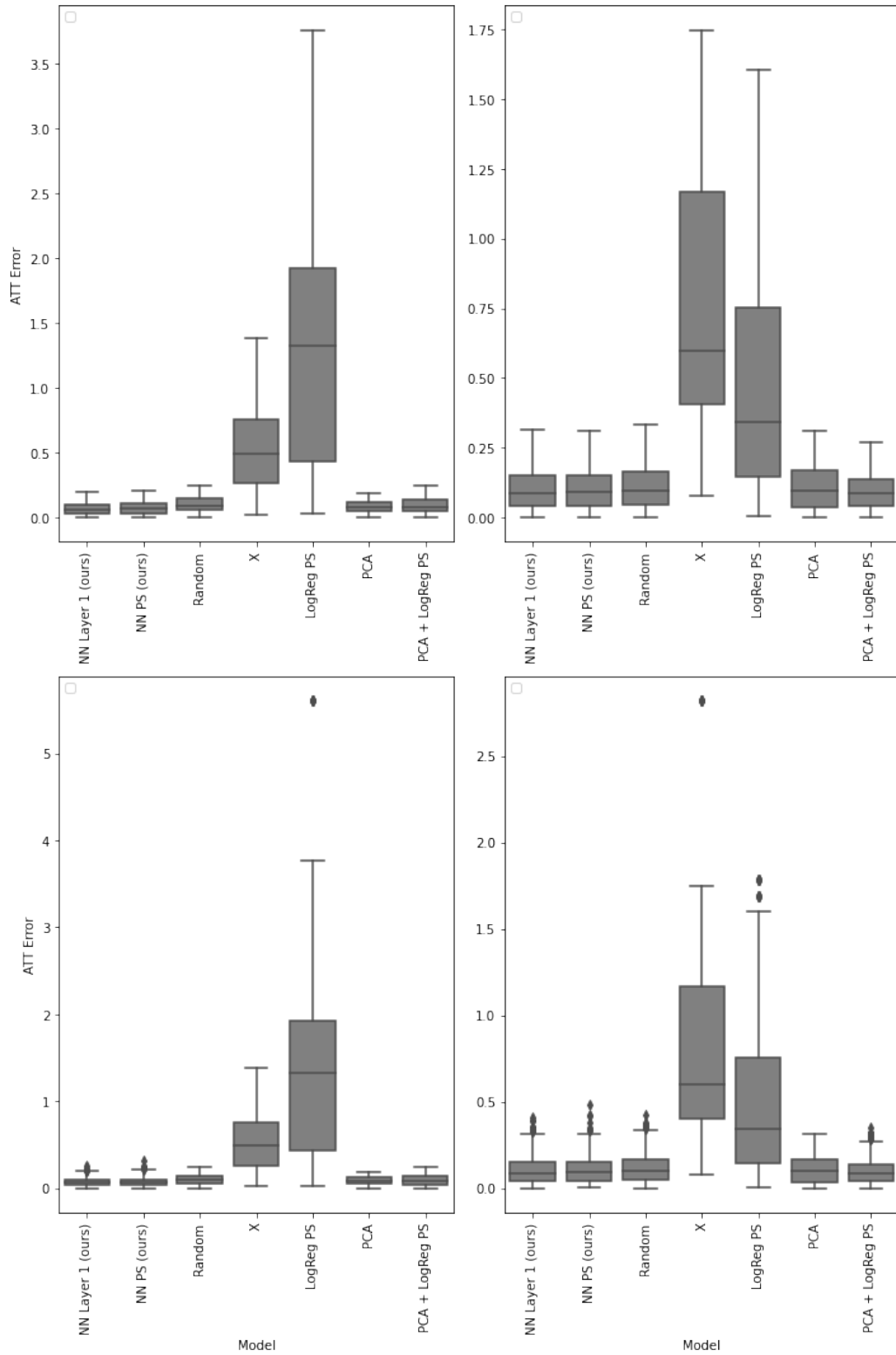


Figure S5: ATT error boxplots on the News dataset: in-sample (left) and hold-out (right), without (up) and with (bottom) outliers. The data points underlying this figure refer to the ATT computed on a dataset version, corresponding to a single draw of the random seed, and a training seed.



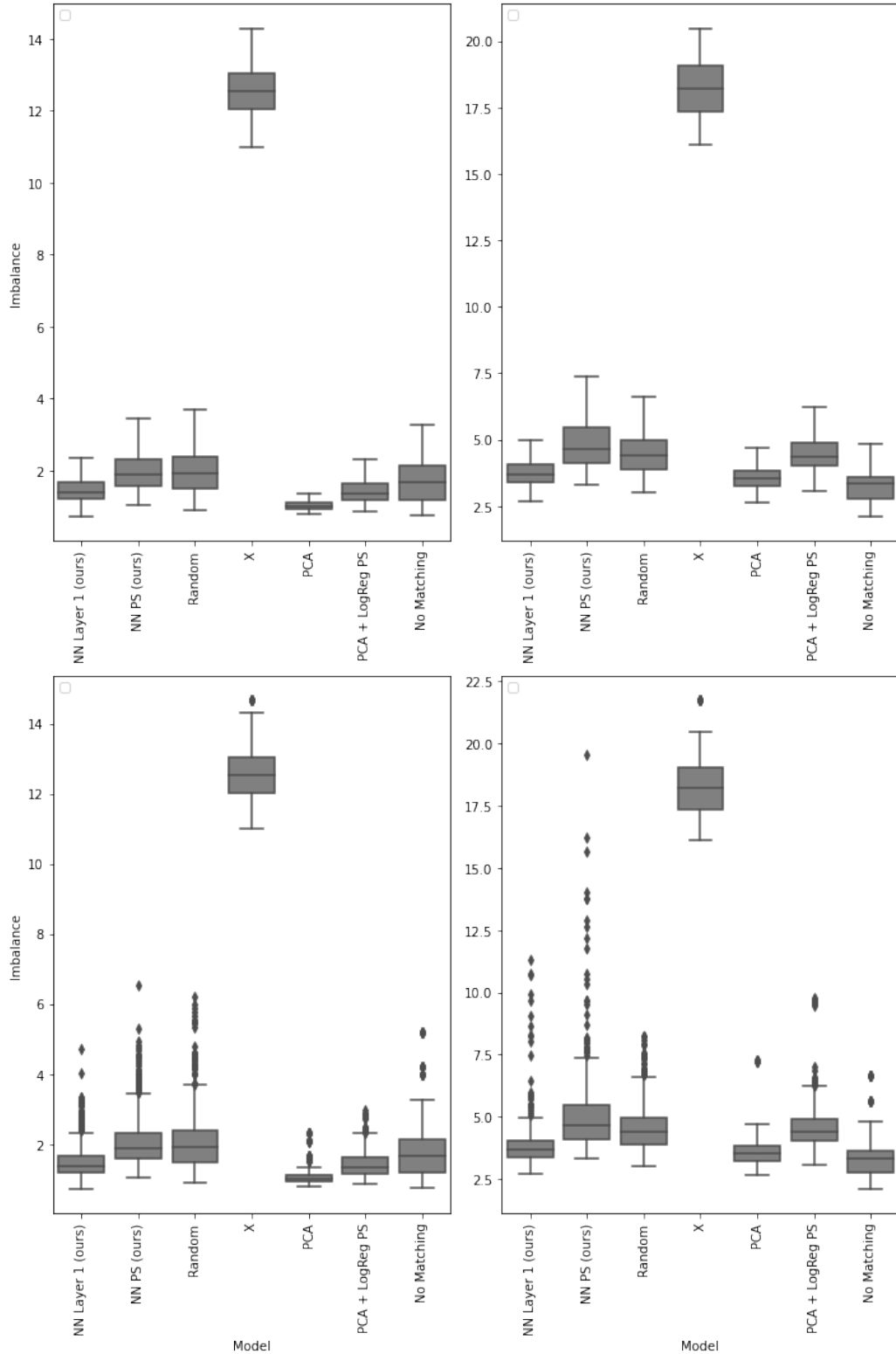


Figure S6: Sample imbalance boxplots on the News dataset: in-sample (left) and hold-out (right), without (up) and with (bottom) outliers. The data points underlying this figure refer to sample imbalance computed on a dataset version, corresponding to a single draw of the random seed, and a training seed. Note that we do not show the boxplot for LogReg PS, whose exceptionally high values were hindering the readability of the Figure.

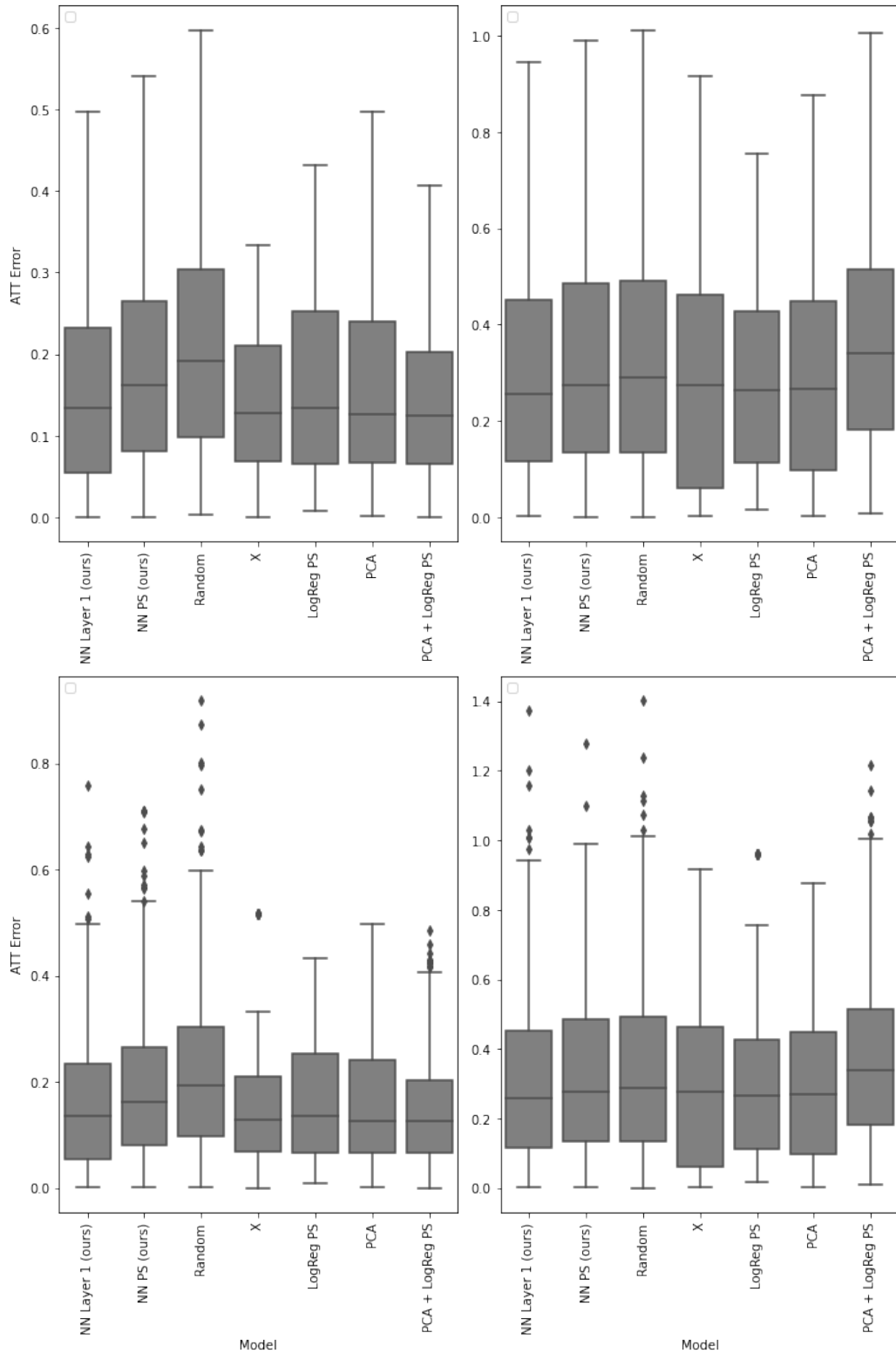


Figure S7: ATT error boxplots on the IHDP dataset: in-sample (left) and hold-out (right), without (up) and with (bottom) outliers. The data points underlying this figure refer to the ATT computed on a dataset version, corresponding to a single draw of the random seed, and a training seed.

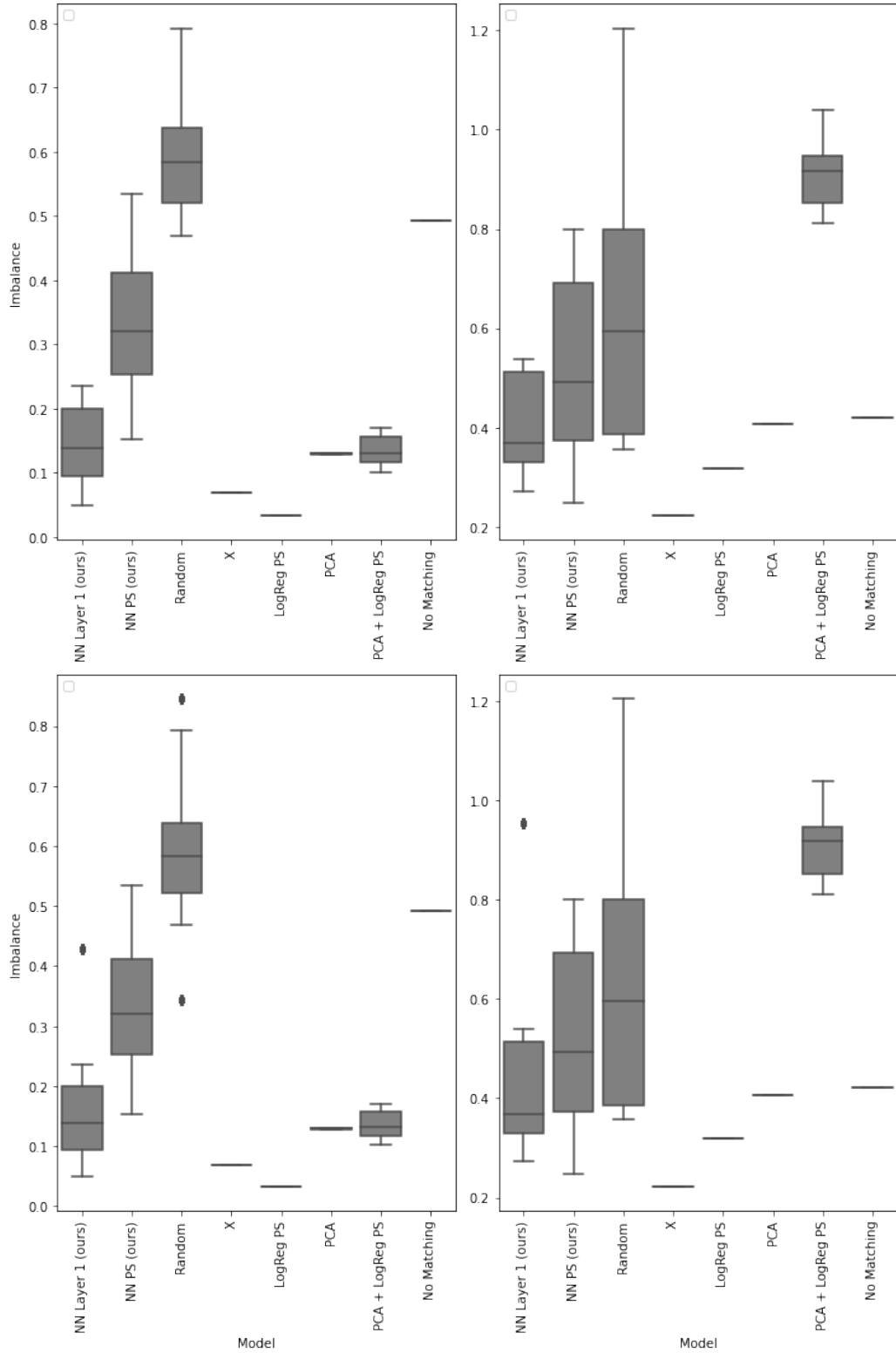


Figure S8: Sample imbalance boxplots on the IHDP dataset: in-sample (left) and hold-out (right), without (up) and with (bottom) outliers. The data points underlying this figure refer to sample imbalance computed on a dataset version, corresponding to a single draw of the random seed, and a training seed.