A novel decomposition to explain heterogeneity in observational and randomized studies of causality

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Abstract

This paper introduces a novel decomposition framework to explain heterogeneity in causal effects observed across different studies, considering both observational and randomized settings. We present a formal decomposition of between-study heterogeneity, identifying sources of variability in treatment effects across studies. The proposed methodology allows for robust estimation of causal parameters under various assumptions, addressing differences in pre-treatment covariate distributions, mediating variables, and the outcome mechanism. Our approach is validated through a simulation study and applied to data from the Moving to Opportunity (MTO) study, demonstrating its practical relevance. This work contributes to the broader understanding of causal inference in multi-study environments, with potential applications in evidence synthesis and policy-making.

1 Introduction

Across different research fields, data fusion is increasingly being used to combine information from multiple databases to improve statistical information and power. Although the ideas behind data fusion are not new, the first formal frameworks for this concept have just been recently developed. Bareinboim and Pearl (2016), for instance, formalized the conditions under which causal findings from a source population could be reasonably extrapolated to another target population. This framework serves as a theoretical base for many data fusion methods such as covariate shift (Uehara et al., 2020), selection bias adjustment (Ferri-García and Rueda, 2020), external validity (Stuart et al., 2011), randomized and observational data combination (Colnet et al., 2024), transported indirect effects (Rudolph et al., 2021), causally interpretable evidence synthesis and

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heterogeneity assessment (Dahabreh et al., 2020; Vo et al., 2019). While most of these methods focus on a setting with two populations, one source and one target, many recent works have also shown the identifiability of a transported or fused causal parameter when multiple data sources are available. See for instance Bareinboim and Pearl (2016), Dahabreh et al. (2023), Li and Luedtke (2023), Sobel et al. (2017), Vo et al. (2019), and Vo et al. (2021).

When there are differences in the effects of the same nominal intervention on the same outcome across studies, there are at least three potential sources of these differences. First, the distribution of pre-treatment covariates that modify the effect of the intervention on the outcome may be different in the different study sites. If this is the only source, the “S-ignorability” assumption (namely, that the counterfactual outcomes are independent of study selection, conditional on observed covariates) enables a simple reweighting approach to understand the difference or “transport” effects to a new population, as in Hotz et al. (2005); Cole and Stuart (2010) and Tipton et al. (2014). However, post-treatment variables (such as mediators) may also drive heterogeneity, and the “S-admissibility” assumption (namely, that for each treatment level, the counterfactual outcome is conditionally independent of the counterfactual study selection, conditional on the counterfactual covariate values) given in Bareinboim and Pearl (2016) provides an alternative way to transport treatment effects in some cases where S-ignorability fails due to post-treatment covariates. (See Pearl (2015) for a helpful discussion about the distinction between these two assumptions.) Additionally, Rudolph et al. (2017) and Rudolph et al. (2021) give robust methods to estimate effect discrepancies due to differences in (possibly sequential) mediating variables. However, pre- and post-treatment variables might not explain all differences in effect estimates across study sites, and the remainder might be attributed to inconsistencies inherent to the study design or implementation (see Sobel et al. (2017); Rudolph et al. (2018a), and Vo et al. (2019)). We are not aware of any non-parametric methods designed to jointly assess heterogeneity arising from pre-treatment covariates, mediating variables, and other causes.

In this paper, we contribute to the data fusion literature by providing a nonparametric method to explain the sources of effect heterogeneity across datasets. In particular, we combine individual-level data from the different datasets under consideration and decompose the effect heterogeneity across datasets into the various contributing sources. Such differences might be due to differences in covariate distributions, differences in mediator distributions, or pure (unmediated) effect modification. Rather than assuming away any of these differences, we propose an approach to estimate the extent to which each contributes to effect heterogeneity through a decomposition of the average treatment effect. Such an analysis is scientifically valuable, especially in the context of multi-site studies where differences in effects across sites are often observed but not fully understood. For example, multiple trials for sepsis treatment with hydrocortisone, as illustrated by the patient-level meta-analysis in Pirracchio et al. (2023), have found different effects of corticosteroids on mortality rates in patients with septic shock, but the sources of these variations remain unclear. Understanding these variations would help determine what factors determine mortality in patients with septic shock when treated with corticosteroids, and, by extension, also what kinds of patients with septic shock should receive corticosteroids. This project is similar in nature to the work of Jin et al. (2023), but those authors were focused on ordinary least squares estimates in randomized trials, restrictions that we do not assume here.

The current paper is structured as follows. In Section 2, we explain our setup and notation and introduce the Moving to Opportunity (MTO) study (Kling et al., 2007; Sanbonmatsu et al., 2011), which provides our motivating example. We then formalize our heterogeneity decompo-
osition mathematically in Section 3. In Section 4, we provide sufficient assumptions for the identification of the components of the decomposition, and in Section 5, we explain how they can be robustly estimated. Section 6 tests the accuracy of the procedure through a simulation study, and Section 7 extends the approach to consider more than two studies at a time. Finally, Section 8 is an analysis of the MTO trial, and Section 9 concludes.

2  Types of effect heterogeneity

To introduce our framework, we will first define some notation. Let $A$ denote a binary treatment of interest, let $W$ denote measured pre-treatment covariates, let $S \in \{0, 1\}$ denote the study source (i.e., which of multiple studies or sites the observation arose from), and let $Y$ denote an outcome of interest. (We first assume only two studies are present and will then generalize our methods to multiple studies.) In addition, we assume that we have measured intermediate variables $M$ as described below. We will assume that the data are generated by the structural causal model (SCM) (Pearl, 2000) below, where some of our results will require that we have measured the intermediate variables $M$, and some others will not. In many applications, it will be the case that both $S = 0$ and $S = 1$ denote randomized studies for which we wish to explain their conflicting results. However, the methodology is developed in general and can be used if either or both $S = 0$ and $S = 1$ are observational studies, under additional identifiability assumptions.

While the causal ordering of $A \rightarrow M \rightarrow Y$ is clear, and $W, S$ are assumed to precede $A$, the ordering of $W$ (baseline covariates) and $S$ (study membership) might be ambiguous. If studies have enrollment criteria that are functions of covariates, then it seems preferable to say that $W$ precedes $S$, whereas if $S$ corresponds to an environment that gives rise to the covariate values in that environment (e.g., a state where particular legislation is rolled out), it may make sense to say that $S$ precedes $W$. In this paper, we will assume that $W$ precedes $S$. The import of this is that when we consider counterfactual values of $S$ (i.e., what would happen to an individual if they were subject to the conditions of a different study), we consider that individual’s same baseline covariate values in the counterfactual. (If $S$ preceded $W$, then switching studies would change the covariate values.) However, the ordering is not crucial if one wants only to consider expressions conditional on $S$ and $W$, rather than counterfactuals. In this paper, we will take the counterfactual point of view.

A structural causal model (SCM) can be defined as a tuple $(\mathbf{U}, \mathbf{V}, \mathbf{F}, \mathbf{P})$ (Bareinboim et al., 2022), where $\mathbf{U}$ are a set of unobserved variables outside the model, $\mathbf{V}$ are the set of variables determined by other variables in the model, $\mathbf{F}$ are a set of (deterministic) functions describing how the elements of $\mathbf{V}$ are determined by previous variables, and $\mathbf{P}$ is a probability distribution over the domain of $\mathbf{U}$. Our specific SCM can be written as follows, where $\mathbf{V} = (W, S, A, M, Y)$.

$$
\begin{align*}
W &= f_W(U_W) \\
S &= f_S(W, U_S) \\
A &= f_A(W, S, U_A) \\
M &= f_M(A, W, S, U_M) \\
Y &= f_Y(M, A, W, S, U_Y).
\end{align*}
$$

(1)

In principle, we leave the distribution $\mathbf{P}$ unrestricted, but restrictions to it will be implied by our
identification assumptions in Section 4.

2.1 Remarks on notation and interpretation

Our definitions below refer to counterfactual values implied by the SCM. For example, $Y(A = a, M = m, S = s)$ denotes the random variable obtained by solving for $Y$ in the SCM when $A, M, S$ were set to the values $a, m, s$, respectively. Where the meaning is clear, we may abbreviate this as $Y(a, m, s)$. (To make this concrete, we note that $Y_i(a, m, s)$ is the final output of the SCM for $W = W_i, S = s, A = a, M = m, (U_W, U_S, U_A, U_M, U_Y) = (U_W, U_S, U_A, U_M, U_Y)_i$.) We will also have occasion to write $M(a, s)$ with similar meaning. In an abuse of notation, arguments may be omitted, so that, for example, $Y(A = a) = Y(a)$ denotes the outcome with the variable $A$ assigned (possibly counterfactually) to $a$ but other variables samples from the assumed SCM. In a similar manner, conditional probability expressions will rely on context and symbols, so that, for example, $P(M = m | w, s, a)$ denotes the probability measure of the random variable $M$ at the point $m$ conditional on the events $W = w, S = s, A = a$. Similarly, $dP(M = m | w, s, a)$ is used for integration with respect to this measure. Furthermore, counterfactuals are not to be interpreted with an interventionist or agential view as variables observed under a hypothetical action (Woodward, 2003; Díaz, 2024). Rather, counterfactuals are to be interpreted merely as mathematical functions that encode relationships between variables. For instance, considering an action whereby a study is set to $S = s$ makes little logical and practical sense, but we can use counterfactuals of the type $Y(a, m, s)$ to study how structural functions such as $f_Y(m, a, w, s, u_Y)$ vary as $a, m,$ and $s$ vary.

2.2 Heterogeneity definitions

To formally isolate sources of heterogeneity, we will start by identifying mathematically when different kinds of heterogeneity can be said to be absent.

In the following definitions, suppose as above that $W$ are pre-treatment covariates, $A$ is the exposure of interest, $S$ is study identity, $Y$ is the outcome of interest, and $M$ is a mediator of the effect of $A$ on $Y$.

**Definition 1.** The structural null hypothesis of no case-mix heterogeneity holds if either of the following is satisfied:

i. The pre-treatment covariates are distributed equally across studies; i.e., if

$$p(W | S = 1) = p(W | S = 0)$$

ii. The study-specific average treatment effect does not depend on $W$; i.e., if

$$E[Y(1, s) - Y(0, s) | w] = E[Y(1, s) - Y(0, s)]$$

for any $s, w$.

**Definition 2.** The structural null hypothesis of no mediator-related effect heterogeneity holds if either of the following is satisfied:
i The study-specific conditional average treatment effect does not depend on \( M \); i.e., if
\[
E[Y(1, m_0, S = 1) - Y(0, m_0, S = 1) \mid W = w] = E[Y(1, m_1, S = 0) - Y(0, m_1, S = 0) \mid W = w]
\]
for any \( m_0, m_1, w \).

ii The mediator is unaffected by study assignment; i.e., if
\[
M(a, S = 1) = M(a, 0)
\]
for any \( a \).

**Definition 3.** The structural null hypothesis of no pure effect modification holds if \( S \) has no direct effect on \( Y \); i.e., for all \( a, m \) we have \( Y(a, m, S = 1) = Y(a, m, S = 0) \).

Note that we use the word “structural” in the definitions above to emphasize a difference between the nature of these conditions and the nature of the parameters defined in Section 3. In particular, as discussed in that section, those parameters could equal zero without the structural null hypotheses holding.

### 2.3 Example: Moving to Opportunity study

The Moving to Opportunity (MTO) study (Kling et al., 2007; Sanbonmatsu et al., 2011) was a randomized trial investigating the effect of granting Section 8 housing vouchers; families living in public housing in high-poverty neighborhoods were randomized to receive these vouchers (or not), which they could use to move out of public housing and into a lower-poverty neighborhood. The families were followed for 10-15 years and evaluated for outcomes related to economic status, educational attainment, and physical and mental health. Of interest to the current paper is that the program was administered in five different US cities (Baltimore, Boston, Chicago, Los Angeles, and New York), and disparate effects have been inferred for each site (Rudolph et al., 2018a,b; Rudolph and Díaz, 2022). As in previous analyses (Rudolph et al., 2018a,b), we exclude the Baltimore study due to the presence of a concurrent housing intervention in that city. In previous research, Rudolph et al. (2018a) found that differences in covariate distributions did not fully explain site-level effect differences for depression and anxiety, and Rudolph et al. (2018b) found that aspects of school experience play a small role in mediating the effect of MTO vouchers on adolescent substance use. In this study, we aim to understand the factors driving heterogeneity in the effect of the intervention on psychiatric outcomes for boys, considering school poverty as a potential mediating variable. In particular, our question is whether the MTO voucher makes a psychiatric diagnosis less likely for boys and if this effect is mediated by the boys’ attending fewer high-poverty schools. A detailed description of the variables of interest and our statistical analysis can be found in Section 8.

### 3 A hierarchical decomposition of between-study effect heterogeneity

With these different sources of heterogeneity in mind, we can decompose observed heterogeneity into its component sources. Note, however, that the null hypothesis definitions in Section 2.2
involve stronger conditions than needed for a value of zero for the corresponding parameter given below.

### 3.1 Case-mix decomposition

Our goal is to develop a methodology to understand and quantify the sources of heterogeneity that may give rise to conflicting effect estimates in different studies. To represent the problem mathematically, we can express the difference in study-specific effects as follows:

\[ \delta := E[Y(A = 1) - Y(A = 0) \mid S = 1] - E[Y(A = 1) - Y(A = 0) \mid S = 0] \]

where each term is the average treatment effect (ATE) within each study. Different factors can cause \( \delta \) to be nonzero; it may be the case that either the study populations differ, or that the treatment has different effects (for similar individuals) in the two studies. We can express this scientific assertion as the following mathematical decomposition:

\[ \delta = \delta_{EH} + \delta_{CM} \]

where

\[ \delta_{EH} := E[Y(A = 1, S = 1) - Y(A = 0, S = 1) \mid S = 0] - E[Y(A = 1, S = 0) - Y(A = 0, S = 0) \mid S = 0] \]

\[ \delta_{CM} := E[Y(A = 1, S = 1) - Y(A = 0, S = 1) \mid S = 1] - E[Y(A = 1, S = 1) - Y(A = 0, S = 1) \mid S = 0] \]

The parameter \( \delta_{EH} \), where the initials stand for “effect heterogeneity,” considers what the difference in treatment effects would be if both studies had a case mix corresponding to the distribution of pre-treatment covariates in study \( S = 0 \). Conversely, \( \delta_{CM} \), where the initials stand for “case mix,” considers what would happen to the difference in treatment effects across studies if the outcome variable (and any mediating variables) were generated according to the mechanisms present in the environment of study \( S = 1 \). For the former parameter, it is the case mix that is “held constant” in some sense, while in the latter case, it is the outcome data-generating mechanism that is held constant. It is not hard to show that \( \delta_{CM} = 0 \) if the structural hypothesis of no case-mix heterogeneity holds, and \( \delta_{EH} = 0 \) if both the structural hypothesis of no mediator-related effect heterogeneity holds and the structural hypothesis of no pure effect modification holds. See Section 3.3 for an example of a calculation of this kind.

### 3.2 Mediator-related variability decomposition

When \( \delta_{EH} \) is non-zero, it is also of interest to understand to what extent the heterogeneity is driven by a mediating variable. For example, MTO was conducted in multiple cities, which had differing levels of school poverty and could plausibly also differ in the extent to which moving with a Section 8 voucher would affect school poverty. Consequently, the mediating variable of school poverty could partially explain discrepancies in the relationship between moving with the voucher on the risk of later psychiatric disorder between cities.
To further decompose $\delta_{EH}$ into these two sources of variability, consider the counterfactual variable $M(a, s)$ that would have been observed for an individual if, possibly contrary to fact, their mediator was assigned using the mechanism that prevailed in study $S = s$ treatment arm $A = a$. By definition, we have that $Y(a) = Y(a, M(a, S))$, so that $\delta_{EM} + \delta_{MV} = \delta_{EH}$, with

$$
\delta_{EM} := \mathbb{E}[Y(A = 1, M(A = 1, S = 1), S = 1) - Y(A = 0, M(A = 0, S = 1), S = 1) | S = 0] - \mathbb{E}[Y(A = 1, M(A = 1, S = 1), S = 0) - Y(A = 0, M(A = 0, S = 1), S = 0) | S = 0]
$$

$$
\delta_{MV} := \mathbb{E}[Y(A = 1, M(A = 1, S = 1), S = 0) - Y(A = 0, M(A = 0, S = 1), S = 0) | S = 0] - \mathbb{E}[Y(A = 1, M(A = 1, S = 0), S = 0) - Y(A = 0, M(A = 0, S = 0), S = 0) | S = 0]
$$

Here we have that $\delta_{MV} = 0$ if the structural hypothesis of no mediator-related effect heterogeneity holds, and $\delta_{EM} = 0$ if the structural hypothesis of no pure effect modification holds.

### 3.3 Example calculation

As an example to illustrate the connections between the parameters defined above and the structural hypotheses of Section 2.2, consider the case that the structural hypothesis of no mediator-related heterogeneity holds, so that for all $a$, we have $M(a, S = 1) = M(a, S = 0) := M_a$. Then $\delta_{EH}$ can be expressed as

$$
\delta_{EH} := \mathbb{E}[Y(A = 1, S = 1) - Y(A = 0, S = 1) | S = 0] - \mathbb{E}[Y(A = 1, S = 0) - Y(A = 0, S = 0) | S = 0]
$$

$$
= \mathbb{E}[Y(A = 1, M(1, 1), S = 1) - Y(A = 0, M(0, 1), S = 1) | S = 0] - \mathbb{E}[Y(A = 1, M(1, 0), S = 0) - Y(A = 0, M(0, 0), S = 0) | S = 0]
$$

$$
= \mathbb{E}[Y(A = 1, M(1, 1), S = 1) - Y(A = 1, M(1, 0), S = 0) | S = 0] - \mathbb{E}[Y(A = 0, M(0, 1), S = 1) - Y(A = 0, M(0, 0), S = 0) | S = 0]
$$

$$
= \mathbb{E}[Y(A = 1, M_1, S = 1) - Y(A = 1, M_1, S = 0) | S = 0] - \mathbb{E}[Y(A = 0, M_0, S = 1) - Y(A = 0, M_0, S = 0) | S = 0]
$$

We can see that, when the structural hypothesis of no mediator-related heterogeneity holds, $\delta_{EH}$ must arise from differences of the form $Y(a, m, 1) - Y(a, m, 0)$. Thus, if $\delta_{EH} \neq 0$, in this scenario, where the structural hypothesis of no mediator-related heterogeneity holds, then the structural null hypothesis of no pure effect modification must fail. Furthermore, it is clear by definition that, $\delta_{MV} = 0$, and thus $\delta_{EH} = \delta_{EM}$.

It is important to note that while the structural null hypotheses imply null values for the parameters defined in this section, the reverse is not necessarily true.
4 Identification of the treatment effect heterogeneity decompositions

4.1 Identification under unconfoundedness conditions

To be able to learn the values of these parameters from data, we will require the following assumptions, which guarantee that there is sufficient random variability in the studies so that the relevant conditional expectations are well-defined.

A1. There exists \( \epsilon > 0 \) such that, for \( a, s \in \{0, 1\} \), \( m \) in the support of \( M \), and with probability 1 over draws of \( W \):

(i) \( \epsilon < P(A = 1 \mid W, S = s) < 1 - \epsilon \), and

(ii) \( \epsilon < P(S = 1 \mid W) < 1 - \epsilon \)

(iii) \( \epsilon < P(M = m \mid W, S = s, A = a) \).

In addition, the results in this section will require some of the following assumptions:

A2 (Conditional exchangeability of study assignment with outcome). For \( a, s = 0, 1 \), assume \( Y(a, M(a, s), s) \perp \perp S \mid W \).

A3 (No unmeasured confounding within study). For all \( a, m, s \), assume \( (Y(a, m), M(a)) \perp \perp A \mid W, S = s \).

A4 (Conditional exchangeability of study assignment with mediator). For all \( a, s \), assume \( M(a, s) \perp \perp S \mid W \).

A5 (Counterfactual independences within study). For all \( a, m, s, s' \), assume \( Y(a, m) \perp \perp M(a, s') \mid (W, S = s) \) and \( Y(a, m) \perp \perp M \mid (W, S = s, A) \).

First, we note that if each study is a randomized controlled trial (RCT), then assumptions A1(i) and A3 are satisfied by randomization, but the other assumptions do not necessarily hold. Also, we have omitted the types of assumptions common in causal inference labeled as “consistency” since we take such statements to be implied by the SCM.

While the preceding assumptions are somewhat difficult to interpret, we can provide somewhat more intuitive conditions. The following are sufficient conditions for A2, A3, A4, and A5 to hold in terms of the errors \( U \) of the structural causal model (1). These conditions allow us to assess the validity of A2-A5 by checking whether common causes are measured.

Proposition 1. The following statements are true:

(i) Assume \( (U_Y, U_M) \perp \perp U_S \mid W \). Then A2 holds.

(ii) Assume \( U_A \perp \perp (U_Y, U_M) \mid W, S = s \). Then A3 holds.

(iii) Assume \( U_S \perp \perp U_M \mid W \). Then A4 holds.

(iv) Assume \( U_Y \perp \perp U_M \mid W, S = s \) and \( U_Y \perp \perp U_M \mid W, S = s, A \). Then A5 holds.
(a) The largest DAG fulfilling the conditions of Eq. 1.

(b) DAG of an RCT fulfilling Eq. 1.

(c) DAG of an RCT that fails to satisfy A4 if the common cause $U$ is unmeasured.

(d) DAG of an RCT that fails to satisfy A5 if the common cause $U$ is unmeasured.

Figure 1: Comparison of Directed Acyclic Graphs (DAGs) illustrating different scenarios related to the conditions of Eq. 1.
Proof These follow from substituting the definitions of the counterfactuals in A2-A5 into the SCM in Eq. 1.

In the following theorem, we will use the quantities
\[ h_s(w) = E(Y \mid W = w, S = s, A = 1) - E(Y \mid W = w, S = s, A = 0), \]
which identify the conditional average treatment effect \( E[Y(1) - Y(0) \mid W = s, S = s] \) under A3 and A1. We also define the parameters
\[ f_a(w) = \int \left[ E(Y \mid w, S = 1, a, m) - E(Y \mid w, S = 0, a, m) \right] dP(M = m \mid w, S = 1, a) \]
\[ d_a(w) = \int E(Y \mid w, S = 0, a, m) \left[ dP(M = m \mid w, S = 1, a) - dP(M = m \mid w, S = 0, a) \right] \]

Theorem 1. Assume A1, A2, and A3. We have
\[ \delta_{CM} = E[h_1(W) \mid S = 1] - E[h_1(W) \mid S = 0], \text{ and} \]
\[ \delta_{EH} = E[h_1(W) - h_0(W) \mid S = 0]. \]
If A4 and A5 hold, then we have
\[ \delta_{EM} = E[f_1(W) - f_0(W) \mid S = 0], \text{ and} \]
\[ \delta_{MV} = E[d_1(W) - d_0(W) \mid S = 0]. \]

Proof See Section S2 in the Supplementary Materials.

4.2 Remarks on Theorem 1

Since the definitions of \( \delta_{CM} \) and \( \delta_{EH} \) do not involve the variable \( M \), one can see that if the identification of only \( \delta_{CM} \) and \( \delta_{EH} \) (and not \( \delta_{MV} \) and \( \delta_{EM} \)) are desired, then the positivity and conditional independence assumptions involving \( M \) are unnecessary.

It is also worth analyzing the situation when A2 fails. In this case, \( \delta_{CM} \) and \( \delta_{EH} \) no longer have the straightforward scientific interpretations given above in terms of structural hypotheses, but the estimated quantities may still be considered and interpreted in other ways. For example, we identified \( \delta_{CM} \) through the intermediate expression
\[ \tilde{\delta}_{CM} := \int E[Y(1) - Y(0) \mid W, S = 1] \left\{ dP(W \mid S = 1) - dP(W \mid S = 0) \right\} \]
If the study assignment is not ignorable, then \( \tilde{\delta}_{CM} \) is no longer the difference in effect sizes if each population were subject to the conditions of study 1. However, \( \tilde{\delta}_{CM} \) still is the difference in effect sizes if study 0 had a conditional average treatment effect (CATE) equal to the CATE of study 1, where the CATE for study \( s \) is defined as \( CATE_s(w) = E[Y(1) - Y(0) \mid W = w, S = s] \), which may still be of interest.
5 Estimation

For the discussion of estimation, it will be useful to define the following expression for a family of parameters.

\[
\theta(s_Y, s_M, s_W) = \int \left[ \mathbb{E}(Y \mid w, s_Y, A = 1, m) \, dP(m \mid w, s_M, A = 1) \right. \\
- \left. \mathbb{E}(Y \mid w, s_Y, A = 0, m) \, dP(m \mid w, s_M, A = 0) \right] \, dP(w \mid s_W).
\]

Then we have

\[
\delta_{CM} = \theta(1, 1, 1) - \theta(1, 1, 0) \\
\delta_{EH} = \theta(1, 1, 0) - \theta(0, 0, 0) \\
\delta_{EM} = \theta(1, 1, 0) - \theta(0, 1, 0) \\
\delta_{MV} = \theta(0, 1, 0) - \theta(0, 0, 0).
\]

We propose an estimator for the general parameter \( \theta(s_Y, s_M, s_W) \), which can then be used to estimate any of the parameters identified above by linear combination. To simplify notation, we may occasionally simply write \( \theta \), keeping the arguments implicit.

To propose an estimator and make inferences about its distribution, we will make use of established semiparametric theory; for reference, one may consult Pfanzagl and Wefelmeyer (1985); Bickel et al. (1993), and Kennedy (2022), the last of which gives a modern overview. In particular, our estimator will make use of the “efficient influence function” (EIF), which can be used to construct robust and efficient estimators. (For the definition of “efficient influence function,” see Section S3.) In Proposition 2, we give the form of the EIF, and in the remainder of this section build the estimator and demonstrate its properties.

**Proposition 2.** The efficient influence function for \( \theta \) in the nonparametric model is equal to

\[
D(O; \eta) = \frac{g_M(A \mid W, s_M, M) \, e_M(s_M \mid W, M)}{g_M(A \mid W, s_Y, M)} \frac{e(s_W \mid W)}{e(s_M \mid W)} \frac{(2A - 1)I(S = s_Y)}{g(A \mid W, s_M) \cdot h(s_W)} \left\{ q_Y(W, s_Y, A, M) - q_M(W, s_Y, s_M, A) \right\}
\]

where we denote \( \eta = (q_Y, q_M, e, e_M, g, g_M, h) \) and

\[
q_Y(w, s_Y, a, m) = \mathbb{E}(Y \mid w, s_Y, a, m) \\
q_M(w, s_Y, s_M, a) = \mathbb{E}[q_Y(W, s_Y, A, M) \mid w, s_M, a] \\
e(s \mid w) = P(s \mid w) \\
e_M(s \mid w, m) = P(s \mid w, m) \\
g(a \mid w, s) = P(a \mid w, s) \\
g_M(a \mid w, s, m) = P(a \mid w, s, m) \\
h(s) = P(s).
\]
Note that this EIF is an extension of the EIF in previous work to enable the construction of efficient estimators in more general settings. In particular, Rudolph and van der Laan (2017) discussed the identification of the intention-to-treat effect under non-adherence in a target population using outcome data from elsewhere. In that setting, the adherence status can be viewed as a single binary mediator that entirely mediates the causal effect of $A$ on $Y$. Here, we allow $M$ to be a vector of multiple mediators of any data type, and these mediators might only partially mediate the effect. In addition, Rudolph and van der Laan (2017) also assumed that the mediator distribution in the target population is known, and the conditional outcome distribution is identical between the source and target populations, assumptions which we do not make here.

The preceding proposition is a corollary of the following lemma, which also serves to characterize the multiple robustness of estimators relying on the influence function above.

**Lemma 1** (von Mises expansion). Let $\theta(F)$ denote the parameter (2) evaluated at an arbitrary distribution $F$. Let $\eta_F$ denote the parameters corresponding to distribution $F$. Then we have

$$\theta(F) - \theta(P) = -E_P[D(O; \eta_F)] + R(\eta_P, \eta_F),$$

where we add the index $P$ to the expectation for clarity, and where $R$ is a second-order term satisfying

$$R(\eta_P, \eta_F) = \int C_1(P, F)[g_{M,P} - g_{M,F}][\{e_P - e_F\} + \{g_P - g_F\} + \{h_P - h_F\}] dP$$

$$+ \int C_2(P, F)[q_{Y,P} - q_{Y,F}][\{e_{M,P} - e_{M,F}\} + \{g_{M,P} - g_{M,F}\}] dP,$$

where $C_1, C_2$ are some random variables that remain bounded as $F \rightarrow P$. (The arguments of the functions have been suppressed to emphasize the structure of the expression; see proof for details.)

**Proof** See Section S4.

The above result has multiple important implications for constructing efficient and flexible estimators of $\theta$. First, notice that a plug-in estimator may be constructed by

(i) fitting a regression of $Y$ on $(A, M, W, S)$,

(ii) using the above regression to predict $q_Y(W, s_Y, A, M)$ by fixing $S = s_Y$ for all units,

(iii) regressing the estimate of $q_Y(W, s_Y, A, M)$ on $(W, S, A)$,

(iv) using the above regression to predict $q_M(W, s_Y, s_M, A)$ by fixing $S = s_M$ for all units,

(v) averaging the above predictions.

In addition, Lemma 1 shows that the error of such a “plug-in estimator” is given by $\theta(\hat{\eta}) - \theta = -E[D(O; \hat{\eta})] + R(\eta, \hat{\eta})$, where $\hat{\eta}$ contains the corresponding estimators of $q_Y$ and $q_M$. This motivates the construction of the “one-step” estimator:

$$\tilde{\theta} = \theta(\hat{\eta}) + \frac{1}{n} \sum_{i=1}^n D(O_i; \hat{\eta})$$

(4)
The error of the one-step estimator is \( \frac{1}{n} \sum_{i=1}^{n} \{ D(O_i; \hat{\eta}) - \mathbb{E}[D(O; \eta)] \} + R(\eta, \hat{\eta}) \). The first term will be controlled under the assumptions of Theorem 2. The second term is a “second-order” error term as given in (3). Thus it can be expected to be small and goes to zero under the following assumption A6.

**A6.** Assume that \( \hat{\eta} \) converges in probability to an element \( \eta_1 \). At least one of the following statements is true.

- (i) \((q_{Y,1}, q_M) = (q_Y, q_M)\)
- (ii) \((q_{M,1}, e_{M,1}; g_{M,1}) = (q_M, e_M, g_M)\)
- (iii) \((q_{Y,1}, e_1, g_1) = (q_Y, e, g)\)
- (iv) \((e_{M,1}, g_{M,1}, e_1, g_1) = (e_M, g_M, e, g)\).

Note that \( h \), the proportion of subjects in each study, is excluded from A6 because it is trivially estimated by an empirical proportion. All the other components of \( \eta \) can be estimated by standard regression models, including flexible machine-learning approaches. In the theorem below, we clarify the conditions for \( \tilde{\theta} \) to be asymptotically normal and efficient.

**Theorem 2.** (Asymptotic normality and efficiency) Assume

(i) Positivity, described in A1 and (i)

(ii) The second-order term \( R(\eta, \hat{\eta}) \) is \( o_P(n^{-1/2}) \) and

(iii) The class of functions \( \{ D(\eta, \theta') : |\theta' - \theta| < \delta, ||\eta - \eta_1|| < \delta \} \) is Donsker for some \( \delta > 0 \) and such that \( P \{ D(\eta, \theta') - D(\eta_1, \theta) \}^2 \rightarrow 0 \) as \( (\eta, \theta') \rightarrow (\eta_1, \theta) \)

then:

\[
\tilde{\theta}(s_Y, s_M, s_W) = \theta(s_Y, s_M, s_W) + \frac{1}{N} \sum_{i=1}^{N} D(O_i, \eta) + o_P(1),
\]

due to which \( \sqrt{N}(\tilde{\theta} - \theta) \xrightarrow{D} N(0, \zeta^2) \), where \( \zeta^2 = V\{D(O, \eta)\} \) is the nonparametric efficiency bound.

**Proof** This is an application of well-known semiparametric theory to Lemma 1. A proof sketch is given in Section S6.

Note that condition (ii) for asymptotic normality in Theorem 2 is satisfied if all components of \( \hat{\eta} \) converge in \( L_2(P) \) norm to their true counterparts in \( \eta \) at \( n^{-1/4} \)-rate or faster. This is the case for many data-adaptive algorithms such as LASSO or highly adaptive LASSO, under certain conditions (Belloni et al., 2015; Benkeser and van der Laan, 2016). An alternative to condition (iii), the “Donsker condition,” is the use of “cross-fitting” (Chernozhukov et al., 2018). In cross-fitting, the data are randomly split into a number of similarly-sized folds, with one fold at a time used as a “validation” set and the others used as “training.” The training sets are used to estimate nuisance functionals, and the validation set is used to evaluate the resulting efficient influence functions. In either case (Donsker assumption or cross-fitting), the sample variance of the efficient influence function can be used to estimate the variance of \( \tilde{\theta} \) and derive confidence intervals based on a normal approximation.
6 Simulation Study

We conducted a Monte Carlo simulation study with multiple settings to illustrate the behavior of our estimators under various conditions. A detailed description of the data-generating mechanisms is provided in Table 1.

Table 1: Description of simulation study

| Aspect | Details |
|--------|---------|
| Sample Size | The sample size, $N$, was varied within the range of $[10^2, 10^4]$. |
| Variables | $W \sim \text{Uniform}(0, 1)$: $W$ is a uniformly distributed random variable between 0 and 1. $S \sim \text{Bernoulli}(\text{clamp}(W, Q, 1 - Q))$: $S$ is a Bernoulli random variable with success probability $\text{clamp}(W, Q, 1 - Q)$, where $\text{clamp}(x, a, b) = \max(a, \min(x, b))$, for $a \leq b$. $A \sim \text{Bernoulli}(\text{ilogit}(S + W + S \times W))$: $A$ is a Bernoulli random variable with success probability given by the inverse logit function of $S + W + S \times W$. $M \sim \text{Bernoulli}(\frac{A + W + B \times S}{3})$: $M$ is a Bernoulli random variable with success probability given by $\frac{A + W + B \times S}{3}$. $Y = A + C \times (1 + S) \times W \times A + M \times A + \epsilon$: $Y$ is the response variable, where $\epsilon \sim \text{N}(0, 1)$ represents normally distributed random noise with mean 0 and variance 1. |
| Settings | $Q \in [0.1, 0.5]$ $B, C \in [0, 1]$ |

These settings allow us to “zero out” certain parts of the estimand. In particular, when $Q$ is 0.5 $\delta_{CM}$ is zero, when $B$ is zero $\delta_{MV}$ is zero, and when $C$ is zero $\delta_{EM}$ is zero. We have used relatively simple linear functions in order to facilitate the analytic calculation of the target estimands, but we estimate them nonparametrically. In particular, we use the Super Learner approach (van der Laan et al., 2007) using a library of estimation strategies consisting of a constant mean value, a generalized linear model, a generalized additive model, extreme gradient boosting, random forest, and multivariate adaptive regression splines.

Results for the simulation study run with 500 replications for each setting are shown in Figure 2; full numeric results can be found in Section S1. The estimators have high accuracy (low MSE), especially when $n$ is large. In large samples, the 95% intervals have nominal coverage, except for a few scenarios where the coverage drops down to around 90%. We note that estimation of standard errors for robust nonparametric estimators via the standard deviation of the empirical influence function is known to be occasionally anti-conservative (see, e.g., Tran et al. (2023)), the development of improved variance estimators is the subject of future work.
Figure 2: Simulation study results. The top plot shows $n \times$ MSE versus sample size; the bottom plot shows coverage probability versus sample size. See Section S1 for full numerical results. The "Scenario" variable refers to different settings as described in Section 1; see Table S2 for a key to this variable.
7 Extension to multiple studies

The challenge of heterogeneity also arises in other research areas such as evidence synthesis and meta-analysis. In this literature, the slightly different focus is on combining multiple exposure effect estimates \( \lambda(1), \ldots, \lambda(K) \) that are obtained from different populations \( 1, \ldots, K \). The heterogeneity across these populations is taken into account in multiple ways. For instance, studies are only meta-analyzed when they are deemed as sufficiently similar. Even when this condition holds, a meta-analysis will not naively combine individual-level data from different studies (whenever such data are available). Instead, it assumes that \( \lambda(1), \ldots, \lambda(K) \) are heterogeneous but all come from an underlying distribution. The target of the analysis is to obtain the mean of such distribution as a summary, and the variance as a measurement of heterogeneity (Higgins et al., 2009).

The above principle of meta-analysis seems to be particularly relevant to a data fusion setting, where it can help suggest a way to extend the decomposition presented above to a scenario with more than two studies. To formalize this, we define \( \theta(s_Y, s_M, s_W) \) as

\[
\theta(s_Y, s_M, s_W) = \int \mathbb{E}[Y(1, M(1, s_M)) - Y(0, M(0, s_M)) \mid W, S = s_Y] \, dP(W \mid S = s_W),
\]

where \((s_Y, s_M, s_W)\) now take values in \(\{1, \ldots, K\}^3\). When \(s_M = s_Y = s_W\), this is the effect in the corresponding study. We let \(S_Y, S_M, \) and \(S_W\) denote three random variables independently and identically distributed in \(\{1, \ldots, K\}\) with known (e.g., uniform) or easy-to-estimate (e.g., empirical of \(S\)) distribution. Let \(P_S\) denote this joint distribution of \(S_Y, S_M, \) and \(S_W\), and let \(\mathbb{E}_S\) and \(\text{Var}_S\) denote expectation and variance with respect to \(P_S\). We define \(\tau^2 = \text{Var}_S[\theta(S_Y, S_M, S_W)]\) as the total between-study variability, and decompose it into their case-mix and effect heterogeneity components by using the law of total variance as \(\tau^2 = \tau_{CM}^2 + \tau_{EH}^2\), where

\[
\tau_{CM}^2 := \mathbb{E}_S[\text{Var}_S[\theta(S_Y, S_M, S_W) \mid S_Y, S_M]]
\]

\[
\tau_{EH}^2 := \text{Var}_S[\kappa(S_Y, S_M)],
\]

where \(\kappa(S_Y, S_M) = \mathbb{E}_S[\theta(S_Y, S_M, S_W) \mid S_Y, S_M]\). Likewise, we decompose \(\tau_{EH}^2\) into a pure effect modification parameter and a mediator variability parameter as \(\tau_{EH}^2 = \tau_{EM}^2 + \tau_{MV}^2\), where

\[
\tau_{EM}^2 := \text{Var}_S[\mathbb{E}_S[\kappa(S_Y, S_M) \mid S_Y]]
\]

\[
\tau_{MV}^2 := \mathbb{E}_S[\text{Var}_S[\kappa(S_Y, S_M) \mid S_Y]].
\]

**Proposition 3.** Assume A1-A5 hold for \(s \in \{1, \ldots, K\}\). Then \(\theta(s_Y, s_M, s_W)\) is identified as in Equation (2).

*Proof* See Section S5.

Given estimators of \(\theta(s_Y, s_M, s_W)\), and noting that \(\tau_{CM}^2, \tau_{EH}^2, \tau_{MV}^2, \) and \(\tau_{EM}^2\) are functions of the distribution of \(\theta(S_Y, S_M, S_W)\), the delta method can be used to derive their standard errors. These derivations are provided in Section S7.
8 Analysis of MTO study

We now apply our proposed methods to data from the Moving to Opportunity study (MTO), conducted by the US Department of Housing and Urban Development 1994-2010, and which we introduced in Section 2.3 (Kling et al., 2007; Sanbonmatsu et al., 2011). There is ample evidence of effect heterogeneity across MTO sites, even qualitative effect heterogeneity; some sites yielded negative effect estimates, while others yielded positive effect estimates (Rudolph et al., 2017, 2018a). This evidence of effect heterogeneity is seen not only for total effects but also for indirect effects (Rudolph et al., 2020, 2021; Rudolph and Díaz, 2022).

When such effect heterogeneity exists, it is natural to want to understand why: what components of the causal process are contributing to such heterogeneity? We address that question here. Specifically, in this analysis, we are interested in understanding contributions to site-level heterogeneity in the effect of moving with the voucher on the risk of developing a psychiatric disorder in adolescence (10-15 years after randomization), using attendance of a lower-poverty school during follow-up as an intermediate variable/mediator, among boys who were younger than 5 years old when their family enrolled in MTO. Using the proposed methods, we decompose the site-level heterogeneity into heterogeneity due to baseline covariates, differences in mediator distributions, or pure effect modification.

Baseline covariates, $W$, included family-level, child-level, and neighborhood characteristics at the time of randomization, collected from 1994 to 1998. Child variables included race/ethnicity, age, history of behavioral problems, and whether the child was ever enrolled in a special class for gifted and talented students. Adult variables included whether the adult was a high school graduate or had their GED, never married, was under 18 when the child was born, was currently working, was currently receiving welfare, perceived the baseline neighborhood as being unsafe at night, was very dissatisfied with the neighborhood, had moved 3 times or more, signed up to participate in MTO so that their child(ren) could attend better quality schools, or had a Section 8 voucher previously. Other variables included whether a household member had a disability, the size of the household (2, 3, or $\geq 4$), and the poverty rate of the baseline neighborhood. Site, $S$, included Boston, Chicago, Los Angeles (LA), and New York City (NYC). Exposure, $A$, was a binary variable indicating whether the family moved with the voucher out of public housing and was collected in the same period as the baseline variables, 90 days after randomization. The mediator, $M$, was a binary variable indicating whether the child had ever attended a school that was not high-poverty (a non-Title I school) over the duration of follow-up—so spanning the time from randomization to the outcome measurement. The outcome, $Y$, was a binary variable indicating whether the boy had any psychiatric disorder in the past year, as defined by the Diagnostic and Statistical Manual of Mental Disorders, Fourth Edition (DSM-IV), collected 2008-2010.

Restricting to boys in the Boston, Chicago, LA, and NYC sites resulted in a rounded sample size of 2,100, with rounded sample sizes of 500 in the Boston site, 600 in the Chicago site, 400 in the LA site, and 600 in the NYC site (any reported sample size must be rounded in accordance with Census rules).

For simplicity in this illustrative example, we use a single imputed dataset (imputed using multiple imputation by chained equations (Van Buuren and Groothuis-Oudshoorn, 2011)). Most baseline variables had no missingness, though race/ethnicity and baseline neighborhood poverty were missing for 2%. The mediator and outcome were missing for 8%. Again, for simplicity in this illustrative example, we did not use the survey weights provided by MTO (Kling et al., 2007; San-
bonmatsu et al., 2011). Consequently, we are ignoring the sampling probability of a child within a multi-child family and making inferences among the boys who were retained through the duration of the study. We use the Super Learner (van der Laan et al., 2007) technique using a library of estimators consisting of a constant mean value, a generalized linear model, extreme gradient boosting, elastic net regression, and multivariate adaptive regression splines.

The current aim is to estimate the proportion of variation in effect estimates that is driven by case-mix differences, mediator distribution differences, and pure effect modification, respectively, following the approach outlined in Sections 5 and 7. The results of our decomposition analysis are shown in Table 2. For site-specific total effect estimates, see Section S9.

Table 2: Results of our analyses. Variances and their S.E. multiplied by 10000. All results were approved for release by the U.S. Census Bureau, authorization number CBDRB-FY22-CES018-013, CBDRB-FY24-CES018-002

| Parameter | Var.  | S.E. of S.D. | %   | S.E. of %  |
|-----------|-------|--------------|-----|------------|
| τ         | 5.102 | 3.418        | 100.000 |           |
| τ_{CM}    | 2.532 | 1.832        | 49.620 | 11.160     |
| τ_{EH}    | 2.570 | 1.770        | 50.380 | 11.160     |
| τ_{EM}    | 0.300 | 0.370        | 5.911  | 5.713      |
| τ_{MV}    | 2.269 | 1.582        | 44.470 | 12.960     |

These results indicate that case-mix and differences in mediator distributions each account for about half of the variation in effect sizes, and pure effect modification accounts for only a small amount. This is useful to know in the current context because it indicates that differences across sites in the total effect of moving with the voucher on the risk of developing a mental health disorder are almost entirely explained by differences in baseline covariate distributions and the distribution in high-vs.-low poverty school attendance.

9 Conclusion

In this paper, we have presented a framework for combining individual-level data across multiple studies to understand the sources of differences in effect estimates. In contrast to other research, we have not assumed that covariate shift fully explains such differences; rather, we have given a decomposition into variation due to covariate shift, mediator shift, and pure effect modification. We have provided a nonparametric and robust algorithm for estimating each component of the decomposition for any number of studies, subject to identification conditions related to positivity and ignorability. Further research may consider more complicated longitudinal data structures or missing data, including the case where different studies collect data on variables that are closely related but not identical. In addition, researchers might be interested in disentangling multiple distinct paths of mediation, which we have not considered here.
10 Acknowledgments

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Supplementary material

S1 Lemma 2

The following lemma will be useful in proving later results.

**Lemma 2.** A3 implies that \( Y(a) \perp \perp \{A, W, S = s\} \).

**Proof** Note that \( Y(a) = Y(a, M(a)) \) and is a composition of the random variables \( Y(a, m) \) and \( M(a) \), which are jointly conditionally independent of \( A \) by the assumption. Concretely,

\[
\text{pr}(Y(a) \mid W, S = s, A) = \text{pr}(Y(a, M(a)) \mid W, S = s, A)
\]

\[
= \int_m \text{pr}(Y(a, m) \mid W, S = s, M(a) = m) \text{pr}(M(a) = m \mid W, S = s, A) \, dm
\]

\[
= \int_m \text{pr}(Y(a) \mid W, S = s, M(a) = m) \text{pr}(M(a) = m \mid W, S = s) \, dm
\]

\[
= \int_m \text{pr}(Y(a) \mid W, S = s) \, dm
\]

where the third line is justified by the joint conditional independence assumption. \( \square \)

S2 Proof of Theorem 1

First, assume \( A_1, A_2, \) and \( A_3 \) for \( s \in \{0, 1\} \); throughout, \( A_1 \) ensures positive probability/probability density of conditioning events. Then, by definition

\[
\delta_{CM} = E[Y(A = 1, S = 1) - Y(A = 0, S = 1) \mid S = 1] - E[Y(A = 1, S = 1) - Y(A = 0, S = 1) \mid S = 0]
\]

\[
= \int \text{E}[Y(A = 1, S = 1) - Y(A = 0, S = 1) \mid W, S = 1] \, dP(W \mid S = 1) - \int \text{E}[Y(A = 1, S = 1) - Y(A = 0, S = 1) \mid W, S = 0] \, dP(W \mid S = 0)]
\]

By \( A_2 \),

\[
= \int \text{E}[Y(A = 1, S = 1) - Y(A = 0, S = 1) \mid W, S = 1] \, dP(W \mid S = 1) - \int \text{E}[Y(A = 1, S = 1) - Y(A = 0, S = 1) \mid W, S = 0] \, dP(W \mid S = 0)]
\]

\[
= \int \text{E}[Y(1) - Y(0) \mid W, S = 1] \, dP(W \mid S = 1)
\]

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\[
\int \mathbb{E}[Y(1) - Y(0) \mid W, S = 1] \, d\mathbb{P}(W \mid S = 0)
\]

\[
\delta_{CM} = \int \mathbb{E}[Y(1) - Y(0) \mid W, S = 1] \{ d\mathbb{P}(W \mid S = 1) - d\mathbb{P}(W \mid S = 0) \}
\]

By A3, using Lemma 2,

\[
= \int \{ \mathbb{E}[Y(1) \mid W, S = 1, A = 1] - \mathbb{E}[Y(0) \mid W, S = 1, A = 0] \} \{ d\mathbb{P}(W \mid S = 1) - d\mathbb{P}(W \mid S = 0) \}
\]

\[
= \int \{ \mathbb{E}[Y(W, S = 1, A = 1)] - \mathbb{E}[Y(W, S = 1, A = 0)] \} \{ d\mathbb{P}(W \mid S = 1) - d\mathbb{P}(W \mid S = 0) \}
\]

Then, we plug in the definition of \( h_s \) to obtain

\[
\delta_{CM} = \mathbb{E}[h_1(W) \mid S = 1] - \mathbb{E}[h_1(W) \mid S = 0]
\]

Next, by definition

\[
\delta_{EH} := \mathbb{E}[Y(A = 1, S = 1) - Y(A = 0, S = 1) \mid S = 0] - \\
\mathbb{E}[Y(A = 1, S = 0) - Y(A = 0, S = 0) \mid S = 0]
\]

\[
= \int \mathbb{E}[Y(A = 1, S = 1) - Y(A = 0, S = 1) \mid W, S = 0] \, d\mathbb{P}(W \mid S = 0) - \\
\int \mathbb{E}[Y(A = 1, S = 0) - Y(A = 0, S = 0) \mid W, S = 0] \, d\mathbb{P}(W \mid S = 0)
\]

By A3,

\[
= \int \left\{ \mathbb{E}[Y(1) - Y(0) \mid W, S = 1] - \mathbb{E}[Y(1) - Y(0) \mid W, S = 0] \right\} \, d\mathbb{P}(W \mid S = 0)
\]

Separating the terms and using A1 and A3 with Lemma 2,

\[
= \int \left\{ \mathbb{E}[Y(W, S = 1, A = 1)] - \mathbb{E}[Y(W, S = 1, A = 0)] \\
- \mathbb{E}[Y(W, S = 0, A = 1)] + \mathbb{E}[Y(W, S = 0, A = 0)] \right\} \, d\mathbb{P}(W \mid S = 0)
\]

\[
= \int \left\{ \mathbb{E}[Y(W, S = 1, A = 1)] - \mathbb{E}[Y(W, S = 1, A = 0)] \\
- \mathbb{E}[Y(W, S = 0, A = 1)] + \mathbb{E}[Y(W, S = 0, A = 0)] \right\} \, d\mathbb{P}(W \mid S = 0)
\]
By definition,
\[
\delta_{EM} = E[Y(A = 1, M(A = 1, S = 1), S = 1) - Y(A = 0, M(A = 0, S = 1), S = 1) | S = 0] -
E[Y(A = 1, M(A = 1, S = 1), S = 0) - Y(A = 0, M(A = 0, S = 1), S = 0) | S = 0]
\]
\[
= \int \left[ E[Y(A = 1, M(A = 1, S = 1), S = 1) - Y(A = 0, M(A = 0, S = 1), S = 1) | W, S = 0] dP(W | S = 0) -
\right.
\]
\[
\left. \int E[Y(A = 1, M(A = 1, S = 1), S = 0) - Y(A = 0, M(A = 0, S = 1), S = 0) | W, S = 0] dP(W | S = 0) \right] dP(W | S = 0)
\]
By A2,
\[
= \int E[Y(A = 1, M(A = 1, S = 1), S = 1) - Y(A = 0, M(A = 0, S = 1), S = 1) | W, S = 1] dP(W | S = 0) -
\]
\[
\int E[Y(A = 1, M(A = 1, S = 1), S = 0) - Y(A = 0, M(A = 0, S = 1), S = 0) | W, S = 0] dP(W | S = 0)
\]
\[
\delta_{EM} = \int \left\{ E \left[ Y(1, M(1, 1)) - Y(0, M(0, 1)) \mid W, S = 1 \right] - \right.
\]
\[
\left. E \left[ Y(1, M(1, 1)) - Y(0, M(0, 1)) \mid W, S = 0 \right] \right\} dP(W \mid S = 0)
\]
Now, take the third term for example:
\[
E \left[ Y(1, M(1, 1)) \mid W, S = 0 \right] = \int E \left[ Y(1, m) \mid M(1, 1) = m, W, S = 0 \right] P(M(1, 1) = m \mid W, S = 0) \, dm
\]
By A5,
\[
= \int E \left[ Y(1, m) \mid W, S = 0 \right] P(M(1, 1) = m \mid W, S = 0) \, dm
\]
By A4,
\[
= \int E \left[ Y(1, m) \mid W, S = 0 \right] P(M(1, 1) = m \mid W, S = 1) \, dm
\]
\[
= \int E \left[ Y(1, m) \mid W, S = 0 \right] P(M(1) = m \mid W, S = 1) \, dm
\]
By A3,
\[
= \int E \left[ Y(1, m) \mid W, S = 0, A = 1 \right] dP(m \mid W, S = 1, A = 1)
\]
By A5,
\[
= \int E \left[ Y(1, m) \mid W, S = 0, A = 1, m \right] dP(m \mid W, S = 1, A = 1)
\]
\[ \mathbb{E}[Y(1, M(1, 1)) | W, S = 0] = \int \mathbb{E}[Y | W, S = 0, A = 1, m] \, dP(m | W, S = 1, A = 1) \]

Expanding the other terms similarly,
\[
\delta_{EM} = \int \left\{ \int \mathbb{E}[Y | W, S = 1, A = 1, m] \, dP(m | W, S = 1, A = 1) \\
- \int \mathbb{E}[Y | W, S = 1, A = 0, m] \, dP(m | W, S = 1, A = 0) \\
- \int \mathbb{E}[Y | W, S = 0, A = 1, m] \, dP(m | W, S = 1, A = 1) \\
+ \int \mathbb{E}[Y | W, S = 0, A = 0, m] \, dP(m | W, S = 1, A = 0) \right\} \, dP(W | S = 0)
\]

Grouping the first term with the third, and the second with the fourth,
\[
= \int \left\{ f_1(W) - f_0(W) \right\} \, dP(W | S = 0) \\
= \mathbb{E}[f_1(W) - f_0(W) | S = 0]
\]

Finally, by definition
\[
\delta_{MV} = \mathbb{E}[Y(A = 1, M(A = 1, S = 1), S = 0) - Y(A = 0, M(A = 0, S = 1), S = 0) | S = 0] - \\
\mathbb{E}[Y(A = 1, M(A = 1, S = 0), S = 0) - Y(A = 0, M(A = 0, S = 0), S = 0) | S = 0]
= \int \mathbb{E}[Y(A = 1, M(A = 1, S = 1), S = 0) - Y(A = 0, M(A = 0, S = 1), S = 0) | W, S = 0] \, dP(W | S = 0) - \\
\int \mathbb{E}[Y(A = 1, M(A = 1, S = 0), S = 0) - Y(A = 0, M(A = 0, S = 0), S = 0) | W, S = 0] \, dP(W | S = 0)
= \int \mathbb{E}[Y(A = 1, M(A = 1, S = 1), S = 0) - Y(A = 0, M(A = 0, S = 1), S = 0) | W, S = 0] \, dP(W | S = 0) - \\
\int \mathbb{E}[Y(A = 1, M(A = 1, S = 0), S = 0) - Y(A = 0, M(A = 0, S = 0), S = 0) | W, S = 0] \, dP(W | S = 0)
\]

\[
\delta_{MV} = \int \left\{ \mathbb{E}[Y(1, M(1, 1)) - Y(0, M(0, 1)) | W, S = 0] \\
- \mathbb{E}[Y(1, M(1, 0)) - Y(0, M(0, 0)) | W, S = 0] \right\} \, dP(W | S = 0)
\]

Manipulating the expressions similarly as above, we can write this as
\[
\delta_{MV} = \int \left\{ \int \mathbb{E}[Y | W, S = 0, A = 1, m] \, dP(m | W, S = 1, A = 1) \\
- \int \mathbb{E}[Y | W, S = 0, A = 0, m] \, dP(m | W, S = 1, A = 0) \\
- \int \mathbb{E}[Y | W, S = 0, A = 1, m] \, dP(m | W, S = 0, A = 1) \\
+ \int \mathbb{E}[Y | W, S = 0, A = 0, m] \, dP(m | W, S = 0, A = 0) \right\} \, dP(W | S = 0)
\]
\[ = \mathbb{E}[d_1(W) - d_0(W) \mid S = 0] \]

### S3 Proof of Proposition 2

Under regularity conditions, this is a corollary of the von Mises representation, which is demonstrated by Lemma 1.

Specifically, note that the definition of the efficient influence function in the nonparametric model is that it must satisfy

\[
\frac{\partial}{\partial \epsilon} \theta(P_\epsilon) \Bigr|_{\epsilon=0} = \mathbb{E}_P[D(O; \eta_P)s_0(O)]
\]

where \( \{P_\epsilon\} \) is a smooth parametric submodel and \( s_0 \) is the score function at \( \epsilon = 0 \). If the von Mises expansion holds, then we have

\[
\theta(P) - \theta(P_\epsilon) = -\mathbb{E}_{P_\epsilon}[D(O; \eta_P)] + R(\eta_P, \eta_P)
\]

Differentiating with respect to \( \epsilon \) yields

\[
-\frac{\partial}{\partial \epsilon} \theta(P_\epsilon) = -\frac{\partial}{\partial \epsilon} \mathbb{E}_{P_\epsilon}[D(O; \eta_P)] + \frac{\partial}{\partial \epsilon} R(\eta_P, \eta_P)
\]

Because \( R \) is second-order, its derivative at zero is zero by the product rule (with the regularity condition that the components of \( \eta \) have bounded first derivatives). Thus,

\[
\frac{\partial}{\partial \epsilon} \theta(P_\epsilon) \Bigr|_{\epsilon=0} = \frac{\partial}{\partial \epsilon} \mathbb{E}_{P_\epsilon}[D(O; \eta_P)] \Bigr|_{\epsilon=0}
\]

\[
= \frac{\partial}{\partial \epsilon} \int D(O; \eta_P) \, dP_\epsilon(O) \Bigr|_{\epsilon=0}
\]

\[
= \int D(O; \eta_P) \frac{\partial}{\partial \epsilon} P_\epsilon(O) \Bigr|_{\epsilon=0} \, d(O)
\]

\[
= \int D(O; \eta_P) \frac{\partial}{\partial \epsilon} P_\epsilon(O) \Bigr|_{\epsilon=0} \, dP(O)
\]

\[
= \int D(O; \eta_P) \frac{\partial}{\partial \epsilon} \log P_\epsilon(O) \Bigr|_{\epsilon=0} \, dP(O)
\]

\[
= \mathbb{E}_P[D(O; \eta_P)s_0(O)]
\]

### S4 Proof of Lemma 1

We will first analyze the following term, denoted \( T_1 \). Throughout, we will use subscripts \( F \) and \( P \) to refer to quantities from each distribution, respectively.

\[
T_1 := \mathbb{E}_P\left\{ \frac{I(S = s_W)}{h_F(s_W)}[q_{M,F}(W, s_Y, s_M, 1) - q_{M,F}(W, s_Y, s_M, 0) - \theta_F] \right\} + \theta_F - \theta_P
\]
\[
\begin{align*}
E_p \left\{ \frac{I(S = s_W)}{h_f(s_W)} \left[ q_{M,F}(W, s_y, s_M, 1) - q_{M,F}(W, s_y, s_M, 0) \right] \right\} - \theta_F & \cdot E_p \{ I(S = s_W) \} + \theta_F - \theta_p \\
= & \quad E_p \left\{ \frac{I(S = s_W)}{h_f(s_W)} \left[ q_{M,F}(W, s_y, s_M, 1) - q_{M,F}(W, s_y, s_M, 0) \right] \right\} - \theta_F + \frac{h_p(s_W)}{h_f(s_W)} + \theta_F - \theta_p \\
= & \quad E_p \left\{ \frac{I(S = s_W)}{h_f(s_W)} \left[ q_{M,F}(W, s_y, s_M, 1) - q_{M,F}(W, s_y, s_M, 0) \right] \right\} - \theta_F + \frac{h_p(s_W)}{h_f(s_W)} + (1 - \theta_F) - \theta_p \\
= & \quad E_p \left\{ \frac{e_p(s_W | W)}{h_f(s_W)} \left[ q_{M,F}(W, s_y, s_M, 1) - q_{M,F}(W, s_y, s_M, 0) \right] \right\} - \theta_F + \frac{h_p(s_W)}{h_f(s_W)} + (1 - \theta_F)(\theta_F - \theta_p) \\
= & \quad E_p \left\{ \frac{e_p(s_W | W)}{h_f(s_W)} \left[ q_{M,F}(W, s_y, s_M, 1) - q_{M,F}(W, s_y, s_M, 0) \right] \right\} - \theta_F + \frac{h_p(s_W)}{h_f(s_W)} + (1 - \theta_F)(\theta_F - \theta_p) \\
= & \quad E_p \left\{ \frac{e_p(s_W | W)}{h_f(s_W)} \left[ q_{M,F}(W, s_y, s_M, 1) - q_{M,F}(W, s_y, s_M, 0) \right] \right\} - \theta_F + \frac{h_p(s_W)}{h_f(s_W)} + (1 - \theta_F)(\theta_F - \theta_p) \\
= & \quad E_p \left\{ \frac{e_p(s_W | W)}{h_f(s_W)} \left[ q_{M,F}(W, s_y, s_M, 1) - q_{M,F}(W, s_y, s_M, 0) \right] \right\} - \theta_F + \frac{h_p(s_W)}{h_f(s_W)} + (1 - \theta_F)(\theta_F - \theta_p) \\
\end{align*}
\]

Next, take

\[
T_2 := E_p \left\{ \frac{e_p(s_W | W)}{h_f(s_W)} \left[ q_{M,F}(W, s_y, s_M, 1) - q_{M,F}(W, s_y, s_M, 0) \right] \right\} - \theta_F + \frac{h_p(s_W)}{h_f(s_W)} + (1 - \theta_F)(\theta_F - \theta_p)
\]

For brevity, we will derive the \( A = 1 \) term and write the \( A = 0 \) term at the end.

\[
E_p \left\{ \frac{e_p(s_W | W)}{e_p(s_M | W)} \cdot \frac{I(A = 1, S = s_M)}{g_f(A | W, s_M) \cdot h_f(s_W)} \left\{ q_{Y,F}(W, s_y, A, M) - q_{M,F}(W, s_y, s_M, A) \right\} \right\} - \ldots
\]

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So far, the teal terms are already second-order, and the red terms combine and factorize to yield

\[
\mathbb{E}_p \left\{ e_F(s_W | W) \cdot \frac{I(A = 1, S = s_M)}{g_F(A | W, s_M) \cdot h_F(s_W)} \{ q_{y,F}(W, s_Y, A, M) - q_{y,P}(W, s_Y, A, m) \} \right\} + \\
\mathbb{E}_p \left\{ e_F(s_W | W) \cdot \frac{I(A = 1, S = s_M)}{g_F(A | W, s_M) \cdot h_F(s_W)} \{ q_{y,F}(W, s_Y, A, M) - q_{y,P}(W, s_Y, A, m) \} \right\} - \ldots \\
\mathbb{E}_p \left\{ e_F(s_W | W) \cdot \frac{I(A = 1, S = s_M)}{g_F(A | W, s_M) \cdot h_F(s_W)} \{ q_{y,F}(W, s_Y, A, M) - q_{y,P}(W, s_Y, A, m) \} \right\} + \\
\mathbb{E}_p \left\{ e_F(s_W | W) \cdot \frac{I(A = 1, S = s_M)}{g_F(A | W, s_M) \cdot h_F(s_W)} \{ q_{y,F}(W, s_Y, A, M) - q_{y,P}(W, s_Y, A, m) \} \right\} - \ldots \\
\mathbb{E}_p \left\{ e_F(s_W | W) \cdot \frac{I(A = 1, S = s_M)}{g_F(A | W, s_M) \cdot h_F(s_W)} \left\{ q_{y,F}(W, s_Y, A, M) - q_{y,P}(W, s_Y, A, M) \right\} \right\} + \\
\mathbb{E}_p \left\{ e_F(s_W | W) \cdot \frac{I(A = 1, S = s_M)}{g_F(A | W, s_M) \cdot h_F(s_W)} \left\{ q_{y,F}(W, s_Y, A, M) - q_{y,P}(W, s_Y, A, M) \right\} \right\} - \ldots \\
\mathbb{E}_p \left\{ e_F(s_W | W) \cdot \frac{I(A = 1, S = s_M)}{g_F(A | W, s_M) \cdot h_F(s_W)} \left\{ q_{y,F}(W, s_Y, A, M) - q_{y,P}(W, s_Y, A, M) \right\} \right\}
\]

So far, the teal terms are already second-order, and the red terms combine and factorize to yield

\[
\mathbb{E}_p \left\{ e_F(s_W | W) - e_F(s_W | W) \right\} \left\{ q_{y,F}(W, s_Y, A, M) - q_{y,P}(W, s_Y, A, M) \right\} + \\
\mathbb{E}_p \left\{ e_F(s_W | W) - e_F(s_W | W) \right\} \left\{ q_{y,F}(W, s_Y, A, M) - q_{y,P}(W, s_Y, A, M) \right\} - \\
\mathbb{E}_p \left\{ e_F(s_W | W) - e_F(s_W | W) \right\} \left\{ q_{y,F}(W, s_Y, A, M) - q_{y,P}(W, s_Y, A, M) \right\} - \\
\mathbb{E}_p \left\{ e_F(s_W | W) - e_F(s_W | W) \right\} \left\{ q_{y,F}(W, s_Y, A, M) - q_{y,P}(W, s_Y, A, M) \right\}
\]

which is also second-order.

The blue terms can be written as

\[
\mathbb{E}_p \left\{ e_F(s_W | W) \cdot \frac{I(A = 1, S = s_M)}{g_F(A | W, s_M) \cdot h_F(s_W)} \{ q_{y,F}(W, s_Y, A, M) - q_{y,P}(W, s_Y, A, M) \} \right\} = \\
\mathbb{E}_p \left\{ e_F(s_W | W) \cdot \frac{e_{M,P}(s_M | W, M)g_{M,P}(1 | W, s_M, M)}{g_f(1 | W, s_M) \cdot h_f(s_W)} \{ q_{y,F}(W, s_Y, 1, M) - q_{y,P}(W, s_Y, 1, M) \} \right\}
\]
and
\[ \mathbb{E}_P \left\{ \frac{e_F(s_W \mid W)}{e_F(s_M \mid W)} \cdot I(A = 0, S = s_M) \cdot g_F(A \mid W, s_M) \cdot h_F(s_W) \{q_{Y,F}(W, s_Y, A, M) - q_{Y,P}(W, s_Y, A, M)\} \right\} = \]
\[ \mathbb{E}_P \left\{ \frac{e_F(s_W \mid W)}{e_F(s_M \mid W)} \cdot e_{M,F}(s_M \mid W, M) g_{M,F}(0 \mid W, s_M) \cdot h_F(s_W) \{q_{Y,F}(W, s_Y, 0, M) - q_{Y,P}(W, s_Y, 0, M)\} \right\} \]

Finally,
\[ T_3 := \mathbb{E}_P \left\{ \frac{g_{M,F}(A \mid W, s_M, M)}{g_{M,F}(A \mid W, s_Y, M)} e_{M,F}(s_M \mid W, M) e_F(s_W \mid W) \cdot (2A - 1)I(S = s_Y) \cdot g_{F}(A \mid W, s_M) h_{F}(s_W) \{q_{Y,F}(W, S, A, M)\} \right\} \]

Again, for brevity, we will simply derive the \( A = 1 \) term since the \( A = 0 \) term is similar with opposite sign.
\[ = \mathbb{E}_P \left\{ \frac{g_{M,F}(A \mid W, s_M, M)}{g_{M,F}(A \mid W, s_Y, M)} e_{M,F}(s_M \mid W, M) e_F(s_W \mid W) \cdot I(A = 1, S = s_Y) \cdot g_{F}(A \mid W, s_M) h_{F}(s_W) \{q_{Y,F}(W, S, A, M)\} \right\} - \]
\[ = \mathbb{E}_P \left\{ \frac{g_{M,F}(A \mid W, s_M, M)}{g_{M,F}(A \mid W, s_Y, M)} e_{M,F}(s_M \mid W, M) e_F(s_W \mid W) \cdot I(A = 1, S = s_Y) \cdot g_{F}(A \mid W, s_M) h_{F}(s_W) \{q_{Y,F}(W, s_Y, 1, M)\} \right\} - \]
\[ = \mathbb{E}_P \left\{ \frac{g_{M,F}(A \mid W, s_M, M)}{g_{M,F}(A \mid W, s_Y, M)} e_{M,F}(s_M \mid W, M) e_F(s_W \mid W) \cdot I(A = 1, S = s_Y) \cdot g_{F}(A \mid W, s_M) h_{F}(s_W) \{q_{Y,F}(W, s_Y, 1, M)\} \right\} - \]
\[ = \mathbb{E}_P \left\{ \frac{g_{M,F}(A \mid W, s_M, M)}{g_{M,F}(A \mid W, s_Y, M)} e_{M,F}(s_M \mid W, M) e_F(s_W \mid W) \cdot I(A = 1, S = s_Y) \cdot g_{F}(A \mid W, s_M) h_{F}(s_W) \{q_{Y,F}(W, s_Y, 1, M)\} \right\} - \]
\[ = \mathbb{E}_P \left\{ \frac{g_{M,F}(A \mid W, s_M, M)}{g_{M,F}(A \mid W, s_Y, M)} e_{M,F}(s_M \mid W, M) e_F(s_W \mid W) \cdot I(A = 1, S = s_Y) \cdot g_{F}(A \mid W, s_M) h_{F}(s_W) \{q_{Y,F}(W, s_Y, 1, M)\} \right\} - \]
\[ = \mathbb{E}_P \left\{ \frac{g_{M,F}(A \mid W, s_M, M)}{g_{M,F}(A \mid W, s_Y, M)} e_{M,F}(s_M \mid W, M) e_F(s_W \mid W) \cdot I(A = 1, S = s_Y) \cdot g_{F}(A \mid W, s_M) h_{F}(s_W) \{q_{Y,F}(W, s_Y, 1, M)\} \right\} - \]
\[ = \mathbb{E}_P \left\{ \frac{g_{M,F}(A \mid W, s_M, M)}{g_{M,F}(A \mid W, s_Y, M)} e_{M,F}(s_M \mid W, M) e_F(s_W \mid W) \cdot I(A = 1, S = s_Y) \cdot g_{F}(A \mid W, s_M) h_{F}(s_W) \{q_{Y,F}(W, s_Y, 1, M)\} \right\} - \]
\[ = \mathbb{E}_P \left\{ \frac{g_{M,F}(A \mid W, s_M, M)}{g_{M,F}(A \mid W, s_Y, M)} e_{M,F}(s_M \mid W, M) e_F(s_W \mid W) \cdot I(A = 1, S = s_Y) \cdot g_{F}(A \mid W, s_M) h_{F}(s_W) \{q_{Y,F}(W, s_Y, 1, M)\} \right\} - \]

...
Here, the teal term is second order, and the brown term combines with the previous brown $A = 1$ term to yield

\[
E_P\left\{g_{M,F}(1) - g_{M,F}(1 | W, s_M) \right\} = \int C * \left((g_{M,P} - g_{M,F}) + (e_{M,P} - e_{M,F})\right) * (q_{Y,F} - q_{Y,P}) \ dP
\]

where the missing factor can be absorbed into $C$ due to L’Hospital’s rule.

S5 Proof of Proposition 3

Consider the expression $E[Y(1, M(1, s_M)) | W, S = s_Y]$, which we can expand as

\[
\int E[Y(1, m) | M(1, s_M) = W, S = s_Y, m] \ P(M(1, s_M) = m | W, S = s_Y) \ d m
\]

By A5,

\[
\int E[Y(1, m) | W, S = s_Y] \ P(M(1, s_M) = m | W, S = s_Y) \ d m
\]

By A4,

\[
\int E[Y(1, m) | W, S = s_Y] \ P(M(1, s_M) = m | W, S = s_M) \ d m
\]

By A3,

\[
\int E[Y(1, m) | W, S = s_Y, A = 1] \ P(M(1) = m | W, S = s_M, A = 1) \ d m
\]

By A5,

\[
\int E[Y(1, m) | W, S = s_Y, A = 1, m] \ P(m | W, S = s_M, A = 1) \ d m
\]

Manipulating $E[Y(0, M(0, s_M)) | W, S = s_Y]$ analogously and integrating over $W$ yields the desired result. Note that throughout the proof, A1 ensures positive probability/probability density of conditioning events.
Proof of Theorem 2

From equation 4, our estimator is given by

\[ \tilde{\theta} = \theta(\hat{\eta}) + \frac{1}{n} \sum_{i=1}^{n} D(O_i; \hat{\eta}) \]

Following Lemma 1,

\[ = \theta - E[D(O; \hat{\eta})] + R(\eta, \hat{\eta}) + \frac{1}{n} \sum_{i=1}^{n} D(O_i; \hat{\eta}) \]

\[ = \theta - E[D(O; \hat{\eta})] + R(\eta, \hat{\eta}) + \frac{1}{n} \sum_{i=1}^{n} D(O_i; \hat{\eta}) + \sum_{i=1}^{n} D(O_i; \eta) - \frac{1}{n} \sum_{i=1}^{n} D(O_i; \eta) \]

Noting that \( E[D(O; \eta)] = 0 \), and letting \( P \) and \( P_n \) denote true and empirical expected values, respectively, we have

\[ \tilde{\theta} = \theta + R(\eta, \hat{\eta}) + (P_n - P)(D(O; \hat{\eta}) - D(O; \eta)) + P_n(D(O; \eta)). \]

By the assumption of the theorem, we have a bound on \( R(\eta, \hat{\eta}) \):

\[ \tilde{\theta} - \theta = P_n(D(O; \eta)) + (P_n - P)(D(O; \hat{\eta}) - D(O; \eta)) + o_P(n^{-1/2}) \]

\[ \sqrt{n}(\tilde{\theta} - \theta) = \sqrt{n}P_n(D(O; \eta)) + \sqrt{n}(P_n - P)(D(O; \hat{\eta}) - D(O; \eta)) + o_P(1) \]

Since the first term on the right-hand side is subject to the central limit theorem, Theorem 2 is proved if \( (P_n - P)(D(O; \hat{\eta}) - D(O; \eta)) = o_P(n^{-1/2}) \). Under assumption (iii) of the theorem, this is true; see Theorem 19.24 of van der Vaart (1998b).

For a full treatment of these concepts, see Kennedy (2016), especially Section 4.2.

Estimators of the variance parameters

Assume we have efficient estimators of \( \theta(s_Y, s_M, s_W) \) for all values of the arguments as well as efficient influence functions calculated for each observation, denoted \( D_i(s_Y, s_M, s_W) \).

We will start with \( \tau_{CM}^2 := E_S[\text{Var}_S[\theta(s_Y, S_M, S_W) \mid S_Y, S_M]]. \) Recall that for \( E_S \) and \( \text{Var}_S \) we use a uniform distribution over \( S \), but the empirical distribution could be used as well. We can write

\[ \text{Var}_S[\theta(s_Y, s_M, S_W)] = \sum_{0 \leq j < i < K} C \cdot (\theta(s_Y, s_M, i) - \theta(s_Y, s_M, j))^2 \]

where \( C = \frac{K-1}{2K-\frac{3}{2}} \). Using the delta method with this expression (see, e.g., van der Vaart (1998a)), the influence function of \( \text{Var}_S[\theta(s_Y, s_M, S_W)] \) can be found by differentiation to equal

\[ D_{\tau_{CM}} := \sum_{0 \leq j < i < K} 2C \cdot (\tilde{\theta}(s_Y, s_M, i) - \tilde{\theta}(s_Y, s_M, j)) \cdot (D(s_Y, s_M, i) - D(s_Y, s_M, j)) \]
Then since $\tau^2_{CM}$ is just an average of these inner variance terms, its efficient influence function is the average of their influence functions. Let this efficient influence function be denoted $D_{\tau^2_{CM}}$. Because we have efficient estimators $\hat{\theta}$, we can construct an efficient plug-in estimator

$$\hat{\tau}^2_{CM} = E_S\{\text{Var}_S[\hat{\theta}(S_Y, S_M, S_W) \mid S_Y, S_M]$$

whose standard error can be approximated as the $n^{-1/2}$-scaled standard deviation of the empirical analog of $D_{\tau^2_{CM}}$. Similar logic holds for $\hat{\tau}^2_{EM}$, $\hat{\tau}^2_{MV}$, and $\hat{\tau}^2_{EH}$.

To decompose the total variance as a percentage, we consider $\tau^2 := \text{Var}_S[\theta(S_Y, S_M, S_W)]$. Similarly, we can write

$$\tau^2 = \sum_{(s_Y, s_M, s_W) \neq (s'_Y, s'_M, s'_W)} C \cdot (\theta(s_Y, s_M, s_W) - \theta(s'_Y, s'_M, s'_W))^2$$

with $C = \frac{K^3 - 1}{2K^3 \cdot \binom{K}{2}}$. This has influence function equal to

$$D_{\tau^2} := \sum_{(s_Y, s_M, s_W) \neq (s'_Y, s'_M, s'_W)} C \cdot (\theta(s_Y, s_M, s_W) - \theta(s'_Y, s'_M, s'_W)) \cdot (D(s_Y, s_M, s_W) - D(s'_Y, s'_M, s'_W)).$$

Using the plug-in estimator $\hat{\tau}^2 = \text{Var}_S[\theta(S_Y, S_M, S_W)]$, the parameter $\tau^2_{CM}/\tau^2$ can be estimated as $\hat{\tau}^2_{CM}/\hat{\tau}^2$. Again by the delta method, this has efficient influence function given by

$$(\tau^2)^{-2}[\tau^2 \cdot D_{\tau^2_{CM}} - \tau^2_{CM} \cdot D_{\tau^2}].$$

The expressions for the other terms of the decomposition are similar. When scaled by 100, these can be used to express the variance decomposition in percentages with standard errors estimated from the empirical standard deviation of the influence function, scaled by $n^{-1/2}$.

Our implementation of all these estimators can be found at https://github.com/bjg345/hetero_decomp.
S8  Simulation tables

Table S1: Simulation results. The target parameters are defined as in Section 3. The columns labeled “MSE” and “CP” are the mean squared error and empirical coverage probabilities for the associated target parameters.

| n  | δCM | δEH | δEM | δMV | n\textsuperscript{3}MSE, δCM | n\textsuperscript{3}MSE, δEH | n\textsuperscript{3}MSE, δEM | n\textsuperscript{3}MSE, δMV | CP, δCM | CP, δEH | CP, δEM | CP, δMV |
|----|-----|-----|-----|-----|-----------------|-----------------|-----------------|-----------------|--------|--------|--------|--------|
| 100 | 0e+00 | 0e+00 | 0e+00 | 0e+00 | 2.3e+01 | 4.5e+01 | 5e+00 | 5.1e+00 | 9.6e-01 | 9.6e-01 | 9.6e-01 | 9.6e-01 |
| 100 | 0e+00 | 0e+00 | 0e+00 | 0e+00 | 6.6e-01 | 2.4e+01 | 2.7e+00 | 3.8e+00 | 9.7e-01 | 9.3e-01 | 9.3e-01 | 9.5e-01 |
| 100 | 0e+00 | 0e+00 | 0e+00 | 0e+00 | 2.6e+01 | 4.6e+01 | 3e+00 | 5.5e+01 | 9.6e-01 | 9.4e-01 | 9.5e-01 | 9.6e-01 |
| 100 | 0e+00 | 0e+00 | 3.3e-01 | 6e-01 | 3.8e+00 | 2.2e+01 | 3.8e+00 | 2.1e+01 | 9.6e-01 | 9.4e-01 | 9.4e-01 | 9.6e-01 |
| 100 | 0e+00 | 3.3e-01 | 3.3e-01 | 4.4e-01 | 4.5e+00 | 4.5e+00 | 6.6e+00 | 8.2e-01 | 9.4e-01 | 9.4e-01 | 9.7e-01 | 9.7e-01 |
| 100 | 0e+00 | 5e-01 | 5e-01 | 0e+00 | 2e+00 | 3.5e+01 | 4e+00 | 5.8e+00 | 9.3e-01 | 8.8e-01 | 8.8e-01 | 9.3e-01 |
| 100 | 0e+00 | 6.6e-01 | 3.3e-01 | 3.3e-01 | 3.3e-01 | 4.2e+01 | 5.1e+00 | 7.7e+01 | 8.4e-01 | 9.2e-01 | 8.6e-01 | 9.3e-01 |
| 100 | 0e+00 | 8.3e-01 | 3.3e-01 | 3.3e-01 | 1e+00 | 3.2e+01 | 5.6e+00 | 2.2e+01 | 9.7e-01 | 9.6e-01 | 9.6e-01 | 9.6e-01 |
| 1000 | 0e+00 | 3.3e-01 | 3.3e-01 | 3.3e-01 | 3.3e-01 | 4e+00 | 6e+00 | 1e+01 | 9.4e-01 | 9.5e-01 | 9.5e-01 | 9.5e-01 |
| 1000 | 0e+00 | 3.3e-01 | 3.3e-01 | 3.3e-01 | 3.3e-01 | 3.2e+01 | 3.5e+00 | 1.6e+01 | 9.3e-01 | 9.4e-01 | 9.4e-01 | 9.4e-01 |
| 1000 | 0e+00 | 3.3e-01 | 3.3e-01 | 3.3e-01 | 3.3e-01 | 1.8e+00 | 2.5e+00 | 2.3e+00 | 1.7e+01 | 9.3e-01 | 9.2e-01 | 9.2e-01 | 9.2e-01 |
| 1000 | 0e+00 | 3.3e-01 | 3.3e-01 | 3.3e-01 | 3.3e-01 | 1.6e+00 | 2.3e+00 | 2.3e+00 | 1.7e+01 | 9.3e-01 | 9.2e-01 | 9.2e-01 | 9.2e-01 |
| 1000 | 0e+00 | 8.3e-01 | 3.3e-01 | 3.3e-01 | 3.3e-01 | 3.3e+01 | 4.2e+01 | 5.1e+00 | 7.7e+01 | 8.4e-01 | 9.2e-01 | 8.6e-01 | 9.3e-01 |
| 1000 | 0e+00 | 8.3e-01 | 3.3e-01 | 3.3e-01 | 3.3e-01 | 3.3e+01 | 4.2e+01 | 5.1e+00 | 7.7e+01 | 8.4e-01 | 9.2e-01 | 8.6e-01 | 9.3e-01 |
| 10000 | 0e+00 | 8.3e-01 | 3.3e-01 | 3.3e-01 | 3.3e-01 | 3.3e+01 | 4.2e+01 | 5.1e+00 | 7.7e+01 | 8.4e-01 | 9.2e-01 | 8.6e-01 | 9.3e-01 |
Table S2: Scenarios and Corresponding Parameter Values

| Scenario | Q   | B    | C    | $\delta_{CM}$ | $\delta_{EH}$ | $\delta_{EM}$ | $\delta_{MY}$ |
|----------|-----|------|------|---------------|---------------|---------------|---------------|
| 1        | 0.10| 0.00 | 0.00 | 0.10         | 0.00          | 0.00          | 0.00          |
| 2        | 0.50| 0.00 | 0.00 | 0.00         | 0.00          | 0.00          | 0.00          |
| 3        | 0.10| 1.00 | 0.00 | 0.10         | 0.33          | 0.00          | 0.33          |
| 4        | 0.50| 1.00 | 0.00 | 0.00         | 0.33          | 0.00          | 0.33          |
| 5        | 0.10| 0.00 | 1.00 | 0.73         | 0.34          | 0.34          | 0.00          |
| 6        | 0.50| 0.00 | 1.00 | 0.00         | 0.50          | 0.50          | 0.00          |
| 7        | 0.10| 1.00 | 1.00 | 0.73         | 0.68          | 0.34          | 0.33          |
| 8        | 0.50| 1.00 | 1.00 | 0.00         | 0.83          | 0.50          | 0.33          |

S9 Site-specific study estimates

| Site    | Estimate of Moving with Voucher on Risk of Developing Psychiatric Disorder | Standard Error |
|---------|--------------------------------------------------------------------------|----------------|
| Boston  | -0.033                                                                   | 0.029          |
| Chicago | -0.048                                                                   | 0.027          |
| LA      | 0.064                                                                    | 0.034          |
| NYC     | 0.194                                                                    | 0.019          |

Table S3: All results were approved for release by the U.S. Census Bureau, authorization number CBDRB-FY25-CES018-001.