
A hierarchical decomposition for explaining ML performance discrepancies

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Abstract

Machine learning (ML) algorithms can often differ in performance across domains. Understanding *why* their performance differs is crucial for determining what types of interventions (e.g., algorithmic or operational) are most effective at closing the performance gaps. *Aggregate decompositions* express the total performance gap as the gap due to a shift in the feature distribution $p(X)$ plus the gap due to a shift in the outcome's conditional distribution $p(Y|X)$. While this coarse explanation is helpful for guiding root cause analyses, it provides limited details and can only suggest coarse fixes involving **all variables** in an ML system. *Detailed decompositions* quantify the importance of **each variable** to each term in the aggregate decomposition, which can provide a deeper understanding and suggest more targeted interventions. Although parametric methods exist for conducting a full hierarchical decomposition of an algorithm's performance gap at the aggregate and detailed levels, current nonparametric methods only cover parts of the hierarchy; many also require knowledge of the entire causal graph. We introduce a nonparametric hierarchical framework for explaining why the performance of an ML algorithm differs across domains, without requiring causal knowledge. Furthermore, we derive debiased, computationally-efficient estimators and statistical inference procedures to construct confidence intervals for the explanations.

1 Introduction

The performance of an ML algorithm can differ across domains due to shifts in the data distribution. Understanding what contributed to this performance gap can help teams choose the most effective corrective action(s), ranging from algorithmic modifications (e.g. model retraining) to operational fixes (e.g. updating data pipelines). Prior works have focused primarily on *aggregate* decompositions, which decompose the performance gap into that due to a shift in the marginal distribution of the input features $p(X)$ (covariate shift [37]) and that due to a shift in the conditional distribution of the outcome $p(Y|X)$ (concept shift or conditional outcome shift) [5, 50, 30, 36, 16]. However, coarse decompositions can only suggest coarse corrective actions, such as investigating data pipelines for all features. The goal of this work is to provide a hierarchical nonparametric framework that first decomposes a performance gap into aggregate terms and then each aggregate term into detailed terms. This helps narrow down the features to investigate and understand how they affect the gap.

If one is willing to make the strong assumption that the expected loss of a model is a linear function of some feature set X , the problem of obtaining *aggregate* and *detailed* decompositions drastically simplifies. This is the key assumption underlying the Oaxaca-Blinder (OB) decomposition, one of the most widely used frameworks in the (income and health) disparities literature [32, 3]. Given an ML

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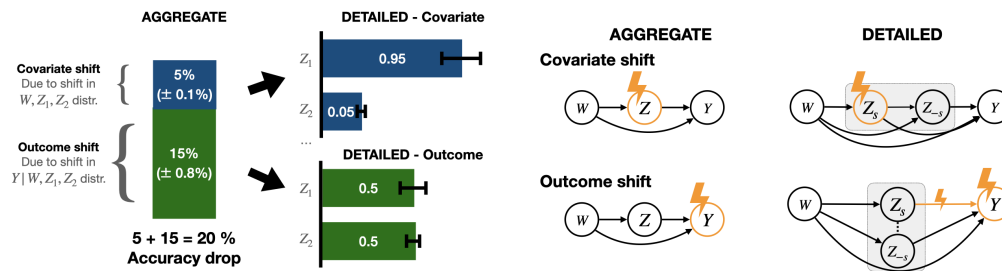


Figure 1: **(left)** Proposed framework called Hierarchical Decomposition of Performance Differences (namely, HDPD) helps to understand performance gaps of an ML algorithm between two domains. It decomposes the overall gap (say, in classification accuracy) into gaps due to shifts in the covariate versus outcome distribution (Aggregate). Then, it quantifies the importance of each feature to the two components (Detailed). **(right)** In terms of directed acyclic graphs, aggregate decompositions describe the effect of shift interventions, for instance, on the outcome Y distribution while keeping all else fixed between domains. Detailed decompositions quantify how well can we explain those shift interventions by more targeted shifts with respect to feature subsets Z_s alone.

model with average loss $\mathbb{E}_D[\ell]$ in domains $D = 0$ and 1 and assuming the linear loss relationship $\mathbb{E}_D[\ell|X] = \beta_D^\top X$, the OB framework decomposes the performance gap at the *aggregate* level into that due to a covariate shift ($\beta_0^\top (\mathbb{E}_1[X] - \mathbb{E}_0[X])$) and that due to a conditional outcome shift ($(\beta_1 - \beta_0)^\top \mathbb{E}_1[X]$). That is, the former is due to a shift in the feature means and the latter is due to a shift in the coefficients. At the *detailed* level, the aggregate terms corresponding to covariate and conditional outcome shifts are further broken down into the contributions from each feature, i.e. $\beta_{0,j} (\mathbb{E}_1[X_j] - \mathbb{E}_0[X_j])$ and $(\beta_{1,j} - \beta_{0,j}) \mathbb{E}_1[X_j]$, respectively. Although the highly intuitive nature of the OB framework has led to its widespread popularity, the terms are difficult to interpret under model misspecification. As such, this work aims to define a similar hierarchical decomposition framework for explaining ML performance disparities, *without making strong parametric assumptions*.

There is currently no unified, nonparametric framework that obtains aggregate and detailed decompositions. Instead, solutions have been proposed for parts of the hierarchy (see Table 1): nonparametric methods exist for the aggregate decomposition [5, 30, 48] and, assuming the causal graph is known, detailed decompositions of the covariate shift [40, 44, 50, 38, 4, 23]. However, the causal graph is unlikely to be known in high-dimensional settings and, more importantly, there are no methods for simultaneously obtaining a detailed decomposition of the conditional outcome shift. There are also methods that do not decompose the performance gap and instead describe distribution shifts in the variables [29] or model explanations [12, 31, 23]. However, such approaches do not quantify how such shifts ultimately contribute to an ML performance gap. We make the following contributions.

- We introduce a **unified hierarchical nonparametric framework** for decomposing the performance gap of an ML algorithm (Fig 1 left). Using the concept of *partial* distribution shifts, we generalize shifts with respect to variable subgroups to encompass not only covariate shifts but also conditional outcome shifts. We then introduce a unified scoring rule for (candidate) partial shifts, which can be used even when the causal graph is not known.
- We derive novel debiased and asymptotically normal estimators for terms in the decomposition, which allow us to construct **confidence intervals (CIs) with asymptotically valid coverage rates**.
- We demonstrate the utility of our framework in **real-world examples** of prediction models for hospital readmission and insurance coverage. Code for reproducing experiments is available at <https://github.com/jjfeng/HDPD>.

2 A unifying framework for explaining performance gaps

Notation. Consider a prediction algorithm $f : \mathcal{X} \subseteq \mathbb{R}^m \rightarrow [0, 1]$ for binary outcomes Y across source and target domains, denoted by $D = 0$ and $D = 1$, respectively. Let the performance of f be quantified in terms of a loss function $\ell : \mathcal{X} \times \{0, 1\} \rightarrow \mathbb{R}$, such as the 0-1 misclassification loss $\mathbb{1}\{f(X) \neq Y\}$. Suppose variables X can be partitioned into disjoint sets $W \in \mathbb{R}^{m_1}$ and $Z = X \setminus W \in \mathbb{R}^{m_2}$, where $m = m_1 + m_2$. Although our framework does not require knowing the causal ordering between variables, the interpretation is more intuitive when W is causally upstream

Table 1: Comparison of HDPD to prior works that decompose ML performance gaps. The distinguishing contribution of this work is that it unifies aggregate and detailed decompositions under a nonparametric framework with uncertainty quantification.

Papers	Aggregate decomp.	Detailed decomp. for		Does not require causal graph	Confidence intervals	Nonparametric
		$p(X)$ -shift	$p(Y X)$ -shift			
Zhang et al. [50]	✓	✓				✓
Cai et al. [5]	✓			✓	✓	✓
Quintas-Martinez et al. [38]	✓	✓			✓	✓
Wu et al. [48]		✓		✓		✓
Liu et al. [30]	✓		✓	✓		✓
Dodd and Pepe [11]			✓	✓	✓	
Oaxaca [32], Blinder [3]	✓	✓	✓	✓	✓	
HDPD (this paper)	✓	✓	✓	✓	✓	✓

of Z and Y (Fig 1 right). Variables Z can be chosen to be mediators or modifiers of the effect of the domain shift D on Y . For instance, if Z are treatment variables and W are baseline variables, one can interpret a covariate shift as a change in the treatment policy and an outcome shift as a change in the treatment effect across the two environments. In absence of any causal knowledge, another option is to choose W as the variables for which one would like the expected loss given W to be invariant across the two environments; this can be useful to promote fairness of ML algorithms across environments. When this invariance does not hold, the framework explains how variables Z contribute to these differences. We refer to W as baseline variables and Z as conditional covariates. Please refer to Appendix C for more discussion on choosing W and Z as well as a summary of notation (Table 2).

Our proposed hierarchical decomposition of an ML performance gap is based on a stratification of distribution shifts into *aggregate* and *partial* shifts. At the aggregate level, the joint distribution of (W, Z, Y) can be factorized with respect to the aggregate variable groups W , Z , and Y , i.e.

$$p_{D_W}(W)p_{D_Z}(Z|W)p_{D_Y}(Y|W, Z), \quad (1)$$

where subscripts D_W , D_Z and D_Y indicate the domain of that factor. An *aggregate shift* substitutes a factor from the source domain in (1) with that from the target domain, i.e. we swap the factor from p_0 to p_1 . A *partial shift* with respect to variable subset s (or an s -partial shift) shifts a factor from the source domain in (1) *only with respect to variable subset s* ; we denote this by swapping a factor from p_0 to p_s . (We keep the precise definition of s -partial shifts purposely vague until Section 2.2.) We denote expectations with respect to the joint distribution (1) as $\mathbb{E}_{D_W D_Z D_Y}$.

The overall performance gap between domains, $\Lambda = \mathbb{E}_{111}[\ell(W, Z, Y)] - \mathbb{E}_{000}[\ell(W, Z, Y)]$, can be decomposed hierarchically as follows. In the Appendix D, we also discuss how this decomposition can be interpreted causally under certain conditions.

Aggregate. At the first level of the hierarchy, the framework quantifies how aggregate shifts contribute to the performance gap individually. This leads to the decomposition $\Lambda = \Lambda_W + \Lambda_Z + \Lambda_Y$, where Λ_W quantifies the impact of a shift in the baseline distribution $p(W)$, Λ_Z quantifies the impact of a shift in the conditional covariate distribution $p(Z|W)$, and Λ_Y quantifies the impact of a shift in the outcome distribution $p(Y|W, Z)$. More concretely,

$$\begin{aligned} \Lambda_W &= \mathbb{E}_{100}[\ell] - \mathbb{E}_{000}[\ell] \\ \Lambda_Z &= \mathbb{E}_{110}[\ell] - \mathbb{E}_{100}[\ell] = \mathbb{E}_{1..}[\underbrace{\mathbb{E}_{..10}[\ell | W] - \mathbb{E}_{..00}[\ell | W]}_{\Delta_{..10}(W)}] \\ \Lambda_Y &= \mathbb{E}_{111}[\ell] - \mathbb{E}_{110}[\ell] = \mathbb{E}_{11.}[\underbrace{\mathbb{E}_{..1}[\ell | W, Z] - \mathbb{E}_{..0}[\ell | W, Z]}_{\Delta_{..0}(W, Z)}]. \end{aligned}$$

The same (or similar) aggregate decompositions have also appeared in prior works [5, 30, 15, 50, 38].

Detailed. At the detailed level, each aggregate term is further broken down into variable-level attributions. The effect of each variable can be isolated using partial shifts. However, because variables can interact to induce complex partial distribution shifts, we define variable importance (VI) using the Shapley attribution framework [41, 6, 31, 17], which has the benefits of satisfying axiomatic properties such as fairness, monotonicity, and full attribution. Thus, given a real-valued value function v that quantifies the contribution of an s -partial shift to an aggregate shift for all

$s \subseteq \{1, \dots, m\}$, the attribution to variable j is the average gain in value when additionally shifting with respect to j , i.e.

$$\phi_j := \frac{1}{m} \sum_{s \subseteq \{1, \dots, m\} \setminus j} \binom{m-1}{|s|}^{-1} \{v(s \cup j) - v(s)\}. \quad (2)$$

Interpretation. Such VI values can help ML teams identify the underlying cause(s) for a performance gap and design targeted operational and/or algorithmic interventions. For instance, a variable with high importance to the conditional covariate shift term Λ_Z may indicate differences in the variable's missingness rates, prevalence, or selection bias across domains. If instead the variable is highly important to the conditional outcome shift term Λ_Y , it may indicate inherent differences in the conditional distribution (i.e. effect modification), differences in measurement error or the way outcome is defined between domains, or omission of variables predictive of the outcome. Finally, note that variable importances should be viewed as *relative* to the variables included in the framework rather than absolute importances, as one cannot include all possible explanatory variables.

To define VI values, **the key question is how to define a value function v that is applicable to different types of s -partial shifts, even when the causal graph is not known.** It turns out that the answer is far from straightforward. The next section discusses how the value function and candidate s -partial shifts must be defined with care.

2.1 Value of partial distribution shifts

When the true causal graph is known, prior works define an s -partial covariate shift as the substitution of nodes s with mechanisms from the target domain and its value $v(s)$ as the difference in the average loss, e.g. $\mathbb{E}_{1s0}[\ell] - \mathbb{E}_{100}[\ell]$ [50, 38]. However, this has a number of limitations: (i) knowing the entire causal graph is often impractical, (ii) in the absence of such a graph, this value function is not a proper scoring rule and can assign high values to partial shifts that contradict the true causal graph (see Example E.1 for details), and (iii) $v(s)$ can be high even if the shift does not induce similar shifts in the loss as the aggregate shift.

Instead, we propose to evaluate candidate s -partial shifts by how closely they approximate aggregate shifts, using a nonparametric extension of the traditional R^2 measure. In the case of conditional covariate shifts, an aggregate shift induces a performance difference of $\Delta_{.10}(W)$ in strata W while a candidate s -partial shift induces a performance difference of $\Delta_{.s0}(W) = \mathbb{E}_{.s0}[\ell|W] - \mathbb{E}_{.00}[\ell|W]$. The value of this s -partial shift is then the percent variation of $\Delta_{.10}$ explained by $\Delta_{.s0}$, i.e.

$$v_Z(s) := 1 - \frac{\mathbb{E}_{1..} \left[(\Delta_{.s0}(W) - \Delta_{.10}(W))^2 \right]}{\mathbb{E}_{1..} [\Delta_{.10}^2(W)]}. \quad (3)$$

Likewise, for conditional outcome shifts, an aggregate shift induces a performance difference of $\Delta_{..1}(W, Z)$ in strata (W, Z) while a candidate s -partial shift induces a performance difference of $\Delta_{..s}(W, Z) = \mathbb{E}_{..s}[\ell|W, Z] - \mathbb{E}_{..0}[\ell|W, Z]$. The value of this s -partial conditional outcome shift is then defined as the percent variation of $\Delta_{..1}$ explained by $\Delta_{..s}$, i.e.

$$v_Y(s) := 1 - \frac{\mathbb{E}_{11.} \left[(\Delta_{..s}(W, Z) - \Delta_{..1}(W, Z))^2 \right]}{\mathbb{E}_{11.} [\Delta_{..1}^2(W, Z)]}. \quad (4)$$

This formulation of the value function in terms of R^2 provides a unified way to score partial conditional covariate and outcome shifts, does not require knowledge of the true causal graph, and is a strictly proper scoring rule under certain conditions (see Appendix E). In general, we expect the highest scoring candidate s -partial shifts to be those that are close to the true causal graph *and* induce large shifts in the ML algorithm's loss. Finally, we acknowledge one caveat with this framework: because some variables must be held out to define the R^2 measure, we cannot score partial shifts in the baseline variables W . We hope to close this gap in future work.

2.2 Candidate partial distribution shifts

We now present the set of candidate partial shifts considered in this work. High-level illustrations for the candidate partial shifts are given in Fig 1 right top; more detailed illustrations are given in

Fig 4 of the Appendix. We emphasize that these are *candidates*, as the true causal graph is not known. While there are certainly other partial shifts that one may consider, many have various disadvantages. As such, we leave the investigation of other partial shifts to future work.

***s*-partial conditional covariate shift:** Suppose Z_{-s} is downstream of Z_s . Then $p_s(z|w) := p_1(z_s|w)p_0(z_{-s}|z_s, w)$. Wu et al. [48] considered a similar proposal.

***s*-partial conditional outcome shift:** Shifting the conditional distribution of Y only with respect to a variable subset Z_s but not Z_{-s} requires care. We cannot simply define $p_s(Y|W, Z)$ as a function of only W and Z_s . Such a definition would imply that an *s*-partial shift has a non-zero effect, even in settings with no shift in the conditional outcome distribution (i.e. $p_1(Y|W, Z) \equiv p_0(Y|W, Z)$).

Instead, we define an *s*-partial outcome shift based on models commonly used in model recalibration/revision [42, 34], where the modified risk (conditional probability of Y) is a function of the risk in the source domain $Q := q(W, Z) := p_0(Y = 1|W, Z)$, W , and Z_s . That is, we define the shift as

$$p_s(y|z, r, w) := p_1(y|z_s, r, w) = \int p_1(y|\tilde{z}_{-s}, z_s, w) p_1(\tilde{z}_{-s}|z_s, q(w, z_s, \tilde{z}_{-s}) = r, w) d\tilde{z}_{-s} \quad (5)$$

By defining the shifted outcome distribution solely as a function of Q , W , and Z_s , any direct effect from Z_{-s} to Y is eliminated and p_s has the desired behavior in the setting where there is no conditional outcome shift.

3 Estimation and statistical inference

Here we discuss estimation and statistical inference for the aggregate terms (Λ_w , Λ_z , and Λ_y), the value functions $v_z(s)$ and $v_y(s)$, and the Shapley-based detailed terms $\phi_{z,j}$ and $\phi_{y,j}$ for $j \in (0, \dots, m_2)$. One approach is to rely on *plug-in* estimators, which plug in estimates of conditional means (also called outcome models) or density ratios [43], which we collectively refer to as nuisance parameters. For instance, one can estimate the conditional means $\mu_{.10}(w) = \mathbb{E}_{.10}[\ell|W]$ and $\mu_{.00}(w) = \mathbb{E}_{.00}[\ell|W]$ using ML and take the empirical mean of $\hat{\mu}_{.10} - \hat{\mu}_{.00}$ with respect to the target domain to get a plug-in estimator for $\Lambda_z = \mathbb{E}_{1..}[\mu_{.10} - \mu_{.00}]$. However, because estimation of the true nuisance parameters using ML typically converge at a rate slower than $n^{-1/2}$, plug-in estimators generally fail to be consistent at a rate of $n^{-1/2}$ and cannot be used to construct CIs [25].

To this end, we use the method of one-step correction from semiparametric inference to derive *debiased* ML estimators [45, 7]. The core idea is to subtract the first-order bias of a plug-in estimator, which requires characterizing the canonical gradient (or efficient influence function) of the estimand [25]. The primary technical contribution in this section is the derivation of debiased estimators for the detailed decompositions. (Estimation and inference for the aggregate decomposition is well-studied, as the aggregate terms can be formulated as average causal effects.) Due to space limitations, this section only presents estimators for the detailed decomposition of the conditional outcome shift. This estimand is particularly interesting, as its unique structure is not amenable to standard techniques for debiasing ML estimators. We refer the reader to the Appendix for derivations, pseudocode, and proofs for all the estimators.

Notation. Let \mathbb{P}_D denote the expectation with respect to domain D . For ease of exposition, suppose the number of IID observations from each domain is the same, denoted by n . We present split-sample estimators, though the results can be readily extended using cross-fitting [7, 25]. Let the data be randomly split into “training” and “evaluation” partitions. Let $\mathbb{P}_{D,n}$ denote the empirical average in the evaluation partition for domain D . All estimated quantities are denoted using hat notation.

3.1 Value of *s*-partial conditional outcome shifts

Here we describe the high-level steps for deriving a debiased estimator for $v_y(s)$, the value of a candidate *s*-partial conditional outcome shift. The following section describes a computationally efficient procedure for combining such estimates to obtain Shapley values.

Standard recipes for deriving asymptotically normal, nonparametric-efficient estimators rely on *pathwise* differentiability of the estimand and analyzing its efficient influence function [25]. However, $v_y(s)$ is not pathwise differentiable because it is a function of (5), which conditions on the source risk $q(w, z)$ equalling some value r . Taking the pathwise derivative of $v_y(s)$ requires taking a derivative

of the indicator function $\mathbb{1}\{q(w, z) = r\}$, which generally does not exist. Given the difficulties in deriving an asymptotically normal estimator for $v_Y(s)$, we propose estimating a close alternative that is pathwise differentiable.

The idea is to replace q in (5) with its binned variant $q_{\text{bin}}(w, z) = \frac{1}{B} \lfloor q(w, z)B + \frac{1}{2} \rfloor$ for some $B \in \mathbb{Z}^+$, which discretizes outputs from q into B disjoint bins. As long as B is sufficiently high, the binned version of the estimand, denoted $v_{Y, \text{bin}}(s)$, is a close approximation to $v_Y(s)$. (We use $B = 20$ in the empirical analyses, which we believe to be sufficient in practice.) The benefit of this binned variant is that the derivative of the indicator function $\mathbb{1}\{q_{\text{bin}}(w, z) = r\}$ is zero almost everywhere as long as observations with source risks exactly equal to a bin edge have measure zero. More formally, we require the following:

Condition 3.1. Let Ξ be the set of (W, Z) such that $q(W, Z)$ falls precisely on some bin edge and is not equal to zero or one. The set Ξ is measure zero.

Under this condition, $v_{Y, \text{bin}}(s)$ is pathwise differentiable and, using one-step correction, we derive a debiased ML estimator that has the unique form of a V-statistic (this follows from the integration over “phantom” \tilde{z}_{-s} in (5)). We represent V-statistics using the operator $\mathbb{P}_{1, n} \tilde{\mathbb{P}}_{1, n}$, which takes the average over all pairs of observations O_i with replacement, i.e. $\frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n g(O_i, O_j)$ for some function g . Calculation of this estimator and its theoretical properties are as follows.

Estimation. Using the training partition, estimate the outcome models $\mu_{..D}(W, Z) = \mathbb{E}_{..D}[\ell|W, Z]$ for $D = 0, 1$, the shifted outcome model $\mu_{..s}(W, Z) = \mathbb{E}_{..s}[\ell|W, Z]$; and the density ratio models $\pi_{110}(W, Z) = p_1(W, Z)/p_0(W, Z)$ and $\pi(W, Z_s, Z_{-s}, Q_{\text{bin}}) = p_1(Z_{-s}|W, Z_s, q_{\text{bin}}(W, Z) = Q_{\text{bin}})/p_1(Z_{-s})$. The outcome and density ratio models can be fit using ML-based regression models and probabilistic classifiers [43], respectively (see Section H for details). The estimator for $v_{Y, \text{bin}}(s)$ is the ratio $\hat{v}_{Y, \text{bin}}(s) = \hat{v}_{Y, n}^{\text{num}}(s)/\hat{v}_{Y, n}^{\text{den}}$, where the numerator and denominator are estimated using the evaluation partition as

$$\begin{aligned} \hat{v}_{Y, n}^{\text{num}}(s) = & \mathbb{P}_{1, n} \hat{\xi}_s(W, Z)^2 + 2 \mathbb{P}_{1, n} \hat{\xi}_s(W, Z)(\ell - \hat{\mu}_{..1}(W, Z)) \\ & - 2 \mathbb{P}_{1, n} \tilde{\mathbb{P}}_{1, n} \hat{\xi}_s(W, Z_s, \tilde{Z}_{-s}) \ell(W, Z_s, \tilde{Z}_{-s}, Y) \hat{\pi}(W, Z_s, \tilde{Z}_{-s}, Q_{\text{bin}}) \\ & + 2 \mathbb{P}_{1, n} \tilde{\mathbb{P}}_{1, n} \hat{\xi}_s(W, Z_s, \tilde{Z}_{-s}) \hat{\mu}_{..s}(W, Z_s, \tilde{Z}_{-s}) \hat{\pi}(W, Z_s, \tilde{Z}_{-s}, Q_{\text{bin}}) \end{aligned} \quad (6)$$

$$\begin{aligned} \hat{v}_{Y, n}^{\text{den}} = & \mathbb{P}_{1, n} (\hat{\mu}_{..1}(W, Z) - \hat{\mu}_{..0}(W, Z))^2 + 2 \mathbb{P}_{1, n} (\hat{\mu}_{..1}(W, Z) - \hat{\mu}_{..0}(W, Z)) (\ell - \hat{\mu}_{..1}(W, Z)) \\ & - 2 \mathbb{P}_{0, n} (\hat{\mu}_{..1}(W, Z) - \hat{\mu}_{..0}(W, Z)) (\ell - \hat{\mu}_{..0}(W, Z)) \hat{\pi}_{110}(W, Z), \end{aligned} \quad (7)$$

where $\hat{\xi}_s(W, Z) = \hat{\mu}_{..1}(W, Z) - \hat{\mu}_{..s}(W, Z)$. Note that the first terms in (6) and (7) are the plug-in estimates, followed by additional terms that correct its bias.

Inference. This estimator is asymptotically normal assuming the estimators for the nuisance parameters converge at a fast enough rate, per the following theorem.

Theorem 3.2. Suppose Condition 3.1 holds. For variable subset s , suppose the density ratios $\pi(W, Z_s, Z_{-s}, Q_{\text{bin}})$ and $\pi_{110}(W, Z)$ are bounded; denominator in case of no shift $v_Y^{\text{den}}(\emptyset) > 0$; estimator $\hat{\pi}$ is consistent; estimators $\hat{\mu}_{..0}$, $\hat{\mu}_{..1}$ and $\hat{\mu}_{..s}$ converge at an $o_p(n^{-1/4})$ rate, and

$$\mathbb{P}_1(\hat{q}_{\text{bin}} - q_{\text{bin}})^2 = o_p(n^{-1}) \quad (8)$$

$$\mathbb{P}_1(\hat{\mu}_{..s} - \hat{\mu}_{..s})(\pi - \hat{\pi}) = o_p(n^{-1/2}), \quad \mathbb{P}_0(\hat{\mu}_{..0} - \hat{\mu}_{..0})(\pi_{110} - \hat{\pi}_{110}) = o_p(n^{-1/2}) \quad (9)$$

Then the estimator $\hat{v}_{Y, \text{bin}}(s)$ is asymptotically normal centered at the estimand $v_{Y, \text{bin}}(s)$.

Note that the product terms in (9) mean that the estimator converges to normal at $n^{-1/2}$ -rate even if one of the nuisance parameters is estimated at a rate slower than $n^{-1/2}$. Hence, it is *multiply-robust* to nuisance model misspecification. A convergence rate of $o_p(n^{-1/4})$ can be achieved by ML estimators in a wide variety of conditions, and such assumptions are commonly used to construct debiased ML estimators. The additional requirement in (8) that \hat{q}_{bin} converges at a $o_p(n^{-1})$ rate is new, but fast or even super-fast convergence rates of *binned* risks is achievable under suitable margin conditions [2] such as Condition G.7 in the Appendix.

3.2 Shapley values

Calculating the exact Shapley value is computationally intractable as it involves an exponential number of terms. However, Williamson and Feng [47] showed that calculating the exact Shapley

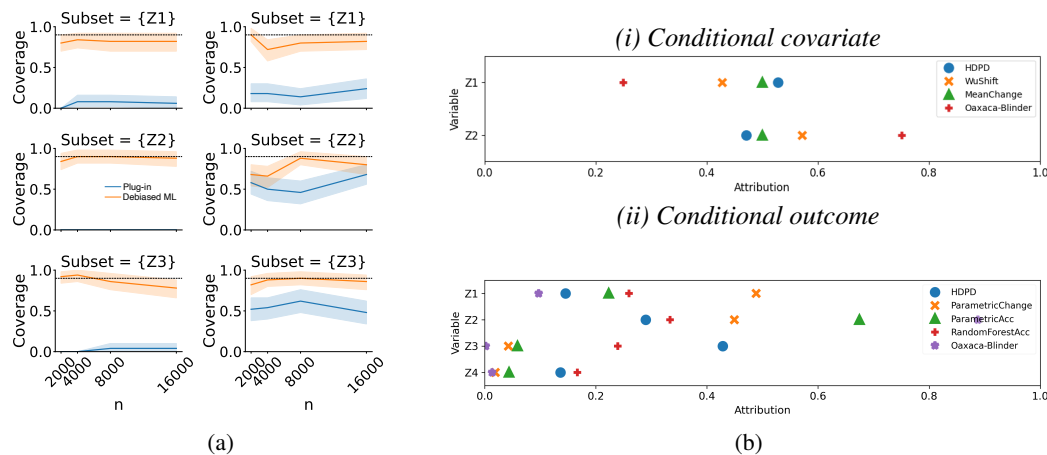


Figure 2: (a) Coverage rates of 90% CIs for value of s -partial shifts for the conditional covariate (first column) and outcome shifts (second column) across dataset sizes n . Dashed horizontal line indicates 90% coverage rate. (b) Comparison of variable importance reported by proposed method HDPD (debiased) versus existing methods for conditional covariate and outcome shift terms.

value is unnecessary for the purposes of statistical inference. Because there is inherent uncertainty in estimates of the value functions $v(s)$, one only needs to sample and estimate the values for enough variable subsets such that the uncertainty due to estimation dominates that due to subset sampling. This leads to a drastic reduction in computation time: Williamson and Feng [47] proves that the number of subsets one needs to sample only needs to be linear or super-linear in the total number of observations n . Using this result, Algorithm 4 outlines a computationally efficient procedure for estimation and inference of the detailed decomposition.

4 Simulation

We now present simulations to show that the proposed procedure achieves the desired coverage rates (Section 4.1) and illustrate how the HDPD framework provides more intuitive explanations of performance gaps (Section 4.2). In all empirical analyses, performance of the ML algorithm is quantified in terms of 0-1 accuracy. Below, we briefly describe the simulation settings; full details are provided in Section I in the Appendix.

4.1 Verifying theoretical properties

We first verify that the inference procedures for the decomposition terms have CIs with coverage close to their nominal rate. We check the coverage of the aggregate decomposition as well as the value of s -partial conditional covariate and partial conditional outcome shifts for $s = \{Z_1\}, \{Z_2\}, \{Z_3\}$. (W, Z_1, Z_2, Z_3) are sampled from independent normal distributions with different means in source and target, while Y is simulated from logistic regression models with different coefficients. CIs for the debiased ML estimator converge to the nominal 90% coverage rate with increasing sample size, whereas those for the naïve plug-in estimator do not (Fig 2a and Fig 6).

4.2 Comparing explanations

We now compare the proposed definitions for the detailed decomposition with existing methods. For the detailed decomposition due to conditional covariate shift, the comparators are:

- **MeanChange** Tests for a difference in means for each feature. Defines importance as $1 - \text{p-value}$.
- **Oaxaca-Blinder**: Fits a linear model of the logit-transformed expected loss with respect to Z in the source domain. Defines importance of Z_i as its coefficient multiplied by the difference in the means of Z_i [32, 3].
- **WuShift** [48]: Defines importance of subset s as change in *overall* performance due to s -partial conditional covariate shifts. Applies Shapley framework to obtain VIs.

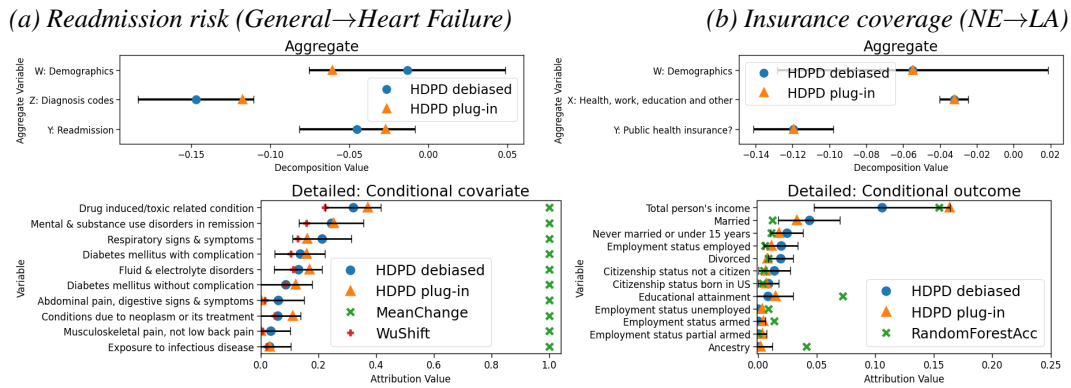


Figure 3: Aggregate and detailed decompositions for performance gaps of (a) a model predicting readmission risk across patient populations and (b) a model predicting insurance coverage across US states. A subset of VI estimates is shown; see full list in Section J in the Appendix.

For the detailed decomposition due to conditional outcome shifts, we compare against:

- **ParametricChange**: Fits a logistic model for Y with interaction terms between domain and Z . Defines importance of Z_i as the coefficient of its interaction term.
- **ParametricAcc**: Same as **ParametricChange** but models the 0-1 loss rather than Y .
- **RandomForestAcc**: Compares VI of random forest models trained on data from both domains with input features D , Z , and W to predict the 0-1 loss.
- **Oaxaca-Blinder**: Fits linear models for the logit-transformed expected loss in each domain. Defines importance of Z_i as its mean in the target domain multiplied by the difference in its coefficients across domains.

Although the proposed method may agree with these other methods on the top features in certain data settings, we highlight important situations where the methods differ.

Conditional covariate. (Fig 2b(i)) We simulate (W, Z_1) from a standard normal distribution, Z_2 from a mixture of two Gaussians whose means depend on the value of Z_1 (i.e. $Z_1 \rightarrow Z_2$), and Y from a logistic regression model depending on (W, Z_1, Z_2) . We induce a shift from the source domain to the target domain by shifting only the distribution of Z_1 , so that $p_1(Z|W) = p_0(Z_2|Z_1, W)p_1(Z_1|W)$. Only the proposed estimator correctly recovers that Z_1 is more important than Z_2 , as the $\{1\}$ -partial conditional covariate shift explains all the variation in performance gaps across strata W (i.e. the corresponding R^2 -based value function $v_z(\{1\})$ is equal to 1). The other methods incorrectly assign higher importance to Z_2 . **MeanChange** only measures shifts but not loss due to shifts, **Oaxaca-Blinder** uses a misspecified linear model, and **WuShift** estimates the performance change due to hypothesized s -partial shifts but does not check if the partial shifts are good explanations in the first place.

Conditional outcome. (Fig 2b(ii)) W and $Z \in \mathbb{R}^4$ are simulated from the same distribution in both domains. Y is generated from a logistic regression model with coefficients for (W, Z_1, \dots, Z_4) as $(0.5, 0.5, 1, 0.3, 0.3)$ in the source and $(0.5, 0.3, 1, 1.3, -0.1)$ in the target. Interestingly, none of the methods have the same ranking of the features. **ParametricChange** identifies Z_1 as having the largest shift on the logit scale, but this does not mean that it is the most important explanation for changes in the loss. According to our decomposition framework, Z_3 is actually the most important for explaining changes in model performance due to outcome shifts. **Oaxaca-Blinder**, **ParametricAcc**, and **RandomForestAcc** have odd behavior. **Oaxaca-Blinder** assigns Z_3 second to the lowest importance and **ParametricAcc** assigns Z_2 the highest importance, likely because they misspecify the outcome models. **RandomForestAcc** likely ranks Z_2 highly because its VI values quantify which variables are good predictors of performance, not performance shift.

A more objective evaluation is to compare the performance of fixes based on the different explanations. To this end, we re-fit the ML algorithm in the target domain with respect to input features Q , W , and the top variables Z_s from each explanation. We find that model revisions based on the proposed method achieve the highest performance gain (Table 3 in Appendix).

5 Real-world data case studies

We now demonstrate applicability of the framework on two datasets with naturally-occurring shifts.

Hospital readmission. Using electronic health record data from the Zuckerberg San Francisco General Hospital, we analyzed performance of a Gradient Boosted Tree (GBT) trained on the general patient population (source) to predict 30-day readmission risk but applied to patients diagnosed with heart failure (HF, target). Features include 4 demographic variables (W) and 16 diagnosis codes (Z). Each domain supplied $n = 3750$ observations from which we keep 20% in the evaluation partition.

Model accuracy drops from 70% to 53% in HF population. From the aggregate decompositions (Fig 3a), we observe that the drop is mainly due to covariate shift. If one performed the standard check to see which variables significantly changed in their mean value (MeanChange), then one would find a significant shift in nearly *every* variable. Little support is offered to identify main drivers of the performance drop. In contrast, the detailed decomposition from the proposed framework estimates diagnoses “Drug-induced or toxic-related condition” and “Mental & substance use disorder in remission” as having the highest estimated contributions to the conditional covariate shift, and most other variables having little to no contribution. Upon discussion with clinicians from this hospital, differences in the top two diagnoses may be explained by (i) substance use being a major cause of HF at this hospital, with over eighty percent of its HF patients reporting current or prior substance use, and (ii) substance use and mental health disorders often occurring simultaneously in this HF patient population. Based on these findings, closing the performance gap may require a mixture of both operational (e.g. care programs centered around substance use) and algorithmic interventions (e.g. reweighting data with respect to the top two features). Finally, CIs from the debiased ML procedure provide valuable information on the uncertainty of the estimates and highlight, for instance, that more data is necessary to determine the true ordering between the top two features. In contrast, existing methods do not provide (asymptotically valid) CIs.

ACS Public Coverage. We analyze a neural network trained to predict whether a person has public health insurance using data from Nebraska in the American Community Survey (source, $n = 3000$), applied to data from Louisiana (target, $n = 6000$). Baseline variables include 3 demographics (sex, age, race), and covariates Z include 31 variables related to health conditions, employment, marital status, citizenship status, and education.

Model accuracy drops from 84% to 66% across the two states. The main driver is the shift in the outcome distribution per the aggregate decomposition (Fig 3b) and the most important contributor to the outcome shift is annual income, perhaps due to differences in cost of living across the two states. Income is significantly more important than all the other variables; the ranking between the remaining variables is unclear. In comparing the performance of targeted model revisions, we find that revising the model based on top variables identified by the proposed procedure leads to AUCs that are better or as good as those based on RandomForestAcc (Table 4 in the Appendix).

6 Prior work

Describing distribution shifts. This line of work focuses on detecting and localizing which distributions shift between datasets [29, 39]. Budhathoki et al. [4] identify the main variables contributing to a distribution shift via a Shapley framework, Kulinski and Inouye [28] fits interpretable optimal transport maps, and Liu et al. [30] finds the region with the largest shift in the conditional outcome distribution. However, these works do not quantify how these shifts contribute to *changes in performance*, the metric of practical importance.

Explaining loss differences across subpopulations. Understanding differences in model performance across subpopulations in a single dataset is similar to understanding differences in model performance across datasets, but the focus is typically to *find* subpopulations with poor performance rather than to explain how distribution shifts contributed to the performance change. Existing approaches include slice discovery methods [35, 22, 10, 13] and structured representations of the subpopulation using e.g. Euclidean balls [1].

Attributing performance changes. Prior works have described similar aggregate decompositions of the performance change into covariate and conditional outcome shift components [5, 36]. To provide more granular explanations of performance shifts, existing works on causal attribution [50, 38] and

mediation analysis [44] quantify the importance of shifts in each variable assuming the causal graph is correctly specified; covariate shifts restricted to variable subsets assuming that the partial shifts follow a particular structure [48]; and conditional shifts in each variable assuming a parametric model [11]. However, the strong assumptions made by these methods make them difficult to apply in practice, and model misspecification can lead to unintuitive interpretations. Furthermore, such methods do not provide hierarchical decompositions, i.e. VIs for each type of shift. Decomposition methods such as Oaxaca-Blinder similarly make strong parametric assumptions [32, 3, 16, 14, 49, 15], which is inappropriate for the complex data settings in ML. In addition, there is no unifying nonparametric framework for decomposing both covariate and outcome shifts, and many methods do not output CIs, which is important when the amount of labeled data from a given domain is limited. A summary of how the proposed framework compares against prior works is shown in Table 1.

7 Discussion

ML algorithms regularly encounter distribution shifts in practice, leading to drops in performance. We present a novel framework that helps ML developers and deployment teams build a more nuanced understanding of the shifts. Compared to past work, the approach provides a nonparametric hierarchical framework for decomposing both conditional covariate and outcome shifts, does not require fine-grained knowledge of the causal relationship between variables, and quantifies the uncertainty of the estimates by constructing confidence intervals. We present real-world case studies to demonstrate how this framework can help diagnose performance drops and guide corrective actions. This framework requires overlapping support of the covariates, which may not always be applicable in practice. In such cases, one solution is to restrict to the common support [5].

Important extensions of this work include decompositions of more complex measures of model performance such as AUC and analyzing other factorizations of the data distribution (e.g. label/prior shifts [27]). For unstructured data (e.g. image and text), the current framework can be applied to low-dimensional embeddings or by extracting interpretable concepts [26]; more work is needed to directly analyze unstructured data. Finally, while the focus of this work is to interpret performance gaps, future work may take this work one step further to design optimal interventions for closing the performance gap.

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A Appendix

Contents of the Appendix are as follows.

- Table 2 collects all the notation used for reference.
- Section B discusses broader impacts of the work.
- Algorithms 1 and 4 provide the steps required for computing the aggregate and detailed decomposition respectively. Detailed decompositions require computing the value of s -partial conditional outcome and conditional covariate shifts which is described in Algorithms 2 and 3.
- Section C discusses considerations for choosing baseline variables W and conditional covariates Z .
- Section D describes a causal interpretation of the aggregate and detailed decompositions as effects of stochastic (or shift) interventions on a structural causal model.
- Section E explain why value functions in prior work give unintuitive attribution and that the R^2 -based value functions are proper scoring rules.
- Section F describes the estimation and inference for aggregate decomposition and detailed decomposition of conditional covariate shift.
- Section G provides the derivations of the results.
- Sections H and I describe the implementation and simulation details.
- Section J provides additional details on the two real world datasets and results.

B Broader impacts

This work presents a method for understanding failures of ML algorithms when they are deployed in settings or populations different from the ones in development datasets. Therefore, the work can be used to suggest ways of improving the algorithms or mitigating their harms. The method is generally applicable to tabular data settings for any classification algorithm, hence, it can potentially be applied across multiple domains where ML is used including medicine, finance, and online commerce.

Care must be taken while interpreting the results. As usual, assumptions underlying the decompositions such as the coarse causal ordering between the variables W , Z , and Y should be validated through domain knowledge.

Algorithm 1 Aggregate decompositions into baseline, conditional covariate, and conditional outcome shifts

Input: Source and target data $\{(W_i^{(d)}, Z_i^{(d)}, Y_i^{(d)})\}_{i=1}^{n_d}$ for $d \in \{0, 1\}$, loss function $\ell(W, Z, Y; f)$.

Output: Performance change due to baseline, conditional covariate, and conditional outcome shifts $\Lambda_W, \Lambda_Z, \Lambda_Y$.

- 1 Split source and target data into training Tr and evaluation Ev partitions. Let n^{Ev} be the total number of data points in the Ev partition.
 - 2 Fit nuisance parameters η_W, η_Z, η_Y , defined in Section G.1, on the Tr partition as outlined in Section H.1.
 - 3 Estimate $\Lambda_W, \Lambda_Z, \Lambda_Y$ using fitted nuisance parameters on the Ev partitions following the equations in Section F.1.
 - 4 Estimate variance of influence functions $\psi_W(d, w, z, y; \hat{\eta}_N)$, $\psi_Z(d, w, z, y; \hat{\eta}_N)$, and $\psi_Y(d, w, z, y; \hat{\eta}_N)$ as defined in (23), (24), and (25), respectively.
 - 5 Compute α -level confidence intervals as $\hat{\Lambda}_N \pm z_{1-\alpha/2} \sqrt{\widehat{\text{var}}(\psi_N(d, w, z, y; \hat{\eta}_N)) / n^{\text{Ev}}}$ for $N \in \{W, Z, Y\}$, where z is the inverse CDF of the standard normal distribution.
 - 6 **return** $\hat{\Lambda}_W, \hat{\Lambda}_Z, \hat{\Lambda}_Y$ and confidence intervals
-

Table 2: Notation

Symbol	Meaning
W, Z, Y	Variables: Baseline, Conditional covariates, Outcome
f	Prediction model being analyzed
$\ell(W, Z, Y)$ or ℓ	Loss function e.g. 0-1 loss
$D = 0$ and $D = 1$	Indicators for source and target domain
p_0, p_1	Probability density (or mass) function for the two domains $D = 0, 1$
p_s	Probability density (or mass) function when only variable subset s shifts from source to target
$\mathbb{E}_{D_0 D_Z D_Y}$	Expectation over the distribution $p_{D_0}(W)p_{D_Z}(Z W)p_{D_Y}(Y W, Z)$
$Q := q(W, Z)$	Source domain risk at W, Z , i.e. $p_0(Y = 1 W, Z)$
Tr and Ev	Training dataset used to fit models and evaluation dataset used to compute decompositions
$\phi_{Z,j}$ and $\phi_{Y,j}$	Shapley values for variable j in the detailed decomposition of conditional covariate and outcome shifts
$v_Z(s)$ and $v_Y(s)$	Value of a subset s for s -partial conditional covariate shift and s -partial outcome shift
$v_Y^{\text{num}}(s)$ and $v_Y^{\text{den}}(s)$	Numerator and denominator of the ratio defined in the value of a subset
Models μ .	Outcome models for the conditional expectation of the loss across different settings
Models π .	Density ratio models for feature densities across datasets
\mathbb{P}	Notation for expectation
$\mathbb{P}_{0,n}$ and $\mathbb{P}_{1,n}$	sample average over source and target data in the evaluation dataset
$\psi(d, w, z, y)$	Influence function defined in the linear approximation of an estimand, see e.g. (22)

Algorithm 2 VALUECONDITIONALOUTCOME(S): Value for s -partial conditional outcome shift for a subset s

Input: Training **Tr** and evaluation **Ev** partitions of source and target data, subset of variables s .

Output: Value for s -partial conditional outcome shift for subset s .

- 1 Fit nuisance parameters $\eta_{Y,s}^{\text{num}}, \eta_Y^{\text{den}}$, defined in Sections G.3, on the **Tr** partitions as outlined in H.2.
- 2 Estimate $v_Y(s)$ by $\hat{v}_Y^{\text{num}}(s)/\hat{v}_Y^{\text{den}}$ where $\hat{v}_Y^{\text{num}}(s)$ is estimated using (6) and \hat{v}_Y^{den} is estimated using (7) on the **Ev** partition.
- 3 Estimate variance of influence function $\psi_{Y,\text{bin},s}(d, w, z, y; \hat{\eta}_{Y,s}^{\text{num}}, \hat{\eta}_Y^{\text{den}})$ as defined in (74).
- 4 Compute α -level confidence interval as $\hat{v}_Y(s) \pm z_{1-\alpha/2} \sqrt{\widehat{\text{var}}(\psi_{Y,\text{bin},s}(d, w, z, y; \hat{\eta}_{Y,s}^{\text{num}}, \hat{\eta}_Y^{\text{den}}))/n^{\text{Ev}}}$.
- 5 **return** $\hat{v}_Y(s)$ and confidence interval

Algorithm 3 VALUECONDITIONALCOVARIATE(S): Value for s -partial conditional covariate shift for a subset s

Input: Training **Tr** and evaluation **Ev** partitions of source and target data, subset of variables s .

Output: Value for s -partial conditional covariate shift for subset s .

- 1 Fit nuisance parameters $\eta_{Z,s}^{\text{num}}$, defined in Sections G.2, on the **Tr** partition, as outlined in H.3.
- 2 Estimate $v_Z(s)$ by $\hat{v}_Z^{\text{num}}(s)/\hat{v}_Z^{\text{num}}(\emptyset)$ using (21) on the **Ev** partition.
- 3 Estimate variance of influence function $\psi_{Z,s}(d, w, z, y; \hat{\eta}_{Z,s}^{\text{num}})$ as defined in (41).
- 4 Compute α -level confidence interval as $\hat{v}_Z(s) \pm z_{1-\alpha/2} \sqrt{\widehat{\text{var}}(\psi_{Z,s}(d, w, z, y; \hat{\eta}_{Z,s}^{\text{num}}))/n^{\text{Ev}}}$.
- 5 **return** $\hat{v}_Z(s)$ and confidence interval

Algorithm 4 Detailed decomposition for conditional outcome and covariate shift

Input: Source and target data $\{(W_i^{(d)}, Z_i^{(d)}, Y_i^{(d)})\}_{i=1}^{n_d}$ for $d \in \{0, 1\}$, loss function $\ell(W, Z, Y; f)$, $\gamma \in \mathbb{R}^+$.

Output: Detailed decomposition for conditional outcome or covariate shift, $\{\phi_{Y,j} : j = 0, \dots, m_2\}$ or $\{\phi_{Z,j} : j = 1, \dots, m_2\}$.

- 1 Split source and target data into training Tr and evaluation Ev partitions. Let n^{Ev} be the total number of data points in the Ev partition.
 - 2 Subsample $\lfloor \gamma n^{\text{Ev}} \rfloor$ subsets from $\mathcal{Z} = \{1, \dots, m_2\}$ with respect to Shapley weights, including \emptyset and \mathcal{Z} , denoted s_1, \dots, s_k .
 - 3 Estimate $v_Y(s) \leftarrow \text{VALUECONDITIONALOUTCOME}(s)$ and $v_Z(s) \leftarrow \text{VALUECONDITIONALCOVARIATE}(s)$ for $s \in s_1, \dots, s_k$.
 - 4 Get estimated Shapley values $\{\phi_{Y,j}\}$ and $\{\phi_{Z,j}\}$ by solving constrained linear regression problems in (7) in Williamson and Feng [47] with value functions $v_Y(s)$ and $v_Z(s)$, respectively.
 - 5 Compute confidence intervals based on the influence functions defined in Theorem 1 in Williamson and Feng [47].
 - 6 **return** Shapley values $\{\phi_{Y,j} : j = 0, \dots, m_2\}$ and $\{\phi_{Z,j} : j = 1, \dots, m_2\}$ and confidence intervals
-

C Considerations for the choice of W and Z variables

We suppose that variables X are partitioned into baseline variables W and conditional covariates Z . We suggest selecting Z to be the variables that may act as mediators of the environment shift and/or variables whose associations with Y are likely to be modified by the environment shift (i.e. effect modification). This selection can be chosen based on a high-level causal graph, where W are variables known to be upstream of Z . For instance, if Z are treatment variables and W are baseline variables, one can interpret a covariate shifts as a change in the treatment policy and an outcome shift as a change in the treatment effect across the two environments.

In the absence of any prior knowledge, another option is to choose W as the variables for which one would like the expected loss given W to be invariant across the two environments; this can be useful to promote fairness of ML algorithms across environments. When this invariance does not hold, the proposed framework explains how variables Z contribute to these differences, which can inform efforts to eliminate performance gaps. This last option is similar to how variables are typically chosen in disparity analyses [21]. For instance, to understand why income differs between males and females controlling for age, one would set domain to $D = \text{gender}$, $W = \text{age}$, and Z as variables that may explain this disparity (e.g. marital status, employment status).

In general, including more variables in W and Z to explain the performance difference is preferable. Nevertheless, there are tradeoffs. For instance, including more variables in W leads to higher variance of $\Delta_{.10}(W)$, so it allows one to better distinguish the relative importance of variables in Z for explaining its variability. On the other hand, when more variables are assigned to W , the performance gap with respect to W ($\Delta_{.10}(W)$) is a more complex function. Thus we may have more uncertainty in our estimate of $\Delta_{.10}(W)$, which may lead to wider confidence intervals for the variable importance values.

D Causal interpretation of aggregate and detailed decompositions

Partial distribution shifts that we define in the framework can be equivalently described as stochastic (or shift) interventions in a structural causal model (SCM) respecting a causal directed acyclic graph (DAG) [8]. To represent an intervention on variable X , we use regime indicator σ_X which means that the conditional probability distribution for X in the SCM has been updated to a new one [9].

Suppose that the source and target data (W, Z, Y) are generated by SCMs respecting the same DAG \mathcal{G} in Figure 4 with no unmeasured confounders. Intervening on a variable in source SCM sets its

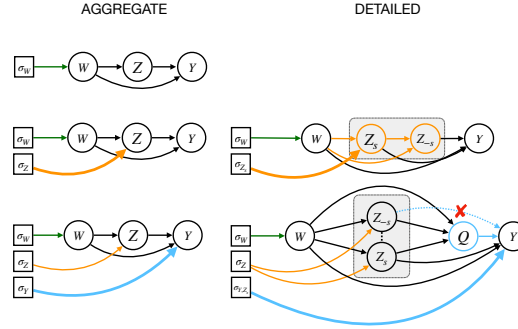


Figure 4: Decomposition framework for explaining the performance gap from source to target domain, visualized through causal directed acyclic graphs. Aggregate decompositions describe the incremental effect of stochastic interventions on each aggregate variable’s distribution at the source with that in the target, indicated by regime indicators σ_W , σ_Z , and σ_Y . Detailed decompositions quantify how well candidate partial distribution shifts explain the variability of performance gaps across strata. The candidate partial shifts considered in this work are shown in the DAGs on the right. An s -partial conditional covariate shift is a stochastic intervention on variable subset Z_s . An s -partial conditional outcome shift is a stochastic intervention on variable Y , in which the conditional outcome distribution fine-tunes the risk in the source domain (indicated by the additional node $Q = p_0(Y = 1|W, Z)$) with respect to Z_s .

conditional distribution to the corresponding one in the target SCM. Under the assumption of no unmeasured confounders, we have

$$p_0(V; \sigma_X) = \prod_{V_i \in V \setminus X} p_0(V_i | pa_G(V_i); \sigma_X) \prod_{V_i \in X} p_1(V_i | pa_G(V_i)) \quad (10)$$

for any variable set V where pa_G denotes parents in \mathcal{G} . Therefore, the target data is obtained by intervening on all the variables $p_0(W, Z, Y; \sigma_W, \sigma_Z, \sigma_Y) = p_1(W, Z, Y)$. Expectation \mathbb{E} is taken over the source distribution or its shifted version based on the specified regime indicator.

Aggregate decompositions can then be written as causal effect of intervening on W, Z, Y incrementally as follows

$$\begin{aligned} \Lambda_W &= \mathbb{E}[\ell | \sigma_W] - \mathbb{E}[\ell] \\ \Lambda_Z &= \mathbb{E}[\ell | \sigma_W, \sigma_Z] - \mathbb{E}[\ell | \sigma_W] \\ \Lambda_Y &= \mathbb{E}[\ell | \sigma_W, \sigma_Z, \sigma_Y] - \mathbb{E}[\ell | \sigma_W, \sigma_Z] \end{aligned}$$

Due to the factorization (10), the above are equivalent to aggregate decompositions presented in Section 2.

For detailed decomposition of the conditional covariate shift, assume the causal DAG in Figure 4 with $Z_s \rightarrow Z_{-s}$ for variable subset s . The s -partial conditional covariate shift is represented by $p_0(V; \sigma_{Z_s})$ and, under the factorization (10), is equivalent to the one considered in Section 2.2. Thus, the performance difference $\Delta_{.s0}(W)$ can be equivalently written as $\mathbb{E}[\ell | W; \sigma_{Z_s}] - \mathbb{E}[\ell | W]$ and $\Delta_{.10}(W)$ as $\mathbb{E}[\ell | W; \sigma_Z] - \mathbb{E}[\ell | W]$. The value function is then

$$v_Z(s) := 1 - \frac{\mathbb{E}[(\Delta_{.s0}(W) - \Delta_{.10}(W))^2; \sigma_W]}{\mathbb{E}[\Delta_{.10}^2(W); \sigma_W]}.$$

The s -partial conditional outcome shift corresponds to a stochastic intervention that changes the distribution of Y to (5). Denoting it as $p_0(V; \sigma_{Y, Z_s})$, the performance difference $\Delta_{..s}(W, Z)$ can be equivalently written as $\mathbb{E}[\ell | W, Z; \sigma_{Y, Z_s}] - \mathbb{E}[\ell | W, Z]$ and $\Delta_{..1}(W, Z)$ as $\mathbb{E}[\ell | W, Z; \sigma_Y] - \mathbb{E}[\ell | W, Z]$. The value function (4) is then

$$v_Y(s) := 1 - \frac{\mathbb{E}[(\Delta_{..s}(W, Z) - \Delta_{..1}(W, Z))^2; \sigma_W, \sigma_Z]}{\mathbb{E}[\Delta_{..1}^2(W, Z); \sigma_W, \sigma_Z]}. \quad (11)$$

E Proper scoring rules for partial distribution shift

Prior works have considered scoring rules for partial distribution shifts in terms of their change in the average loss [48]. For instance, for conditional covariate shifts, prior works have considered scoring rules of the form

$$\mathbb{E}_{1s0}[\ell] - \mathbb{E}_{100}[\ell] = \int \ell(Y, f(Z, W)) (p_s(z|w) - p_0(z|w)) p_1(w) dz dw. \quad (12)$$

However, in the absence of a detailed causal graph, we show that this can lead to unintuitive attributions. Consider the following counterexample. We drop W from the data example for simplicity of exposition.

Example E.1. Consider the following data-generating process with random variables Z_1 and Z_2 , a real-valued outcome Y , and loss function as squared error $\ell = (f(Z_1, Z_2) - Y)^2$:

$$Z_1 \sim N(D + 1, 1) \quad (13)$$

$$Z_2 = |Z_1| \quad (14)$$

$$\epsilon \sim N(0, 1) \quad (15)$$

$$Y = Z_1 + Z_2 + \epsilon \mathbb{1}\{Z_1 \leq 0\} \quad (16)$$

where $D = 0$ and $D = 1$ correspond to the source and target domains, respectively. Suppose the ML model is the optimal model for minimizing the expected loss in the source domain, i.e. $f(Z_1, Z_2) = Z_1 + Z_2$. Consider the following candidate partial distribution shifts for explaining the performance change, where Option 1 hypothesizes Z_1 causes Z_2 and Option 2 hypothesizes Z_2 causes Z_1 .

(Option 1) For $s = \{1\}$, $p_s(Z) = p_1(Z_1)p_0(Z_2|Z_1)$

(Option 2) For $s = \{2\}$, $p_s(Z) = p_1(Z_2)p_0(Z_1|Z_2)$

Per the given data-generating process, the partial shift in Option 1 exactly corresponds to the true (aggregate) dataset shift; thus we would expect it to have a higher value than Option 2. Nevertheless, the MSE resulting from Option 2's shift is 0.5 (the marginal distribution of Z_1 under Option 2 is symmetric around 0). In contrast, the MSE resulting from Option 1's shift is the probability that a standard normal variable is less than -1, which is 0.159.

In Example E.1, scoring rule (12) assigns a higher value to a partial shift that contradicts the true causal graph than even the true aggregate shift, because the rule *assumes* the hypothesized dataset shift is true. Consequently, (12) is not a *proper* scoring rule. In contrast, the proposed value functions described in Section 2.1 are.

More formally, we extend the traditional definition for a proper scoring rule [18] to the context of explaining performance changes as follows. Let a scoring function $\chi : O_0 \times O_1 \times Q$ be defined as a function of source observation $O_0 = (W_0, Z_0, Y_0)$, target observation $O_1 = (W_1, Z_1, Y_1)$, and candidate shift probability model Q . A scoring rule χ is proper with respect to the set of distribution shift models \mathcal{F} if the following holds: for any true model of the post-shift data distribution $p^*(W, Z, Y) \in \mathcal{F}$, the expectation of the scoring function $\chi(O_0, O_1, p^*)$ with respect to $O_0 \sim p_0$ and $O_1 \sim p^*$ is always no smaller than the expectation of $\chi(O_0, O_1, p)$ for any $p \in \mathcal{F}$, i.e.

$$\mathbb{E}_{p_0, p^*}[\chi(O_0, O_1, p^*)] \geq \mathbb{E}_{p_0, p^*}[\chi(O_0, O_1, p)] \quad \forall p \in \mathcal{F} \quad (17)$$

Moreover, we say that χ is strictly proper if (17) holds with equality iff $p = p^*$.

Let \mathcal{F}_Z be the set of candidate s -partial conditional covariate shifts $p_{\cdot s0}$ and \mathcal{F}_Y be the set of candidate s -partial conditional outcome shifts $p_{\cdot s}$, i.e.

$$\mathcal{F}_Z = \{p_{\cdot s0}(y, z|w) = p_0(y|z, w)p_s(z|w) : s \subseteq \{1, \dots, m_2\}\}$$

$$\mathcal{F}_Y = \{p_s(y|z, w) : s \subseteq \{1, \dots, m_2\}\}.$$

Then, v_Z defined in (3) is a proper scoring rule with respect to \mathcal{F}_Z , as v_Z attains its largest value when $\Delta_{\cdot s0} \equiv \Delta_{\cdot 10}$, which holds when $p_{\cdot s0}$ matches the true covariate-only distribution shift model $p_{\cdot 10}$. Similarly, v_Y defined in (4) is a proper scoring rule with respect to \mathcal{F}_Y . Moreover, these are *strictly* proper scoring rules as long as the conditional expectation of the losses of candidate distribution shifts are not adversarially aligned. That is, under the assumptions that

$$\mathbb{E}_{\cdot s0}[\ell|W] \equiv \mathbb{E}_{\cdot 10}[\ell|W] \iff p_{\cdot s0} \equiv p_{\cdot 10} \quad \forall p_{\cdot s0} \in \mathcal{F}_Z \quad (A.1)$$

$$\mathbb{E}_{\cdot s}[\ell|W, Z] \equiv \mathbb{E}_{\cdot 1}[\ell|W, Z] \iff p_{\cdot s} \equiv p_{\cdot 1} \quad \forall p_{\cdot s} \in \mathcal{F}_Y \quad (A.2)$$

v_Z and v_Y are strictly proper scoring rules with respect to \mathcal{F}_Z and \mathcal{F}_Y , respectively. As the candidate distribution shifts considered in this work are functionals of the observed distribution shift and observed distribution shifts are unlikely to be adversarial in many real-world situations, Assumptions (A.1) and (A.2) are likely reasonable in practice.

F Estimation and Inference

Let $\{(W_i^{(d)}, Z_i^{(d)}, Y_i^{(d)}) : i = 1, \dots, n_d\}$ denote n_d independent and identically distributed (IID) observations from the source and target domains $d = 0$ and 1 , respectively. Let a fixed fraction of the data be partitioned towards “training” (Tr) and the remaining to “evaluation” (Ev); let n_{Ev} be the number of observations in the evaluation partition. Let \mathbb{P}_d denote the expectation with respect to domain d and $\mathbb{P}_{d,n}$ denote the empirical average over observations in partition Ev from domain $d = \{0, 1\}$.

F.1 Aggregate decomposition

The aggregate decomposition terms can be formulated as an average treatment effect, a well-studied estimand in causal inference, where domain D corresponds to treatment. As such, one can use augmented inverse probability weighting (AIPW) to define debiased ML estimators of the aggregate decomposition terms (e.g. Kang and Schafer [24]). We review estimation and inference for these terms below.

Estimation. Using the training data, estimate outcome models $\mu_{\cdot 00}(W) = \mathbb{E}_{\cdot 00}[\ell | W = w]$ and $\mu_{\cdot \cdot 0}(W, Z) = \mathbb{E}[\ell | W, Z]$ and density ratio models $\pi_{100}(W) = p_1(W)/p_0(W)$ and $\pi_{110}(W, Z) = p_1(W, Z)/p_0(W, Z)$. The debiased ML estimators for $\Lambda_W, \Lambda_Z, \Lambda_Y$ are

$$\begin{aligned}\hat{\Lambda}_W &= \mathbb{P}_{0,n}(\ell - \hat{\mu}_{\cdot 00}(W)) \hat{\pi}_{100}(W) + \mathbb{P}_{1,n} \hat{\mu}_{\cdot 00}(W) - \mathbb{P}_{0,n} \ell \\ \hat{\Lambda}_Z &= \mathbb{P}_{0,n}(\ell - \hat{\mu}_{\cdot \cdot 0}(W, Z)) \hat{\pi}_{110}(W, Z) + \mathbb{P}_{1,n} \hat{\mu}_{\cdot \cdot 0}(W, Z) \\ &\quad - \mathbb{P}_{0,n}(\ell - \hat{\mu}_{\cdot 00}(W)) \hat{\pi}_{100}(W) - \mathbb{P}_{1,n} \hat{\mu}_{\cdot 00}(W) \\ \hat{\Lambda}_Y &= \mathbb{P}_{1,n} \ell - \mathbb{P}_{0,n}(\ell - \hat{\mu}_{\cdot \cdot 0}(W, Z)) \hat{\pi}(W, Z) - \mathbb{P}_{1,n} \hat{\mu}_0(W, Z)\end{aligned}$$

Inference. Assuming the estimators for the outcome and density ratio models converge at a fast enough rate, the AIPW estimators for the aggregate decomposition terms are asymptotically linear and, thus, facilitate the construction of CIs.

Theorem F.1. Suppose π_{100} and π_{110} are bounded; estimators $\hat{\mu}_{\cdot 00}$, $\hat{\pi}_{\cdot \cdot 0}$, $\hat{\pi}_{100}$, and $\hat{\pi}_{110}$ are consistent; and

$$\begin{aligned}\mathbb{P}_0(\hat{\mu}_{\cdot 00} - \mu_{\cdot 00})(\hat{\pi}_{100} - \pi_{100}) &= o_p(n^{-1/2}) \\ \mathbb{P}_0(\hat{\mu}_{\cdot \cdot 0} - \mu_{\cdot \cdot 0})(\hat{\pi}_{110} - \pi_{110}) &= o_p(n^{-1/2}).\end{aligned}$$

Then $\hat{\Lambda}_Y$, $\hat{\Lambda}_Z$, and $\hat{\Lambda}_W$ are asymptotically linear estimators of their respective estimands.

F.2 Value of s -partial conditional covariate shifts

Estimation. Using the training partition, estimate the density ratio $\pi_{1s0}(z_s, w) = p_1(z_s, w)/p_0(z_s, w)$ and the outcome models

$$\mu_{\cdot 0-s0}(z_s, w) = \mathbb{E}_{\cdot 00}[\ell | z_s, w] = \int \int \ell p_0(y | w, z) p_0(z_{-s} | z_s, w) dy dz_{-s} \quad (18)$$

$$\mu_{\cdot \cdot 10}(w) = \mathbb{E}_{\cdot 10}[\ell | w] \quad (19)$$

$$\mu_{\cdot s0}(w) = \mathbb{E}_{\cdot s0}[\ell | w] = \int \int \int \ell p_0(y | w, z) p_0(z_{-s} | z_s, w) p_1(z_s | w) dy dz_{-s} dz_s, \quad (20)$$

in addition to the other nuisance models previously mentioned. We propose the estimator $\hat{v}_Z(s) = \hat{v}_Z^{\text{num}}(s)/\hat{v}_Z^{\text{den}}$, where

$$\begin{aligned}\hat{v}_Z^{\text{num}}(s) := & \mathbb{P}_{1,n}(\hat{\mu}_{\cdot s0}(W) - \hat{\mu}_{\cdot 10}(W))^2 \\ & + 2\mathbb{P}_{0,n}(\hat{\mu}_{\cdot s0}(W) - \hat{\mu}_{\cdot 10}(W))(\ell - \hat{\mu}_{\cdot 0-s0}(W, Z_s))\hat{\pi}_{1s0}(W, Z_s) \\ & - 2\mathbb{P}_{0,n}(\hat{\mu}_{\cdot s0}(W) - \hat{\mu}_{\cdot 10}(W))(\ell - \hat{\mu}_{\cdot 0}(W, Z))\hat{\pi}_{110}(W, Z) \\ & + 2\mathbb{P}_{1,n}(\hat{\mu}_{\cdot s0}(W) - \hat{\mu}_{\cdot 10}(W))(\hat{\mu}_{\cdot 0-s0}(W, Z_s) - \hat{\mu}_{\cdot s0}(W)) \\ & - 2\mathbb{P}_{1,n}(\hat{\mu}_{\cdot s0}(W) - \hat{\mu}_{\cdot 10}(W))(\hat{\mu}_{\cdot 0}(W, Z) - \hat{\mu}_{\cdot 10}(W))\end{aligned}\quad (21)$$

and $\hat{v}_Z^{\text{den}} := \hat{v}_Z^{\text{num}}(\emptyset)$.

Inference. The estimator is asymptotically normal as long as the outcome and density ratio models are estimated at a fast enough rate defined formally as follows.

Condition F.2. For variable subset s , suppose the following holds

- $\mathbb{P}_0(\mu_{001}(W) - \mu_{01}(W))^2$ is bounded
- $\mathbb{P}_0(\mu_{\cdot 0-s0}(Z_s, W) - \hat{\mu}_{\cdot 0-s0}(Z_s, W))(\hat{\pi}_{1s0}(Z_s, W) - \pi_{1s0}(Z_s, W)) = o_p(n^{-1/2})$
- $\mathbb{P}_0(\mu_{\cdot 0}(W, Z) - \hat{\mu}_{\cdot 0}(W, Z))(\hat{\pi}_{110}(W, Z) - \pi_{110}(W, Z)) = o_p(n^{-1/2})$
- $\mathbb{P}_1(\hat{\mu}_{\cdot s0}(W) - \mu_{\cdot s0}(W))^2 = o_p(n^{-1/2})$
- $\mathbb{P}_1(\hat{\mu}_{\cdot 10}(W) - \mu_{\cdot 10}(W))^2 = o_p(n^{-1/2})$
- (Positivity) $p_0(z_s, w) > 0$ and $p_0(w, z) > 0$ almost everywhere, such that the density ratios $\pi_{1s0}(w, z_s)$ and $\pi_{110}(w, z)$ are well-defined and between $(0, 1)$.

Theorem F.3. For variable subset s , suppose $v_Z^{\text{den}}(s) > 0$ and Condition F.2 hold. Then the estimator $\hat{v}_Z(s)$ is asymptotically normal.

G Proofs

Notation. For all proofs, we will write \mathbb{P} to mean expectation on the evaluation partition (and likewise for the empirical version) for notational simplicity.

Overview of derivation strategy. We first present the general strategy for proving asymptotic normality of the estimators for the decompositions. Details on nonparametric debiased estimation can be found in texts such as Tsiatis [45] and Kennedy [25].

Let $v(\mathbb{P})$ be a pathwise differentiable quantity that is a function of the true regular (differentiable in quadratic mean) probability distribution \mathbb{P} over random variable O . For instance, v in the case of mean is defined as $v(\mathbb{P}) := \mathbb{E}_{O \sim \mathbb{P}(O)}[O]$. Let $\hat{\mathbb{P}}$ denote an arbitrary regular estimator of \mathbb{P} , such as the maximum likelihood estimator. The plug-in estimator is then defined as $v(\hat{\mathbb{P}})$.

The von-Mises expansion of the functional v (which linearizes v in analogy to the first-order Taylor expansion), given it is pathwise differentiable, gives

$$v(\hat{\mathbb{P}}) - v(\mathbb{P}) = -\mathbb{P} \psi(o; \hat{\mathbb{P}}) + R(\hat{\mathbb{P}}, \mathbb{P}). \quad (22)$$

Here, the function ψ is called an influence function (or a functional gradient of v at $\hat{\mathbb{P}}$). $R(\hat{\mathbb{P}}, \mathbb{P})$ is a second-order remainder term. The one-step corrected estimators we consider have the form of $v(\hat{\mathbb{P}}) + \mathbb{P}_n \psi(o; \hat{\mathbb{P}})$ where \mathbb{P}_n denotes a sample average. Following the expansion above, the one-step corrected estimator can be analyzed as follows,

$$\begin{aligned}& \left(v(\hat{\mathbb{P}}) + \mathbb{P}_n \psi(o; \hat{\mathbb{P}}) \right) - v(\mathbb{P}) \\ &= (\mathbb{P}_n - \mathbb{P}) \psi(o; \hat{\mathbb{P}}) + R(\hat{\mathbb{P}}, \mathbb{P}) \\ &= (\mathbb{P}_n - \mathbb{P}) \psi(o; \mathbb{P}) + (\mathbb{P}_n - \mathbb{P})(\psi(o; \hat{\mathbb{P}}) - \psi(o; \mathbb{P})) + R(\hat{\mathbb{P}}, \mathbb{P})\end{aligned}$$

Our goal will be to analyze each of the three terms and to show that they are asymptotically negligible at \sqrt{n} -rate, such that the one-step corrected estimator satisfies

$$\left(v(\hat{\mathbb{P}}) + \mathbb{P}_n \psi(o; \hat{\mathbb{P}})\right) - v(\mathbb{P}) = \mathbb{P}_n \psi(o; \mathbb{P}) + o_p(n^{-1/2}),$$

where we used the property of influence functions that they have zero mean. Thus the one-step corrected estimator is asymptotically normal with mean $v(\mathbb{P})$ and variance $\text{var}(\psi(o; \mathbb{P}))/n$, which allows for the construction of CIs. In the following proofs, we present the influence functions without derivations; see Kennedy [25] and Hines et al. [20] for strategies for deriving influence functions.

G.1 Aggregate decompositions

Let the nuisance parameters in the one-step estimators $\Lambda_W, \Lambda_Z, \Lambda_Y$ be denoted by $\eta_W = (\mu_{\cdot 00}, \pi_{100})$, $\eta_Z = (\mu_{\cdot 0}, \mu_{\cdot 00}, \pi_{110})$, $\eta_Y = (\mu_{\cdot 0}, \pi_{110})$ respectively. Denote the estimated nuisances by $\hat{\eta}_W, \hat{\eta}_Z, \hat{\eta}_Y$. The canonical gradients for the three estimands are

$$\begin{aligned} \psi_W(d, w, z, y; \eta_W) &= [(\ell(w, z, y) - \mu_{\cdot 00}(w)) \pi_{100}(w) - \ell(w, z, y)] \frac{\mathbb{1}\{d=0\}}{p(d=0)} \\ &\quad + \mu_{\cdot 00}(w) \frac{\mathbb{1}\{d=1\}}{p(d=1)} - \Lambda_W \end{aligned} \quad (23)$$

$$\begin{aligned} \psi_Z(d, w, z, y; \eta_Z) &= [(\ell(w, z, y) - \mu_{\cdot 0}(w, z)) \pi_{110}(w, z)] \frac{\mathbb{1}\{d=0\}}{p(d=0)} + \mu_{\cdot 0}(w, z) \frac{\mathbb{1}\{d=1\}}{p(d=1)} \\ &\quad - [(\ell(w, z, y) - \mu_{\cdot 00}(w)) \pi_{100}(w)] \frac{\mathbb{1}\{d=0\}}{p(d=0)} + \mu_{\cdot 00}(w) \frac{\mathbb{1}\{d=1\}}{p(d=1)} - \Lambda_Z \end{aligned} \quad (24)$$

$$\begin{aligned} \psi_Y(d, w, z, y; \eta_Y) &= (\ell(w, z, y) - \mu_{\cdot 0}(w, z)) \frac{\mathbb{1}\{d=1\}}{p(d=1)} \\ &\quad - [(\ell(w, z, y) - \mu_{\cdot 0}(w, z)) \pi_{110}(w, z)] \frac{\mathbb{1}\{d=0\}}{p(d=0)} - \Lambda_Y. \end{aligned} \quad (25)$$

Theorem G.1 (Theorem F.1). *Under conditions outlined in Theorem F.1, the one-step corrected estimators for the aggregate decomposition terms, baseline, conditional covariate, and conditional outcome $\hat{\Lambda}_W, \hat{\Lambda}_Z$, and $\hat{\Lambda}_Y$, are asymptotically linear, i.e.*

$$\hat{\Lambda}_N - \Lambda_N = \mathbb{P}_n \psi_N + o_p(n^{-1/2}) \quad \forall N \in \{W, Z, Y\}. \quad (26)$$

Proof. The estimands $\Lambda_W, \Lambda_Z, \Lambda_Y$ have similarities to the standard average treatment effect (ATE) in the causal inference literature (see [25, Example 2]). Hence, the estimators and their asymptotic properties directly follow. For treatment T , outcome O , and confounders C , the mean outcome under $T = 1$ among the population with $T = 0$ is identified as

$$\phi = \int op(o|c, t=1)p(c|t=0)dodc \quad (27)$$

and its one-step corrected estimator can be derived from the canonical gradient of ϕ , which takes the following form after plugging in the estimates of the nuisance models:

$$\hat{\phi}_n = \mathbb{P}_n \left\{ \frac{\mathbb{1}\{T=1\}}{\Pr(T=1)} \hat{\pi}(c) (O - \hat{\mu}_1(c)) + \frac{\mathbb{1}\{T=0\}}{\Pr(T=0)} \hat{\mu}_1(c) \right\}$$

satisfies

$$\hat{\phi}_n - \phi = \mathbb{P}_n \left\{ \frac{\mathbb{1}\{T=1\}}{\Pr(T=1)} \pi(c) (O - \mu_1(c)) + \frac{\mathbb{1}\{T=0\}}{\Pr(T=0)} \mu_1(c) - \phi \right\} + o_p(n^{-1/2})$$

where $\mu_1(c) = \mathbb{E}[o|c, t=1]$ and $\pi(c) = p(c|t=0)/p(c|t=1)$ as long as the following conditions hold:

- $p(c|t=1) > 0$ almost everywhere such that the density ratios $\pi(c)$ are well-defined and bounded,

- $\mathbb{P}_1(\hat{\mu}_1 - \mu_1)(\hat{\pi} - \pi) = o_p(n^{-1/2})$.

We establish the estimators and their influence functions by showing that they can all be viewed as mean outcomes of the form (27).

Baseline term Λ_w . The first term $\mathbb{E}_{100}[\ell(w, z, y)]$ is a mean outcome with respect to $p(\ell(w, z, y)|w, d = 0)p(w|d = 1)$, which is the same as that in (27) but with $\ell(w, z, y)$ as the outcome, w as the confounder, and d as the (flipped) treatment. The second term $\mathbb{E}_{000}[\ell(w, z, y)]$ is a simple average over $D = 0$ population whose influence function is the $\ell(w, z, y)$ itself.

Conditional covariate term Λ_z . First term $\mathbb{E}_{110}[\ell(w, z, y)]$ is the mean outcome with respect to $p(\ell(w, z, y)|w, z, d = 0)p(w, z|d = 1)$, where the chief difference is (w, z) is the confounder. Second term $\mathbb{E}_{100}[\ell(w, z, y)]$ is also a mean outcome, as discussed above.

Conditional outcome term Λ_y . First term $\mathbb{E}_{111}[\ell(w, z, y)]$ is a simple average over the $D = 1$ population. \square

G.2 Value of s -partial conditional covariate shifts

Let nuisance parameters in the one-step estimator $v_{Z,s}^{\text{num}}$ be denoted $\eta_{Z,s}^{\text{num}} = (\mu_{\cdot s0}, \mu_{\cdot 10}, \mu_{\cdot 0-s0}, \mu_{001}, \mu_{\cdot \cdot 0}, \pi_{1s0}, \pi_{110})$ and the set of estimated nuisances by $\hat{\eta}_{Z,s}^{\text{num}}$. The canonical gradient of $v_Z^{\text{num}}(s)$ is

$$\begin{aligned} \psi_{Z,s}^{\text{num}}(D, W, Z, Y; \eta_{Z,s}^{\text{num}}) &= (\mu_{\cdot s0}(W) - \mu_{\cdot 10}(W))^2 \frac{\mathbb{1}\{D = 1\}}{\Pr(D = 1)} \\ &\quad + 2(\mu_{\cdot s0}(W) - \mu_{\cdot 10}(W))(\ell - \mu_{\cdot 0-s0}(W, Z_s))\pi_{1s0}(W, Z_s) \frac{\mathbb{1}\{D = 0\}}{\Pr(D = 0)} \\ &\quad - 2(\mu_{\cdot s0}(W) - \mu_{\cdot 10}(W))(\ell - \mu_{\cdot \cdot 0}(W, Z))\pi_{110}(W, Z) \frac{\mathbb{1}\{D = 0\}}{\Pr(D = 0)} \\ &\quad + 2(\mu_{\cdot s0}(W) - \mu_{\cdot 10}(W))(\mu_{\cdot 0-s0}(W, Z_s) - \mu_{\cdot s0}(W)) \frac{\mathbb{1}\{D = 1\}}{\Pr(D = 1)} \\ &\quad - 2(\mu_{\cdot s0}(W) - \mu_{\cdot 10}(W))(\mu_{\cdot \cdot 0}(W, Z) - \mu_{\cdot 10}(W)) \frac{\mathbb{1}\{D = 1\}}{\Pr(D = 1)} \\ &\quad - v_Z^{\text{num}}(s). \end{aligned} \quad (28)$$

Lemma G.2. Under Condition F.2, $\hat{v}_Z^{\text{num}}(s)$ satisfies

$$\hat{v}_Z^{\text{num}}(s) - v_Z^{\text{num}}(s) = \mathbb{P}_n \psi_{Z,s}^{\text{num}}(D, W, Z, Y; \eta_{Z,s}^{\text{num}}) + o_p(n^{-1/2}) \quad (29)$$

$$\hat{v}_Z^{\text{den}} - v_Z^{\text{den}} = \mathbb{P}_n \psi_{Z,\emptyset}^{\text{num}}(D, W, Z, Y; \eta_{Z,s}^{\text{num}}) + o_p(n^{-1/2}) \quad (30)$$

Proof. Consider the following decomposition

$$\begin{aligned} &\hat{v}_Z^{\text{num}}(s) - v_Z^{\text{num}}(s) \\ &= (\mathbb{P}_n - \mathbb{P})\psi_{Z,s}^{\text{num}}(D, W, Z, Y; \eta_{Z,s}^{\text{num}}) \end{aligned} \quad (31)$$

$$+ (\mathbb{P}_n - \mathbb{P})(\psi_{Z,s}^{\text{num}}(D, W, Z, Y; \hat{\eta}_{Z,s}^{\text{num}}) - \psi_{Z,s}^{\text{num}}(W, Z, Y; \eta_{Z,s}^{\text{num}})) \quad (32)$$

$$+ \mathbb{P}(\psi_{Z,s}^{\text{num}}(D, W, Z, Y; \hat{\eta}_{Z,s}^{\text{num}}) - \psi_{Z,s}^{\text{num}}(D, W, Z, Y; \eta_{Z,s}^{\text{num}})) \quad (33)$$

We note that (32) converges to a normal distribution per CLT assuming the variance of $\psi_{Z,s}^{\text{num}}$ is finite. The empirical process term (32) is asymptotically negligible, as the nuisance parameters $\eta_{Z,s}^{\text{num}}$ are estimated using a separate training data split from the evaluation data and [25, Lemma 1] states that

$$(\mathbb{P}_n - \mathbb{P})(\psi_{Z,s}^{\text{num}}(D, W, Z, Y; \hat{\eta}_{Z,s}^{\text{num}}) - \psi_{Z,s}^{\text{num}}(D, W, Z, Y; \eta_{Z,s}^{\text{num}})) = o_p(n^{-1/2})$$

as long as estimators for all nuisance parameters are consistent. We now establish that the remainder term (33) is also asymptotically negligible. Integrating with respect to Y , we have that

$$\begin{aligned}
 (33) = & \mathbb{P} 2(\hat{\mu}_{\cdot s0}(W) - \hat{\mu}_{\cdot 10}(W)) \times \left((\mu_{\cdot 0-s0}(Z_s, W) - \hat{\mu}_{\cdot 0-s0}(Z_s, W)) \hat{\pi}_{1s0}(W, Z_s) \frac{\mathbb{1}\{D=0\}}{p(D=0)} \right. \\
 & + (\hat{\mu}_{\cdot 0-s0}(Z_s, W) - \hat{\mu}_{\cdot s0}(W)) \frac{\mathbb{1}\{D=1\}}{p(D=1)} \\
 & - (\mu_{\cdot \cdot 0}(W, Z) - \hat{\mu}_{\cdot \cdot 0}(W, Z)) \hat{\pi}_{110}(W, Z) \frac{\mathbb{1}\{D=0\}}{p(D=0)} \\
 & \left. - (\hat{\mu}_{\cdot \cdot 0}(W, Z) - \hat{\mu}_{\cdot 10}(W)) \frac{\mathbb{1}\{D=1\}}{p(D=1)} \right) \\
 & + \mathbb{P}((\hat{\mu}_{\cdot s0}(W) - \hat{\mu}_{\cdot 10}(W))^2 - (\mu_{\cdot s0}(W) - \mu_{\cdot 10}(W))^2) \frac{\mathbb{1}\{D=1\}}{p(D=1)} \tag{34}
 \end{aligned}$$

$$\begin{aligned}
 & + \mathbb{P}((\hat{\mu}_{\cdot s0}(W) - \hat{\mu}_{\cdot 10}(W))^2 - (\mu_{\cdot s0}(W) - \mu_{\cdot 10}(W))^2) \frac{\mathbb{1}\{D=1\}}{p(D=1)} \tag{35} \\
 = & \mathbb{P} 2(\hat{\mu}_{\cdot s0}(W) - \hat{\mu}_{\cdot 10}(W)) \times \left((\mu_{\cdot 0-s0}(Z_s, W) - \hat{\mu}_{\cdot 0-s0}(Z_s, W)) (\hat{\pi}_{1s0}(W, Z_s) - \pi_{1s0}(W, Z_s)) \frac{\mathbb{1}\{D=0\}}{p(D=0)} \right. \\
 & + (\mu_{\cdot 0-s0}(Z_s, W) - \hat{\mu}_{\cdot 0-s0}(Z_s, W)) \pi_{1s0}(W, Z_s) \frac{\mathbb{1}\{D=0\}}{p(D=0)} \\
 & + (\hat{\mu}_{\cdot 0-s0}(Z_s, W) - \hat{\mu}_{\cdot s0}(W)) \frac{\mathbb{1}\{D=1\}}{p(D=1)} \\
 & - (\mu_{\cdot \cdot 0}(W, Z) - \hat{\mu}_{\cdot \cdot 0}(W, Z)) (\hat{\pi}_{110}(W, Z) - \pi_{110}(W, Z)) \frac{\mathbb{1}\{D=0\}}{p(D=0)} \\
 & - (\mu_{\cdot \cdot 0}(W, Z) - \hat{\mu}_{\cdot \cdot 0}(W, Z)) \pi_{110}(W, Z) \frac{\mathbb{1}\{D=0\}}{p(D=0)} \\
 & \left. - (\hat{\mu}_{\cdot \cdot 0}(W, Z) - \hat{\mu}_{\cdot 10}(W)) \frac{\mathbb{1}\{D=1\}}{p(D=1)} \right) \\
 & + \mathbb{P}((\hat{\mu}_{\cdot s0}(W) - \hat{\mu}_{\cdot 10}(W))^2 - (\mu_{\cdot s0}(W) - \mu_{\cdot 10}(W))^2) \frac{\mathbb{1}\{D=1\}}{p(D=1)} \tag{36}
 \end{aligned}$$

$$+ \mathbb{P}((\hat{\mu}_{\cdot s0}(W) - \hat{\mu}_{\cdot 10}(W))^2 - (\mu_{\cdot s0}(W) - \mu_{\cdot 10}(W))^2) \frac{\mathbb{1}\{D=1\}}{p(D=1)} \tag{37}$$

From convergence conditions in Condition F.2, this simplifies to

$$\begin{aligned}
 (33) = & \mathbb{P} 2(\hat{\mu}_{\cdot s0}(W) - \hat{\mu}_{\cdot 10}(W)) \times \left((\mu_{\cdot 0-s0}(Z_s, W) - \hat{\mu}_{\cdot 0-s0}(Z_s, W)) \pi_{1s0}(W, Z_s) \frac{\mathbb{1}\{D=0\}}{p(D=0)} \right. \\
 & + (\hat{\mu}_{\cdot 0-s0}(Z_s, W) - \hat{\mu}_{\cdot s0}(W)) \frac{\mathbb{1}\{D=1\}}{p(D=1)} \\
 & - (\mu_{\cdot \cdot 0}(W, Z) - \hat{\mu}_{\cdot \cdot 0}(W, Z)) \pi_{110}(W, Z) \frac{\mathbb{1}\{D=0\}}{p(D=0)} \\
 & \left. - (\hat{\mu}_{\cdot \cdot 0}(W, Z) - \hat{\mu}_{\cdot 10}(W)) \frac{\mathbb{1}\{D=1\}}{p(D=1)} \right) \\
 & + \mathbb{P}((\hat{\mu}_{\cdot s0}(W) - \hat{\mu}_{\cdot 10}(W))^2 - (\mu_{\cdot s0}(W) - \mu_{\cdot 10}(W))^2) \frac{\mathbb{1}\{D=1\}}{p(D=1)} \tag{38}
 \end{aligned}$$

$$+ \mathbb{P}((\hat{\mu}_{\cdot s0}(W) - \hat{\mu}_{\cdot 10}(W))^2 - (\mu_{\cdot s0}(W) - \mu_{\cdot 10}(W))^2) \frac{\mathbb{1}\{D=1\}}{p(D=1)} \tag{39}$$

$$+ o_p(n^{-1/2}), \tag{40}$$

Given the true density ratios, we can further simplify the expectations over $D=0$ weighted by the density ratios in the expression above to expectations over $D=1$. By definition of $\mu_{\cdot 0-s0}(Z_s, W)$ in

(18) and $\mu_{\cdot s0}(W)$ in (20) and the definition of $\mu_{\cdot 0}(W, Z)$ and $\mu_{\cdot 10}(W)$ in Section F.1, (33) simplifies to

$$(33) = \mathbb{P}_1 2(\hat{\mu}_{\cdot s0}(W) - \hat{\mu}_{\cdot 10}(W))(\mu_{\cdot s0}(W) - \hat{\mu}_{\cdot s0}(W)) \\ - \mathbb{P}_1 2(\hat{\mu}_{\cdot s0}(W) - \hat{\mu}_{\cdot 10}(W))(\mu_{\cdot 10}(W) - \hat{\mu}_{\cdot 10}(W)) \\ + \mathbb{P}_1 (\hat{\mu}_{\cdot s0}(W) - \hat{\mu}_{\cdot 10}(W))^2 - (\mu_{\cdot s0}(W) - \mu_{\cdot 10}(W))^2 \\ + o_p(n^{-1/2}),$$

which is $o_p(n^{-1/2})$ as long as the convergence conditions in Condition F.2 hold.

As the denominator v_Z^{den} is equal to the numerator $v_Z^{\text{num}}(\emptyset)$, it follows that the one-step estimator for the denominator \hat{v}_Z^{den} is asymptotically linear with influence function $\psi_{Z,\emptyset}^{\text{num}}$. \square

Proof for Theorem F.3. Combining Lemma G.2 and the Delta method [46, Theorem 3.1], the estimator $\hat{v}_Z(s) = \hat{v}_Z^{\text{num}}(s)/\hat{v}_Z^{\text{den}}$ is asymptotically linear

$$\frac{\hat{v}_Z^{\text{num}}(s)}{\hat{v}_Z^{\text{den}}} - \frac{v_Z^{\text{num}}(s)}{v_Z^{\text{den}}} = \mathbb{P}_n \psi_{Z,s}(D, W, Z, Y; \eta_{Z,s}^{\text{num}}, \eta_Z^{\text{den}}) + o_p(n^{-1/2}),$$

with influence function

$$\psi_{Z,s}(D, W, Z, Y; \eta_{Z,s}^{\text{num}}, \eta_Z^{\text{den}}) = \frac{1}{v_Z^{\text{den}}} \psi_{Z,s}^{\text{num}}(D, W, Z, Y; \eta_{Z,s}^{\text{num}}) - \frac{v_Z^{\text{num}}(s)}{(v_Z^{\text{den}})^2} \psi_Z^{\text{den}}(D, W, Z, Y; \eta_Z^{\text{den}}), \quad (41)$$

where $\psi_{Z,s}^{\text{num}}(D, W, Z, Y; \eta_{Z,s}^{\text{num}})$ is defined in (28) and $\psi_Z^{\text{den}}(D, W, Z, Y; \eta_Z^{\text{den}}) = \psi_{Z,\emptyset}^{\text{num}}(D, W, Z, Y; \eta_{Z,\emptyset}^{\text{num}})$.

Accordingly, the estimator asymptotically follows the normal distribution,

$$\sqrt{n}(\hat{v}_Z(s) - v_Z(s)) \rightarrow_d N(0, \text{var}(\psi_{Z,s}(D, W, Z, Y; \eta_{Z,s}^{\text{num}}, \eta_Z^{\text{den}}))) \quad (42)$$

\square

G.3 Value of s -partial conditional outcome shifts

Let the nuisance parameters in $v_{Y,\text{bin}}^{\text{num}}$ be denoted $\eta_{Y,s}^{\text{num}} = (Q_{\text{bin}}, \mu_{\cdot 1}, \mu_{\cdot s}, \pi)$ and its estimate as $\hat{\eta}_{Y,s}^{\text{num}}$.

We represent the one-step corrected estimator for $v_{Y,\text{bin}}^{\text{num}}(s)$ as the V-statistic

$$\hat{v}_{Y,\text{bin}}^{\text{num}}(s) = \mathbb{P}_{1,n} \tilde{\mathbb{P}}_{1,n} (\hat{\mu}_{\cdot 1}(W, Z) - \hat{\mu}_{\cdot s}(W, Z))^2 \quad (43)$$

$$+ 2\mathbb{P}_{1,n} \tilde{\mathbb{P}}_{1,n} (\hat{\mu}_{\cdot 1}(W, Z) - \hat{\mu}_{\cdot s}(W, Z)) (\ell - \mu_{\cdot 1}(W, Z)) \quad (44)$$

$$- 2\mathbb{P}_{1,n} \tilde{\mathbb{P}}_{1,n} \left[(\hat{\mu}_{\cdot 1}(W, Z_s, \tilde{Z}_{-s}) - \hat{\mu}_{\cdot s}(W, Z_s, \tilde{Z}_{-s})) \right. \\ \left. (\ell(W, Z_s, \tilde{Z}_{-s}, Y) - \mu_{\cdot s}(W, Z_s, \tilde{Z}_{-s})) \pi(\tilde{Z}_{-s}, Z_s, W, q_{\text{bin}}(W, Z)) \right] \quad (45)$$

$$= \mathbb{P}_{1,n} \tilde{\mathbb{P}}_{1,n} h(W, Z, Y, \tilde{W}, \tilde{Z}, \tilde{Y}; \hat{\eta}_{Y,s}^{\text{num}}). \quad (46)$$

In more detail, the conditions in Theorem 3.2 are as follows.

Condition G.3. For variable subset s , suppose the following hold

- $\pi(W, Z_s, Z_{-s}, Q_{\text{bin}})$ is bounded
- $\hat{\pi}$ is consistent
- $\mathbb{P}_1 (\hat{\mu}_{\cdot 0} - \mu_{\cdot 0})^2 = o_p(n^{-1/2})$
- $\mathbb{P}_1 (\hat{\mu}_{\cdot 1} - \mu_{\cdot 1})^2 = o_p(n^{-1/2})$
- $\mathbb{P}_1 (\hat{\mu}_{\cdot s} - \mu_{\cdot s})^2 = o_p(n^{-1/2})$

- $\mathbb{P}_1 (\hat{q}_{bin} - q_{bin})^2 = o_p(n^{-1})$
- $\mathbb{P}_1 (\hat{\mu}_{..s} - \mu_{..s}) (\hat{\pi} - \pi) = o_p(n^{-1/2})$.

Lemma G.4. Assuming Condition G.3 holds, $\hat{v}_{Y,bin}^{num}$ is an asymptotically linear estimator for $v_{Y,bin}^{num}$, i.e.

$$\hat{v}_{Y,bin}^{num}(s) - v_{Y,bin}^{num}(s) = \mathbb{P}_{1,n} \psi_{Y,s}^{num}(D, W, Z, Y; \eta_{Y,s}^{num}) + o_p(n^{-1/2}), \quad (47)$$

with influence function

$$\begin{aligned} \psi_{Y,s}^{num}(d, w, z, y; \eta_{Y,s}^{num}) = & (\mu_{..1}(w, z) - \mu_{..s}(w, z))^2 \\ & + 2(\mu_{..1}(w, z) - \mu_{..s}(w, z)) [\ell(w, z, y) - \mu_{..1}(w, z)] \\ & - 2\mathbb{P}_1 \left[(\mu_{..1}(w, z_s, Z_{-s}) - \mu_{..s}(w, z_s, Z_{-s})) \right. \\ & \quad \left. [\ell(w, z_s, Z_{-s}, y)) - \mu_{..s}(w, z_s, Z_{-s})] \pi(Z_{-s}, z_s, w, q_{bin}(w, z)) \right] \\ & - v_{Y,bin}^{num}(s). \end{aligned} \quad (48)$$

Proof. Defining the symmetrized version of h in (46) as $h_{sym}(W, Z, Y, \tilde{W}, \tilde{Z}, \tilde{Y}) = \frac{h(W, Z, Y, \tilde{W}, \tilde{Z}, \tilde{Y}) + h(\tilde{W}, \tilde{Z}, \tilde{Y}, W, Z, Y)}{2}$, we rewrite the estimator as

$$\hat{v}_{Y,bin}^{num}(s) = \mathbb{P}_{1,n} \tilde{\mathbb{P}}_{1,n} h_{sym}(W, Z, Y, \tilde{W}, \tilde{Z}, \tilde{Y}; \hat{\eta}_{Y,s}^{num}).$$

Per Theorem 12.3 in [46], the Hájek projection of $\hat{v}_{Y,bin}^{num}(s)$ is

$$\begin{aligned} \hat{v}_{Y,bin}^{num}(s) &= \sum_{i=1}^n \mathbb{P}_1 \left[\mathbb{P}_{1,n} \tilde{\mathbb{P}}_{1,n} h_{sym}(W, Z, Y, \tilde{W}, \tilde{Z}, \tilde{Y}; \hat{\eta}_{Y,s}^{num}) - \tilde{v}_Y^{num}(s) \mid X_i, Y_i \right] \\ &= \sum_{i=1}^n \mathbb{P}_1 \left[h_{sym}(X_i, Y_i, X^{(2)}, Y^{(2)}; \hat{\eta}_{Y,s}^{num}) - \tilde{v}_Y^{num}(s) \mid X_i, Y_i \right] \\ &= \sum_{i=1}^n h_{sym,1}(X_i, Y_i; \hat{\eta}_{Y,s}^{num}) \end{aligned}$$

where $\tilde{v}_Y^{num}(s) = \mathbb{P}_1 \tilde{\mathbb{P}}_1 h_{sym}(W, Z, Y, \tilde{W}, \tilde{Z}, \tilde{Y}; \hat{\eta}_{Y,s}^{num})$.

Consider the decomposition

$$\begin{aligned} \hat{v}_{Y,bin}^{num}(s) - v_{Y,bin}^{num}(s) &= \mathbb{P}_{1,n} \tilde{\mathbb{P}}_{1,n} h_{sym}(W, Z, Y, \tilde{W}, \tilde{Z}, \tilde{Y}; \hat{\eta}_{Y,s}^{num}) - \mathbb{P}_1 \tilde{\mathbb{P}}_1 h_{sym}(W, Z, Y, \tilde{W}, \tilde{Z}, \tilde{Y}; \eta_{Y,s}^{num}) \\ &= \mathbb{P}_{1,n} \tilde{\mathbb{P}}_{1,n} h_{sym}(W, Z, Y, \tilde{W}, \tilde{Z}, \tilde{Y}; \hat{\eta}_{Y,s}^{num}) - \mathbb{P}_{1,n} [h_{sym,1}(X, Y; \hat{\eta}_{Y,s}^{num}) + \tilde{v}_Y^{num}(s)] \end{aligned} \quad (49)$$

$$+ (\mathbb{P}_{1,n} - \mathbb{P}_1) (h_{sym,1}(X, Y; \hat{\eta}_{Y,s}^{num}) + \tilde{v}_Y^{num}(s) - h_{sym,1}(X, Y) - v_Y^{num}(s)) \quad (50)$$

$$+ (\mathbb{P}_{1,n} - \mathbb{P}_1) (h_{sym,1}(X, Y) + v_Y^{num}(s)) \quad (51)$$

$$+ \mathbb{P}_1 (h_{sym,1}(X, Y; \hat{\eta}_{Y,s}^{num}) + \tilde{v}_Y^{num}(s) - h_{sym,1}(X, Y; \eta_{Y,s}^{num}) - v_Y^{num}(s)). \quad (52)$$

We analyze each term in turn.

Term (49): Suppose $\mathbb{P}_1 h_{sym}^2(W, Z, Y, \tilde{W}, \tilde{Z}, \tilde{Y}; \hat{\eta}_{Y,s}^{num}) < \infty$. Via a straightforward extension of the proof in Theorem 12.3 in van der Vaart [46], one can show that

$$\frac{\text{var} \left(\mathbb{P}_{1,n} \tilde{\mathbb{P}}_{1,n} h_{sym}(W, Z, Y, \tilde{W}, \tilde{Z}, \tilde{Y}; \hat{\eta}_{Y,s}^{num}) \right)}{\text{var} \left(\mathbb{P}_{1,n} h_{sym,1}(W, Z, Y; \hat{\eta}_{Y,s}^{num}) \right)} \rightarrow_p 1.$$

Then by Theorem 11.2 in van der Vaart [46] and Slutsky's lemma, we have

$$\mathbb{P}_{1,n} \tilde{\mathbb{P}}_{1,n} h_{sym} \left(W, Z, Y, \tilde{W}, \tilde{Z}, \tilde{Y}; \hat{\eta}_{Y,s}^{\text{num}} \right) - \mathbb{P}_{1,n} \left[h_{sym,1} \left(W, Z, Y; \hat{\eta}_{Y,s}^{\text{num}} \right) + \bar{v}_Y^{\text{num}}(s) \right] = o_p \left(n^{-1/2} \right).$$

Term (50): We perform sample splitting to estimate the nuisance parameters and calculate the estimator for $\hat{v}_Y^{\text{num}}(s)$. Then by Lemma 1 in Kennedy [25], we have that

$$(\mathbb{P}_{1,n} - \mathbb{P}_1) \left(h_{sym,1} \left(W, Z, Y; \hat{\eta}_{Y,s}^{\text{num}} \right) + \bar{v}_Y^{\text{num}}(s) - h_{sym,1} \left(W, Z, Y; \eta_{Y,s}^{\text{num}} \right) - v_Y^{\text{num}}(s) \right) = o_p(n^{-1/2})$$

as long as the estimators for the nuisance parameters are consistent.

Term (51): This term $(\mathbb{P}_{1,n} - \mathbb{P}_1) \left(h_{sym,1} \left(W, Z, Y; \hat{\eta}_{Y,s}^{\text{num}} \right) + v_Y^{\text{num}}(s) \right) = (\mathbb{P}_{1,n} - \mathbb{P}_1) h_{sym,1} \left(W, Z, Y; \eta_{Y,s}^{\text{num}} \right)$ follows an asymptotic normal distribution per CLT.

Term (52): We will show that this bias term is asymptotically negligible. For notational simplicity, let $\hat{\xi}(W, Z_s, Z_{-s}) = \hat{\mu}_{\cdot 1}(W, Z) - \hat{\mu}_{\cdot s}(W, Z)$.

$$\begin{aligned} & \mathbb{P}_1 \tilde{\mathbb{P}}_1 \left(h_{sym} \left(W, Z, Y, \tilde{W}, \tilde{Z}, \tilde{Y}; \hat{\eta}_{Y,s}^{\text{num}} \right) + \bar{v}_Y^{\text{num}}(s) - h_{sym} \left(W, Z, Y, \tilde{W}, \tilde{Z}, \tilde{Y}; \eta_{Y,s}^{\text{num}} \right) - v_Y^{\text{num}}(s) \right) \\ &= \mathbb{P}_1 \tilde{\mathbb{P}}_1 \left(h \left(W, Z, Y, \tilde{W}, \tilde{Z}, \tilde{Y}; \hat{\eta}_{Y,s}^{\text{num}} \right) - h \left(W, Z, Y, \tilde{W}, \tilde{Z}, \tilde{Y}; \eta_{Y,s}^{\text{num}} \right) \right) \\ &= \mathbb{P}_1 \left(\hat{\mu}_{\cdot 1}(W, Z) - \hat{\mu}_{\cdot s}(W, Z) \right)^2 - \mathbb{P}_1 \left(\mu_{\cdot 1}(W, Z) - \mu_{\cdot s}(W, Z) \right)^2 \\ & \quad + 2\mathbb{P}_1 \left(\hat{\mu}_{\cdot 1}(W, Z) - \hat{\mu}_{\cdot s}(W, Z) \right) \left[\mu_{\cdot 1}(W, Z) - \mu_{\cdot 1}(W, Z) \right] \\ & \quad - 2\mathbb{P}_1 \tilde{\mathbb{P}}_1 \left\{ \left(\hat{\mu}_{\cdot 1}(W, Z_s, \tilde{Z}_{-s}) - \hat{\mu}_{\cdot s}(W, Z_s, \tilde{Z}_{-s}) \right) \left[\ell(W, Z_s, \tilde{Z}_{-s}, Y) - \hat{\mu}_{\cdot s}(W, Z_s, \tilde{Z}_{-s}) \right] \right. \\ & \quad \left. \hat{\pi} \left(\tilde{Z}_{-s}, Z_s, W, \hat{q}_{\text{bin}}(W, Z) \right) \right\} \\ &= \mathbb{P}_1 \left(\hat{\mu}_{\cdot 1}(W, Z) - \hat{\mu}_{\cdot s}(W, Z) \right)^2 - \mathbb{P}_1 \left(\mu_{\cdot 1}(W, Z) - \mu_{\cdot s}(W, Z) \right)^2 \\ & \quad + 2\mathbb{P}_1 \left(\hat{\mu}_{\cdot 1}(W, Z) - \hat{\mu}_{\cdot s}(W, Z) \right) \left[\mu_{\cdot 1}(W, Z) - \hat{\mu}_{\cdot 1}(W, Z) \right] \\ & \quad - 2\mathbb{P}_1 \tilde{\mathbb{P}}_1 \hat{\xi}(W, Z_s, \tilde{Z}_{-s}) \left[\mu_{\cdot s}(W, Z_s, \tilde{Z}_{-s}) - \hat{\mu}_{\cdot s}(W, Z_s, \tilde{Z}_{-s}) \right] \hat{\pi} \left(\tilde{Z}_{-s}, Z_s, W, \hat{q}_{\text{bin}}(W, Z) \right) \\ & \quad - 2\mathbb{P}_1 \tilde{\mathbb{P}}_1 \left\{ \hat{\xi}(W, Z_s, \tilde{Z}_{-s}) \left[\ell(W, Z_s, \tilde{Z}_{-s}, Y) - \hat{\mu}_{\cdot s}(W, Z_s, \tilde{Z}_{-s}) \right] \right. \\ & \quad \left. \left[\hat{\pi} \left(\tilde{Z}_{-s}, Z_s, W, \hat{q}_{\text{bin}}(W, Z) \right) - \hat{\pi} \left(\tilde{Z}_{-s}, Z_s, W, q_{\text{bin}}(W, Z) \right) \right] \right\} \\ &= \mathbb{P}_1 \left(\mu_{\cdot s}(W, Z) - \hat{\mu}_{\cdot s}(W, Z) \right) \left(\hat{\mu}_{\cdot 1}(W, Z) - \hat{\mu}_{\cdot s}(W, Z) + \mu_{\cdot 1}(W, Z) - \mu_{\cdot s}(W, Z) \right) \quad (53) \\ & \quad + \mathbb{P}_1 \left(\hat{\mu}_{\cdot 1}(W, Z) - \mu_{\cdot 1}(W, Z) \right) \left(\mu_{\cdot 1}(W, Z) - \mu_{\cdot s}(W, Z) - \hat{\mu}_{\cdot 1}(W, Z) + \hat{\mu}_{\cdot s}(W, Z) \right) \quad (54) \\ & \quad - 2\mathbb{P}_1 \tilde{\mathbb{P}}_1 \hat{\xi}(W, Z_s, \tilde{Z}_{-s}) \left[\mu_{\cdot s}(W, Z_s, \tilde{Z}_{-s}) - \hat{\mu}_{\cdot s}(W, Z_s, \tilde{Z}_{-s}) \right] \hat{\pi} \left(\tilde{Z}_{-s}, Z_s, W, \hat{q}_{\text{bin}}(W, Z) \right) \quad (55) \\ & \quad - 2\mathbb{P}_1 \tilde{\mathbb{P}}_1 \left\{ \hat{\xi}(W, Z_s, \tilde{Z}_{-s}) \left[\ell(W, Z_s, \tilde{Z}_{-s}, Y) - \hat{\mu}_{\cdot s}(W, Z_s, \tilde{Z}_{-s}) \right] \right. \\ & \quad \left. \left[\hat{\pi} \left(\tilde{Z}_{-s}, Z_s, W, \hat{q}_{\text{bin}}(W, Z) \right) - \hat{\pi} \left(\tilde{Z}_{-s}, Z_s, W, q_{\text{bin}}(W, Z) \right) \right] \right\}. \quad (56) \end{aligned}$$

Note that (56) is $o_p(n^{-1/2})$ under the assumed convergence rates for \hat{q}_{bin} . In addition, (54) is $o_p(n^{-1/2})$, under the assumed convergence rates for $\hat{\mu}_{\cdot 1}$ and $\hat{\mu}_{\cdot s}$.

Analyzing the remaining summands (53) + (55), we note that it simplifies as follows:

$$\begin{aligned}
& \mathbb{P}_1 (\mu_{..s}(X) - \hat{\mu}_{..s}(X)) (\hat{\mu}_{..1}(X) - \hat{\mu}_{..s}(X) + \mu_{..1}(X) - \mu_{..s}(X)) \\
& - 2\mathbb{P}_1 \tilde{\mathbb{P}}_1 \left\{ \hat{\xi}(W, Z_s, \tilde{Z}_{-s}) \left[\mu_{..s}(W, Z_s, \tilde{Z}_{-s}) - \hat{\mu}_{..s}(W, Z_s, \tilde{Z}_{-s}) \right] \right. \\
& \quad \left. \left(\hat{\pi} \left(\tilde{Z}_{-s}, Z_s, W, q_{\text{bin}}(W, Z) \right) - \pi \left(\tilde{Z}_{-s}, Z_s, W, q_{\text{bin}}(W, Z) \right) \right) \right\} \\
& - 2\mathbb{P}_1 \tilde{\mathbb{P}}_1 \hat{\xi}(W, Z_s, \tilde{Z}_{-s}) \left[\mu_{..s}(W, Z_s, \tilde{Z}_{-s}) - \hat{\mu}_{..s}(W, Z_s, \tilde{Z}_{-s}) \right] \pi \left(\tilde{Z}_{-s}, Z_s, W, q_{\text{bin}}(W, Z) \right) \\
& = \mathbb{P}_1 (\mu_{..s}(X) - \hat{\mu}_{..s}(X)) (\mu_{..1}(X) - \hat{\mu}_{..1}(X) - \mu_{..s}(X) + \hat{\mu}_{..s}(X)) \\
& - 2\mathbb{P}_1 \tilde{\mathbb{P}}_1 \left\{ \hat{\xi}(W, Z_s, \tilde{Z}_{-s}) \left[\mu_{..s}(W, Z_s, \tilde{Z}_{-s}) - \hat{\mu}_{..s}(W, Z_s, \tilde{Z}_{-s}) \right] \right. \\
& \quad \left. \left[\hat{\pi} \left(\tilde{Z}_{-s}, Z_s, W, q_{\text{bin}}(W, Z) \right) - \pi \left(\tilde{Z}_{-s}, Z_s, W, q_{\text{bin}}(W, Z) \right) \right] \right\},
\end{aligned}$$

which is $o_p(n^{-1/2})$, under the assumed convergence rates for $\hat{\mu}_{..s}$, $\hat{\mu}_{..1}$, and $\hat{\pi}$. \square

Condition G.5 (Convergence conditions for \hat{v}_Y^{den}). *Suppose the following holds*

- $\mathbb{P}_1(\mu_{..1} - \mu_{..0} - (\hat{\mu}_{..1} - \hat{\mu}_{..0}))^2 = o_p(n^{-1/2})$
- $\mathbb{P}_0(\mu_{..0} - \hat{\mu}_{..0})(\pi_{110} - \hat{\pi}_{110}) = o_p(n^{-1/2})$
- $\mathbb{P}_0(\mu_{..1} - \mu_{..0})^2$ is bounded
- (Positivity) $p(w, z|d = 0) > 0$ almost everywhere, such that the density ratios $\pi_{110}(w, z)$ are well-defined and bounded.

Let the nuisance parameters in the one-step estimator v_Y^{den} be denoted by $\eta_Y^{\text{den}} = (\mu_{..0}, \mu_{..1}, \pi_{110})$ and the set of estimated nuisances by $\hat{\eta}_Y^{\text{den}}$.

Lemma G.6. *Assuming Condition G.5 holds, then \hat{v}_Y^{den} is an asymptotically linear estimator for v_Y^{den} , i.e.*

$$\hat{v}_Y^{\text{den}} - v_Y^{\text{den}} = \mathbb{P}_n \psi_Y^{\text{den}}(D, W, Z, Y; \eta_Y^{\text{den}}) + o_p(n^{-1/2})$$

with influence function

$$\psi_Y^{\text{den}}(D, W, Z, Y; \eta_Y^{\text{den}}) = (\mu_{..1}(W, Z) - \mu_{..0}(W, Z))^2 \frac{\mathbb{1}\{D = 1\}}{p(D = 1)} \quad (57)$$

$$+ 2(\mu_{..1}(W, Z) - \mu_{..0}(W, Z))(\ell - \mu_{..1}(W, Z)) \frac{\mathbb{1}\{D = 1\}}{p(D = 1)} \quad (58)$$

$$- 2(\mu_{..1}(W, Z) - \mu_{..0}(W, Z))(\ell - \mu_{..0}(W, Z))\pi_{110}(W, Z) \frac{\mathbb{1}\{D = 0\}}{p(D = 0)} \quad (59)$$

$$- v_Y^{\text{den}}. \quad (60)$$

Proof. Consider the following decomposition of bias in the one-step corrected estimate

$$\begin{aligned} & \hat{v}_Y^{\text{den}} - v_Y^{\text{den}} \\ & = (\mathbb{P}_n - \mathbb{P})\psi_Y^{\text{den}}(D, W, Z, Y; \eta_Y^{\text{den}}) \end{aligned} \quad (61)$$

$$+ (\mathbb{P}_n - \mathbb{P})(\psi_Y^{\text{den}}(D, W, Z, Y; \hat{\eta}_Y^{\text{den}}) - \psi_Y^{\text{den}}(D, W, Z, Y; \eta_Y^{\text{den}})) \quad (62)$$

$$+ \mathbb{P}(\psi_Y^{\text{den}}(D, W, Z, Y; \hat{\eta}_Y^{\text{den}}) - \psi_Y^{\text{den}}(D, W, Z, Y; \eta_Y^{\text{den}})) \quad (63)$$

We observe that (61) converges to a normal distribution per CLT assuming that the variance of ψ_Y^{den} is finite. The empirical process term (62) is asymptotically negligible since the nuisance parameters η_Y^{den} are evaluated on an separate evaluation data split from the training data used for estimation.

In addition assuming that the estimators for the nuisance parameters are consistent, Kennedy [25, Lemma 1] states that

$$(\mathbb{P}_n - \mathbb{P})(\psi_Y^{\text{den}}(D, W, Z, Y; \hat{\eta}_Y^{\text{den}}) - \psi_Y^{\text{den}}(D, W, Z, Y; \eta_Y^{\text{den}})) = o_p(n^{-1/2}).$$

We now show that the remainder term (63) is also asymptotically negligible. Substituting the influence function and integrating with respect to Y , (63) becomes

$$(63) = \mathbb{P}(\hat{\mu}_{..1}(W, Z) - \hat{\mu}_{..0}(W, Z) - (\mu_{..1}(W, Z) - \mu_{..0}(W, Z)))^2 \frac{\mathbb{1}(D=1)}{p(D=1)} \quad (64)$$

$$+ 2\mathbb{P}(\hat{\mu}_{..1}(W, Z) - \hat{\mu}_{..0}(W, Z) - (\mu_{..1}(W, Z) - \mu_{..0}(W, Z))) (\mu_{..1}(W, Z) - \mu_{..0}(W, Z)) \frac{\mathbb{1}(D=1)}{p(D=1)} \quad (65)$$

$$+ 2\mathbb{P}(\hat{\mu}_{..1}(W, Z) - \hat{\mu}_{..0}(W, Z)) (\mu_{..1}(W, Z) - \hat{\mu}_{..1}(W, Z)) \frac{\mathbb{1}\{D=1\}}{p(D=1)} \quad (66)$$

$$- 2\mathbb{P}(\hat{\mu}_{..1}(W, Z) - \hat{\mu}_{..0}(W, Z)) (\mu_{..0}(W, Z) - \hat{\mu}_{..0}(W, Z)) \hat{\pi}_{110}(W, Z) \frac{\mathbb{1}\{D=0\}}{p(D=0)} \quad (67)$$

$$= \mathbb{P}(\hat{\mu}_{..1}(W, Z) - \hat{\mu}_{..0}(W, Z) - (\mu_{..1}(W, Z) - \mu_{..0}(W, Z)))^2 \frac{\mathbb{1}(D=1)}{p(D=1)} \quad (68)$$

$$+ 2\mathbb{P}(\mu_{..0}(W, Z) - \hat{\mu}_{..0}(W, Z)) (\mu_{..1}(W, Z) - \mu_{..0}(W, Z)) \frac{\mathbb{1}(D=1)}{p(D=1)} \quad (69)$$

$$- 2\mathbb{P}(\hat{\mu}_{..1}(W, Z) - \hat{\mu}_{..0}(W, Z)) (\mu_{..0}(W, Z) - \hat{\mu}_{..0}(W, Z)) (\hat{\pi}_{110}(W, Z) - \pi_{110}(W, Z)) \frac{\mathbb{1}\{D=0\}}{p(D=1)} \quad (70)$$

$$- 2\mathbb{P}(\hat{\mu}_{..1}(W, Z) - \hat{\mu}_{..0}(W, Z)) (\mu_{..0}(W, Z) - \hat{\mu}_{..0}(W, Z)) \pi_{110}(W, Z) \frac{\mathbb{1}\{D=0\}}{p(D=0)} \quad (71)$$

$$= \mathbb{P}(\hat{\mu}_{..1}(W, Z) - \hat{\mu}_{..0}(W, Z) - (\mu_{..1}(W, Z) - \mu_{..0}(W, Z)))^2 \frac{\mathbb{1}(D=1)}{p(D=1)} \quad (72)$$

$$- 2\mathbb{P}(\hat{\mu}_{..1}(W, Z) - \hat{\mu}_{..0}(W, Z)) (\mu_{..0}(W, Z) - \hat{\mu}_{..0}(W, Z)) (\hat{\pi}_{110}(W, Z) - \pi_{110}(W, Z)) \frac{\mathbb{1}\{D=0\}}{p(D=0)} \quad (73)$$

Thus the remainder term is $o_p(n^{-1/2})$ if Condition G.5 holds. \square

Proof for Theorem 3.2. Combining Lemmas G.4, G.6, and the Delta method [46, Theorem 3.1], the estimator $\hat{v}_{Y,\text{bin}}(s) = \hat{v}_{Y,\text{bin}}^{\text{num}}(s)/\hat{v}_Y^{\text{den}}$ is asymptotically linear

$$\frac{\hat{v}_{Y,\text{bin}}^{\text{num}}(s)}{\hat{v}_Y^{\text{den}}} - \frac{v_{Y,\text{bin}}^{\text{num}}(s)}{v_Y^{\text{den}}} = \mathbb{P}_n \psi_{Y,\text{bin},s}(D, W, Z, Y; \eta_{Y,s}^{\text{num}}, \eta_Y^{\text{den}}) + o_p(n^{-1/2}),$$

with influence function

$$\psi_{Y,\text{bin},s}(D, W, Z, Y; \eta_{Y,s}^{\text{num}}, \eta_Y^{\text{den}}) = \frac{1}{v_Y^{\text{den}}} \psi_{Y,s}^{\text{num}}(D, W, Z, Y; \eta_{Y,s}^{\text{num}}) - \frac{v_{Y,\text{bin}}^{\text{num}}(s)}{(v_Y^{\text{den}})^2} \psi_Y^{\text{den}}(D, W, Z, Y; \eta_Y^{\text{den}}), \quad (74)$$

where $\psi_{Y,s}^{\text{num}}$ and ψ_Y^{den} are defined in (48) and (60).

Accordingly, the estimator follows a normal distribution asymptotically,

$$\sqrt{n}(\hat{v}_Y(s) - v_Y(s)) \rightarrow_d N(0, \text{var}(\psi_{Y,\text{bin},s}(D, W, Z, Y; \eta_{Y,s}^{\text{num}}, \eta_Y^{\text{den}}))) \quad (75)$$

\square

Remark on super-fast convergence of \hat{q}_{bin} . One of the conditions in Condition G.3 states that the \hat{q}_{bin} converges at $o_p(n^{-1})$ rate. While this seems restrictive, binned risk converges exponentially under suitable margin conditions presented in Audibert and Tsybakov [2]. In particular, consider the following margin condition which is a relaxation of Condition 3.1.

Condition G.7. For all bin edges b except $b \in \{0, 1\}$, the set $\Xi_\epsilon = \{x : |q(x) - b| \leq \epsilon\}$ is measure zero for some $\epsilon > 0$.

Suppose the function q belongs to the Hölder class $\Sigma(\beta, L, \mathbb{R}^d)$ for positive integer β and $L > 0$ (see definition in Audibert and Tsybakov [2]), the marginal law of X satisfies the strong density assumption, and the margin condition G.7 is satisfied. Then the rate of convergence of \hat{q}_{bin} is exponential, i.e.

$$\mathbb{E}(\hat{q}_{\text{bin}}(X) - q_{\text{bin}}(X))^2 \leq C_1 \exp(-C_2 n) \quad (76)$$

for constants $C_1, C_2 > 0$ that do not depend on n .

Remark on value of s -partial conditional outcome shift. Unlike the case of s -partial conditional covariate shift, note that $v_Y(\emptyset)$ may be non-zero when the risk in the target domain is a recalibration (i.e. temperature-scaling) of the risk in the source domain [34, 19]. For instance, there may be general environmental factors such that readmission risks in the target domain are uniformly lower.

H Implementation details

Here we describe how the nuisance parameters can be estimated in each of the decompositions. In general, density ratio models can be estimated via a standard reduction to a classification problem where a probabilistic classifier is trained to discriminate between source and target domains [43].

Note on computation time. Shapley value computation can be parallelized over the subsets. For high-dimensional tabular data, grouping together variables can further reduce computation time (and increase interpretability).

H.1 Aggregate decompositions

Density ratio models. Using direct importance estimation [43], density ratio models $\pi_{100}(W)$ and $\pi_{110}(W, Z)$ can be estimated by fitting classifiers on the combined source and target data to predict $D = 0$ or 1 from features W and (W, Z) , respectively.

Outcome models. The outcome models $\mu_{..0}(W)$ and $\mu_{..0}(W, Z)$ can be fit in a number of ways. One option is to estimate the conditional distribution of the outcome (i.e. $p_0(Y|W)$ or $p_0(Y|W, Z)$) using binary classifiers, from which one can obtain an estimate of the conditional expectation of the loss. Alternatively, one can estimate the conditional expectations of the loss directly by fitting regression models.

H.2 Detailed decomposition for s -partial outcome shift

Density ratio models. The density ratio $\pi(W, Z_s, Z_{-s}, Q) = p_1(Z_{-s}|W, Z_s, q(W, Z) = Q)/p_1(Z_{-s})$ in (6) can be estimated as follows. Create a second (“phantom”) dataset of the target domain in which Z_{-s} is independent of Z_s by permuting the original Z_{-s} in the target domain. Compute q_{bin} for all observations in the original dataset and the permuted dataset. Concatenate the original dataset from the target domain with the permuted dataset. Train a classifier to predict if an observation is from the original versus the permuted dataset.

Outcome models. The outcome models $\mu_{..1}$ and $\mu_{..s}(W, Z)$ can be similarly fit by estimating the conditional distributions $p_0(Y|W, Z)$ and $p_s(Y|W, Z, q_{\text{bin}}(W, Z))$ on the target domain, and then taking expectation of the loss.

Computing U-statistics. Calculating the double average $\mathbb{P}_{1,n} \tilde{\mathbb{P}}_{1,n}$ in the estimator requires evaluating all n^2 pairs of data points in target domain. This can be computationally expensive, so a good approximation is to subsample the inner average. We take 2000 subsamples. We did not see large changes in the bias of the estimates compared to calculating the exact U-statistics.

H.3 Detailed decomposition for s -partial conditional outcome shift

Density ratio models. The ratio $\pi_{1s0}(W, Z_s) = p_1(W, Z_s)/p_0(W, Z_s)$ can be similarly fit using direct importance estimation.

Outcome models. We require the following models.

- $\mu_{\cdot 0-s0}(z_s, w) = \mathbb{E}_{\cdot 00}[\ell|z_s, w]$, defined in (18), can be estimated by regressing loss against w, z_s on the source domain.
- $\mu_{\cdot 10}(w) = \mathbb{E}_{\cdot 10}[\ell|w]$, defined in (19), can be estimated by regressing $\mu_{\cdot 0}(w, z)$ against w in the target domain.
- $\mu_{\cdot s0}(w) = \mathbb{E}_{\cdot s0}[\ell|z_s, w]$, defined in (20), can be estimated by regressing $\mu_{\cdot 0-s0}(z_s, w)$ against w in the target domain.

For all models, we use cross-validation to select among model types and hyperparameters. Model selection is important so that the convergence rate conditions for the asymptotic normality results are met.

I Simulation details

Data generation: We generate synthetic data under two settings. For the coverage checks in Section 4.1, all features are sampled independently from a multivariate normal distribution. The mean of the (W, Z) in the source and target domains are $(0, 2, 0.7, 3)$ and $(0, 0, 0, 0)$, respectively. The outcome in the source and target domains are simulated from a logistic regression model with coefficients $(0.3, 1, 0.5, 1)$ and $(0.3, 0.1, 0.5, 1.4)$.

In the second setting for baseline comparisons in Figure 2b(ii), each feature in $W \in \mathbb{R}$ and $Z \in \mathbb{R}^5$ is sampled independently from the rest from a uniform distribution over $[-1, 1]$. The binary outcome Y is sampled from a logistic regression model with coefficients $(0.2, 0.4, 2, 0.25, 0.1, 0.1)$ in source and $(0.2, -0.4, 0.8, 0.1, 0.1, 0.1)$ in target.

In both the settings, we analyze performance gap of logistic regression models fit on a held-out source dataset.

Sample-splitting: We fit all models on 80% of the data points from both source and target datasets which is the Tr partition, and keep the remaining 20% for computing the estimators which is the Ev partition.

Model types: We use `scikit-learn` implementations for all models [33]. We use 3-fold cross validation to select models. For density models, we fit random forest classifiers and logistic regression models with polynomial features of degree 3. We clip the predicted probabilities from the density model for π at 10^{-6} to avoid very large density weights. Depending on whether the target outcome in outcome models is binary or real-valued, we fit random forest classifiers or regressors, and logistic regression or linear regression models with ridge penalty. Specific hyperparameter ranges for the grid search are provided in the code.

Computing time and resources: Computation for the VI estimates can be quite fast, as Shapley value computation can be parallelized over the subsets and the number of unique variable subsets sampled in the Shapley value approximation is often quite small. For instance, for the ACS Public Coverage case study with 34 features, the unique subsets is 131 even when the number of sampled subsets is 3000, and it takes around 160 seconds to estimate the value of a single variable subset. All experiments are run on a 2.60 GHz processor with 8 CPU cores.

J Data analysis details

Synthetic. We describe accuracy of the ML algorithm after it is retrained with the top k features and predictions from the original model (Table 3). Proposed method results in the revised model with highest gain in accuracy and AUC. Figure 5 shows the aggregate and detailed decompositions for the simulation setup in Section 4.1. Figure 6 shows the coverage rates of 90% CIs for the aggregate decompositions.

Hospital readmission. Using data from the electronic health records of a large safety-net hospital in the US, we analyzed the transferability of performance measures of a Gradient Boosted Tree (GBT) trained to predict 30-day readmission risk for the general patient population (source) but applied to patients diagnosed with heart failure (target). Each of the source and target datasets have 3750 observations for analyzing the performance gap. The GBT is trained on a held-out sample of 18,873 points from the general population. Features include 4 demographic variables (W) and 16 diagnosis

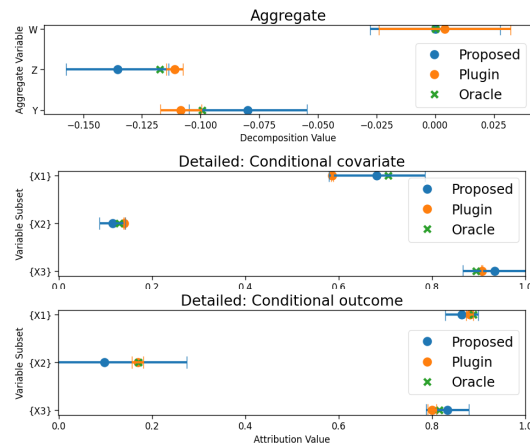


Figure 5: Sample estimates and CIs for simulation from Section 4.1. Proposed is debiased ML estimator for HDPD.

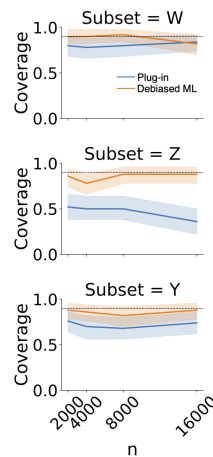


Figure 6: Coverage rates of 90% CIs for the aggregate decomposition terms for the simulation setup in Section 4.1.

Table 3: Accuracy and AUC for the revised model with respect to the top $k = \{1, 2, 3\}$ variables identified by different methods. Proposed method leads to a model with highest improvement in performance, thus, reducing the performance gap. We compare against two additional baselines that are outperformed by the proposed method: retraining a model on the target data with all features (AUC 0.89, Acc 0.84) and retraining on a weighted source-target data where loss for each point in source and target is weighted by a tuned parameter α and $1 - \alpha$ respectively (AUC 0.89, Acc 0.85).

Method	AUC-1	Acc-1	AUC-2	Acc-2	AUC-3	Acc-3
ParametricChange	0.87	0.82	0.87	0.82	0.91	0.86
ParametricAcc	0.87	0.82	0.87	0.82	0.91	0.86
RandomForestAcc	0.87	0.82	0.87	0.82	0.91	0.86
OaxacaBlinder	0.87	0.82	0.87	0.82	0.87	0.82
HDPD (proposed)	0.91	0.86	0.91	0.86	0.91	0.86

Table 4: Difference in AUCs between the revised insurance prediction model with respect to the top k variables identified by the proposed versus RandomForestAcc procedures (Diff AUC- k = Proposed – RandomForestAcc). 95% CIs are shown.

k	Diff AUC- k	Lower CI	Upper CI
1	0.000	0.000	0.000
2	0.006	0.001	0.010
3	-0.002	-0.007	0.002
4	0.004	-0.002	0.008
5	-0.001	-0.006	0.003
6	-0.002	-0.008	0.003
7	0.007	0.002	0.011
8	0.006	0.001	0.010

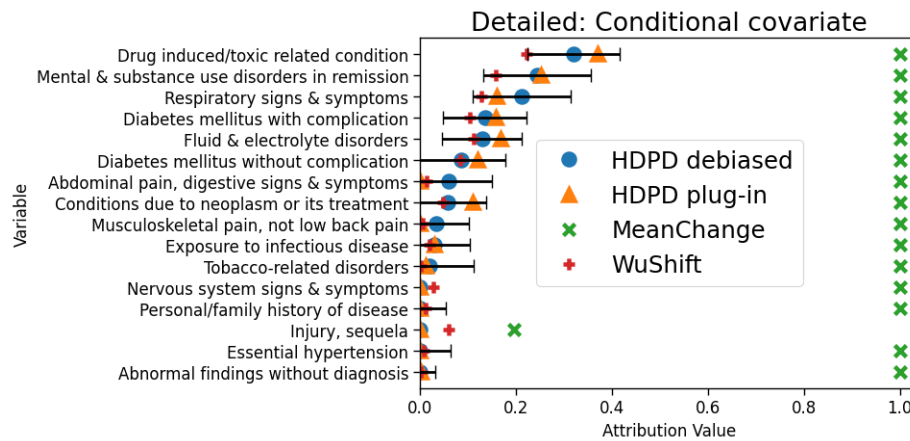


Figure 7: Detailed decompositions for the performance gap of a model predicting hospital readmission in HF population. Plot shows values for the full set of 16 variables.

codes (Z). While training, we reweigh samples by class weights to address class imbalance. Figure 7 shows the detailed decomposition of conditional covariate shift for the dataset.

ACS Public Coverage. We extract data from the American Community Survey (ACS) to predict whether a person has public health insurance. The data only contains persons of age less than 65 and having an income of less than \$30,000. We analyze a neural network (MLP) trained on data from Nebraska (source) to data from Louisiana (target) given 3000 and 6000 observations from the source and target domains, respectively. Another 3300 from source for training the model. Figure 8 shows the detailed decomposition of conditional outcome shift for the dataset. Table 4 shows the difference in AUCs for the revised models based on top features from the proposed method versus RandomForestAcc method.

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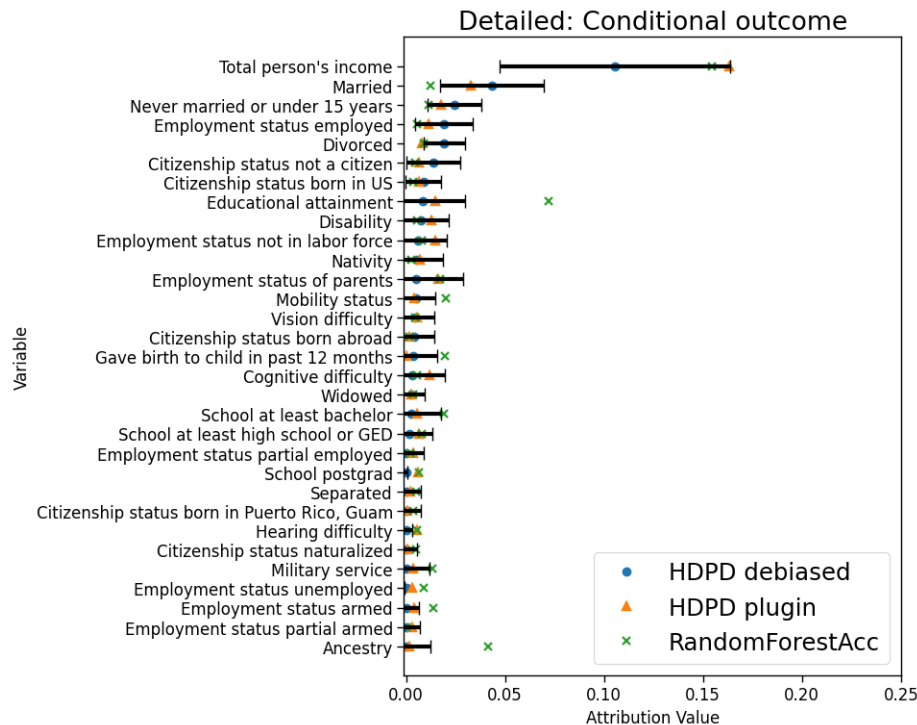


Figure 8: Detailed decompositions for the performance gap of a model predicting insurance coverage prediction across two US states (NE → LA). Plot shows values for the full set of 31 covariates.

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