Mahalanobis balancing: a multivariate perspective on approximate covariate balancing

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Abstract
In the past decade, various exact balancing-based weighting methods were introduced to the causal inference literature. Exact balancing greatly alleviates the issues of extreme weights and model misspecification of inverse probability weighting. It directly eliminates covariate imbalance by imposing balancing constraints in a certain optimization problem. The optimization problem can nevertheless be infeasible when there is bad overlap between the covariate distributions or when the covariates are high-dimensional. Recently, approximate balancing was proposed as an alternative balancing framework, which resolves the feasibility issue by using inequality moment constraints. In each of these constraints, covariate imbalance is bounded by a threshold parameter. However, it can be difficult to select the threshold parameters particularly when the number of constraints is large. Moreover, moment constraints may not fully capture the discrepancy of covariate distributions. In this paper, we propose Mahalanobis balancing, which approximately balances covariate distributions from a multivariate perspective. We use a single quadratic constraint to control overall imbalance with a threshold parameter, which can be tuned by a simple selection procedure. We show that the dual problem of Mahalanobis balancing is an $\ell_2$ norm-based regularized regression problem, and establish interesting connection to propensity score models. We further generalize Mahalanobis balancing to the high-dimensional scenario. We derive asymptotic properties and make extensive comparison with existing balancing methods in the numerical studies.

Keyword: causal inference, Mahalanobis distance, multivariate imbalance, overlap, propensity score

1 Introduction
Inference about causation gains increasing attention in medical science, economics, computer science, and many other disciplines. Propensity score (Rosenbaum and Rubin, 1983), the probability

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of receiving a treatment or exposure conditional on the confounders, plays a central role in causal inference for observational studies. There are several classes of propensity score-based methods in practitioners’ toolkit, including matching, weighting, and subclassification. We focus on weighting in this article (Rosenbaum, 1987; Robins et al., 1994; Hirano et al., 2003). Inverse probability weighting and its doubly robust version are the most commonly used weighting methods. They explicitly estimate the propensity score via a parametric or nonparametric model (e.g., Hirano et al., 2003). However, as demonstrated by Kang and Schafer (2007) and related articles, inverse probability weighting is prone to misspecification of the propensity score model, and it may produce extreme weights. Moreover, covariate balance may not be attained after reweighting.

In the past decade, numerous robust weighting methods have been proposed, which aim to provide protection against extreme weights and model misspecification by directly balancing covariates in the estimation procedure. Hainmueller (2012) introduced the entropy balancing method, which optimizes the entropy loss function subject to a set of balancing constraints. The balancing constraints enforce the weighted moments in the control group to be equal to the unweighted counterparts in the treated group, and thus finite-sample exact balance is achieved. The balanced weights are then used to reweight the subjects in the control group to produce a weighted estimator of the average treatment effect on the treated. This method has close connection to the literature of survey sampling, missing data, and machine learning (e.g., Dehejia and Wahba, 1999; Graham et al., 2012; Mohri et al., 2018). Zhao and Percival (2017) derived the asymptotic properties of entropy balancing. In particular, he revealed that entropy balancing is doubly robust. Imai and Ratkovic (2014) considered parametric propensity score model and solved the likelihood score function together with the balancing constraints simultaneously to produce covariate balancing parameter estimation for the propensity score model. Fan et al. (2021) presented an improved version of this covariate balancing propensity score method. Chan et al. (2016) constructed a class of calibration weighting estimators by minimizing a certain distance measure subject to balancing constraints. Empirical likelihood and exponential tilting belong to this class. Yiu and Su (2018) proposed to eliminate the association between treatment and covariates in the weight construction procedure. Hazlett (2020) recommended to construct balancing constraints from the kernel viewpoint. Josey et al. (2021b) proposed the Bregman distance framework which unifies many existing methods.

A common feature of these balancing methods is that balancing conditions are directly imposed as equality constraints in a certain convex optimization problem. That is, they are exact balancing methods. Exact balancing is capable of producing stable weights. It is more robust to model misspecification compared to inverse probability weighting in many circumstance. Recently, exact balancing has received great attention in applied disciplines. For example, it was used as a cornerstone in the integrative analysis of randomized clinical trial and observational study (Lee et al., 2021), and in the analysis of transportability of trial results to a target population (Josey et al., 2021a). Nevertheless, in the bad-overlap scenario where there is limited overlap between the covariate distributions in the treated and control groups, or in the high-dimensional scenario where the number of constraints is large, exact balancing performs poorly. Even worse, the infeasibility issue may occur.

To alleviate the feasibility problem, Zubizarreta (2015) and Wang and Zubizarreta (2020) proposed minimal dispersion approximately balancing weights (MDABW) as an approximate balancing framework, which relaxes the balancing conditions by using inequality constraints instead. The inequality constraints are obtained by controlling the univariate dispersion for each covariate with a separate threshold parameter. Wang and Zubizarreta (2020) showed that the dual problem for MDABW is a weighted $\ell_1$ norm-based regularized regression problem. There are other robust balancing methods which may not suffer the feasibility problem. For example, Wong and Chan (2018) minimized covariate imbalance directly by the regularized kernel regression method. Zhao
proposed a general balancing framework using tailored loss functions. Li et al. (2018) and Ma and Wang (2020) provided insights about robust weighting from different perspectives.

In general, covariate balancing becomes more difficult in the high-dimensional scenario, because the overlap in the covariate distributions tends to be much worse as the dimensionality increases. We refer to D’Amour et al. (2021) for a formal discussion of the overlap condition in the high-dimensional scenario. Regularization plays a key role in high-dimensional analysis, and it has been adapted to covariate balancing recently. Among others, Athey et al. (2018), Ning et al. (2020), and Tan (2020a,b) addressed the high-dimensional balancing problems using regularization techniques. We term them as the high-dimensional regularized balancing methods. Many of these methods involved outcome models and thus cannot be categorized as pure data preprocessing procedures. Interestingly, Athey et al. (2018); Zhao (2019); Tan (2020b) established tight connections to the MDABW method.

The common feature of the existing exact and approximate balancing methods is that they all directly impose covariate imbalance as the moment constraints. There are potential limitations to use the moment constraints. For example, MDABW controls covariate dispersion by thresholding the absolute difference of the weighted average of each covariate in the treated group and the sample average. This is equivalent to bound the weighted absolute standardized mean difference (ASMD) for each covariate, where the ASMD is a commonly used univariate imbalance measure in observation studies and will be discussed in Section 2. Hence, univariate approximate balancing is achieved. However, univariate approximate balancing does not guarantee overall balance especially in the bad-overlap or high-dimensional scenario, as demonstrated in the numerical studies. Another potential issue is that there is no principled way to select the threshold parameters simultaneously, because decreasing imbalance of some covariate by shrinking the threshold parameter may reversely increase imbalance of other covariates. Even when optimal threshold parameters are obtained for all covariates, it does not imply that overall imbalance is under control particularly in the high-dimensional setting. Moreover, the theoretical results for MDABW (Wang and Zubizarreta, 2020) require that the number of balancing constraints is much smaller than the sample size. Extension of MDABW to handle high-dimensional constraints remains an open work.

The limitations of univariate approximate balancing can be greatly resolved by monitoring and controlling overall covariate balance from the multivariate perspective. Multivariate imbalance measures of the overall difference in covariate distributions are widely used in the matching literature (e.g. Iacus et al., 2011, 2012; Diamond and Sekhon, 2013; Imbens and Rubin, 2015). Nevertheless, they are largely neglected in the covariate balancing literature. In this paper, we highlight the importance of multivariate imbalance. In deed, our numerical studies suggest that controlling univariate imbalance without considering multivariate imbalance in reweighting can be insufficient to delineate overall imbalance, and treatment effect estimation can be seriously biased.

In this paper, we propose a multivariate balancing approach, Mahalanobis balancing, to tackle the aforementioned difficulties of univariate approximate balancing. We optimize a prespecified loss function (e.g., entropy or empirical likelihood) subject to a single quadratic inequality constraint, where we directly control multivariate imbalance in the covariate distributions. We use a generalized version of Mahalanobis distance to measure overall imbalance in the covariate distributions. A sufficient small value of this imbalance measure suggests that the covariates are approximately balanced from the multivariate perspective. We study the primal optimization problem by utilizing the Fenchel duality theory (e.g. Bertsekas, 2016; Mohri et al., 2018). We show that the dual problem is an unconstrained regularized regression problem with an $\ell_2$ norm regularizer. Off-the-shelf convex optimization algorithms can be employed to solve the dual problem. We adopt the BFGS quasi-Newton algorithm to obtain the solution of the dual problem in this paper.

The key difference of Mahalanobis balancing and MDABW is that Mahalanobis balancing con-
trols multivariate imbalance measure directly as an inequality constraint in an constrained optimization problem. Hence, multivariate approximate balance is monitored and controlled. This simple idea has important consequences that make Mahalanobis balancing a highly competitive balancing method. First, there is a single threshold parameter attached to the quadratic inequality constraint in Mahalanobis balancing, and thus the issue of tuning multiple threshold parameters of the MDABW method is greatly alleviated. Second, there are situations where univariate balance holds but the covariate distributions are still imbalanced. MDABW does not work well in these situations as illustrated in the numerical studies. In contrast, Mahalanobis balancing explicitly constrains multivariate imbalance and substantially improves the empirical performance of MDABW in these situations. Third, Mahalanobis balancing is not restricted to the low-dimensional situation. In particular, we propose a high-dimensional version of Mahalanobis balancing where the idea of multivariate imbalance is further exploited. The simulations show that it is competitive to the state-of-the-art high-dimensional regularized balancing methods (e.g., Athey et al., 2018; Ning et al., 2020; Tan, 2020b) in important settings. In comparison, MDABW requires that the number of constraints is small.

The rest of the paper is organized as follows. In Section 2, we introduce necessary notations, existing imbalance measures, and balancing methods. In Section 3, we present the proposed Mahalanobis balancing method, and make extension to the high-dimensional situation. Asymptotic properties of Mahalanobis balancing are studied. In Section 4, we make extensive comparison of Mahalanobis balancing to the existing balancing methods in numerical studies. We make conclusion and discussion in the final section. Proofs and additional numerical results are available in the online Supplementary Material. The codes to implement Mahalanobis balancing are available in Github via the link: https://yimindai0521.github.io/MBalance/.

2 Notation and Preliminary

2.1 The framework

Consider a simple random sample of $n$ subjects from a population. Let $T$ be a binary treatment indicator with $T = 1$ if the subject is treated and $T = 0$ otherwise. Let $X = (X_1, \cdots, X_p)^\top$ be a $p$-dimensional vector of pre-treatment covariates. Let $Y$ be the univariate outcome. The observed data are $\{(X_i, T_i, Y_i) : i = 1, \cdots, n\}$, which are $n$ independent and identically distributed copies of the triplet $(X, T, Y)$. Under the potential outcome framework (e.g. Imbens and Rubin, 2015), we define a pair of potential outcomes $\{Y(0), Y(1)\}$ for each subject if he were not treated or treated. The observed outcome is $Y = (1 - T) Y(0) + T Y(1)$.

We impose the following strong ignorability and overlap assumptions for identification and inference of the average treatment effect.

**Assumption 1** (Strong Ignorability). $\{Y(0), Y(1)\} \perp T \mid X$.

Here, $\perp$ denotes independence. Assumption 1 states that the potential outcomes $\{Y(0), Y(1)\}$ are independent of the treatment indicator $T$ given pre-treatment covariates $X$, which implies that there are no unmeasured confounders that may cause selection bias. The probability $\pi(X) = \Pr(T = 1 \mid X)$ is the propensity score function. Assumption 1 implies $\pi(X)$ is a balancing score (Rosenbaum and Rubin, 1983) in the sense that $\{Y(0), Y(1)\} \perp T \mid \pi(X)$. Under Assumption 1, the average treatment effect is identifiable.

Moreover, to ensure that there are informative observations for treatment effect estimation, we impose the overlap assumption:
Assumption 2 (Overlap). \( 0 < Pr(T = 1 \mid X) < 1 \) for any \( X \) in its support.

In this paper, the causal estimand of interest is the average treatment effect (ATE), defined by \( \tau = E\{Y(1) - Y(0)\} = \mu_1 - \mu_0 \), where \( \mu_j = E\{Y(j)\} \), \( j = 0, 1 \). The proposed method can be adapted to other causal estimands, e.g., average treatment effect on the treated. Under Assumption 1, \( \tau = E\{\mu_1(X) - \mu_0(X)\} \), where \( \mu_j(X) = E\{Y(j) \mid X\} \), \( j = 0, 1 \).

A generic reweighting scheme constructs weights \( w = (w_1, \ldots, w_n)^\top \) by exploiting the sampled data and possibly external information from the population, and then estimate the ATE by \( \hat{\tau} = \sum_{i=1}^{n} T_i w_i Y_i - \sum_{i=1}^{n} (1 - T_i) w_i Y_i \). The covariate balancing methods introduced in Section 1 explicitly balance the covariates in the reweighting procedure and produce a set of balanced weights.

### 2.2 Imbalance measures

A set of pre-specified basis functions, denoted by \( \phi_1(X), \ldots, \phi_K(X) \), can be used instead of the original covariates \( X \) in the construction of balanced weights (e.g., Hainmueller, 2012; Imai and Ratkovic, 2014; Wang and Zubizarreta, 2020). In Section 3, we discuss the choices of the basis functions. Define \( \Phi(X) = (\phi_1(X), \ldots, \phi_K(X))^\top \) to be a vector of the basis functions, which is an \( \mathbb{R}^p \to \mathbb{R}^K \) feature mapping.

Assessment of covariate balance is crucial in the inference of causal effects. Many imbalance measures are proposed and widely used in the literature. The absolute standardized mean difference (ASMD) is the most popular univariate imbalance measure (Imbens and Rubin, 2015). The ASMD for \( \phi_k(X) \) is expressed as

\[
\text{ASMD}_k = \frac{|\bar{\phi}_{k,1} - \bar{\phi}_{0,k}| \sqrt{s_{1,k}^2 + s_{0,k}^2}}{2}
\]

where \( \bar{\phi}_{j,k} = \sum_{i=1}^{n} I(T_i = j)\phi_k(X_i)/n_j \) and \( s_j^2 = \sum_{i=1}^{n} I(T_i = j)(\phi_k(X_i) - \bar{\phi}_{j,k})^2/(n_j - 1) \) are the treatment-specific sample mean and sample variance, \( j = 0, 1 \). Here, \( I(\cdot) \) is the indicator function, and \( n_1 \) and \( n_0 \) are the sample sizes of the treated and control groups, respectively. The ASMD is an affinely invariant univariate measure of the location difference in the two groups.

When the ASMD for a basis function does not exceed a pre-specified threshold parameter \( \delta \), then this basis function is considered to be approximately balanced (Imbens and Rubin, 2015). Common choices of \( \delta \) are 0.1, 0.2 and 0.25 (e.g. Stuart et al., 2013; Xie et al., 2019). Our simulation studies show that even when all basis functions are on average approximately balanced in the sense that the average ASMD is smaller than the threshold, say \( \delta = 0.1 \), the average treatment effect estimation is still severely biased. This can be explained by that the ASMD is a univariate imbalance measure which cannot fully characterize multivariate imbalance. There are directions of imbalance that are missed by \( \text{ASMD}_1, \ldots, \text{ASMD}_K \).

To assess the imbalance for all covariates or basis functions simultaneously, overall imbalance measures need to be used instead. The squared Mahalanobis distance (MD) (Imbens and Rubin, 2015) is the most commonly used multivariate imbalance measure, given by

\[
\text{MD} = (\Phi_1 - \Phi_0)^\top \left( \frac{\hat{\Sigma}_1 + \hat{\Sigma}_0}{2} \right)^{-1} (\Phi_1 - \Phi_0),
\]

where \( \Phi_j = (\bar{\phi}_{j,1}, \ldots, \bar{\phi}_{j,K})^\top, j = 0, 1 \), and \( \hat{\Sigma}_1 \) and \( \hat{\Sigma}_0 \) are the sample covariance matrices of \( \phi(X) \) in the treated and control groups, respectively. The MD was used in Mahalanobis distance matching...
(e.g. Imbens and Rubin, 2015) to determine the closeness of subjects in the treated and control groups. Moreover, it was adapted to the genetic matching method (Diamond and Sekhon, 2013), which aims at minimizing a generalized version of MD to optimize postmatching covariate balance. The \( \ell_1 \) distance-based measure proposed by Iacus et al. (2011) is another example of multivariate imbalance measure, which motivates a class of matching methods with the monotonic imbalance bounding property. Iacus et al. (2012) derived the coarsened exact matching method from this class, and emphasized the importance of optimizing multivariate balance in matching. Zhu et al. (2018) proposed to use the Kernel distance as a multivariate imbalance measure. Huling and Mak (2020) studied the energy distance as an imbalance measure.

### 2.3 Exact balancing v.s. approximate balancing

The existing covariate balancing methods usually achieve exact balance by imposing a set of equality balancing constraints

\[
\sum_{i=1}^{n} w_i T_i \phi_k(X_i) = \bar{\phi}_k, \\
and \ \sum_{i=1}^{n} w_i (1 - T_i) \phi_k(X_i) = \bar{\phi}_k, \ k = 1, \cdots, K, \tag{3}
\]

in the construction of the weights \( w_1, \cdots, w_n \), where \( \bar{\phi}_k = \sum_{i=1}^{n} \phi_k(X_i)/n \). These constraints enforce the basis functions to be exactly balanced in the first moment after reweighting. Examples of exact balancing methods include entropy balancing (Hainmueller, 2012), covariate balancing propensity score (Imai and Ratkovic, 2014), and calibration weighting (Chan et al., 2016), among others.

Define a weighted version of the ASMD by

\[
\text{ASMD}_k^w = \frac{\left| \sum_{i=1}^{n} w_i T_i \phi_k(X_i) - \sum_{i=1}^{n} w_i (1 - T_i) \phi_k(X_i) \right|}{\sqrt{s^2_{1,k} + s^2_{0,k}}/2}, \ k = 1, \cdots, K. \tag{4}
\]

The ASMD\(_k^w\) is a weighted univariate imbalance measure that quantifies remaining imbalance for the \( k \)th basis function \( \phi_k \) after reweighting. It is a generic measure to assess the balancing performance of any weighting methods. It is straightforward that the equality balancing constraints (3) lead to that \( \text{ASMD}_k^w = 0 \) for all \( k = 1, \cdots, K \). Therefore, finite-sample univariate exact balance is achieved by the exact balancing methods. In comparison, inverse probability weighting does not possess this attractive property.

When exact balancing is not attainable in the bad-overlap situation, the MDABW method (Zubizarreta, 2015; Wang and Zubizarreta, 2020) can be used instead. The balanced weights for the treated group \( \{i : T_i = 1\} \) are the global minimum of the following optimization problem:

\[
\begin{align*}
\text{minimize}_{w} & \sum_{i=1}^{n} T_i f(w_i) \\
\text{subject to} & \left| \sum_{i=1}^{n} w_i T_i \phi_k(X_i) - \bar{\phi}_k \right| \leq \delta_k, k = 1, \cdots, K, \tag{5}
\end{align*}
\]

where \( f(\cdot) \) is a pre-specified loss function, and \( \delta_1, \cdots, \delta_K \geq 0 \) are the threshold parameters. Because the constraints are imposed separately for the basis functions, MDABW is a univariate approximate balancing method. The choices of \( f(\cdot) \) is discussed in Section 3. Similarly, the weights for the control group \( \{i : T_i = 0\} \) can be obtained by replacing \( T_i \) with \( 1 - T_i \) in the optimization problem (5).
Without loss of generality, we normalize the basis function \( \phi_k(X_i) \) to be \( \phi_k(X_i) / \sqrt{s_{1,k}^2 + s_{0,k}^2} / 2 \) in the optimization problem (5). It is clear that \( \text{ASMD}_k^w \leq 2\delta_k \) for \( k = 1, \cdots, K \). A small value of \( \delta_k \), say 0.1, indicates that the \( \phi_k \) is approximately balanced (Stuart et al., 2013; Xie et al., 2019). However, it is difficult to define optimality for all the thresholds \( (\delta_1, \cdots, \delta_K) \) even in the low-dimensional setting, because decreasing univariate imbalance for some bad-overlap basis function may inevitably increase imbalance for other basis functions. Correlation of the basis functions are not taken into account in Problem (5). Tuning a large number of parameters is very time-consuming. In fact, there is lack of guideline on tuning these parameters simultaneously. These potential issues of univariate approximate balancing motivate Mahalanobis balancing in the following section.

We define the following Mahalanobis imbalance measure (MIM) as a weighted version of the squared Mahalanobis distance:

\[
\text{MIM}^w = \left\{ \sum_{i=1}^{n} w_i T_i (X_i) - \sum_{i=1}^{n} w_i (1 - T_i) (X_i) \right\}^\top \left( \hat{\Sigma}_1 + \hat{\Sigma}_0 / 2 \right)^{-1} \\
\times \left\{ \sum_{i=1}^{n} w_i T_i (X_i) - \sum_{i=1}^{n} w_i (1 - T_i) (X_i) \right\},
\]

(6)

which can be used to measure the remaining overall imbalance after reweighting. Note that univariate exact balance is equivalent to multivariate exact balance, in the sense that \( \text{ASMD}_k^w = 0 \) for all \( k = 1, \cdots, K \) is equivalent to \( \text{MIM}^w = 0 \). However, we remark that univariate approximate balance does not imply multivariate approximate balance, because it is possible that the \( \text{ASMD}_k^w \) is small for all \( k = 1, \cdots, K \) but the \( \text{MIM}^w \) is very large, as illustrated in the simulations.

3 Proposed Methodology

3.1 Mahalanobis balancing

To alleviate the aforementioned limitations of univariate approximate balancing, we propose the Mahalanobis balancing (MB) method. The key idea is to directly control multivariate imbalance in the optimization problem. Hence, MB is a multivariate approximate balancing method. Specifically, Mahalanobis balancing obtains the balanced weights for the treated group by solving the convex optimization problem:

\[
\begin{align*}
\text{minimize:} & \quad \sum_{i=1}^{n} T_i f(w_i) \\
\text{subject to:} & \quad w_i \geq 0, \quad i \in \{ j : T_j = 1 \}; \\
& \quad \sum_{i=1}^{n} T_i w_i \{ \Phi(X_i) - \bar{\Phi} \} \top W \sum_{i=1}^{n} T_i w_i \{ \Phi(X_i) - \bar{\Phi} \} \leq \delta,
\end{align*}
\]

(7)

where \( f(\cdot) \) is a convex loss function, \( \Phi(X) \) is a vector of basis functions defined in Section 2.2, \( \bar{\Phi} = \sum_{i=1}^{n} \Phi(X_i) / n \), \( W \) is a user-specified \( K \times K \) positive-definite weight matrix, and \( \delta \geq 0 \) is a threshold parameter. The MB weights are normalized for the treated subjects, i.e., \( w_i^{MB} = w_i / \sum_{i=1}^{n} T_i w_i \). Similarly, the MB weights in the control group can be obtained.

The role of each \( w_i \) is to down-weigh or up-weigh the deviation of \( \Phi(X_i) \) from the pooled-sample mean \( \bar{\Phi} \). The pre-specified matrix \( W \) weighs the relative importance of the basis functions \( \phi_1(\cdot), \cdots, \phi_K(\cdot) \) and their interactions. In this paper, we consider two choices of \( W \): (i) the diagonal matrix \( W_1 = \{ \text{diag}((\hat{\Sigma}_1 + \hat{\Sigma}_0) / 2) \}^{-1} \), where its main diagonal contains the inverse diagonal elements of \( (\hat{\Sigma}_1 + \hat{\Sigma}_0) / 2 \); (ii) \( W_2 = \{ (\Sigma_1 + \Sigma_0) / 2 \}^{-1} \). We use \( W_2 \) when \( K \) is not large and the basis functions
are not highly correlated. Otherwise, we prefer \( W_1 \).

For a set of normalized balanced weights, we define the generalized Mahalanobis imbalance measure (GMIM) in the treated group:

\[
\text{GMIM}_1^w = \left\{ \sum_{i=1}^{n} T_i w_i \Phi(X_i) - \bar{\Phi} \right\}^\top W \left\{ \sum_{i=1}^{n} T_i w_i \Phi(X_i) - \bar{\Phi} \right\} .
\]  

(8)

Similar, we define GMIM\(_0^w\) for the control group. The GMIM\(_1^w\) measures the remaining multivariate difference of the basis functions in the treated group and the sample average \( \bar{\Phi} \) after reweighting. Note that GMIM\(_1^w\) is the normalized version of the constraint \( \sum_{i=1}^{n} T_i w_i \Phi(X_i) - \bar{\Phi} \) in Problem (7). Therefore, the quadratic constraint in Problem (7) restricts the unnormalized remaining multivariate imbalance in the treated group such that it does not exceed \( \delta \). The GMIM\(_w\) has similar interpretation for the control group. When Problem (7) is feasible with \( \delta = 0 \), then MB reduces to an exact balancing method. When Problem (7) is infeasible with \( \delta = 0 \), we need to tune a positive \( \delta \) to directly control GMIM\(_1^w\) and GMIM\(_0^w\) and thus optimize multivariate balance.

We remark that we prefer to minimize GMIM\(_1^w\) and GMIM\(_0^w\) separately rather than minimize the Mahalanobis imbalance measure MIM\(_w\) for the following reasons. First, it allows us to easily obtain balanced weights from two separate optimization problems. When \( (\Sigma_1 + \Sigma_0)/2 \) is positive-definite and \( W = W_2 \), it holds that \( \sqrt{\text{MIM}_1^w} \leq \sqrt{\text{GMIM}_1^w} + \sqrt{\text{GMIM}_0^w} \). Therefore, by minimizing GMIM\(_1^w\) and GMIM\(_0^w\), the Mahalanobis imbalance measure MIM\(_w\) is under control. More importantly, compared to MIM\(_w\), GMIM\(_w\) and GMIM\(_w\) are more relevant to assess the multivariate balancing performance of any weighting method. This is because a very small value of MIM\(_w\) does not imply that the weighted basis functions \( \sum_{i=1}^{n} T_i w_i \Phi(X_i) \) and \( \sum_{i=1}^{n} (1-T_i) w_i \Phi(X_i) \) are close to the sample average \( \bar{\Phi} \). That is, it is possible that the weighted distributions in the two groups are close to each other, but meanwhile each of them is quite different from the distribution in the population. In the simulations, we show that this phenomenon frequently occurs in the bad-overlap situation for the covariate balancing propensity score method, which directly balances the moments of the covariates between the two groups.

Next, we discuss the choices of the loss function \( f(\cdot) \), including the entropy function \( f(x) = x \log(x) \) (Hainmueller, 2012), the negative of empirical likelihood \( f(x) = -\log(x) \), the quadratic function \( f(x) = (x - 1/n)^2 \) by Zubizarreta (2015), the distance measure by Chan et al. (2016), and the Bregman distance by Josey et al. (2021b). We prefer the entropy function \( f(x) = x \log(x) \) in this paper for its stable performance and theoretical properties.

The choice of the basis functions is important for the consistency of the balancing methods (e.g. Zhao and Percival, 2017), which generally requires that the linear combination of the \( \phi_k(\cdot) \)'s coincides with the linear predictor in the propensity score or the outcome model. The default choice is the first and second moments of \( X \), and sometimes the interaction terms are included. Motivated by the theory of Reproducing Kernel Hilbert Space (RKHS), as was explored in several related work (Wong and Chan, 2018; Zhao, 2019; Hazlett, 2020), we also consider the alternative choice \( \Phi(X) = (K(X, X_1), \cdots, K(X, X_n))^\top \) in the high-dimensional setting where the dimension of the covariates \( p \) is large compared to sample size \( n \). Here, \( K(\cdot, \cdot) \) is a pre-specified kernel function (e.g., Mohri et al., 2018), and the number of basis functions is \( K = n \).

In the following, we study the dual of the primal optimization problem (7). By the Fenchel duality theory (Bertsekas, 2016; Mohri et al., 2018), we show that the dual problem is equivalent to fitting a regularized propensity score model with an \( \ell_2 \) norm penalty. In Theorem 1, we formally establish the connection between Mahalanobis balancing and \( \ell_2 \) shrinkage estimation of a propensity score model.
We define some additional notations. Let $W^{1/2}$ be the Cholesky decomposition of $W$ such that $W = (W^{1/2})^T W^{1/2}$. Let $\|\theta\|_2 = \sqrt{\theta_1^2 + \cdots + \theta_K^2}$ be the $\ell_2$ norm for an arbitrary $K$-dimensional vector $\theta = (\theta_1, \ldots, \theta_K)^T$. The quadratic inequality constraint in Problem (7) can then be rewritten as $\|\sum_{i=1}^n T_i w_i W^{1/2} (\Phi(X_i) - \bar{\Phi})\|_2 \leq \sqrt{\delta}$. Let $\hat{f}(p) = f(p)$ if $p \geq 0$, and $\hat{f}(p) = +\infty$, otherwise. Define a convex set $\mathcal{C} \subseteq \mathbb{R}^K$ such that $\mathcal{C} = \{ u \in \mathbb{R}^K : \|u\|_2 \leq \sqrt{\delta} \}$. Define $I_C(u) = 0$ if $u \in \mathcal{C}$, and $I_C(u) = +\infty$ otherwise. Then, Problem (7) is equivalent to the following unconstrained optimization problem:

$$\min_{w \in \mathbb{R}^n} \sum_{i=1}^n T_i \hat{f}(w_i) + I_C \left( \sum_{i=1}^n T_i w_i W^{1/2} (\Phi(X_i) - \bar{\Phi}) \right). \quad (9)$$

**Theorem 1.** Assume that the function $f(\cdot)$ is convex and continuously differentiable. Let $(\hat{f}')^{-1}(\cdot)$ denote the inverse function of the first derivative of $\hat{f}(\cdot)$. Let $\hat{f}^*(\cdot)$ be the conjugate function of $\hat{f}(\cdot)$. Assume that $\max_i \|W^{1/2} \Phi(X_i)\|_\infty$ is finite. The dual of Problem (9) is the following unconstrained optimization problem:

$$\min_{\theta \in \mathbb{R}^K} \sum_{i=1}^n T_i \hat{f}^* \left( \theta^T W^{1/2} (\Phi(X_i) - \bar{\Phi}) \right) + \sqrt{\delta}\|\theta\|_2. \quad (10)$$

Let $\hat{w} = (\hat{w}_1, \ldots, \hat{w}_n)^T$ be the primal solution of Problem (7) and $\hat{\theta} = (\hat{\theta}_1, \ldots, \hat{\theta}_K)^T$ be the dual solution of Problem (10). The $\hat{w}_i$ can be expressed as a function of $\hat{\theta}$:

$$\hat{w}_i = (\hat{f}')^{-1} \left( \hat{\theta}^T W^{1/2} (\Phi(X_i) - \bar{\Phi}) \right), \quad i = 1, \ldots, n. \quad (11)$$

We discuss the implication of Theorem 1 for $f(x) = x \log(x)$, the entropy function as used in entropy balancing (Hainmueller, 2012). The dual problem (10) becomes

$$\min_{\theta \in \mathbb{R}^K} \sum_{i=1}^n T_i \exp \left\{ \hat{\theta}^T W^{1/2} (\Phi(X_i) - \bar{\Phi}) - 1 \right\} + \sqrt{\delta}\|\theta\|_2,$$

and the estimated weight is $\hat{w}_i = \exp \left\{ \hat{\theta}^T W^{1/2} (\Phi(X_i) - \bar{\Phi}) - 1 \right\}$. The estimated MB weight is then obtained by normalization:

$$\hat{w}_i^{MB} = \frac{\hat{w}_i}{\sum_{j:T_j=1} \hat{w}_j} = \frac{\exp \left\{ \hat{\theta}^T W^{1/2} \Phi(X_i) \right\}}{\sum_{j:T_j=1} \exp \left\{ \hat{\theta}^T W^{1/2} \Phi(X_j) \right\}}, \text{ for all } i \in \{ j : T_j = 1 \}. \quad (12)$$

When the propensity score $\pi(x) = \Pr(T = 1 \mid x)$ follows the log model: $\log(\pi(x; \beta)) = \beta^T \Phi(x)$, the inverse probability weight $1/\{n \pi(X_i; \beta)\}$ coincides with the expression of the unnormalized weight $\hat{w}_i$ when $\Phi(\cdot)$ includes an intercept. Moreover, the stabilized inverse probability weight $\pi^{-1}(X_i; \beta)/\{\sum_{j:T_j=1} \pi^{-1}(X_j; \beta)\}$ coincides with the expression of the MB weight $\hat{w}_i^{MB}$. There is a one-to-one correspondence of the dual parameters $\hat{\theta}$ and the coefficients $\beta$ in the propensity score model $\pi(x; \beta)$: $\beta = (W^{1/2})^T \hat{\theta}$. Therefore, solving the dual problem (10) is equivalent to fitting an $\ell_2$ norm-based regularized generalized linear model with the logarithm as the link function.

We briefly discuss other choices of the loss function. When $f(x) = -\log(x)$, which is the negative of empirical likelihood (e.g. Chan et al., 2016), then $\hat{f}^*(x) = -\log(-x) - 1$ for $x > 0$. When the loss function is the quadratic function $f(x) = (x - 1/n)^2$ by Zubizarreta (2015), the distance measure by Chan et al. (2016), or the Bregman distance by Josey et al. (2021b), the conjugate function is more
complicated. We refer the readers to the monograph by Bertsekas (2016) for an extensive discussion of the conjugate functions. We recommend the entropy loss function \( f(x) = x \log(x) \) in Mahalanobis balancing for its theoretical properties (Zhao and Percival, 2017) and stable performance in our numerical experience.

Different values of the threshold parameter \( \delta \) introduces various degrees of bias to the \( \theta \) estimation. More conservative \( \theta \) value indicates larger bias but the MB weights are usually more stable. Consequently, the ATE estimation is more biased but exhibits less variability. Hence, selection of \( \delta \) affects the bias-variance trade-off for treatment effect estimation. In Section 3.2, we make comparison of the proposed method to existing balancing methods from the perspective of ATE estimation. In Section 3.4, we discuss selection of \( \delta \) in details.

### 3.2 A comparison with existing balancing methods

When exact balancing is feasible, the balanced weights by entropy balancing (Hainmueller, 2012; Zhao and Percival, 2017) also have the expression in equation (12). The \( \theta \) estimation of entropy balancing is nevertheless different because it does not involve regularization. In the bad-overlap or high-dimensional situation, entropy balancing is usually infeasible or very unstable. These issues are alleviated by Mahalanobis balancing. Its primal problem is always feasible if \( W \) is positive-definite and \( \phi(X_i) \) is bounded for all \( i \) in the treated group and \( k = 1, \cdots, K \). By regularizing the dual parameters \( \theta \) with the \( \ell_2 \) norm, Mahalanobis balancing stabilizes the estimated weights. The amount of regularization is determined by the tuning parameter \( \delta \), which controls the level of residual multivariate imbalance after reweighting. In contrast to entropy balancing which enforces finite-sample univariate exact balance, Mahalanobis balancing maintains finite-sample multivariate approximate balance.

Next, we make comparison from the outcome modelling perspective. Write

\[
Y_i(1) = E\{Y(1) \mid X_i\} + \epsilon_{1i} = \mu_1(X_i) + \epsilon_{1i}.
\]

Assume that the \( \epsilon_{1i} \) are independent with mean zero and finite variance. Let \( \hat{w}_1, \cdots, \hat{w}_n \) be the normalized weights estimated by an arbitrary weighting method, and \( \hat{\tau}_1 = \sum_{i=1}^n T_i \hat{w}_i Y_i \) be the resulting weighted estimator of \( \tau_1 = E\{Y(1)\} \). It follows that (Wong and Chan, 2018)

\[
\hat{\tau}_1 - \tau_1 = \sum_{i=1}^n T_i \hat{w}_i \mu_1(X_i) - \frac{1}{n} \sum_{i=1}^n \mu_1(X_i) + \frac{1}{n} \sum_{i=1}^n T_i \hat{w}_i \epsilon_{1i} + \frac{1}{n} \sum_{i=1}^n \mu_1(X_i) - E\{Y(1)\}.
\]

A good weighting method should control or minimize the magnitudes of \( A_1 \) and \( A_2 \). Covariate balancing does not utilize outcome information in the construction of the weights \( \hat{w}_1, \cdots, \hat{w}_n \), and thus the magnitude of the term \( A_2 \) is negligible. If the linear outcome model \( \mu_1(X) = \beta_1^T \Phi(X) \) holds (e.g., Athey et al., 2018), then

\[
A_1 = \beta_1^T \left( \sum_{i=1}^n T_i \hat{w}_i \Phi(X_i) - \bar{\Phi} \right).
\]

The exact balancing methods (e.g., Hainmueller, 2012; Imai and Ratkovic, 2014; Chan et al., 2016; Fan et al., 2021) impose \( \sum_{i=1}^n T_i \hat{w}_i \Phi(X_i) = \bar{\Phi} \), and thus \( A_1 \) is exactly zero. In the bad-overlap or high-dimensional situation, exact balancing is infeasible, and the term \( A_1 \) cannot be fully eliminated. The MDABW method (Zubizarreta, 2015; Wang and Zubizarreta, 2020) bounds the \( k \)th component
of \( \sum_{i=1}^{n} T_i \tilde{w}_i \Phi(X_i) - \bar{\Phi} \) by a threshold parameter \( \delta_k, k = 1, \ldots, K \). Therefore, \( |A_1| \leq |\beta_1^T \delta| \), where \( \delta = (\delta_1, \ldots, \delta_K)^T \), suggesting that \( A_1 \) is controlled by the MDABW method. Note that by the Cauchy-Schwarz inequality, the term \( A_1 \) is bounded by
\[
|A_1| \leq \|\beta_1^T W^{-1/2}\|_2 \times \|W^{1/2}(\sum_{i=1}^{n} T_i \tilde{w}_i \Phi(X_i) - \bar{\Phi})\|_2 = \|\beta_1^T W^{-1/2}\|_2 \times \text{GMIM}_i^{\tilde{w}}.
\]

This provides us an intuitive guideline for the selection of the threshold parameter \( \delta \) in the proposed MB method. A good choice of \( \delta \) should make \( \text{GMIM}_i^{\tilde{w}} \) small enough so that the term \( A_1 \) is under control. We provide more details in Section 3.4.

Moreover, some balancing methods also control the magnitudes of \( A_1^2 \) and \( A_2^2 \). The approximately residual balancing method (Athey et al., 2018), the covariate functional balancing method (Wong and Chan, 2018), and the MDABW method, among others, achieve this goal with different techniques. The consensus is that the \( \|\tilde{w}\|_2 \) should be small, because it implies that \( A_2^2 \) is controlled by the Cauchy-Schwarz inequality. The balancing methods differ in the way of handling \( A_1^2 \). The covariate functional balancing method directly minimizes \( A_1^2 \) with the regularization term \( \|\tilde{w}\|_2^2 \), whereas the approximately residual balancing method concern \( \|A_1\|_2^2 \) with the regularization term \( \|\tilde{w}\|_2^2 \), and the MDABW method controls \( A_1^2 \) by \( A_1^2 \leq (\beta_1^T \delta)^2 \).

Intuitively, Mahalanobis balancing stabilizes the estimated weights by the \( \ell_2 \) norm regularizer in the estimation of the dual parameters \( \theta \). In the Supplementary Material, we show that \( \|\tilde{w}\|_2 = O_p(n^{-1/2}) \), and thus \( A_2^2 \) is controlled. Furthermore, by tuning \( \delta \) to make the GMIM measure small, the term \( A_1^2 \) is also small. We remark that a key advantage of Mahalanobis balancing compared to the MDABW method is that it does not need to tune a potentially large number of parameters to control the magnitudes of \( A_1 \) and \( A_2 \) and their second orders.

### 3.3 Asymptotic properties

The proposed Mahalanobis balancing method estimates the average treatment effect by \( \hat{\Phi}^{MB} = \sum_{i=1}^{n} T_i \tilde{w}_i^{MB} Y_i - \sum_{i=1}^{n} (1 - T_i) \tilde{w}_i^{MB} Y_i \), where the \( \tilde{w}_i^{MB} \) are the estimated MB weights obtained by normalizing the weights \( \tilde{w}_i \) in equation (11) with a fixed \( \delta \). In this subsection, we prove that this MB-based ATE estimator is doubly robust and semiparametrically efficient under mild regularity conditions. The proofs are given in the Supplementary Material.

**Assumption 3.** Assume the following conditions:

1. The optimization problem \( \min_{\theta \in \Theta} E[\hat{f}^* (\theta^T W^{1/2} (\Phi(X_i) - E\{\Phi(X)\}))] \) has a unique global minimizer for \( \theta \), where \( \theta \in \text{int}(\Theta) \), and \( \Theta \) is a compact parameter space for \( \theta \).
2. \( \delta = o(n) \).
3. \( (\hat{f}^*)^{-1}(\cdot) = \hat{f}^*(\cdot) \). Moreover, \( f(\cdot) \) is twice continuously differentiable.
4. The conjugate function \( f^*(\cdot) \) satisfies the property that if \( f^*(\theta^T W^{1/2} (\Phi(X) - E\{\Phi(X)\})) = C + f^*(\theta^T W^{1/2} (\Phi(X) - E\{\Phi(X)\})) \), for some constant \( C \) for all \( X \), then \( \theta^* = \theta \).
5. \( E\{\exp(a \theta^T W^{1/2} (\Phi(X) - E\{\Phi(X)\}) | T = t)\} < \infty \) for all \( \theta \in \Theta \) and \( t = 0, 1 \), where \( a = 1, 2, 3 \). Moreover, \( \text{Var}(\Phi(X)) < \infty \) and \( \text{Var}(\Phi(X) | T = t) < \infty \) and \( t = 0, 1 \).
6. The noises \( \epsilon_{1i} = Y_i(1) - E\{Y_i(1) | X_i\} \) and \( \epsilon_{0i} = Y_i(0) - E\{Y_i(0) | X_i\}, i = 1, \ldots, n \) are mutually independent and sub-Gaussian, and they are independent of \( X \).
7. \( \eta \leq \pi(X) \leq 1 - \eta \), where \( 0 < \eta < 1/2 \).

Assumption (3.1) is a standard requirement for consistency of the ATE estimator. Assumption (3.2) requires that the threshold parameter \( \delta \) should not be large. Assumptions (3.3) and (3.4) are satisfied by the common choices \( f(x) = x \log(x), -\log(x) \) or \( (x - 1/n)^2 \). Assumptions (3.5) and
Assumption 4. The entropy function is the loss function. When the loss function is the entropy function, these three conditions are automatically satisfied. These conditions are satisfied when the loss function is the entropy function. The third condition \( \delta \) is needed for double robustness of the ATE estimator. Assumption (3.7) is the strict overlap assumption.

Theorem 2. Suppose that Assumptions 1-3 hold, then the MB-based ATE estimator \( \hat{\tau}^{MB} \) is doubly robust in the sense that:

(i). If the propensity score satisfies \( 1/\pi(X) = C \cdot \hat{f}^*(\theta^T W^{1/2}(\Phi(X) - \bar{\Phi})) \) for some constant \( C \) for all \( X \), then \( \hat{\tau}^{MB} - \tau = O_p(n^{-1/2}) \);

(ii). If the conditional potential outcomes \( E\{Y(1)|X\} \) and \( E\{Y(0)|X\} \) are linear combinations of the basis functions \( \Phi(X) = (\phi_1(X), \cdots, \phi_K(X))^T \), then \( \hat{\tau}^{MB} - \tau = O_p(n^{-1/2}) \) when at least one of the following two statements is true: (a). The loss function is the entropy function; (b). The following conditions hold: \( \sum_{i=1}^n T_i (\hat{w}_i^{MB})^3/\|T \hat{w}^{MB}\|_2^3 = o_p(1), \sum_{i=1}^n (1 - T_i)(\hat{w}_i^{MB})^3/\|(1 - T)\hat{w}_i^{MB}\|_2^3 = o_p(1), \|\hat{w}_i^{MB}\|_2^2 = O_p(n^{-1}) \), and \( \sum_{i=1}^n T_i \hat{w}_i^{MB} \{\Phi(X_i) - \bar{\Phi}\} W \sum_{i=1}^n T_i \hat{w}_i^{MB} \{\Phi(X_i) - \bar{\Phi}\} = O_p(n^{-1}) \), \( \sum_{i=1}^n (1 - T_i) \hat{w}_i^{MB} \{\Phi(X_i) - \bar{\Phi}\} = O_p(n^{-1}) \), \( \sum_{i=1}^n (1 - T_i) \hat{w}_i^{MB} \{\Phi(X_i) - \bar{\Phi}\} W \sum_{i=1}^n (1 - T_i) \hat{w}_i^{MB} \{\Phi(X_i) - \bar{\Phi}\} = O_p(n^{-1}) \).

Here, \( \|T \hat{w}^{MB}\|_2 = \sqrt{\sum_{i=1}^n T_i (\hat{w}_i^{MB})^2} \) and \( \|(1 - T)\hat{w}^{MB}\|_2 = \sqrt{\sum_{i=1}^n (1 - T_i)(\hat{w}_i^{MB})^2} \). Note that the constant \( C \) may depend on the sample size. In particular, when \( C = n \), then it implies that the unnormalized MB weight in equation (11) satisfies \( \hat{w}_i = 1/\{n \pi(X_i)\} \) by Assumption (3.3). The first two conditions in statement (b) require that the weights should be smoothly distributed and no extremely large weights are allowed. Roughly speaking, it means that the weights should be stable. These conditions are satisfied when the loss function is the entropy function. The third condition in statement (b) requires that multivariate imbalance is asymptotically negligible after reweighting. When the loss function is the entropy function, these three conditions are automatically satisfied.

Next, we prove the semiparametric efficiency property for the MB-based ATE estimator when the entropy function is the loss function.

Assumption 4. Assume the following conditions:

(4.1). Suppose that \( 1/\pi(X) = C_1 \cdot \hat{f}^*(m^*(X)) \) for some constant \( C_1 \) for all \( X \), where \( m^*(\cdot) \in \mathcal{M} \) and \( \mathcal{M} \) is a set of smooth functions satisfying log \( n_{\varepsilon}(\varepsilon, \mathcal{M}, L_2(P)) \leq C_2(1/\varepsilon)^{k_1} \). Here, \( C_2 \) is a positive constant, \( k_1 > 1/2 \), and \( n_{\varepsilon}(\varepsilon, \mathcal{M}, L_2(P)) \) denotes the covering number of \( \mathcal{M} \) by \( \varepsilon \)-brackets.

(4.2). \( \hat{f}^*(m^*(X)) \) is Lipschitz in \( \mathcal{X} \), where \( \mathcal{X} \) is the domain of covariate \( X \).

(4.3). There exists an \( \theta^* \) such that sup \( \varepsilon \in \mathcal{X} \|\theta^T \Phi(x) - m^*(x)\|_2 = o_p(1) \).

(4.4). The conditional potential outcomes \( E\{Y(1)|X\} \) and \( E\{Y(0)|X\} \) are linear combinations of the basis functions \( \Phi(X) = (\phi_1(X), \cdots, \phi_K(X))^T \).

Assumption (4.1) requires that the complexity of the function class is sufficiently smooth. Wang and Zubizarreta (2020) noted that the Hölder class with smoothness parameter \( s \) with \( s/K > 1/2 \) satisfies this condition (see also van der Vaart and Wellner, 1996; Fan et al., 2021). Assumption (4.2) bounds the second derivative of the function \( f^*(\cdot) \). Assumption (4.3) requires that the \( m^*(\cdot) \) can be approximated by the linear span of the basis functions. It is similar to Assumption 1.6 by Wang and Zubizarreta (2020). Assumption (4.4) is a standard condition for semiparametric efficiency.

Theorem 3. Suppose that Assumptions 1-4 hold, then the MB-based ATE estimator reaches the semiparametric efficiency bound.

3.4 Tuning parameter selection

If the normalization constraint \( \sum_{i=1}^n T_i w_i = 1 \) is incorporated in Problem (7), then it may be infeasible when \( \delta \) is small. We instead normalize the weights only after solving Problem (7). This
guarantees that Problem (7) is always feasible for any \( \delta > 0 \) under the mild condition that \( W \) is positive-definite and \( \phi_k(X_i) \) is bounded for any \( i \) and \( k \). This allows us to freely try a set of grid points and select the best \( \delta \) that minimizes multivariate imbalance. In contrast to the MDABW method, there is no resampling techniques in the selection procedure.

Now, we present the selection of \( \delta \) in details. First, set up a set of positive values \( D \) for \( \delta \) selection. We use \( D = \{10^{-k} : k = 0, 1, \cdots, 6\} \) in the simulations and application. The algorithm for selection of \( \delta \) is as follows:

**Algorithm 1. Selection of \( \delta \):**

- **For each** \( \delta \in D \):
  - Compute the dual parameters \( \hat{\theta} \) by solving Problem (10);
  - Compute the weights \( \hat{w}_i \) using (11);
  - Obtain the Mahalanobis balancing weights by normalization: \( \hat{w}_i^{MB} = \hat{w}_i / \sum_{j:T_j = 1} \hat{w}_j; \)
  - Calculate GMIM\(_i^\nu\) in (8) using the \( \hat{w}_i^{MB} \);
  - Output \( \delta^* \) that minimizes GMIM\(_i^\nu\).

Similarly, we select the optimal threshold parameter for the control group by minimizing GMIM\(_i^\nu_0\). Let \( (\hat{w}_1^{MB}, \cdots, \hat{w}_n^{MB}) \) be the resulting MB weights corresponding to the optimal threshold parameters. The average treatment effect is then estimated by \( \hat{\tau}^{MB} = \sum_{i=1}^n T_i \hat{w}_i^{MB} Y_i - \sum_{i=1}^n (1 - T_i) \hat{w}_i^{MB} Y_i \).

Our empirical experience is that the ATE estimation is not sensitive to the choice of tuning parameter if \( \delta \) is small enough. In the Supplementary Material, the simulations reveal that the outputs of ATE estimation and imbalance measures are quite similar when \( \delta \leq 10^{-4} \). Therefore, if computation cost is a concern, we suggest to use a fixed small value for \( \delta \) in practise, say \( \delta = 10^{-4} \).

### 3.5 High-dimensional Mahalanobis balancing

In the high-dimensional setting where \( K \) is large compared to the sample size \( n \), balancing all basis functions becomes a difficult problem even when each of the unadjusted basis functions is approximately balanced. The difficulty can be partly explained from the multivariate perspective: when the basis functions are mutually independent, the squared Mahalanobis distance increases linearly with \( K \), and hence multivariate imbalance can be hardly controlled. Exact balancing is infeasible, and univariate approximate balancing becomes more difficult to obtain optimal high-dimensional threshold parameters.

Mahalanobis balancing is still feasible in the high-dimensional situation under the mild conditions that the weight matrix is positive-definite and the basis functions are bounded. Moreover, it still only needs to tune one threshold parameter. By minimizing multivariate imbalance to some extent, Mahalanobis balancing generally produces more balanced weights and less biased ATE estimation compared to univariate approximate balancing.

We provide asymptotic property for the MB-based ATE estimator in the high-dimensional situation. We choose the entropy function as the loss function.

**Assumption 5.** Assume the following conditions:

1. \( (5.1) \). The dimension of covariate \( p = n^{1-2\alpha} \), where \( 0 \leq \alpha \leq 1/2 \).
2. \( (5.2) \). \(|\theta^TW^{1/2}(E\{\Phi(X)\} - E\{\Phi(X) \mid T = t\})| \leq \gamma \log(n) \) for all \( \theta \in \Theta \) and \( t = 0, 1 \), where \( \gamma > 0 \).
3. \( (5.3) \). \( \mu_j(X) = \beta_j\Phi(X) \) with \( \|\beta_j\|_2 = O(n^{1-2\alpha}) \), \( j = 0, 1 \).
4. \( (5.4) \). \( \delta = O(n^{2\alpha}) \), where \( s \geq 0 \).
Assumption (5.1) restricts the dimension $p$. It is allowed to increase with the sample size $n$, but should not exceed $n$. Assumption (5.2) adds some additional assumption on $W^{1/2}(E\{\Phi(X)\} - E\{\Phi(X) \mid T = t\})$. It is satisfied, for instance, when $\|\theta\|_2 \leq \gamma \log(n)$ and $\|E\{\Phi(X) \mid T = t\} - E\{\Phi(X)\}\|_2 \leq 1$, or when the $\theta$ is sparse. Assumption (5.3) imposes linear outcome models where the magnitude of the coefficients is not too large. Assumption (5.4) requires that $\delta$ should not be large.

**Theorem 4.** Suppose that Assumptions 1, 2, 3, 5 hold, then $\hat{\tau}^{MB} - \tau = O_p(n^{-1/2}) + O_p(n^{s+\gamma-2\alpha})$.

It suggests that $\delta$ should be small, so we set $s = 0$. According to Theorem 4, when $\gamma - 2\alpha \leq -1/2$, the MB-based ATE estimator is consistent. Moreover, this theorem illustrates the difficulty of ATE estimation in high-dimensional setting. For example, when $p = n$ and $\gamma > 0$, then Theorem 4 no longer guarantees the consistency of the MB-based ATE estimator.

When the true propensity score model is not sparse, Mahalanobis balancing outperforms the state-of-the-art high-dimensional regularized balancing methods (Athey et al., 2018; Ning et al., 2020; Tan, 2020a,b) in the simulation studies. Therefore, Mahalanobis balancing is preferred over univariate approximate balancing and high-dimensional regularized balancing in this situation. When the true propensity score model is sparse, the performance of Mahalanobis balancing is not entirely satisfactory. This is not surprising because the high-dimensional regularized balancing methods commonly select a sparse subset of basis functions by $\ell_1$ or elastic net regularization. In contrast, the $\ell_2$ regularization in the dual problem (10) suggests that Mahalanobis balancing does not automatically perform variable selection.

In the sparse setting, we propose the high-dimensional Mahalanobis balancing method, which performs selection of basis functions before producing balanced weights. It substantially improves the performance of Mahalanobis balancing in the sparse setting.

Recall that we write $X = (X_1, \cdots, X_p)^T$. In the high-dimensional setting, we use the trivial feature mapping: $\Phi(X) = X$ and $K = p$. In high-dimensional Mahalanobis balancing, we select a subset of the covariates $X$ with dimension $K_0$, where $K_0 \leq p$. The following algorithm gives a principled way for subset selection. Let $ASMD_j$ be the absolute standard mean deviation for $X_j$ defined in equation (1), $j = 1, \cdots, p$. Rank $X_1, \cdots, X_p$ as $X_{(1)}, \cdots, X_{(p)}$ such that $X_{(1)}$ has the largest ASMD value, $X_{(2)}$ has the second largest ASMD value, and so forth.

**Algorithm 2.** High-dimensional Mahalanobis balancing

For each step $j \in \{1, \cdots, p\}$:

1. Apply Algorithm 1 to obtain the MB weights $\hat{w}^{MB}_j$ using $\Phi(X) = (X_{(1)}, \cdots, X_{(j)})^T$;
2. Calculate $\text{GMIM}_i^w$ in (8) using the $\hat{w}^{MB}_j$, and define $\text{GMIM}_{i,j}^w = \text{GMIM}_i^w / j$;
3. Add $(j, \text{GMIM}_{i,j}^w)$ to the $x$-$y$ plot;
4. Observe whether there is a kink at $(j, \text{GMIM}_{i,j}^w)$:
   - If no, let $j = j + 1$;
   - If yes, stop and output $K_0 = j − 1$.

We then use $\Phi(X) = (X_{(1)}, \cdots, X_{(K_0)})^T$ and the MB weights at step $K_0$ for high-dimensional Mahalanobis balancing. Similarly, we obtain the MB weights for the control group. The average treatment effect is then estimated by the weighted difference of the outcomes.

The rationale of Algorithm 2 hinges on the adjusted multivariate imbalance measure $\text{GMIM}_{i,j}^w$. It represents the average contribution of the $j$ most imbalanced covariates to the residual multivariate imbalance after MB weighting. If it remains stable as $j$ increases, then MB is capable of controlling multivariate imbalance. However, if there is a kink at Step $j$, it implies that adding the $j$th
imbalanced covariate greatly increases the multivariate imbalance measure, and thus is harmful to the overall imbalance. That is, MB starts to lose control of overall imbalance at Step $j$. Therefore, we stop and choose the outputs at Step $j - 1$. The kink usually occurs when $K_0 = O(\sqrt{p})$ in the numerical studies. If there is no kink for all $j = 1, \cdots, p$, it suggests that the performance of MB is acceptable even if all $p$ covariates are included. One may choose $K_0 = p$ in this situation, or $K_0 = \sqrt{p}$ if a small subset of covariates is preferred.

Algorithm 2 tends to select covariates that exhibit large univariate imbalance. The number of covariates is determined by their average contribution to overall imbalance. Algorithm 2 may not work well when the unselected imbalanced covariates are correlated with the outcomes, because selection bias may occur in this situation. To alleviate this issue, one may construct bias-corrected ATE estimation by augmenting the simple weighted outcome difference with an outcome model.

### 3.6 Alternative formulations of Mahalanobis balancing

Asymptotic theory of Mahalanobis balancing becomes much more difficult in the ultra high-dimensional setting with $K \gg n$. For example, the general high-dimensional regularized M-estimation theory does not apply (Wainwright, 2019) because the $\ell_2$ norm regularizer $\|\theta\|_2$ in the dual problem (10) is not decomposable. Another potential concern of the $\ell_2$ norm is that the gradient computation of the dual problem (10) might be unstable in the ultra high-dimensional setting. These problems can be resolved by employing the squared $\ell_2$ norm $\|\theta\|_2^2$ instead, but it does not lead to a primal problem similar to Problem (7).

Our numerical experience reveals that the dual problem (10) can be easily solved using the standard BFGS algorithm together with Algorithm 2 even in the ultra high-dimensional setting, because Algorithm 2 usually selects a small subset of covariates. Therefore, we stick to use the $\ell_2$ norm $\|\theta\|_2$ in the high-dimensional setting in this paper.

Next, we discuss the formulation of Mahalanobis balancing when the normalization constraint is added to Problem (7). Note that without the normalization constraint, Problem (7) is equivalent to an unconstrained optimization problem with a sum of independent terms plus a regularizer, and thus it can be viewed as a regularized M-estimation problem. When the normalization constraint is inserted, the dual problem is no longer a regularized M-estimation problem. Using the entropy function as the loss function, the optimization problem is

$$\begin{align*}
\text{minimize } & \quad \sum_{i=1}^n T_i w_i \log(w_i) \\
\text{subject to: } & \quad w_i \geq 0, \quad i \in \{j : T_j = 1\}; \\
& \quad \sum_{i=1}^n T_i w_i = 1; \\
& \quad \sum_{i=1}^n T_i \{w_i \Phi(X_i) - \bar{\Phi}\}^\top W \sum_{i=1}^n T_i \{w_i \Phi(X_i) - \bar{\Phi}\} \leq \delta.
\end{align*}$$

By the Fenchel duality theory, the corresponding dual problem is

$$\begin{align*}
\text{minimize } & \quad -\log \left[ \sum_{i=1}^n T_i \exp \left\{ \theta^\top W^{1/2} \Phi(X_i) \right\} \right] + \theta^\top W^{1/2} \Phi + \sqrt{\delta} \|\theta\|_2.
\end{align*}$$

The estimated weight for subject $i$ in the treated group is

$$\hat{w}_i^{MB} = \frac{\exp \left\{ \hat{\theta}^\top W^{1/2} \Phi(X_i) \right\}}{\sum_{i:T_i=1} \exp \left\{ \hat{\theta}^\top W^{1/2} \Phi(X_i) \right\}}, \quad \text{for all } i \in \{j : T_j = 1\},$$
where \( \hat{\theta} \) is solved from the dual problem. No further normalization is needed. We remark that when \( \delta = 0 \), then the dual problem reduces to that by entropy balancing (Hainmueller, 2012; Zhao and Percival, 2017). Therefore, Mahalanobis balancing with the normalization constraint is a direct generalization of entropy balancing, in the sense that it regularizes the dual parameters \( \theta \) by entropy balancing with the \( \ell_2 \) norm.

The parameter \( \delta \) is more difficult to tune when the normalization constraint is inserted. In particular, a small \( \delta \) tends to make the primal problem infeasible in the bad overlap and high-dimensional settings. A tentative selection strategy is to examine the feasibility of the primal problem by varying \( \delta \) from 0 to \( D \) with a small step, say \( D = 10 \) and \( d = 0.05 \). Resampling (e.g. Wang and Zubizarreta, 2020) is then applied to each feasible case to evaluate the out-of-sample balancing performance. The \( \delta \) is chosen as the value that minimizes the out-of-sample multivariate imbalance. Further investigation of alternative formulations of Mahalanobis balancing is warranted.

4 Numerical Studies

In this section, we compare Mahalanobis balancing to three classes of existing balancing methods for ATE estimation in numerical studies. The first class consists of exact balancing methods, including entropy balancing (EB) (Hainmueller, 2012) implemented with the R package \texttt{Weightit}, covariate balancing propensity score (CBPS) (Imai and Ratkovic, 2014) implemented with the R package \texttt{CBPS}, and calibration weighting (CAL) (Athey et al., 2018) implemented with the R package \texttt{ATE}. The second class consists of univariate approximate balancing methods, among which the MDABW method (Wang and Zubizarreta, 2020) is implemented with the R package \texttt{sbw}. The third class consists of high-dimensional regularized balancing methods, including two versions of regularized calibrated estimation (RCAL1 and RCAL2) (Tan, 2020a,b) implemented with the R package \texttt{RCAL}, approximately residual balancing (ARB) (Athey et al., 2018) implemented with the R package \texttt{balanceHD}, and high-dimensional covariate balancing propensity score (hdCBPS) (Ning et al., 2020) implemented with the R package \texttt{CBPS}. We also report the unadjusted ATE estimator using the sample difference in the outcomes (Unad).

For each method, we report the bias (Bias) of ATE estimation, Monte Carlo standard deviation (SD), root mean squared error (RMSE), Monte Carlo average of the sample mean of ASMD\(_k\), \( k = 1, \ldots, K \) (meanASMD) as a univariate imbalance measure, and the generalized Mahalanobis imbalance measure (GMIM) \( \text{GMIM}_W = \text{GMIM}_1^W + \text{GMIM}_0^W \) with \( W_1 \) as the weight matrix aiming to quantify residual multivariate imbalance after reweighting.

4.1 The low-dimensional settings

In this subsection, we assess the performance of two Mahalanobis balancing methods using \( W_1 = [\text{diag}((\Sigma_1 + \Sigma_0)/2)]^{-1} \) (denoted by MB), or \( W_2 = [(\Sigma_1 + \Sigma_0)/2]^{-1} \) (denoted by MB2) as the weight matrix, and make comparison with exact balancing (EB, CBPS, CAL) and univariate approximate balancing (MDABW). We consider four scenarios. For each scenario, we conduct 1000 Monte Carlo simulations. The sample size is set to be \( n = 200 \) for the first three scenarios and \( n = 1000 \) for the fourth scenario. Table 1 summarizes the outputs. The Supplementary Material provides more detailed information.

In Scenario A, we consider the situation where both propensity score and outcome models are misspecified. This setting similar to that of Kang and Schafer (2007). For each simulation, we first generate a standard normal random vector \( Z = (Z_1, \ldots, Z_p)^\top \) with \( p = 10 \) for each observation, and then generate the covariates \( X \) from \( X_1 = \exp(Z_1/2), X_2 = Z_2/(1 + \exp(Z_1)), X_3 = (Z_1Z_3 + 0.6)^3, X_4 = (Z_2 + Z_4 + 20)^2, X_j = Z_j, j = 5, \ldots, 10 \). The outcome is generated from the linear
Table 1: Simulation outputs in the low-dimensional settings.

| Scenario | $n,K=(200,10)$: both propensity score and outcome models are misspecified. | $n,K=(200,45)$: the confounders are the interaction of covariates. | $n,K=(200,10)$: covariate means are very different. | $n,K=(1000,10)$: sample sizes are very imbalanced across treatment groups. |
|----------|--------------------------------------------------------------------------|-----------------------------------------------------------------|-------------------------------------------------|---------------------------------------------------------------------|
|          | **Unad** | **MB** | **MB2** | **MDABW** | **CBPS** | **CAL** | **EB** | **Unad** | **MB** | **MB2** | **MDABW** | **CBPS** | **CAL** | **EB** | **Unad** | **MB** | **MB2** | **MDABW** | **CBPS** | **CAL** | **EB** | **Unad** | **MB** | **MB2** | **MDABW** | **CBPS** | **CAL** | **EB** |
| **Bias** | -2.19    | -0.10  | -0.10  | -0.10     | -0.10    | -0.10   | -0.10  | 7.27     | -0.09  | 2.58   | 1.49     | 3.60    | -       | -      | 15.03    | 0.21  | 0.26  | 1.88     | -3.01 | -       | -      | -5.88    | -0.16 | -0.15  | -1.36    | -0.74 | -       | -      |
| **SD**   | 3.09     | 3.22   | 3.22   | 3.23      | 3.29     | 3.21    | 3.21   | 4.80     | 1.33   | 2.73   | 1.80     | 5.98    | -       | -      | 15.26    | 0.80  | 0.85  | 1.69     | 0.70  | -       | -      | -5.98    | 0.46  | 0.45   | 0.82     | 0.40  | -       | -      |
| **RMSE** | 3.77     | 3.22   | 3.22   | 3.23      | 3.29     | 3.21    | 3.21   | 8.74     | 1.33   | 3.74   | 2.33     | 6.98    | -       | -      | 15.26    | 0.83  | 0.89  | 2.53     | 3.10  | -       | -      | -5.98    | 0.49  | 0.47   | 1.59     | 0.84  | -       | -      |
| **meanASMD** | 0.15    | 0.00   | 0.00   | 0.01      | 0.00     | 0.00    | 0.00   | 0.22     | 0.05   | 0.10   | 0.11     | 0.18    | -       | -      | 1.00     | 0.02  | 0.02  | 0.13     | 0.00  | -       | -      | -0.85    | 0.01  | 0.01   | 0.09     | 0.00  | -       | -      |
| **GMIM** | 0.21     | 0.00   | 0.00   | 0.02      | 0.00     | 0.00    | 0.00   | 2.13     | 0.11   | 0.77   | 0.56     | 3.16    | -       | -      | 5.18     | 0.02  | 0.02  | 0.15     | 2.20  | -       | -      | -4.98    | 0.01  | 0.01   | 0.09     | 0.00  | -       | -      |

regression model using $Z$: $Y = 210 + (1.5T - 0.5)(13.7Z_1 + 13.7Z_2 + 13.7Z_3 + 13.7Z_4) + \epsilon$, where $\epsilon$ is a standard normal variable and is independent of $(T,Z)$. The treatment indicator is generated from $T \sim \text{Bernoulli}(\pi(Z))$, where $\pi(Z) = 1/(1 + \exp(0.5Z_1 + 0.1Z_4))$. The $Z$ are latent variables and the $X$ are observed instead. Linear outcome model and logistic propensity model with $X$ as the covariates are implemented. Both regression models are misspecified. In this scenario, $\Phi(X) = X$, and $K = p = 10$. The distributions of $X$ are not quite discrepant between the two treatment groups, and thus Scenario A is a good-overlap setting. The exact balancing methods are applicable.

The MB and MB2 methods and other balancing methods produce similar outputs. They all successfully remove covariate imbalance and produce almost identical ATE estimates. The RMSEs of MB, MB2, CAL, and EB are somewhat smaller than those of MDABW and CBPS. We conclude that Mahalanobis balancing maintains the advantages of the exact balancing methods in Scenario A. Moreover, the computation cost of Mahalanobis balancing is less than 0.5% than that of MDABW. This is because MDABW needs 1000 bootstraps for each possible tuning parameter and is time-consuming.

In Scenario B, we first generate $T \sim \text{Bernoulli}(0.5)$ for each observation. If $T = 1$, the covariate is generated from $X \sim N(1,\Sigma_1)$, where $\text{Cov}(X_j,X_k) = 2^{-I(j\neq k)}$; if $T = 0$, then the covariate is
generated from $X \sim N(1, \Sigma_0)$, where $Cov(X_j, X_k) = I(j = k)$. Set $p = 10$. This data generation procedure allows us to delineate the discrepancy of covariate distributions between the treated and control groups: the mean and variance are the same, but the interaction terms are very different. The observed outcome is generated from $Y = (1 + T)(X_1 + \cdots + X_{10}) + (1 + T)(X_1X_2 + X_2X_3 + \cdots + X_9X_{10} + X_{10}X_1) + \epsilon$, where $\epsilon \sim N(0, 1)$. The first two moments of $X$ are well balanced. In contrast, the interaction terms are strong confounders. We set $\Phi(X) = \{X_jX_k : 1 \leq j < k \leq 10\}$ and thus $K = 45$.

Because the covariance structures are highly dissimilar in the treated and control groups, Scenario B is a bad-overlap setting. In fact, both EB and CAL do not admit solutions. In comparison, MB is able to approximately balance the interaction terms. The two imbalance measures of MB are substantially lower than those of MDABW and CBPS. Furthermore, MB significantly improves ATE estimation of exact balancing and univariate approximate balancing because it exhibits much smaller bias and RMSE than those of MDABW and CBPS. Nevertheless, MB2 performs unsatisfactorily because these interaction terms are highly correlated and thus the weight matrix $W_2$ is unstable. We recommend MB over MB2 in this situation.

In Scenario C, the covariate means are highly different in the two groups. Set $p = 10$. We first generate $T \sim Bernoulli(0.5)$ for each observation. If $T = 1$, the covariate is generated from $X \sim N(1, \Sigma_1)$; otherwise, $X \sim N(0, \Sigma_0)$. The covariance matrices $\Sigma_1$ and $\Sigma_0$ are the same as those in Scenario B. The observed outcome is generated from $Y = (1 + T)(X_1 + \cdots + X_{10}) + \epsilon$, where $\epsilon \sim N(0, 1)$. In this scenario, $\Phi(X) = X$, and $K = 10$. Scenario C is a bad-overlap setting, because the covariate distributions are quite different such that the optimization problems of EB and CAL are infeasible. MDABW exhibits much less bias compared to CBPS, but it has larger standard deviation. The proposed MB and MB2 methods have smallest multivariate imbalance. MB and MB2 produce much less biased ATE estimation than MDABW and CBPS. The RMSEs are much smaller.

In Scenario D, the sample sizes are highly imbalanced. This situation is commonly seen in cohort studies when the exposure is rare and the control sample is very large. We fix the expected sample size of the treated group to be 50, and the control group has a sample size of roughly 950. Set $\Phi(X) = X$ and $K = p = 10$. The covariates are simulated by $X \sim N(1, I_{10\times10})$. The treatment indicator is simulated from $T \sim Bernoulli(\pi(X))$ with $\pi(X) = 1/(1 + 19\exp(X_1 + \cdots + X_{10} - 10))$. The outcome is simulated from $Y = (1 + T)(X_1 + \cdots + X_{10}) + \epsilon$, where $\epsilon \sim N(0, 1)$. Again, this is a bad-overlap setting. EB and CAL are infeasible. In contrast to Scenario C, the ATE estimate of CBPS is less biased than that of MDABW. The RMSE of CBPS is also smaller. MB and MB2 greatly outperform MDABW and CBPS in terms of bias, RMSE, and GMIM, although their meanASMDs are slightly larger than that of CBPS.

Finally, we remark that although CBPS is an exact balancing method, it is still applicable in the bad-overlap settings as in Scenarios B, C, and D. This is because it employs the generalized method of moments for parameter estimation, which still works even when the moment constraints are not met exactly. CBPS achieves lowest standard deviation and meanASMD in Scenarios C and D, but it has enormous bias, RMSE, and GMIM. Large GMIM value implies that the weighted average of the basis functions in each group is highly different from the pooled-sample average. It implies that the covariate distributions in each group (that is, the conditional distributions of $X|T = 1$ and $X|T = 0$) are still highly dissimilar to the distribution of $X$ in the population after CBPS reweighting, leading to large estimation bias. Therefore, GMIM accurately recognizes multivariate imbalance between each group and the pooled-sample after reweighting and is predictive of the performance of balancing methods for treatment effect estimation. We recommend to use GMIM instead of ASMD to assess residual covariate imbalance in the bad-overlap settings.
Table 2: Simulation outputs in the high-dimensional settings.

| Scenario E with \((n, p) = (200, 100)\): sparse propensity score model. | Unad | MB | kernelMB | hdMB | MDABW | RCAL1 | RCAL2 | ARB | hdCBPS |
|---|---|---|---|---|---|---|---|---|---|
| Bias | -3.44 | -0.85 | -0.92 | -0.01 | -2.13 | -0.48 | -0.47 | -0.22 | -0.19 |
| SD | 0.36 | 0.30 | 0.29 | 0.32 | 1.11 | 0.32 | 0.31 | 0.27 | 0.37 |
| RMSE | 3.47 | 0.90 | 0.96 | 0.32 | 2.39 | 0.58 | 0.57 | 0.35 | 0.38 |
| meanASMD | 0.16 | 0.07 | 0.08 | 0.14 | 0.15 | 0.15 | 0.16 | - | - |
| GMIM | 4.35 | 0.53 | 0.71 | 4.19(0.00)* | 2.12 | 2.17 | 3.43 | - | - |

| Scenario E with \((n, p) = (200, 500)\): sparse propensity score model. | Unad | MB | kernelMB | hdMB | MDABW | RCAL1 | RCAL2 | ARB | hdCBPS |
|---|---|---|---|---|---|---|---|---|---|
| Bias | -3.46 | -2.46 | -2.49 | 0.00 | -3.43 | -0.76 | -0.76 | -0.43 | -0.38 |
| SD | 0.37 | 0.33 | 0.33 | 0.35 | 0.37 | 0.29 | 0.29 | 0.25 | 0.40 |
| RMSE | 3.48 | 2.48 | 2.52 | 0.35 | 3.45 | 0.81 | 0.81 | 0.48 | 0.55 |
| meanASMD | 0.12 | 0.10 | 0.10 | 0.22 | 0.12 | 0.12 | 0.13 | - | - |
| GMIM | 7.32 | 5.15 | 5.30 | 36.26(0.00) | 7.28 | 7.36 | 7.43 | - | - |

| Scenario F with \((n, p) = (200, 100)\): dense propensity score model. | Unad | MB | kernelMB | hdMB | MDABW | RCAL1 | RCAL2 | ARB | hdCBPS |
|---|---|---|---|---|---|---|---|---|---|
| Bias | -1.35 | -0.35 | -0.31 | -0.55 | -0.91 | -0.76 | -0.75 | -0.54 | -0.86 |
| SD | 0.21 | 0.23 | 0.22 | 0.39 | 0.39 | 0.30 | 0.30 | 0.23 | 0.23 |
| RMSE | 1.36 | 0.42 | 0.38 | 0.68 | 0.99 | 0.82 | 0.81 | 0.59 | 0.89 |
| meanASMD | 0.20 | 0.07 | 0.08 | 0.16 | 0.15 | 0.20 | 0.20 | - | - |
| GMIM | 3.53 | 0.64 | 0.82 | 4.87(0.00) | 1.86 | 3.03 | 3.20 | - | - |

| Scenario F with \((n, p) = (200, 500)\): dense propensity score model. | Unad | MB | kernelMB | hdMB | MDABW | RCAL1 | RCAL2 | ARB | hdCBPS |
|---|---|---|---|---|---|---|---|---|---|
| Bias | -0.33 | -0.23 | -0.22 | -0.27 | -0.33 | -0.32 | -0.33 | -0.27 | -0.34 |
| SD | 0.17 | 0.17 | 0.17 | 0.33 | 0.17 | 0.18 | 0.18 | 0.19 | 0.17 |
| RMSE | 0.37 | 0.29 | 0.28 | 0.43 | 0.37 | 0.37 | 0.37 | 0.33 | 0.39 |
| meanASMD | 0.12 | 0.10 | 0.10 | 0.22 | 0.12 | 0.18 | 0.13 | - | - |
| GMIM | 7.29 | 5.13 | 5.28 | 34.55(0.00) | 7.26 | 7.38 | 7.52 | - | - |

*If we use \(\Phi(X) = X\) to compute the GMIM for the hdMB method, then \(\text{GMIM}^w = 4.19\); if we use \(\Phi(X) = (X_{(1)}, \ldots, X_{(K_0)})^\top\) by Algorithm 2, then \(\text{GMIM}^w = 0.00\).

4.2 The high-dimensional settings

In this subsection, we assess the performance of three Mahalanobis balancing methods in the high-dimensional setting. The MB method was described in Section 4.1. High-dimensional Mahalanobis balancing (hdMB) was described in Section 3.5, where \(\Phi(X) = (X_{(1)}, \ldots, X_{(K_0)})^\top\) and \(K_0\) is selected by Algorithm 2. We also consider kernel-based Mahalanobis balancing (kernelMB), where we use \(\Phi(X) = (K(X, X_1), \ldots, K(X, X_n))^\top\) with \(K(\cdot, \cdot)\) set to be the Gaussian kernel. We compare them with four high-dimensional regularized balancing methods (RCAL1, RCAL2, ARB, hdCBPS). We do not report imbalance measures for ARB and hdCBPS, because they utilize outcome information in weight construction. For all methods except kernelMB, we set \(\Phi(X) = X\) and thus \(K = p\). In each scenario, we consider \((n, p) = (200, 100)\) or \((200, 500)\). Table 2 summarizes the outputs.

In Scenario E, we generate the observed data from \(X \sim N(0, \Sigma)\) where \(\text{Cov}(X_j, X_k) = 2^{-|j-k|}\). The treatment assignment is generated by \(T \sim \text{Bernoulli}(\pi(X))\) with \(\pi(X) = 1/(1 + \exp(X_1 + \sum_{j=2}^{6} X_j/2))\). Therefore, treatment assignment is correlated with a sparse subset of covariates. The outcome is generated from \(Y = T(\sum_{j=1}^{5} X_j) + (1 - T)(\sum_{j=2}^{5} X_j/2) + \epsilon\).

Both MB and kernelMB have low bias, small standard deviation, and small imbalance measures when \((n, p) = (200, 100)\), implying that they are capable of approximately balancing covariates when the covariate dimension is substantially smaller than the sample size. When \((n, p) = (200, 500)\), MB and kernelMB have quite large GMIM values, and their biases are larger than those of the
high-dimensional regularized balancing methods but are smaller than that of MDABW. The hdMB method controls multivariate imbalance for the selected covariates, though its GMIM value is enormous when all covariates are taken into account. It achieves lower bias and RMSE compared to MDABW and all high-dimensional regularized balancing methods (RCAL1, RCAL2, ARB, hdCBPS). In conclusion, the hdMB method is recommended over MB and kernelMB when the true propensity score model is sparse. It is competitive to the existing high-dimensional regularized balancing methods.

In Scenario F, data generation of the covariates is the same as that of Scenario E. The treatment index is generated by 
\[ T \sim Bernoulli(\pi(X)) \]
with 
\[ \pi(X) = \frac{1}{1 + \exp(X_1 + \sum_{j=2}^{5} X_j/2 + 10\sum_{j=6}^{p} X_j/p)} \].

Therefore, treatment assignment is correlated with all covariates. We name it as a dense propensity score model. The outcome is generated from 
\[ Y = T(10\sum_{j=1}^{p} X_j/p) + (1 - T)(5\sum_{j=1}^{p} X_j/p) + \epsilon. \]

Both MB and kernelMB have lower bias and smaller standard deviation compared to hdMB and MDABW. The high-dimensional regularized balancing methods (RCAL1, RCAL2, ARB, hdCBPS) have larger biases than MB and kernelMB. This is not surprising because they are not tailored for the dense propensity score scenario. The kernelMB method performs better than MB, suggesting that kernel approximation can be beneficial. Both MB and kernelMB produce much more balanced weights when \((n, p) = (200, 100)\), because their GMIM values are much smaller than other methods. However, multivariate imbalance is difficult to control when the true propensity score model is dense with \((n, p) = (200, 500)\), which is the most challenging situation in the simulation studies. The MB and kernelMB methods are recommended for their lowest biases and RMSEs, and smallest meanASMDs and GMIMs.

Additional simulations with a misspecified outcome model are displayed in the Supplementary Material. Mahalanobis balancing does not use outcome information, and thus it is more robust to model misspecification compared to ARB and hdCBPS. It substantially improves the performance of ARB and hdCBPS in terms of bias and root mean square error in this situation.

4.3 Application

We revisit a dataset from the National Supported Work program (Dehejia and Wahba, 1999). The National Supported Work program is a labor training program implemented in the 1970s by providing work experience to selected individuals. The data consist of a National Supported Work experimental group with sample size 185 and a nonexperimental comparison group from the Panel Study of Income Dynamics with sample size 429. We regard them as the treated and control groups, respectively. The outcome variable \(Y\) is the post-intervention earning measured in Year 1978.

The covariates include four numeric covariates \(age, education, earn1974, earn1975\), four binary variables \(married, black, nodegree\) and \(hispanic\), and sixteen interaction terms between the numeric covariates and the binary variables. In addition, we include the quotient \(education/age\), which represents the possible nonlinear effect of \(age\) at each level of \(education\). Table 3 shows the results. 500 bootstrap resamples are used to calculate the standard error for all methods.

This is a bad-overlap setting, as the EB method by Hainmueller (2012) and the CAL method by Chan et al. (2016) fail to output ATE estimation. This can be explained by that the distribution of the covariate \(education/age\) is highly disimilar between the two groups. The CBPS method by Imai and Ratkovic (2014) substantially reduces univariate and multivariate imbalance compared to the unadjusted method. MDABW performs worse than CBPS in the sense that it has larger residual univariate and multivariate imbalance after reweighting. In comparison, the proposed Mahalanobis balancing methods produce most balanced weights as they have smallest ASMD and GMIM values, although they have larger standard error. The Mahalanobis balancing methods are recommended.
Table 3: Data analysis of National Supported Work program

|       | UnAD | MB   | MB2  | MDABW | CBPS  | CAL  | EB  |
|-------|------|------|------|-------|-------|------|-----|
| ATE   | -620.37 | 1693.18 | 1697.52 | 1075.22 | 1173.15 | -    | -   |
| SE    | 29.83 | 106.88 | 106.86 | 57.00  | 61.78  | -    | -   |
| maxASMD | 1.34  | 0.28  | 0.21  | 1.00   | 0.23   | -    | -   |
| medASMD | 0.23  | 0.00  | 0.00  | 0.07   | 0.02   | -    | -   |
| meanASMD | 0.53  | 0.01  | 0.01  | 0.08   | 0.03   | -    | -   |
| GMIM  | 2.04  | 0.00  | 0.00  | 0.21   | 0.14   | -    | -   |

when balanced weights are in demand. We conclude that the training program significantly increases the postintervention earning adjusting for the aforementioned covariates.

5 Concluding Remarks

In this paper, we proposed Mahalanobis balancing. It produces balanced weights by solving a convex optimization problem with a quadratic constraint that represents multivariate imbalance. We further extended it to the high-dimensional setting. Different choices of the basis functions were examined in the simulations. We compared Mahalanobis balancing with the exact balancing, univariate approximate balancing, and high-dimensional regularized balancing methods in extensive numerical studies, and found that Mahalanobis balancing generally led to more balanced weights and less biased ATE estimation.

The proposed Mahalanobis balancing methods can be easily extended to the situation with multiple treatment arms. Other causal estimands, such as average treatment effect on the control (ATC), can be also estimated using Mahalanobis balancing, though some modification is needed. For example, when ATC is of interest, one needs to replace $\bar{\Phi}$ with the sample average of $\Phi(X)$ in the control group in Problem (7) to obtain Mahalanobis balancing weights.

Our method can be used to address the transportability and generalizability issues in data integration and data fusion. Recently, exact balancing methods were applied to these interesting problems (e.g., Lee et al., 2021; Josey et al., 2021b). Nevertheless, the trial population and the target population usually exhibit high degree of discrepancy, and there can be a large number of confounders. In these situations, exact balancing may be infeasible, and Mahalanobis balancing is a better choice.

In the numerical studies, we used entropy as the loss function. One may further investigate the performance of Mahalanobis balancing using other loss functions (e.g., Chan et al., 2016; Josey et al., 2021b). One may extend Mahalanobis balancing to incorporate other multivariate imbalance measures, e.g., energy distance (Huling and Mak, 2020) and Kernel distance (Zhu et al., 2018).

Supplementary Material

The online Supplementary Material includes the proofs and additional simulation studies.
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Lemma and Proof

Lemma 1 is similar to Lemma 8 by Athey et al. (2018), but the assumptions are different.

**Lemma 1.** (Weight Behaviour I) Suppose that $\sum_{\{i: T_i = 1\}} w_i^3 / \|w\|_2^3 = o_p(1)$ and that the $\varepsilon_{1i}$ are sub-Gaussian. Then, as $n \to \infty$,

$$
\frac{1}{\|w\|_2^2} \sum_{\{i: T_i = 1\}} w_i \varepsilon_{1i} \overset{d}{\to} N(0, \sigma^2),
$$

where $\sigma^2 = \text{Var}(\varepsilon_{1i})$.

**Proof.** Since the MB weights do not utilize the outcomes, the $\varepsilon_{1i}$ are independent of the $w_i$ given the $X_i$. Therefore,

$$
E\{ \sum_{\{i: T_i = 1\}} w_i \varepsilon_{1i} | w_i, T_i = 1 \} = 0 \quad \text{and} \quad \text{Var}\{ \sum_{\{i: T_i = 1\}} w_i \varepsilon_{1i} | w_i, T_i = 1 \} = \sigma^2 \|w\|_2^2.
$$

Since the $\varepsilon_{1i}$ are sub-Gaussian,

$$
E\{ \sum_{\{i: T_i = 1\}} (w_i \varepsilon_{1i})^3 | w_i, T_i = 1 \} \leq C \sum_{\{i: T_i = 1\}} w_i^3
$$

for some positive constant $C$. Therefore,

$$
\frac{E\{ \sum_{\{i: T_i = 1\}} (w_i \varepsilon_{1i})^2 | w_i, T_i = 1 \}}{\text{Var}\{ \sum_{\{i: T_i = 1\}} w_i \varepsilon_{1i} | w_i, T_i = 1 \}^{3/2}} = O\left( \sum_{\{i: T_i = 1\}} w_i^3 / \|w\|_2^3 \right) = o_p(1),
$$

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Hence, the Lyapunov condition is verified, and the proof is completed by applying Lyapunov’s central limit theorem.

The next lemma asserts that the MB weights are stable when the entropy loss function is employed.

**Lemma 2.** (Weight Behaviour II) Suppose that the entropy loss function is used. Assume that $E\{\exp(a\theta^TW^{1/2}\Phi(X) - E\{\Phi(X) | T = 1\}) | T = 1\} \leq K_a$ for all $\theta \in \Theta$, where $K_a$ is some positive constant, $a = 1, 2, 3$. Assume that $\theta^TW^{1/2}(\Phi(X) - E\{\Phi(X) | T = 1\})$ is sub-Gaussian. Then the following properties hold for the MB weights:

$$\sum_{i:T_i=1} (\hat{w}_i^{MB})^a = O_p(n^{1-a}), \text{ for } a = 1, 2, 3;$$

$$\max_{i:T_i=1} \hat{w}_i^{MB} = O_p(n^{-1/2}).$$

**Proof.** When the entropy loss function is employed,

$$\hat{w}_i^{MB} = \frac{\exp\left\{\hat{\theta}^TW^{1/2}\Phi(X_i)\right\}}{\sum_{j:T_j=1} \exp\left\{\hat{\theta}^TW^{1/2}\Phi(X_j)\right\}} = \frac{\exp\left\{\hat{\theta}^TW^{1/2}\Phi(X_i)\right\}}{n_1E\left[\exp\left\{\hat{\theta}^TW^{1/2}\Phi(X)\right\} | T = 1\right]}(1 + o_p(1))$$

$$\leq \frac{\exp\left\{\hat{\theta}^TW^{1/2}\Phi(X_i)\right\}}{n_1\exp\left(\hat{\theta}^TW^{1/2}E\{\Phi(X) | T = 1\}\right)}(1 + o_p(1))$$

$$= \frac{1}{n_1}\exp\left(\hat{\theta}^TW^{1/2}[\Phi(X_i) - E\{\Phi(X) | T = 1\}]\right)(1 + o_p(1))$$

$$= O_p(n^{-1}).$$

Therefore,

$$\sum_{i:T_i=1} (\hat{w}_i^{MB})^a = \frac{1}{n_1^a} \sum_{i:T_i=1} \exp\left(a\hat{\theta}^TW^{1/2}[\Phi(X_i) - E\{\Phi(X) | T = 1\}]\right)(1 + o_p(1))$$

$$= n_1^{1-a}E\{\exp(a\theta^TW^{1/2}\Phi(X) - E\{\Phi(X) | T = 1\}) | T = 1\}(1 + o_p(1))$$

$$= n_1^{1-a}K_a(1 + o_p(1))$$

$$= O_p(n^{1-a}).$$

Moreover, by the maximal inequality (e.g., Rigollet and Hütter, 2015), we obtain that

$$Pr\left(\max_{i:T_i=1} \frac{1}{n_1}\exp\left(\hat{\theta}^TW^{1/2}(\Phi(X_i) - E\{\Phi(X) | T = 1\})\right) \geq \frac{1}{n_1}\exp(t)\right) \leq n_1 \exp\left(-\frac{t^2}{2\sigma^2}\right).$$

Set $t = \sqrt{2}\sigma \log(n_1^{1/2}s)$, we have $\max_{i:T_i=1} \hat{w}_i^{MB} = O_p(n^{-1/2}).$

The following lemma shows the asymptotic property for the solution $\hat{\theta}$ of the MB dual problem.
Lemma 3. Assume that \(1/\pi(X) = C \ast f^* (\theta^* W 1/2 (\Phi(X) - \bar{\Phi}))\) for some \(\theta^* \in \text{int}(\Theta)\) and some constant \(C\) for all \(X\). Suppose that Assumption 3 holds. Then \(\hat{\theta}\) is consistent for \(\theta^*\). Moreover, \(\hat{\theta}\) is asymptotically normal.

**Proof.** The first order optimality condition for the dual problem is

\[
\sum_{i=1}^{n} T_i \hat{f}^* \left( \hat{\theta}^T W 1/2 (\Phi(X_i) - \bar{\Phi}) \right) (\Phi_j(X_i) - \bar{\Phi}_j) + \sqrt{\delta} \frac{\theta_j}{\|\theta\|_2} = 0, \quad j = 1, \ldots, K,
\]

where \(\Phi_j(X_i), \bar{\Phi}_j,\) and \(\hat{\theta}_j\) are the \(j\)th components of \(\Phi(X_i), \bar{\Phi},\) and \(\hat{\theta}\), respectively. Write

\[
\hat{\theta} = \frac{1}{n} \sum_{i=1}^{n} \psi(X_i; T; \theta) = \frac{1}{n} \sum_{i=1}^{n} T_i \hat{f}^* \left( \theta^T W 1/2 (\Phi(X_i) - E\{\Phi(X)\}) \right) (\Phi(X_i) - E\{\Phi(X)\}),
\]

which is a set of \(K\) estimating functions. Note that

\[
E \{\psi(X_i; T; \theta)\} = E \{E (\psi(X; T; \theta)) \mid X\}
= E \left[ \pi(X) \hat{f}^* \left( \theta^* W 1/2 (\Phi(X) - E\{\Phi(X)\}) \right) W 1/2 (\Phi(X) - E\{\Phi(X)\}) \right].
\]

For the above conditional expectation to be zero, it must be true that

\[
\pi(X) \hat{f}^* \left( \theta^* W 1/2 (\Phi(X) - E\{\Phi(X)\}) \right)
\]

is a constant for any \(X\). By the assumption that \(1/\pi(X) = C \ast f^* (\theta^* W 1/2 (\Phi(X) - \bar{\Phi}))\), we obtain that \(\theta^*\) is the unique solution of \(E \{\psi(X_i; T; \theta)\} = 0\). Therefore, by the estimating equation theory (Van der Vaart, 1998), the solution of the estimating equations

\[
\frac{1}{n} \sum_{i=1}^{n} \psi(X_i; T; \theta) = 0,
\]

denoted by \(\hat{\theta}\), is asymptotically consistent for \(\theta^*\). Moreover, by the assumption that \(\delta = o(n)\), we obtain \(\frac{1}{n} \sqrt{n} \frac{\partial \psi}{\|\theta\|_2} = o_p(n^{-1/2})\) for any \(\theta \in \text{int}(\Theta)\). Therefore, the difference between \(\hat{\theta}\) and \(\hat{\theta}\) is asymptotically negligible, and thus \(\hat{\theta}\) is asymptotically consistent for \(\theta^*\). Furthermore, by Taylor expansion, we obtain that as \(n \to \infty\),

\[
\sqrt{n} (\hat{\theta} - \theta^*) \xrightarrow{d} N(0, \Sigma),
\]

where \(\Sigma = \left\{ E(\frac{\partial \psi}{\partial \theta^T}) \right\}^{-1} \mathbb{E}(\psi\psi^T) \left\{ E(\frac{\partial \psi}{\partial \theta}) \right\}^{-1} \).

The following lemma asserts that the MB weight is close to the unknown inverse probability weight. The proof is similar to arguments by Lee et al. (2021).

Lemma 4. (Weight Behaviour III) Assume that \(1/\pi(X) = C \ast f^* (\theta^* W 1/2 (\Phi(X) - \bar{\Phi}))\) for some \(\theta^* \in \text{int}(\Theta)\) and some constant \(C\) for all \(X\). Suppose that Assumption 3 holds. Then the following property holds:

\[
n \hat{w}_i^{MB} = \frac{1}{\pi(X_i)} + O_p(n^{-\frac{1}{2}}).
\]
Proof.

\[
\frac{1}{n} \sum_{i=1}^{n} T_i \tilde{f}' \left( \hat{\theta}^\top W^{1/2} \left( \Phi(X_i) - \bar{\Phi} \right) \right) = \frac{1}{n} \sum_{i=1}^{n} T_i \tilde{f}' \left( \hat{\theta}^\top W^{1/2} \left( \Phi(X_i) - E(\Phi(X)) \right) \right) + O_p(n^{-\frac{1}{2}})
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} T_i \tilde{f}' \left( \theta^* W^{1/2} \left( \Phi(X_i) - E(\Phi(X)) \right) \right) + O_p(n^{-\frac{1}{2}})
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} T_i \tilde{f}' \left( \frac{\Phi(X_i) - E(\Phi(X))}{C\pi(X_i)} \right) + O_p(n^{-\frac{1}{2}})
\]

\[
= \frac{1}{C} + o_p(1).
\]

Therefore,

\[
n\hat{w}_{i,MB} = \frac{\tilde{f}' \left( \hat{\theta}^\top W^{1/2} \left( \Phi(X_i) - \bar{\Phi} \right) \right)}{\frac{1}{n} \sum_{i:T_i=1} \tilde{f}' \left( \hat{\theta}^\top W^{1/2} \left( \Phi(X_i) - \bar{\Phi} \right) \right)}
\]

\[
= \frac{\tilde{f}' \left( \theta^* W^{1/2} \left( \Phi(X_i) - E(\Phi(X)) \right) \right) + O_p(n^{-1/2})}{1/C + o_p(1)}
\]

\[
= \frac{1}{\pi(X_i)} + O_p(n^{-\frac{1}{2}}).
\]

\[
\Box
\]

Proof for Theorem 1

Proof. We utilize the Fenchel duality theorem (Mohri et al., 2018, Theorem B.39). Without loss of generability, suppose that subjects \( i = 1, \ldots, n_1 \) are in the treated group, and subjects \( i = n_1 + 1, \ldots, n \) are in the control group. The primal problem (7) is

\[
\text{minimize } \sum_{w \in \mathbb{R}^{n_1}} \tilde{f}(w_i) + I_C \left( \sum_{i=1}^{n_1} w_i W^{1/2}(\Phi(X_i) - \bar{\Phi}) \right),
\]
where \( w = (w_1, \ldots, w_{n_1})^\top \). Let \( F(w) = \sum_{i=1}^{n_1} \tilde{f}(w_i) \). The conjugate function of \( F \) is given by

\[
F^*(w) = \sup_v \left( \sum_{i=1}^{n_1} w_i v_i - F(v) \right) 
= \sup_v \sum_{i=1}^{n_1} (w_i v_i - \tilde{f}(v_i)) 
= \sup_{v_1, \ldots, v_{n_1} \geq 0} \sum_{i=1}^{n_1} (w_i v_i - f(v_i)) 
= \sum_{i=1}^{n_1} \sup_{v_i \geq 0} (w_i v_i - f(v_i)) 
= \sum_{i=1}^{n_1} \tilde{f}^*(w_i).
\]

Note that if the normalization constraint is added to the primal problem, then the conjugate function \( F^* \) is no longer additive. Let \( g(\theta) = I_C(\theta) \), for any \( \theta \in \mathbb{R}^K \). The conjugate function of \( g \) is given by

\[
g^*(\theta) = \sup_u \left( \sum_{k=1}^K \theta_k u_k - I_C(u) \right) 
= \sup_{\|u\|_2 \leq \sqrt{\delta}} \left( \sum_{k=1}^K \theta_k u_k \right) 
= \sup_{\|u\|_2 \leq \sqrt{\delta}} (\|\theta\|_2 \|u\|_2) 
= \sqrt{\delta} \|\theta\|_2.
\]

Define the mapping \( A : \mathbb{R}^{n_1} \rightarrow \mathbb{R}^K \) such that \( Aw = \sum_{i=1}^{n_1} w_i W^{1/2}(\Phi(X_i) - \bar{\Phi}) \). Then \( A \) is a bounded linear map. Let \( A^* \) be the adjoint operator of \( A \). Then for all \( \theta = (\theta_1, \ldots, \theta_K)^\top \in \mathbb{R}^K \),

\[
A^* \theta = \left( \sum_{k=1}^K \theta_k W^{1/2}(\Phi_k(X_1) - \bar{\Phi}_k), \ldots, \sum_{k=1}^K \theta_k W^{1/2}(\Phi_k(X_{n_1}) - \bar{\Phi}_k) \right)^\top 
= (\theta^\top W^{1/2}(\Phi(X_1) - \bar{\Phi}), \ldots, \theta^\top W^{1/2}(\Phi(X_{n_1}) - \bar{\Phi}))^\top.
\]

Define \( \theta_0 = Aw_0 = \sum_{i=1}^{n_1} W^{1/2}(\Phi(X_i) - \bar{\Phi})/n_i^a \), where \( w_0 = (1/n_1^a, \ldots, 1/n_{n_1}^a)^\top \). Here, we choose \( a \) to be sufficiently large such that \( \|\theta_0\|_2 < \sqrt{\delta} \). Since each component of \( w_0 \) is non-negative, \( w_0 \in dom(F) \), where \( dom(F) \) denotes the domain of \( F \). Therefore, \( \theta_0 \in A(dom(F)) \). Since \( \|\theta_0\|_2 < \sqrt{\delta} \), we obtain that \( g(\theta_0) = 0 \) and \( g \) is continuous at \( \theta_0 \). Therefore, \( \theta_0 \in A(dom(F)) \cap cont(g) \), implying that \( A(dom(F)) \cap cont(g) \neq \emptyset \), where \( cont(g) \) is the set of continuous points of \( g \). Therefore, the strong duality condition of the Fenchel duality theorem is verified. Moreover,

\[
F(A^* \theta) + g^*(-\theta) = \sum_{i=1}^{n_1} \tilde{f}^*(-\theta^\top W^{1/2}(\Phi(X_i) - \bar{\Phi})) + \sqrt{\delta} \|\theta\|_2.
\]
The Fenchel duality theorem leads to that

\[
\min_{w \in \mathbb{R}^{n_1}} \sum_{i=1}^{n_1} \hat{f}(w_i) + I_C \left( \sum_{i=1}^{n_1} w_i W^{1/2} (\Phi(X_i) - \Phi) \right)
\]

\[
= \min_{\theta \in \mathbb{R}^K} \sum_{i=1}^{n_1} \hat{f}^* \left( \theta^T W^{1/2} (\Phi(X_i) - \Phi) \right) + \sqrt{\delta} \| \theta \|_2.
\]

Furthermore, since the strong duality condition holds, equality of the Fenchel’s inequality (Mohri et al., 2018, Prop. 38) holds, leading to that \( A^* \hat{\theta} \) is a subgradient of \( F \) at \( \hat{w} \). That is, \( A^* \hat{\theta} = F'(\hat{w}) \), or equivalently,

\[
\hat{\theta}^T W^{1/2} (\Phi(X_i) - \Phi) = \hat{f}'(\hat{w}_i).
\]

Therefore, \( \hat{w}_i = \left( \hat{f}'^* \right)^{-1} (\hat{\theta}^T W^{1/2} (\Phi(X_i) - \Phi)) \), \( i = 1, \ldots, n_1 \).

\[ \square \]

**Proof for Theorem 2**

*Proof.* We only need to show that \( \hat{\tau}^T_{MB} = \tau_1 + O_p(n^{-1/2}) \), where \( \hat{\tau}^T_{MB} = \sum_{i:T_i=1} \hat{w}_i Y_i \). First, assume the propensity score satisfies that \( 1/\pi(X) = C * \hat{f}^* (\theta^* W^{1/2} (\Phi(X) - \Phi)) \) for some \( \theta^* \in \text{int}(\Theta) \) and some constant \( C \). By Lemma 3,

\[
\sum_{i:T_i=1} \hat{w}_i MB Y_i = \sum_{i:T_i=1} \left( \hat{w}_i MB - \frac{1}{n\pi(X_i)} \right) Y_i + \sum_{i:T_i=1} \frac{Y_i}{n\pi(X_i)}
\]

\[
= \sum_{i:T_i=1} O_p(n^{-3/2})O_p(1) + O_p(n^{-1/2}) + \tau_1.
\]

Therefore, \( \hat{\tau}_1 - \tau_1 = O_p(n^{-1/2}) \).

Second, we assume that the conditional potential outcome \( E\{Y(1)|X\} = \beta^T W^{1/2} \Phi(X) \) with parameter \( \beta \), \( \sum_{i:T_i=1} (\hat{w}_i MB) \beta / \| \hat{w}_i MB \|_2^2 = o_p(1) \), and \( \| \hat{w}_i MB \|_2^2 = O_p(n^{-1}) \). Note that the following decomposition holds:

\[
\sum_{i:T_i=1} \hat{w}_i MB Y_i - \tau_1 = \beta^T \sum_{i:T_i=1} \hat{w}_i MB W^{1/2} (\Phi(X_i) - \Phi) + \sum_{i:T_i=1} \hat{w}_i MB \epsilon_i
\]

\[ + \frac{1}{n} \sum_{i=1}^n \beta^T W^{1/2} \Phi(X_i) - \tau_1. \]

Let the \( \hat{w}_i \) be the unnormalized MB weights. By Assumption 3.5,

\[
\sum_{i:T_i=1} \hat{w}_i = \sum_{i:T_i=1} \exp \left( \theta^T W^{1/2} \left( \Phi(X_i) - \Phi \right) \right) = O_p(n).
\]

Therefore,

\[
|\beta^T \sum_{i:T_i=1} \hat{w}_i MB W^{1/2} (\Phi(X_i) - \Phi)| \leq \| \beta \|_2 \| \sum_{i:T_i=1} \hat{w}_i MB W^{1/2} (\Phi(X_i) - \Phi) \|_2
\]

\[
= \| \beta \|_2 \sqrt{\delta} \sum_{i:T_i=1} \hat{w}_i W^{1/2} (\Phi(X_i) - \Phi) \|_2 / \sum_{i:T_i=1} \hat{w}_i
\]

\[
\leq \| \beta \|_2 \sqrt{\delta} \sum_{i:T_i=1} \hat{w}_i
\]

\[
= o_p(n^{-1/2}).
\]

By Lemma 1, we have \( \frac{1}{\| \hat{w}_i MB \|_2^2} \sum_{i:T_i=1} \hat{w}_i MB \epsilon_i = O_p(1) \). Therefore, by the assumption that \( \| \hat{w}_i MB \|_2^2 = O_p(n^{-1}) \), we obtain \( \sum_{i:T_i=1} \hat{w}_i MB \epsilon_i = O_p(\| \hat{w}_i MB \|_2) = O_p(n^{-1/2}) \). Finally,

\[
\frac{1}{n} \sum_{i=1}^n \beta^T W^{1/2} \Phi(X_i) - \tau_1 = O_p(n^{-1/2}). \text{ Therefore, } \hat{\tau}_1 - \tau_1 = O_p(n^{-1/2}). \text{ The double robustness property is proved.} \]
Proof of Theorem 3

Proof. To simplify the notations, let $\pi_i = \pi(X_i)$. Write $E\{Y(1)|X\} = \mu_1(X) = \beta^T X^{1/2} \Phi(X)$ with parameter $\beta$. Then the following decomposition holds:

$$
\hat{\tau}_1 - \tau_1 = \sum_{i=1}^{n} T_i \hat{w}^{MB}_i Y_i - \tau_1
$$

$$= \sum_{i=1}^{n} T_i \left( \hat{w}^{MB}_i - \frac{1}{n \pi_i} \right) (Y_i - \mu_1(X_i)) + \sum_{i=1}^{n} \frac{T_i}{n \pi_i} (Y_i - \mu_1(X_i))
$$

$$+ \sum_{i=1}^{n} \left( T_i \hat{w}^{MB}_i - \frac{1}{n} \right) \beta^T X^{1/2} \Phi(X_i) + \left( \frac{1}{n} \sum_{i=1}^{n} \mu_1(X_i) - \tau_1 \right)
$$

$$= A_1 + R_1 + A_2 + R_2.$$

Following the empirical process arguments by Wang and Zubizarreta (2020) and Fan et al. (2021), it holds that $A_1 = o_p(n^{-1/2})$. Next,

$$A_2 = \sum_{i=1}^{n} T_i \hat{w}^{MB}_i \left( \beta^T X^{1/2} \Phi(X_i) - \frac{1}{n} \sum_{i=1}^{n} \beta^T X^{1/2} \Phi(X_i) \right)
$$

$$\leq \|\beta\|_2 \|\hat{w}^{MB}_i X^{1/2} \Phi(X_i) - \Phi \|_2 + o_p(1)
$$

$$\leq \|\beta\|_2 \sqrt{\delta} \sum_{i:T_i=1} \hat{w}_i
$$

$$= o_p(n^{-1/2}).$$

The $R_1$ and $R_2$ are regular and asymptotically linear, and they determine the asymptotic expansion of $\hat{\tau}_1 - \tau_1$. Similar expansion holds for $\hat{\tau}_0 - \tau_0$. Using these asymptotic expansions, it is easy to verify that the semiparametric efficiency bound for ATE estimation is attained. 

\[ \square \]

Proof for Theorem 4

By the assumption for $\theta^T X^{1/2} (E\{\Phi(X_i)\} - E\{\Phi(X_i) \mid T = 1\})$, we obtain

$$\exp(\theta^T X^{1/2} (E\{\Phi(X_i)\} - E\{\Phi(X_i) \mid T = 1\})) = o_p(n^\gamma).$$

It follows that

$$\|\sum_{i:T_i=1} \hat{w}^{MB}_i X^{1/2} (\Phi(X_i) - \Phi)\|_2 \leq \sqrt{\delta} \sum_{i:T_i=1} \hat{w}^{MB}_i X^{1/2} (\Phi(X_i) - \Phi) \|_2 + o_p(1))$$

$$= O_p(n^{s-1/2}).$$

Therefore,

$$|\beta^T \sum_{i:T_i=1} \hat{w}^{MB}_i X^{1/2} (\Phi(X_i) - \Phi)| \leq \|\beta\|_2 \|\sum_{i:T_i=1} \hat{w}^{MB}_i X^{1/2} (\Phi(X_i) - \Phi)\|_2 \|_2 \leq O_p(n^{s-1/2}).$$

By Lemmas 1 and 2, $\sum_{i:T_i=1} \hat{w}^{MB}_i \epsilon_i = O_p(\|\hat{w}^{MB}\|_2) = O_p(n^{-1/2})$. Here, the condition $\sum_{i:T_i=1} w_i^3/\|w\|^3 = o_p(1)$ holds. Moreover,

$$\frac{1}{n} \sum_{i=1}^{n} \beta^T X^{1/2} \Phi(X_i) - \tau_1 = \frac{1}{n} \sum_{i=1}^{n} \mu_1(X_i) - \tau_1 = O_p(n^{-1/2}).$$
Therefore,

\[
\hat{\tau}_1^{MB} - \tau_1 = \beta^\top \sum_{i: T_i = 1} \hat{w}_i^{MB} W^{1/2}(\Phi(X_i) - \bar{\Phi}) + \sum_{i: T_i = 1} \hat{w}_i^{MB} \epsilon_{1i} + \frac{1}{n} \sum_{i=1}^n \beta^\top W^{1/2} \epsilon_{1i} - \tau_1 = O_p(n^{-1/2}) + O_p(n^{s+\gamma-2\alpha}).
\]

**Additional Information for Numerical Studies**

We provide more information about the numerical studies in the main article. In particular, we display the results of MB and MB2 by varying \((\delta_1, \delta_0)\), where \(\delta_1\) and \(\delta_0\) are the threshold parameters for the treated and control groups, respectively. The outputs show that both MB and MB2 are not sensitive to the choice of the threshold parameters if the parameter values are small enough. The results are summarized in Table S1.
Table S1: Performance of MB and MB2 by varying \((\delta_1, \delta_0)\) in Scenarios A, C, D

| Scenario | Bias | SD   | RMSE | maxASMD | meanASMD | medASMD | GMIM |
|----------|------|------|------|---------|----------|---------|------|
| Scenario A | \(\delta_1 = \delta_0 = 1\) | | | | | | |
| MB       | -0.25| 3.16 | 3.17 | 0.11    | 0.01     | 0.01    | 0.00 |
| MB2      | -0.24| 3.16 | 3.17 | 0.11    | 0.01     | 0.01    | 0.00 |
| \(\delta_1 = \delta_0 = 10^{-2}\) | | | | | | | |
| MB       | -0.11| 3.21 | 3.21 | 0.05    | 0.00     | 0.00    | 0.00 |
| MB2      | -0.11| 3.21 | 3.21 | 0.05    | 0.00     | 0.00    | 0.00 |
| \(\delta_1 = \delta_0 = 10^{-4}\) | | | | | | | |
| MB       | -0.10| 3.22 | 3.22 | 0.03    | 0.00     | 0.00    | 0.00 |
| MB2      | -0.10| 3.22 | 3.22 | 0.03    | 0.00     | 0.00    | 0.00 |
| \(\delta_1 = \delta_0 = 10^{-6}\) | | | | | | | |
| MB       | -0.10| 3.22 | 3.22 | 0.03    | 0.00     | 0.00    | 0.00 |
| MB2      | -0.10| 3.22 | 3.22 | 0.03    | 0.00     | 0.00    | 0.00 |
| Scenario C | \(\delta_1 = \delta_0 = 10^{-2}\) | | | | | | |
| MB       | 0.26 | 0.81 | 0.85 | 0.39    | 0.02     | 0.01    | 0.02 |
| MB2      | 0.37 | 0.86 | 0.94 | 0.30    | 0.03     | 0.01    | 0.03 |
| \(\delta_1 = \delta_0 = 10^{-4}\) | | | | | | | |
| MB       | 0.21 | 0.80 | 0.83 | 0.36    | 0.02     | 0.00    | 0.02 |
| MB2      | 0.26 | 0.85 | 0.89 | 0.27    | 0.02     | 0.00    | 0.02 |
| Scenario D | \(\delta_1 = \delta_0 = 10^{-2}\) | | | | | | |
| MB       | -0.24| 0.46 | 0.49 | 0.15    | 0.01     | 0.00    | 0.01 |
| MB2      | -0.21| 0.45 | 0.52 | 0.17    | 0.01     | 0.00    | 0.00 |
| \(\delta_1 = \delta_0 = 10^{-4}\) | | | | | | | |
| MB       | -0.16| 0.46 | 0.49 | 0.13    | 0.01     | 0.00    | 0.00 |
| MB2      | -0.15| 0.45 | 0.47 | 0.17    | 0.01     | 0.00    | 0.00 |
Additional Simulation for Model Misspecification

We consider high-dimensional situation with \((n, p) = (200, 100)\) when the outcome model is misspecified as a linear model. The data generation procedure of the covariates is the same as in Scenario E.

In the Scenario M1, we consider a sparse propensity score model

\[
\pi(X_i) = \frac{1}{1 + \exp(X_{i1} + \sum_{j=2}^{6} X_{ij}/2)},
\]

and a nonlinear outcome model

\[
Y_i = 2T_i \left( \sum_{j=1}^{6} X_{ij} + \sum_{j=1}^{6} X_{ij}^2 \right) + (1 - T_i) \left( \sum_{j=1}^{6} X_{ij} + \sum_{j=1}^{6} X_{ij}^2 \right) + \epsilon_i,
\]

where \(\epsilon_i\) is a standard normal random variable.

In the Scenario M2, we consider a dense propensity score model

\[
\pi(X_i) = \frac{1}{1 + \exp(X_{i1} + \sum_{j=2}^{5} X_{ij}/2 + \sum_{j=6}^{100} X_{ij}/10)},
\]

and a nonlinear outcome model

\[
Y_i = T_i \left( \sum_{j=1}^{100} X_{ij} + \sum_{j=1}^{50} X_{ij}^2 \right)/10 + (1 - T_i) \left( \sum_{j=1}^{100} X_{ij} + \sum_{j=1}^{50} X_{ij}^2 \right)/20 + \epsilon_i.
\]

Table S2 gives the results. We observe that MB and hdMB have best performance in Scenario M1, and kernelMB has best performance in Scenario M2. Mahalanobis balancing does not use information of the outcomes, and thus is robust in these scenarios.
Table S2: Model misspecification scenarios

| Scenario M1 | Bias  | SD    | RMSE  | maxASMD | meanASMD | medianASMD | GMIM |
|-------------|-------|-------|-------|---------|----------|-------------|------|
| Unad        | -3.45 | 0.50  | 3.49  | 1.54    | 0.16     | 0.10        | 3.22 |
| MB          | -1.47 | 0.61  | 1.59  | 0.58    | 0.06     | 0.05        | 0.52 |
| kernelMB    | -1.52 | 0.56  | 1.62  | 0.80    | 0.08     | 0.06        | 0.71 |
| hdMB        | -0.72 | 0.73  | 1.03  | 1.25    | 0.14     | 0.10        | 4.19 |
| MDABW       | -2.50 | 0.96  | 2.68  | 1.54    | 0.14     | 0.11        | 2.12 |
| RCAL1       | -1.68 | 0.6   | 1.79  | 1.10    | 0.15     | 0.11        | 2.17 |
| RCAL2       | -1.67 | 0.60  | 1.78  | 1.49    | 0.15     | 0.11        | 2.76 |
| ARB         | -1.22 | 0.55  | 1.34  | -       | -        | -           | -    |
| hdCBPS      | -1.68 | 0.61  | 1.80  | -       | -        | -           | -    |

| Scenario M2 | Bias  | SD    | RMSE  | maxASMD | meanASMD | medianASMD | GMIM |
|-------------|-------|-------|-------|---------|----------|-------------|------|
| Unad        | -1.35 | 0.36  | 1.40  | 1.30    | 0.20     | 0.17        | 3.53 |
| MB          | -0.50 | 0.48  | 0.68  | 0.56    | 0.07     | 0.06        | 0.64 |
| kernelMB    | -0.35 | 0.37  | 0.51  | 0.74    | 0.08     | 0.07        | 0.82 |
| hdMB        | -0.70 | 0.69  | 0.98  | 1.28    | 0.16     | 0.11        | 4.87 |
| MDABW       | -1.02 | 0.51  | 1.14  | 1.30    | 0.15     | 0.14        | 1.86 |
| RCAL1       | -1.20 | 0.41  | 1.27  | 0.93    | 0.20     | 0.18        | 3.03 |
| RCAL2       | -1.19 | 0.41  | 1.26  | 1.24    | 0.20     | 0.18        | 3.18 |
| ARB         | -0.78 | 0.45  | 0.90  | -       | -        | -           | -    |
| hdCBPS      | -1.21 | 0.42  | 1.28  | -       | -        | -           | -    |
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