Causal Mediation in Natural Experiments

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Abstract

Natural experiments are a cornerstone of applied economics, providing settings for estimating causal effects with a compelling argument for treatment ignorability. Economists are often interested in understanding the mechanisms through which causal treatment effects operate, and Causal Mediation (CM) methods achieved this by estimating how much of the treatment effect operates through a proposed mediator. The most popular approach to CM relies on assumptions which are unrealistic in natural experiment settings: assuming the mediator is conditionally ignorable — in addition to the ignorability argument for the initial treatment. This paper shows that this approach leads to biased inference, solving for explicit bias terms when the mediator is not ignorable. Using the case of a Roy model for a mediator, I show that individuals' selection based on expected gains and costs is inconsistent with mediator ignorability without implausible behavioural assumptions, suggesting bias would be large in practice. I consider a control function approach, which overcomes these hurdles under structural assumptions, using cost of mediator take-up as an instrument. Simulations confirm that this method corrects for persistent bias in conventional CM estimates, though require large sample sizes for correct inference. This approach gives applied researchers an alternative method to estimate CM effects when they can only establish a credible argument for randomisation of the initial treatment, as is common in natural experiments.

Keywords: Direct/indirect effects, quasi-experiment, selection, control function.
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Economists use natural experiments to credibly answer social questions, without the trouble of guiding randomisation of what they study. Did Vietnam-era military service lead to income losses? Does access to health insurance lead to employment gains? Do transfer payment lead to measurable long-run economic gains? Quasi-experimental variation gives methods to answer these questions, but give no indication of how these effects came about. Causal Mediation (CM) aims to estimate the mechanisms behind causal treatment effects, by estimating how much of the treatment effect operates through a proposed mediator. For example, how much of the (causal) gain from a transfer payment came from individuals choosing to attend higher education? This paper shows that the conventional approach to estimating CM effects is inappropriate in a natural experiment setting, giving a theoretical framework for how large bias terms are in the real world, and an approach to correctly estimate CM effects under structural assumptions.

This paper starts by answering the following question: what does a selection-on-observables CM approach actually estimate when the mediator is not ignorable? Estimates for the average direct and indirect effects are contaminated by bias terms — a sum of selection bias and non-parametric group differences. I then show how this bias operates in an applied regression framework, with bias coming from a correlated error term, showing that the bias term grows larger with the degree of unexplained selection. If individuals have been choosing whether to partake in a mediator based on expected costs and benefits (i.e., following a rational maximisation process), then assuming the mediator is ignorable gives unlikely implications for choice behaviour. This means the identifying assumption for conventional CM methods are unlikely to hold, and likely lead to biased inference in natural experiment settings.

I consider an alternative control function approach to estimating mediation effects. This approach solves the identification problem by instead placing a structural assumption for selection into the mediator (monotonicity), and assumes the researcher has a valid instrument for mediator take-up. These assumptions may hold in real-world natural experiment settings.

Mediator monotonicity is in-line with conventional theories for selection-into-treatment, and is accepted widely in many applications using an instrumental variables research design. The existence of a valid instrument is a stronger assumption, which will not hold in every applied example, though is important to avoid parametric assumptions. The most compelling example is using data on the cost of mediator take-up as a first-stage instrument, if it varies between individuals for exogenous reasons and is strong in explaining compliance. Using an instrument avoids parametric assumptions on unexplained mediator selection, though limits the wider applicability of the method. This approach is not perfect: it is computationally demanding, and requires large sample sizes for non-parametric estimation steps. Additionally, it provides no harbour for estimating CM effects if the core structural assumptions do not hold true.

The most popular approach to CM estimates direct and indirect effects by assuming that a treatment is ignorable, and then assuming that a mediator is ignorable conditional on the treatment assignment (Imai, Keele & Yamamoto 2010). This approach arose in the statistics literature, and is widely used in epidemiology, medicine, and psychology to estimate mediation effects in observational studies. The applied economics literature has not picked up this practice, partially in an understanding that these assumptions are invalid in most observational settings. Indeed, a new strand of the econometric literature has developed estimators for CM effects under overlapping quasi-experimental research designs (Deuchert, Huber & Schelker 2019, Frölich & Huber 2017), a partial identification approach (Flores & Flores-Lagunes 2009), or testing full mediation through observed channels (Kwon & Roth 2024) — see Huber (2020) for an overview. The new literature has arisen in partial acknowledgement that a conventional selection-on-observables approach to CM in an applied setting can lead to biased inference, and needs alternative methods for credible inference in many cases. This paper makes this part explicit, showing exactly how a conventional approach to CM in a natural experiment can fail in practice.

This paper considers the case when it is not credible to assume the mediator is ignorable (e.g., none of the research designs above apply), leveraging classic labour economic theory for selection-into-treatment to identify direct and indirect effects. A selection-on-observables approach to CM in this setting suffers from bias of the same flavour as classic selection bias (Heckman, Ichimura, Smith & Todd 1998), plus additional bias from group differences. The group differences-bias is a non-parametric version of bad controls bias, which has only previously been studied in a linear setting (Cinelli, Forney & Pearl 2024, Ding & Miratrix 2015).

Throughout, I use the Roy (1951) model as a benchmark for judging the Imai, Keele & Yamamoto (2010) mediator ignorability assumption in a natural experiment setting, and find it unlikely to hold in practice.[1] This motivates a solution to the identification problem inspired by classic labour economic work, which also uses the Roy model as a benchmark (Heckman 1979, Heckman & Honore 1990). I follow the lead of these papers by using a control function approach to correct for the bias developed above. This approach assumes mediator monotonicity, to ensure the mediator follows a selection model (Vytlacil 2002), and a valid instrument for mediator take-up, to avoid parametric assumptions on unobserved selection (Heckman & Navarro-Lozano 2004). Doing so is as an extension of using instruments to identify CM effects — as noted by Frölich & Huber (2017).[2] Using a control function to estimate CM effects builds on the influential Imai, Keele & Yamamoto (2010) approach, marrying the CM literature with labour economic theory on selection-into-treatment for the first time.

This paper proceeds as follows. Section 1 introduces CM, and develops expressions for the bias in mediation estimates in natural experiments. Section 2 describes this bias in

[1] An alternative method to estimate CM effects is ensuring sequential ignorability holds by a running randomised controlled trial for both treatment and mediator at the same time. This setting has been considered in the literature previously, in theory (Imai, Tingley & Yamamoto 2013) and in practice (Ludwig, Kling & Mullainathan 2011).

[2] Indeed, this paper does not improve on control function methods in any way, instead noting its applicability in this setting. See Frölich & Huber (2017) for the newest development of control function methods with instruments, and Imbens (2007) for a general overview of the approach.

applied settings with (1) a regression framework, (2) a setting with selection based on costs and benefits. Section 3 solves the identification problem with a control function, assuming a mediator follows a selection model and a researcher observes exogenous variation in cost of mediator take-up, and gives simulation evidence. Section 4 concludes.

1 Direct and Indirect Effects

Causal mediation decomposes causal effects into two channels, through a mediator (indirect effect) and through all other paths (direct effect). To develop notation for direct and indirect effects, write Z_i for an exogenous binary treatment, D_i a binary mediator, and Y_i an outcome for individuals $i = 1, \ldots, n$.[3] The outcomes are a sum of their potential outcomes.[4]

$$\begin{aligned} D_i &= Z_i D_i(1) + (1 - Z_i) D_i(0), \\ Y_i &= Z_i Y_i(1, D_i(1)) + (1 - Z_i) Y_i(0, D_i(0)). \end{aligned}$$

Assume Z_i is ignorable.[5]

$$Z_i \perp\!\!\!\perp D_i(z), Y_i(z', d), \text{ for } z, z', d = 0, 1$$

There are only two average effects which are identified (without additional assumptions).

[3]Other literatures use different notation. For example, Imai, Keele & Yamamoto (2010) write T_i, M_i, Y_i for the randomised treatment, mediator, and outcome, respectively. I use Z_i, D_i, Y_i to stick to the instrumental variables notation Angrist, Imbens & Rubin (1996), more familiar in empirical economics (Angrist & Pischke 2009).

[4]This paper exclusively focuses on the binary case. See Huber, Hsu, Lee & Lettry (2020) for a discussion of CM with continuous treatment and/or mediator, and the assumptions required.

[5]This assumption can hold conditional on covariates. To simplify notation in this section, leave the conditional part unsaid, as it changes no part of the identification framework.

1. The average first-stage refers to the effect of the treatment on mediator, $Z \to D$.

$$\mathbb{E}\left[D_i \,|\, Z_i = 1\right] - \mathbb{E}\left[D_i \,|\, Z_i = 0\right] = \mathbb{E}\left[D_i(1) - D_i(0)\right]$$

It common in the economics literature to assume that Z influences D in at most one direction, $\Pr\left(D_i(1) \geq D_i(0)\right) = 1$ — monotonicity (Imbens & Angrist 1994). I assume monotonicity (and its conditional variant) holds through-out to simplify notation.[6]

2. The reduced-form effect refers to the effect of the treatment on outcome, $Z \to Y$, and is also known as the intent-to-treat effect in experimental settings, or total effect in causal mediation literature.

$$\mathbb{E}\left[Y_i \,|\, Z_i = 1\right] - \mathbb{E}\left[Y_i \,|\, Z_i = 0\right] = \mathbb{E}\left[Y_i(1, D_i(1)) - Y_i(0, D_i(0))\right]$$

In this setting, Z_i affects outcome Y_i directly, and indirectly via the $D_i(Z_i)$ channel, with no reverse causality. Figure 1 visualises the design, where the direction arrows denote the causal direction (and no reverse causality). On the other hand, mediation aims to decompose the reduced form effect of $Z \to Y$ into these two separate pathways.

$$\text{Average Indirect Effect (AIE), } D(Z) \to Y: \quad \mathbb{E}\left[Y_i(Z_i, D_i(1)) - Y_i(Z_i, D_i(0))\right]$$
$$\text{Average Direct Effect (ADE), } Z \to Y: \quad \mathbb{E}\left[Y_i(1, D_i(Z_i)) - Y_i(0, D_i(Z_i))\right]$$

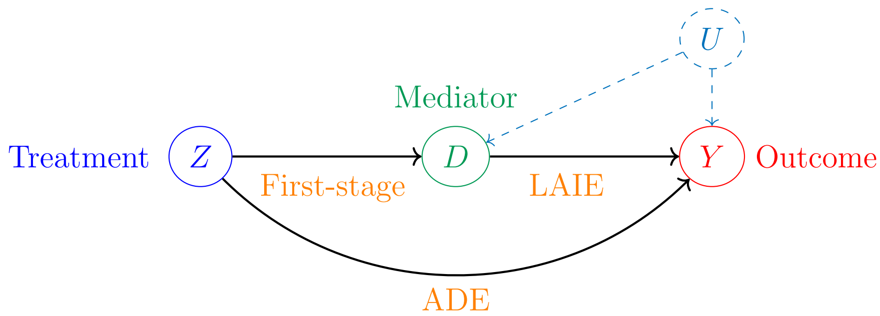
These effects are not separately identified without further assumptions.

1.1 Identifying Causal Mediation (CM) Effects

The conventional approach to estimating direct and indirect effects assumes both Z_i and D_i are ignorable, conditional on a set of control variables $\boldsymbol{X}_i$.

[6] Assuming monotonicity also brings closer to the IV notation, and has other beneficial implications in this setting (see Section 3).

Figure 1: Structural Causal Model for Causal Mediation.



Note: This figures shows the structural causal model behind causal mediation. LAIE refers to the AIE (i.e., effect of the mediator $D \to Y$) local to Z compliers, so that AIE = average first-stage × LAIE. Unobserved confounder U represents this paper's focus on the case that D_i is not ignorable, by showing an implied unobserved confounder. Subsection 2.1 formally defines U in this set-up.

Definition 1. *Sequential Ignorability (Imai, Keele & Yamamoto 2010).*

$$Z_i \perp\!\!\!\perp D_i(z), Y_i(z', d) \;\mid\; \boldsymbol{X}_i, \qquad \text{for } z, z', d = 0, 1 \tag{1}$$

$$D_i \perp\!\!\!\perp Y_i(z', d) \;\mid\; \boldsymbol{X}_i, Z_i = z', \qquad \text{for } z', d = 0, 1 \tag{2}$$

Sequential ignorability assumes that the initial treatment Z_i is assigned randomly, conditional on $\boldsymbol{X}_i$. It then also assumes that, after Z_i is assigned, that D_i is assigned randomly conditional $\boldsymbol{X}_i, Z_i$. If sequential ignorability, 1(1) and 1(2), holds then the direct and indirect effects are identified by two-stage mean differences, after conditioning on $\boldsymbol{X}_i$.[7]

[7] Imai, Keele & Yamamoto (2010) show a general identification statement; I show identification in terms of two-stage regression, which is more familiar in economics. This reasoning is in line with G-computation reasoning (Robins 1986); Subsection A.1 states the Imai, Keele & Yamamoto (2010) identification result, and then develops the two-stage regression notation which holds as a consequence of sequential ignorability.

$$\mathbb{E}_{D_i=d',\boldsymbol{X}_i}\left[\underbrace{\mathbb{E}\left[Y_i \mid Z_i=1, D_i=d', \boldsymbol{X}_i\right] - \mathbb{E}\left[Y_i \mid Z_i=0, D_i=d', \boldsymbol{X}_i\right]}_{\text{Second-stage regression, } Y_i \text{ on } Z_i \text{ holding } D_i \text{ constant}}\right] = \underbrace{\mathbb{E}\left[Y_i(1, D_i(Z_i)) - Y_i(0, D_i(Z_i))\right]}_{\text{Average Direct Effect (ADE)}}$$

$$\mathbb{E}_{Z_i=z',\boldsymbol{X}_i}\left[\underbrace{\left(\mathbb{E}\left[D_i \mid Z_i=1, \boldsymbol{X}_i\right] - \mathbb{E}\left[D_i \mid Z_i=0, \boldsymbol{X}_i\right]\right)}_{\text{First-stage regression, } D_i \text{ on } Z_i} \times \underbrace{\left(\mathbb{E}\left[Y_i \mid Z_i=z', D_i=1, \boldsymbol{X}_i\right] - \mathbb{E}\left[Y_i \mid Z_i=z', D_i=0, \boldsymbol{X}_i\right]\right)}_{\text{Second-stage regression, } Y_i \text{ on } D_i \text{ holding } Z_i \text{ constant}}\right]$$

$$= \underbrace{\mathbb{E}\left[Y_i(Z_i, D_i(1)) - Y_i(Z_i, D_i(0))\right]}_{\text{Average Indirect Effect (AIE)}}$$

I refer to the estimands on the left-hand side as Causal Mediation (CM) estimands. These estimands are typically estimated with linear models, with resulting estimates composed from OLS estimates (Imai, Keele & Yamamoto 2010). While this is the most common approach in the applied literature, I do not assume the linear model. Linearity assumptions are unnecessary to my analysis; it suffices to note that heterogeneous treatment effects and non-linear confounding would bias OLS estimates of CM estimands in the same manner that is well documented elsewhere (see e.g., Angrist 1998, Słoczyński 2022). This section focuses on problems that plague CM in practice, regardless of estimation method.

1.2 Bias in Causal Mediation Estimates

Applied research may use a natural experiment to justify the treatment Z_i is ignorable, justifying assumption 1(1). Rarely does research relying on a quasi-experimental research design employ an additional, overlapping identification design for D_i to justify assumption 1(2) as part of the analysis. One might consider using conventional CM methods to estimate direct and indirect effects, and learn about the mechanisms behind the treatment effect under study.This approach leads to biased estimates, and contaminates inference regarding direct and indirect effects.

Theorem 1. *Absent an identification strategy for the mediator, causal mediation estimates are at risk of selection bias. Suppose 1(1) holds, but 1(2) does not. Then CM estimands are* *contaminated by selection bias and group difference terms.*

Proof. See Subsection A.2 for the extended proof. □

Below I present the relevant selection bias and group difference terms, omitting the conditional on $\boldsymbol{X}_i$ notation for brevity.

For the direct effect: CM estimand = ADE + selection bias + group differences.

$$\mathbb{E}_{D_i=d'}\Big[\mathbb{E}\left[Y_i \,|\, Z_i = 1, D_i = d'\right] - \mathbb{E}\left[Y_i \,|\, Z_i = 0, D_i = d'\right]\Big]$$

$$= \mathbb{E}\left[Y_i(1, D_i(Z_i)) - Y_i(0, D_i(Z_i))\right]$$

$$+ \mathbb{E}_{D_i=d'}\Big[\mathbb{E}\left[Y_i(0, D_i(Z_i)) \,|\, D_i(1) = d'\right] - \mathbb{E}\left[Y_i(0, D_i(Z_i)) \,|\, D_i(0) = d'\right]\Big]$$

$$+ \mathbb{E}_{D_i=d'}\left[\Big(1 - \Pr\left(D_i(1) = d'\right)\Big)\begin{pmatrix}\mathbb{E}\left[Y_i(1, D_i(Z_i)) - Y_i(0, D_i(Z_i)) \,|\, D_i(1) = d'\right] \\ - \mathbb{E}\left[Y_i(1, D_i(Z_i)) - Y_i(0, D_i(Z_i)) \,|\, D_i(0) = 1 - d'\right]\end{pmatrix}\right]$$

For the indirect effect: CM estimand = AIE + selection bias + group differences.

$$\mathbb{E}_{Z_i=z'}\left[\Big(\mathbb{E}\left[D_i \,|\, Z_i = 1\right] - \mathbb{E}\left[D_i \,|\, Z_i = 0\right]\Big) \times \Big(\mathbb{E}\left[Y_i \,|\, Z_i = z', D_i = 1\right] - \mathbb{E}\left[Y_i \,|\, Z_i = z', D_i = 0\right]\Big)\right]$$

$$= \mathbb{E}\left[Y_i(Z_i, D_i(1)) - Y_i(Z_i, D_i(0))\right]$$

$$+ \Pr\left(D_i(1) = 1, D_i(0) = 0\right)\Big(\mathbb{E}\left[Y_i(Z_i, 0) \,|\, D_i = 1\right] - \mathbb{E}\left[Y_i(Z_i, 0) \,|\, D_i = 0\right]\Big)$$

$$+ \Pr\left(D_i(1) = 1, D_i(0) = 0\right) \times$$

$$\left[\begin{array}{l}\Big(1 - \Pr\left(D_i = 1\right)\Big)\begin{pmatrix}\mathbb{E}\left[Y_i(Z_i, 1) - Y_i(Z_i, 0) \,|\, D_i = 1\right] \\ - \mathbb{E}\left[Y_i(Z_i, 1) - Y_i(Z_i, 0) \,|\, D_i = 0\right]\end{pmatrix} \\ + \left(\dfrac{1 - \Pr\left(D_i(1) = 1, D_i(0) = 0\right)}{\Pr\left(D_i(1) = 1, D_i(0) = 0\right)}\right)\begin{pmatrix}\mathbb{E}\left[Y_i(Z_i, 1) - Y_i(Z_i, 0) \,|\, D_i(1) = 0 \text{ or } D_i(0) = 1\right] \\ - \mathbb{E}\left[Y_i(Z_i, 1) - Y_i(Z_i, 0)\right]\end{pmatrix}\end{array}\right]$$

The selection bias terms come from systematic differences between groups who do and do not take the mediator ($D_i = 0$ versus $D_i = 1$), differences not fully unexplained by $\boldsymbol{X}_i$. These selection bias terms would equal to zero if the mediator was ignorable 1(2), but do not necessarily average to zero if not. The group differences represent the fact that a matching estimator gives an average effect on the treated group and, when selection-on-observables does not hold, this is systematically different from the average effect (Heckman et al. 1998).[8,9] The group differences term is a non-parametric framing of the bias from controlling for intermediate outcomes, previously studied only in a linear setting (i.e., bad controls in Cinelli et al. 2024, or M-bias in Ding & Miratrix 2015).

2 Causal Mediation in Applied Settings

In this section, I further develop the issue of selection in causal mediation estimates. First, I show the non-parametric bias terms from above can be written as omitted variables bias in a regression framework. Second, I show how selection bias operates in an applied model for selection into a mediator based on costs and benefits.

2.1 Regression Framework

Inference for CM effects can be written in a regression framework, showing how correlation between the error term and the mediator persistently biases estimates. Write $Y_i(Z, D)$ as a sum of observed factors $Z_i, \boldsymbol{X}_i$ and unobserved factors, $U_{1,i}, U_{0,i}$ (following the notation of Heckman & Vytlacil 2005). For $z', d' = 0, 1$, put $\mu_{d'}(z'; \boldsymbol{X}_i) = \mathbb{E}\left[Y_i(z', d') \,|\, \boldsymbol{X}\right]$, to give a

[8]The group differences term is longer for the AIE estimate, because the indirect effect is comprised from the effect of D_i local to Z_i compliers; a matching estimator gets the average effect on treated, and the longer term adjusts for differences with the complier average effect.

[9]The selection-on-observables approach could, instead, focus on the average effect on treated populations (as do Keele, Tingley & Yamamoto 2015). This runs into a problem of comparisons: CM estimates would give average effects on different treated groups. The CM estimand for the ADE on treated gives the ADE local to the $Z_i = 1$ treated group, and local to the $D_i = 1$ group for the AIE. In this way, these ADE and AIE on treated terms are not comparable to each other, so I focus on the true averages to avoid these misaligned comparisons.

representation of the ADE and AIE.

$$\text{ADE} = \mathbb{E}\left[Y_i(Z_i, D_i(1)) - Y_i(Z_i, D_i(0))\right] = \mathbb{E}\Big[\Big(D_i(1) - D_i(0)\Big) \times \Big(\mu_1(Z_i; \boldsymbol{X}_i) - \mu_0(Z_i; \boldsymbol{X}_i)\Big)\Big],$$
$$\text{AIE} = \mathbb{E}\left[Y_i(1, D_i(Z_i)) - Y_i(0, D_i(Z_i))\right] = \mathbb{E}\Big[\mu_{D_i}(1; \boldsymbol{X}_i) - \mu_{D_i}(0; \boldsymbol{X}_i)\Big].$$

Then define the error terms.

$$U_{0,i} = Y_i(Z_i, 0) - \mu_0(Z_i; \boldsymbol{X}_i), \quad U_{1,i} = Y_i(Z_i, 1) - \mu_1(Z_i; \boldsymbol{X}_i)$$

With this notation, observed data Z_i, D_i, Y_i take the following representation, which characterises direct effects, indirect effects, and selection bias.

$$D_i = \phi + \pi Z_i + \varphi(\boldsymbol{X}_i) + \eta_i \tag{3}$$

$$Y_i = \alpha + \beta D_i + \gamma Z_i + \delta Z_i D_i + \zeta(\boldsymbol{X}_i) + \underbrace{(1 - D_i)\, U_{0,i} + D_i U_{1,i}}_{\text{Correlated error term.}} \tag{4}$$

First-stage (3) is identified, with $\phi, \varphi(\boldsymbol{X}_i)$ the intercept, and π the average rate of compliance (which may depend on $\boldsymbol{X}_i$). Second-stage (4) is not identified thanks to omitted variables bias. $\alpha, \zeta(\boldsymbol{X}_i)$ are the intercept terms, and β, γ, δ are values that comprise mediation effects — all whose values may depend on $\boldsymbol{X}_i$, see Subsection A.3 for full definitions. $(1 - D_i)\, U_{0,i} + D_i U_{1,i}$ is the possibly correlated error term, which disrupts identification. The ADE and AIE are averages of these coefficients.[10]

$$\text{ADE:}\ \ \mathbb{E}\left[Y_i(1, D_i(Z_i)) - Y_i(0, D_i(Z_i))\right] = \mathbb{E}\left[\gamma + \delta D_i\right],$$
$$\text{AIE:}\ \ \mathbb{E}\left[Y_i(Z_i, D_i(1)) - Y_i(Z_i, D_i(0))\right] = \mathbb{E}\left[\pi\left(\beta + \delta Z_i\right)\right].$$

[10] The AIE, in fact, refers only to treatment gains among $D_i(z)$ compliers, so has the more complicated form $\mathbb{E}\Big[\pi \times \mathbb{E}\left[\beta + \delta Z_i \,|\, D_i(1) = 1, D_i(0) = 0\right]\Big]$. The formula above skips the local to compliers part, to keep with regression notation.

By construction, $U_i = U_{0,i} - U_{1,i}$ is an unobserved confounder. The regression estimates of second-stage (4) give unbiased estimates only if D_i is also conditionally ignorable: $D_i \perp\!\!\!\perp U_i$. If not, then regression estimates suffer from omitted variables bias if they do not adjust for the unobserved confounder U_i.

2.2 Selection on Costs and Benefits

CM is at risk of bias because $D_i \perp\!\!\!\perp U_i$ is unlikely to hold in applied settings. Without an identification strategy for D_i (in addition to one for Z_i), bias will persist, given how we conventionally think of selection into treatment.

Consider a model where individual i selects into a mediator based on costs and benefits, after $Z_i, \boldsymbol{X}_i$ have been assigned. Write C_i for individual i's costs of taking mediator D_i, and $\mathbb{1}\{.\}$ for the indicator function. The Roy model has i taking the mediator if the benefits exceed the costs.

$$D_i\left(z'\right) = \mathbb{1}\left\{\underbrace{Y_i\left(z', 1\right) - Y_i\left(z', 0\right)}_{\text{Benefits}} \geq \underbrace{C_i}_{\text{Costs}}\right\}, \quad \text{for } z' = 0, 1$$

The Roy model provides a robust and intuitive framework for analysing selection mechanisms because it captures the fundamental economic principle of decision-making based on costs and benefits in terms of the outcome observed (Roy 1951, Heckman & Honore 1990). If the outcome Y_i is a measure of income, and the mediator a choice of taking education, then it models an individual choice to attend more education in terms of gaining a higher income.[11] This makes it particularly useful as a base case when studying causal mediation, where selection into the mediator may be driven by private information (unobserved by the researcher). Additionally, the Roy model aligns well with many real-world settings, such as education or labour market participation, where decisions are based on a comparison of

[11] If the choice is made for a sum of outcomes, then a simple extension of the framework to a utility maximisation model maintains the same spirit. See Heckman & Honore (1990) for this approach.

expected outcomes across alternatives. By using the Roy model as a benchmark, I explore the practical limits of the mediator ignorability assumption.

Decompose the costs into its mean and unobserved error, as above $C_i(Z_i) = \mu_C(Z_i; \boldsymbol{X}_i) + U_{C,i}$, and collect the mean benefits, $\mu \coloneqq \mu_1 - \mu_0$. So we can write the first-stage selection equation separated by observed means and unobserved errors.

$$D_i(z') = \mathbb{1}\left\{\mu(z'; \boldsymbol{X}_i) - \mu_C(z'; \boldsymbol{X}_i) \geq U_{C,i} - U_i\right\}, \quad \text{for } z' = 0, 1$$

If selection is Roy style, and the mediator is ignorable, then unobserved benefits play no part in selection. The only driver in differences in selection are differences in costs (and not benefits).

$$\mathbb{E}\left[D_i(z') \,|\, U_i = u\right] = \mathbb{E}\left[D_i(z') \,|\, U_i = u'\right]$$

For all u', u in the range of the distribution of $U_i = U_{1,i} - U_{0,i}$. This could, for example, hold if $U_{0,i}, U_{1,i}$ are degenerate conditional on $\boldsymbol{X}_i$.[12]

This means than the vector of control variables $\boldsymbol{X}_i$ must be incredibly rich. Together, $\boldsymbol{X}_i$ and unobserved cost differences $U_{C,i}$ must explain selection into D_i one hundred percent. In the Roy model framework, however, individuals make decisions about mediator take-up based on gains, which the researcher may not observe fully. These unobservables are unlikely to be fully captured by any observable control set $\boldsymbol{X}_i$.[13] Consequently, the assumption of mediator ignorability is implausible in most practical settings (absent a separate research design for D_i).

[12] This statement holds by a simple proof by contradiction: suppose there are u', u such that the statement does not hold, then D_i cannot be ignorable.

[13] In a similar sense, Huber, Kloiber & Laffers (2024) give a method to test the implications of sequential ignorability (requiring an instrument).

3 Solving Identification with a Control Function

If your goal is to estimate CM effects, and you could control for unobserved selection terms $U_{0,i}, U_{1,i}$, then you would. This ideal example would yield unbiased estimates. The control function method takes this insight seriously, providing conditions to model the implied unobserved confounding by $U_{0,i}, U_{1,i}$, and then control for it.[14]

Suppose the vector of control variables $\boldsymbol{X}_i$ has at least two entries; denote $\boldsymbol{X}_i^{\text{IV}}$ as one entry in the vector, and $\boldsymbol{X}_i^-$ as the remaining rows.

Definition 2. *Control function assumptions.*

$$\Pr\left(D_i(1) \geq D_i(0) \,|\, \boldsymbol{X}_i\right) = 1 \tag{5}$$

$$\boldsymbol{X}_i^{IV} \textit{ has the property } \frac{\partial \mu(\boldsymbol{X}_i)}{\partial \boldsymbol{X}_i^{IV}} = 0 < \frac{\partial D_i(z')}{\partial \boldsymbol{X}_i^{IV}}, \text{ for } z' = 0, 1. \tag{6}$$

Assumption 2(5) is the (conditional) monotonicity assumption (Imbens & Angrist 1994), which is untestable but acceptable in many empirical applications. Assumption 2(6) is assuming that an instrument exists, which satisfies an exclusion restriction (i.e., not impacting mediator gains μ), and has a non-zero influence on the mediator (i.e., strong first-stage). The exclusion restriction is untestable, and must be guided by domain-specific knowledge; strength of the first-stage is testable, and must be justified with data by methods common in the instrumental variables literature.

Write K_i for the error in predicting the mediator with observed data, as a function of the instrument $\boldsymbol{X}_i^{\text{IV}}$ and remaining controls $\boldsymbol{X}_i^-$. K_i serves as the control function in this setting.

$$K_i = D_i - \mathbb{E}\left[D_i \,\middle|\, Z_i, \boldsymbol{X}_i^{\text{IV}}, \boldsymbol{X}_i^-\right]$$

Theorem 2. *If 2(5) and 2(6) hold, then the average potential outcomes are identified by a*

[14] This section does not improve on the control function approach, instead only noting its utility to solve the identification problem of CM in a natural experiment setting.

control function approach.

$$\mathbb{E}\left[Y_i \,\middle|\, Z_i = z', D_i = d', \boldsymbol{X}_i^-, K_i\right] = \mathbb{E}\left[Y_i(z', d') \,\middle|\, \boldsymbol{X}_i^-, K_i\right], \quad \textit{for } z', d' = 0, 1.$$

Proof. Special case of Imbens & Newey (2009, Theorem 1); see Subsection A.4. □

Assumption 2(5) guarantees that mediator $D_i(.)$ can be represented by a selection model (Vytlacil 2002), and 2(6) pins down a control function to identify the selection model. The approach exploits the fact that the bias terms, coming from correlated the errors in Subsection 2.1, can be estimated in a first-stage regression and included as controls in the second-stage.

If the underlying selection model had been a Roy model, the control function approach captures the unobserved benefits to taking mediator (independent of observed controls), and thus driving take-up of the mediator. By incorporating the selection term derived from the first-stage model, the approach adjusts for the unobserved confounding from unobserved gains. By contrast, assuming the mediator was ignorable would have been assuming that there are no unobserved benefits to the mediator take-up, so that there is no bias in the second-stage to account for.

The instrument is key to avoid distributional assumptions on the unobserved errors terms. In the Roy model, the exclusion restriction can be satisfied in one key way: having an instrument for cost of mediator take up μ_C. If the instrument $\boldsymbol{X}_i^{\mathrm{IV}}$ enters the cost function μ_C, and not the benefits function μ, then it satisfies the exclusion restriction. In an applied world, $\boldsymbol{X}_i^{\mathrm{IV}}$ can be data that explain cost differences in taking D_i, unrelated to other demographic information. If a researcher is looking into higher education as a proposed mediator, then data which explains different costs of attending university (unrelated to education gains) can serve this role. This is the logic behind the Card (1993) distance-instrument, and can be extended to a CM setting with education as the mediator.

3.1 Estimation

In practice, the approach relies on estimating the control function K_i, then including this in the second-stage as a control, and accounting for the estimation error for these in the standard errors. These reliances come with major concerns. First, it is imperative that the control function is estimated correctly, so it is necessary to employ a non-parametric approach to estimate the first-stage. Second, the error terms enters the outcome equation (4) linearly, but is an unknown function (possibly non-linear) of the control function; thus, the second-stage must be estimated semi-parametrically.[15] Lastly, the standard errors must account for estimation uncertainty in the above two non-parametric steps.

These concerns are worth noting, because non-parametric regression is computationally demanding, and requires large samples for estimator convergence. Furthermore, these are estimated in two steps, so that the concerns are of greater importance. Otherwise, small sample bias properties could even dominate the bias terms identified in Theorem 1.[16] It is beyond the scope of this paper to develop the optimal procedure here, but these concerns are important. For applied research aiming to estimate CM effects, the control function method is only appropriate in extremely large sample sizes, such as applications using administrative sources or biobanks.

With these concerns in mind, I propose the following method to estimate CM effects with a control function approach:

1. Estimate the first-stage, $\mathbb{E}\left[D_i \,\middle|\, Z_i, \boldsymbol{X}_i^{\mathrm{IV}}, \boldsymbol{X}_i^{-}\right]$ with a non-parametric estimator (e.g., a probability forest, or fully interacted OLS specification).

2. Calculate estimates of the control function, $\widehat{K}_i = D_i - \widehat{\mathbb{E}}\left[D_i \middle| Z_i, \boldsymbol{X}_i^{\mathrm{IV}}, \boldsymbol{X}_i^{-}\right]$.

[15] In practice this can be done by adding a polynomial for the estimated control function into the outcome regression, or a splines approach, etc.

[16] See (Imbens & Newey 2009, Section 6) for a full discussion of the asymptotic theory of a control function estimator.

3. Estimate the second-stage with OLS (including an interaction term between Z_i and D_i), and a semi-parametric regressor of the control function. $l(.)$ is a semi-parametric nuisance function, so can be approximated with a spline specification, for example.

$$\mathbb{E}\left[Y_i \middle| Z_i, D_i, \boldsymbol{X}_i^-, \widehat{K}_i\right] = \beta D_i + \gamma Z_i + \delta Z_i D_i + l\left(\widehat{K}_i\right)$$

Estimate the ADE from this second-stage.

$$\widehat{\text{ADE}} = \mathbb{E}\left[\widehat{\mathbb{E}}\left[Y_i \middle| Z_i = 1, D_i, \boldsymbol{X}_i^-, \widehat{K}_i\right] - \widehat{\mathbb{E}}\left[Y_i \middle| Z_i = 0, D_i, \boldsymbol{X}_i^-, \widehat{K}_i\right]\right]$$

4. Estimate the second-stage with weighted-least squares, including a control function with (estimated) κ-weights (Abadie 2003).

$$\widehat{\kappa}_i = 1 - \frac{(1 - Z_i) D_i}{1 - \widehat{\Pr}\left(Z_i = 1 \middle| \boldsymbol{X}_i^-, \boldsymbol{X}_i^{\text{IV}}\right)} - \frac{Z_i (1 - D_i)}{\widehat{\Pr}\left(Z_i = 1 \middle| \boldsymbol{X}_i^-, \boldsymbol{X}_i^{\text{IV}}\right)}$$

$$\mathbb{E}\left[\widehat{\kappa}_i Y_i \middle| Z_i, D_i, \boldsymbol{X}_i^-, \widehat{K}_i\right] = \beta D_i + \gamma Z_i + \delta Z_i D_i + l\left(\widehat{K}_i\right)$$

Estimate the AIE from this second-stage.

$$\widehat{\text{AIE}} = \mathbb{E}\left[\begin{array}{l} \left(\widehat{\mathbb{E}}\left[D_i \middle| Z_i = 1, \boldsymbol{X}_i^{\text{IV}}, \boldsymbol{X}_i^-\right] - \widehat{\mathbb{E}}\left[D_i \middle| Z_i = 1, \boldsymbol{X}_i^{\text{IV}}, \boldsymbol{X}_i^-\right]\right) \\ \times \left(\widehat{\mathbb{E}}\left[\widehat{\kappa}_i Y_i \middle| Z_i, D_i = 1, \boldsymbol{X}_i^-, \widehat{K}_i\right] - \widehat{\mathbb{E}}\left[\widehat{\kappa}_i Y_i \middle| Z_i, D_i = 0, \boldsymbol{X}_i^-, \widehat{K}_i\right]\right) \end{array}\right]$$

5. Bootstrap across steps 1 through 4, to calculate standard errors for the respective ADE and AIE estimates.

3.2 Simulation Evidence

The following simulation gives an example to show how this method works in practice. Suppose data observed to the researcher $Z_i, D_i, Y_i, \boldsymbol{X}_i$ are drawn from the following data generating processes, for $i = 1, \dots, N$.

$$Z_i \sim \text{Binom}\,(0.5)\,, \quad \boldsymbol{X}_i^- \sim N(4, 1), \quad \boldsymbol{X}_i^{\text{IV}} \sim \text{Binom}\,(0.5)\,,$$
$$[U_{0,i}, U_{1,i}]' \sim \text{BivariateNormal}\,(0, 0, \sigma_0, \sigma_1, \rho)\,, \quad U_{C,i} \sim N(0, 0.25).$$

$N = 10,000$ allows the large sample properties of the approach to operate; indeed, smaller sample sizes may not.

Suppose each i chooses to take mediator D_i based on the costs and benefits (i.e., a Roy model), with following definitions for each $z', d' = 0, 1$.

$$\mu_{d'}\left(z'; \boldsymbol{X}_i\right) = \boldsymbol{X}_i^- + \left(z' + d' + z'd'\right), \;\; \mu_C\left(z'; \boldsymbol{X}_i\right) = 3z' + \boldsymbol{X}_i^- - \boldsymbol{X}_i^{\text{IV}}.$$

Following Section 2, these data have the following outcome equations:

$$D_i = \mathbb{1}\left\{-3Z_i - \boldsymbol{X}_i^{\text{IV}} + \boldsymbol{X}_i^- \geq U_{0,i} - U_{1,i}\right\},$$
$$Y_i = Z_i + D_i + Z_i D_i + \boldsymbol{X}_i^- + (1 - D_i)\,U_{0,i} + D_i U_{1,i}.$$

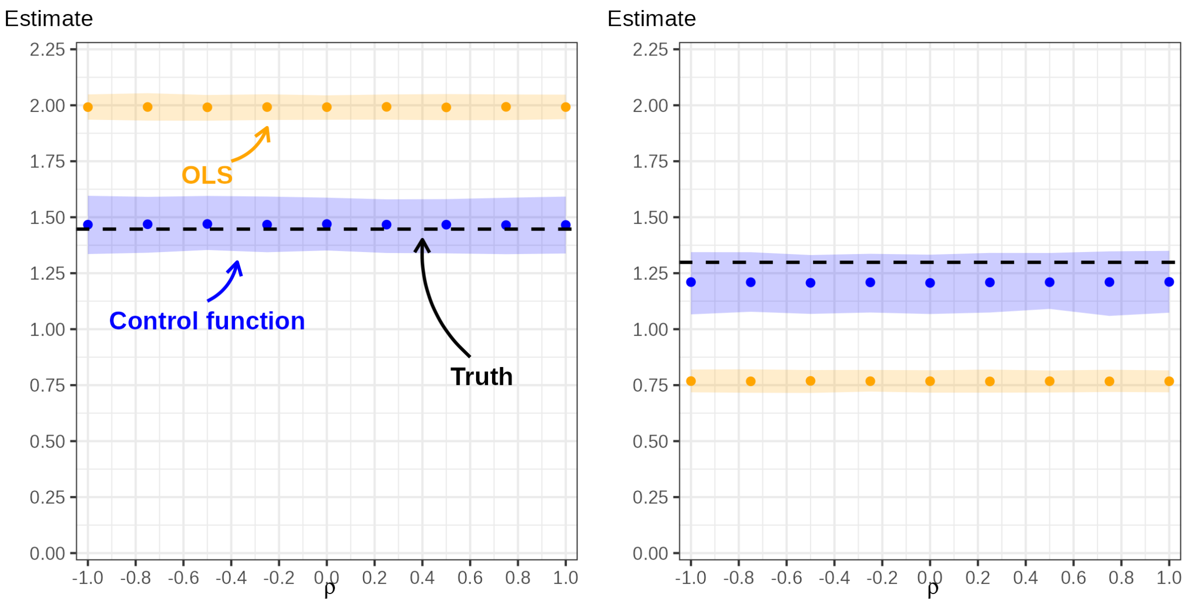
In this setting the error terms $U_{i,0}, U_{i,1}$ determine the bias in OLS estimates of the ADE and AIE, so the bias varies for different values of the DGP parameters $\rho \in [-1, 1]$ and $\sigma_0, \sigma_1 \geq 0$.

Figure 2 shows the control function estimates against estimates calculated by standard OLS, showing 95% confidence intervals calculated from bootstrapped standard errors (from 1,000 bootstrap replications). The OLS approach implicitly asssumes that the mediator is ignorable (when it is not), so its point estimates over and under-estimate the ADE and AIE, respectively; the distance between the OLS estimates and the true values are the underlying bias terms derived in Theorem 1. The control function approach improves on OLS estimates by correcting for the bias terms, with confidence regions overlapping the true values.[17] This

[17]The code behind this simulation estimates the first-stage with an interacted OLS specification, and splines included for the continuous regression. The second-stage is an OLS specification, with estimated

Figure 2: OLS versus Control Function Estimates of CM Effects.

(a) ADE. **(b)** AIE.



Note: These figures show the OLS and control function estimates of the ADE and AIE, for $N = 10,000$ sample size. The black dashed line is the true value, points are points estimates from data simulated with a given ρ value and $\sigma_0 = 1, \sigma_1 = 2$, and shaded regions are the 95% confidence intervals. Orange are the OLS estimates, blue the control function approach.

correction was not free: the standard errors are significantly greater in a control function approach than OLS, and exhibit small sample bias (for reasons mentioned above). In this manner, this simulation shows the pros and cons of using the control function approach to estimating CM effects in practice.

4 Summary and Concluding Remarks

This paper has studied a selection-on-observables approach to CM in a natural experiment setting. I have shown the pitfalls of using the most popular methods for estimating direct and indirect effects without a clear case for the mediator being ignorable. Using the Roy model as a benchmark, a mediator is unlikely to be ignorable in natural experiment settings, and the bias terms likely crowd out inference regarding CM effects.

control function included (with splines) as a linear control.

This paper has contributed to the growing CM literature in economics, integrating labour economic theory for how individuals select into as a way of judging CM methods. It has drawn on the classic literature, and pointed to already-in-use control function methods as a compelling way of estimating direct and indirect effects in a natural experiment. Further research could build on this approach by suggesting efficiency improvements, adjustments for common statistical irregularities (say, cluster dependence), or integrating the control function as an additional robustness in the growing double robustness literature (Huber 2020, Bia, Huber & Lafférs 2024).

This paper has not lit the way for applied researchers to use CM methods unabashedly, with or without a control function adjustment. The structural assumptions are strong and large sample sizes are needed; if the assumptions are broken, then the control function method does not improve on a naïve selection-on-observables approach to CM estimates. And yet, there are likely settings in which the structural assumptions are credible. Mediator monotonicity aligns well with economic theory in many cases, and it is plausible for researchers to study big data settings with exogenous variation in mediator take-up costs. In these cases, this paper opens the door to identifying mechanisms behind treatment effects in natural experiment settings.

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A Appendix

Any comments or suggestions may be sent to me at seh325@cornell.edu, or raised as an issue on the Github project.

A.1 Identification in Causal Mediation

Imai, Keele & Yamamoto (2010, Theorem 1) states that the direct and indirect effects are identified under sequential ignorability, at each level of $Z_i = 0, 1$. For $z' = 0, 1$:

$$\mathbb{E}\left[Y_i(1, D_i(z')) - Y_i(0, D_i(z'))\right] = \int\int \Big(\mathbb{E}\left[Y_i \,|\, Z_i = 1, D_i, \boldsymbol{X}_i\right] - \mathbb{E}\left[Y_i \,|\, Z_i = 0, D_i, \boldsymbol{X}_i\right]\Big) dF_{D_i \,|\, Z_i = z', \boldsymbol{X}_i} dF_{\boldsymbol{X}_i},$$

$$\mathbb{E}\left[Y_i(z', D_i(1)) - Y_i(z', D_i(0))\right] = \int\int \mathbb{E}\left[Y_i \,|\, Z_i = z', D_i, \boldsymbol{X}_i\right] \Big(dF_{D_i \,|\, Z_i = 1, \boldsymbol{X}_i} - dF_{D_i \,|\, Z_i = 0, \boldsymbol{X}_i}\Big) dF_{\boldsymbol{X}_i}.$$

I focus on the averages, which are identified by consequence of the above.

$$\mathbb{E}\left[Y_i(1, D_i(Z_i)) - Y_i(0, D_i(Z_i))\right] = \mathbb{E}_{Z_i}\left[\mathbb{E}\left[Y_i(1, D_i(z')) - Y_i(0, D_i(z')) \,|\, Z_i = z'\right]\right]$$
$$\mathbb{E}\left[Y_i(Z_i, D_i(1)) - Y_i(Z_i, D_i(0))\right] = \mathbb{E}_{Z_i}\left[\mathbb{E}\left[Y_i(z', D_i(1)) - Y_i(z', D_i(0)) \,|\, Z_i = z'\right]\right]$$

My estimand for the average direct effect is a simple rearrangement of the above. The estimand for the average indirect effect relies on a different sequence, relying on (1) sequential ignorability, (2) conditional monotonicity. These give (1) identification of, and equivalence between, LADE conditional on $\boldsymbol{X}_i$ and ADE conditional on $\boldsymbol{X}_i$, (2) identification of the complier score.

$$
\begin{aligned}
&\mathbb{E}\left[Y_i(Z_i, D_i(1)) - Y_i(Z_i, D_i(0)) \,|\, \boldsymbol{X}_i\right] \\
&= \Pr\left(D_i(1) = 1, D_i(0) = 0 \,|\, \boldsymbol{X}_i\right) \mathbb{E}\left[Y_i(Z_i, 1) - Y_i(Z_i, 0) \,|\, D_i(1) = 1, D_i(0) = 0, \boldsymbol{X}_i\right] \\
&= \Pr\left(D_i(1) = 1, D_i(0) = 0 \,|\, \boldsymbol{X}_i\right) \mathbb{E}\left[Y_i(Z_i, 1) - Y_i(Z_i, 0) \,|\, \boldsymbol{X}_i\right] \\
&= \Big(\mathbb{E}\left[D_i \,|\, Z_i = 1, \boldsymbol{X}_i\right] - \mathbb{E}\left[D_i \,|\, Z_i = 0, \boldsymbol{X}_i\right]\Big) \mathbb{E}\left[Y_i(Z_i, 1) - Y_i(Z_i, 0) \,|\, \boldsymbol{X}_i\right] \\
&= \Big(\mathbb{E}\left[D_i \,|\, Z_i = 1, \boldsymbol{X}_i\right] - \mathbb{E}\left[D_i \,|\, Z_i = 0, \boldsymbol{X}_i\right]\Big)\Big(\mathbb{E}\left[Y_i \,|\, Z_i, D_i = 1, \boldsymbol{X}_i\right] - \mathbb{E}\left[Y_i \,|\, Z_i, D_i = 0, \boldsymbol{X}_i\right]\Big)
\end{aligned}
$$

Monotonicity is not technically required for the above. Breaking monotonicity would not change the identification of any of the above; it would be the same except replacing the complier score with a complier or defier score, $\Pr\left(D_i(1) \neq D_i(0) \,|\, \boldsymbol{X}_i\right) = \mathbb{E}\left[D_i \,|\, Z_i = 1, \boldsymbol{X}_i\right] - \mathbb{E}\left[D_i \,|\, Z_i = 0, \boldsymbol{X}_i\right]$.

A.2 Bias in Mediation Estimates

Suppose that Z_i is ignorable conditional on $\boldsymbol{X}_i$, but D_i is not.

A.2.1 Bias in Direct Effect Estimates

To show that the conventional approach to mediation gives an estimate for the ADE with selection and group difference-bias, start with the components of the conventional estimands. This proof starts with the relevant expectations, conditional on a specific value of $\boldsymbol{X}_i$. For each $d' = 0, 1$.

$$\begin{aligned}
\mathbb{E}\left[Y_i \mid Z_i = 1, D_i = d', \boldsymbol{X}_i\right] =& \mathbb{E}\left[Y_i(1, D_i(Z_i)) \mid D_i(1) = d', \boldsymbol{X}_i\right], \\
\mathbb{E}\left[Y_i \mid Z_i = 0, D_i = d', \boldsymbol{X}_i\right] =& \mathbb{E}\left[Y_i(0, D_i(Z_i)) \mid D_i(0) = d', \boldsymbol{X}_i\right]
\end{aligned}$$

And so

$$\begin{aligned}
&\mathbb{E}\left[Y_i \mid Z_i = 1, D_i = d', \boldsymbol{X}_i\right] - \mathbb{E}\left[Y_i \mid Z_i = 0, D_i = d', \boldsymbol{X}_i\right] \\
=& \mathbb{E}\left[Y_i(1, D_i(Z_i)) \mid D_i(1) = d', \boldsymbol{X}_i\right] - \mathbb{E}\left[Y_i(0, D_i(Z_i)) \mid D_i(0) = d', \boldsymbol{X}_i\right] \\
=& \mathbb{E}\left[Y_i(1, D_i(Z_i)) - Y_i(0, D_i(Z_i)) \mid D_i(1) = d', \boldsymbol{X}_i\right] \\
&+ \mathbb{E}\left[Y_i(0, D_i(Z_i)) \mid D_i(1) = d', \boldsymbol{X}_i\right] - \mathbb{E}\left[Y_i(0, D_i(Z_i)) \mid D_i(0) = d', \boldsymbol{X}_i\right]
\end{aligned}$$

The final term is a sum of the ADE, conditional on $D_i(1) = d'$, and a selection bias term — difference in baseline terms between the (partially overlapping) groups for whom $D_i(1) = d'$ and $D_i(0) = d'$.

To reach the final term, note the following.

$$\begin{aligned}
&\mathbb{E}\left[Y_i(1, D_i(Z_i)) - Y_i(0, D_i(Z_i)) \mid \boldsymbol{X}_i\right] \\
=& \mathbb{E}\left[Y_i(1, D_i(Z_i)) - Y_i(0, D_i(Z_i)) \mid D_i(1) = d', \boldsymbol{X}_i\right] \\
&+ \Big(1 - \Pr\left(D_i(1) = d' \mid \boldsymbol{X}_i\right)\Big) \begin{pmatrix} \mathbb{E}\left[Y_i(1, D_i(Z_i)) - Y_i(0, D_i(Z_i)) \mid D_i(1) = d', \boldsymbol{X}_i\right] \\ - \mathbb{E}\left[Y_i(1, D_i(Z_i)) - Y_i(0, D_i(Z_i)) \mid D_i(1) = 1 - d', \boldsymbol{X}_i\right] \end{pmatrix}
\end{aligned}$$

The second term is a difference term between the average and the average for relevant complier groups.

Collect everything together, as follows.

$$\begin{aligned}
&\mathbb{E}\left[Y_i \mid Z_i = 1, D_i = d', \boldsymbol{X}_i\right] - \mathbb{E}\left[Y_i \mid Z_i = 0, D_i = d', \boldsymbol{X}_i\right] \\
=& \underbrace{\mathbb{E}\left[Y_i(1, D_i(Z_i)) - Y_i(0, D_i(Z_i)) \mid \boldsymbol{X}_i\right]}_{\text{ADE, conditional on } \boldsymbol{X}_i} \\
&+ \underbrace{\mathbb{E}\left[Y_i(0, D_i(Z_i)) \mid D_i(1) = d', \boldsymbol{X}_i\right] - \mathbb{E}\left[Y_i(0, D_i(Z_i)) \mid D_i(0) = d', \boldsymbol{X}_i\right]}_{\text{Selection bias}} \\
&+ \underbrace{\Big(1 - \Pr\left(D_i(1) = d' \mid \boldsymbol{X}_i\right)\Big) \begin{pmatrix} \mathbb{E}\left[Y_i(1, D_i(Z_i)) - Y_i(0, D_i(Z_i)) \mid D_i(1) = d', \boldsymbol{X}_i\right] \\ - \mathbb{E}\left[Y_i(1, D_i(Z_i)) - Y_i(0, D_i(Z_i)) \mid D_i(1) = 1 - d', \boldsymbol{X}_i\right] \end{pmatrix}}_{\text{group difference-bias}}
\end{aligned}$$

The proof is achieved by applying the expectation across $D_i = d'$, and $\boldsymbol{X}_i$.

A.2.2 Bias in Indirect Effect Estimates

To show that the conventional approach to mediation gives an estimate for the AIE with selection and group difference-bias, start with the definition of the ADE — the direct effect among compliers times the size of the complier group.

This proof starts with the relevant expectations, conditional on a specific value of $\boldsymbol{X}_i$.

$$\begin{aligned}&\mathbb{E}\left[Y_i(Z_i, D_i(1)) - Y_i(Z_i, D_i(0)) \,|\, \boldsymbol{X}_i\right] \\ =& \Pr\left(D_i(1) = 1, D_i(0) = 0 \,|\, \boldsymbol{X}_i\right) \mathbb{E}\left[Y_i(Z_i, 1) - Y_i(Z_i, 0) \,|\, D_i(1) = 1, D_i(0) = 0, \boldsymbol{X}_i\right]\end{aligned}$$

When D_i is not ignorable, the bias comes from estimating the second term, $\mathbb{E}\left[Y_i(Z_i, 1) - Y_i(Z_i, 0) \,|\, D_i(1) = 1, D_i(0) = 0, \boldsymbol{X}_i\right]$.

For each $z' = 0, 1$.

$$\begin{aligned}\mathbb{E}\left[Y_i \,|\, Z_i = z', D_i = 1, \boldsymbol{X}_i\right] =& \mathbb{E}\left[Y_i(z', 1) \,|\, D_i = 1, \boldsymbol{X}_i\right], \\ \mathbb{E}\left[Y_i \,|\, Z_i = z', D_i = 0, \boldsymbol{X}_i\right] =& \mathbb{E}\left[Y_i(z', 0) \,|\, D_i = 0, \boldsymbol{X}_i\right]\end{aligned}$$

So compose the CM estimand, as follows.

$$\begin{aligned}&\mathbb{E}\left[Y_i \,|\, Z_i = z', D_i = 1, \boldsymbol{X}_i\right] - \mathbb{E}\left[Y_i \,|\, Z_i = z', D_i = 0, \boldsymbol{X}_i\right] \\ =& \mathbb{E}\left[Y_i(z', 1) \,|\, D_i = 1, \boldsymbol{X}_i\right] - \mathbb{E}\left[Y_i(z', 0) \,|\, D_i = 0, \boldsymbol{X}_i\right] \\ =& \mathbb{E}\left[Y_i(z', 1) - Y_i(z', 0) \,|\, D_i = 1, \boldsymbol{X}_i\right] + \mathbb{E}\left[Y_i(z', 0) \,|\, D_i = 1, \boldsymbol{X}_i\right] - \mathbb{E}\left[Y_i(z', 0) \,|\, D_i = 0, \boldsymbol{X}_i\right]\end{aligned}$$

The final term is a sum of the AIE, among the treated group $D_i = 1$, and a selection bias term — difference in baseline terms between the groups $D_i = 1$ and $D_i = 0$.

The AIE is the direct effect among compliers times the size of the complier group, so we need to compensate for the difference between the treated group $D_i = 1$ and complier group $D_i(1) = 1, D_i(0) = 0$.

Start with the difference between treated group's average and overall average.

$$\begin{aligned}&\mathbb{E}\left[Y_i(z', 1) - Y_i(z', 0) \,|\, D_i = 1, \boldsymbol{X}_i\right] \\ =& \mathbb{E}\left[Y_i(z', 1) - Y_i(z', 0) \,|\, \boldsymbol{X}_i\right] \\ &+ \Big(1 - \Pr\left(D_i = 1 \,|\, \boldsymbol{X}_i\right)\Big) \begin{pmatrix} \mathbb{E}\left[Y_i(z', 1) - Y_i(z', 0) \,|\, D_i = 1, \boldsymbol{X}_i\right] \\ - \mathbb{E}\left[Y_i(z', 1) - Y_i(z', 0) \,|\, D_i = 0, \boldsymbol{X}_i\right] \end{pmatrix}\end{aligned}$$

Then the difference between the compliers' average and the overall average.

$$\begin{aligned}&\mathbb{E}\left[Y_i(z', 1) - Y_i(z', 0) \,|\, D_i(1) = 1, D_i(0) = 0, \boldsymbol{X}_i\right] \\ =& \mathbb{E}\left[Y_i(z', 1) - Y_i(z', 0) \,|\, \boldsymbol{X}_i\right] \\ &+ \frac{1 - \Pr\left(D_i(1) = 1, D_i(0) = 0 \,|\, \boldsymbol{X}_i\right)}{\Pr\left(D_i(1) = 1, D_i(0) = 0 \,|\, \boldsymbol{X}_i\right)} \begin{pmatrix} \mathbb{E}\left[Y_i(z', 1) - Y_i(z', 0) \,|\, D_i(1) = 0 \text{ or } D_i(0) = 1, \boldsymbol{X}_i\right] \\ - \mathbb{E}\left[Y_i(z', 1) - Y_i(z', 0) \,|\, \boldsymbol{X}_i\right] \end{pmatrix}\end{aligned}$$

Collect everything together, as follows.

$$
\begin{aligned}
&\mathbb{E}\left[Y_i \,|\, Z_i = z', D_i = 1, \boldsymbol{X}_i\right] - \mathbb{E}\left[Y_i \,|\, Z_i = z', D_i = 0, \boldsymbol{X}_i\right] \\
=& \underbrace{\mathbb{E}\left[Y_i(z', D_i(1)) - Y_i(z', D_i(0)) \,|\, \boldsymbol{X}_i\right]}_{\text{AIE, conditional on } \boldsymbol{X}_i, Z_i = z'} \\
&+ \underbrace{\mathbb{E}\left[Y_i(z', 0) \,|\, D_i = 1, \boldsymbol{X}_i\right] - \mathbb{E}\left[Y_i(z', 0) \,|\, D_i = 0, \boldsymbol{X}_i\right]}_{\text{Selection bias}} \\
&+ \underbrace{\left[\begin{array}{l}
\Big(1 - \Pr\left(D_i = 1 \,|\, \boldsymbol{X}_i\right)\Big)\begin{pmatrix}\mathbb{E}\left[Y_i(z', 1) - Y_i(z', 0) \,|\, D_i = 1, \boldsymbol{X}_i\right] \\ - \mathbb{E}\left[Y_i(z', 1) - Y_i(z', 0) \,|\, D_i = 0, \boldsymbol{X}_i\right]\end{pmatrix} \\
+ \dfrac{1 - \Pr\left(D_i(1) = 1, D_i(0) = 0 \,|\, \boldsymbol{X}_i\right)}{\Pr\left(D_i(1) = 1, D_i(0) = 0 \,|\, \boldsymbol{X}_i\right)}\begin{pmatrix}\mathbb{E}\left[Y_i(z', 1) - Y_i(z', 0) \,|\, D_i(1) = 0 \text{ or } D_i(0) = 1, \boldsymbol{X}_i\right] \\ - \mathbb{E}\left[Y_i(z', 1) - Y_i(z', 0) \,|\, \boldsymbol{X}_i\right]\end{pmatrix}
\end{array}\right]}_{\text{group difference-bias}}
\end{aligned}
$$

The proof is finally achieved by multiplying by the complier score, $\Pr\left(D_i(1) = 1, D_i(0) = 0 \,|\, \boldsymbol{X}_i\right) = \mathbb{E}\left[D_i \,|\, Z_i = 1, \boldsymbol{X}_i\right] - \mathbb{E}\left[D_i \,|\, Z_i = 0, \boldsymbol{X}_i\right]$, then applying the expectation across $Z_i = z'$, and $\boldsymbol{X}_i$.

A.3 A Regression Framework for Direct and Indirect Effects

Put $\mu_D(Z; \boldsymbol{X}) = \mathbb{E}\left[Y_i(Z, D) \,|\, \boldsymbol{X}\right]$ and $U_{D,i} = Y_i(Z, D) - \mu_D(Z; \boldsymbol{X})$, so we have the following expressions.

$$
Y_i(Z_i, 0) = \mu_0(Z_i; \boldsymbol{X}_i) + U_{0,i}, \quad Y_i(Z_i, 1) = \mu_1(Z_i; \boldsymbol{X}_i) + U_{1,i}
$$

$U_{0,i}, U_{1,i}$ are error terms with unknown distributions, mean independent of $Z_i, \boldsymbol{X}_i$ by definition — but possibly correlated with D_i.

Z_i is independent of potential outcomes, so that $U_{0,i}, U_{1,i} \perp\!\!\!\perp Z_i$. Thus, the first-stage regression of $Z \to Y$ has unbiased estimates.

$$
\begin{aligned}
D_i &= Z_i D_i(1) + (1 - Z_i) D_i(0) \\
&= D_i(0) + Z_i \left[D_i(1) - D_i(0)\right] \\
&= \underbrace{\mathbb{E}\left[D_i(0) \,|\, \boldsymbol{X}_i\right]}_{\text{Intercept}} + \underbrace{Z_i \mathbb{E}\left[D_i(1) - D_i(0)\right]}_{\text{Regressor}} \\
&\quad + \underbrace{D_i(0) - \mathbb{E}\left[D_i(0) \,|\, \boldsymbol{X}_i\right] + Z_i\Big(D_i(1) - D_i(0) - \mathbb{E}\left[D_i(1) - D_i(0) \,|\, \boldsymbol{X}_i\right]\Big)}_{\text{Mean-zero independent error term, since } Z_i \perp\!\!\!\perp D_i \,|\, \boldsymbol{X}_i} \\
&=: \phi + \pi Z_i + \varphi(\boldsymbol{X}_i) + \eta_i
\end{aligned}
$$

$$
\implies \mathbb{E}\left[D_i \,|\, Z_i, \boldsymbol{X}_i\right] = \phi + \pi Z_i + \varphi(\boldsymbol{X}_i), \text{ and thus unbiased estimates since } Z_i \perp\!\!\!\perp \phi, \eta_i.
$$

Z_i is also assumed independent of potential outcomes $Y_i(., .)$, so that $U_{0,i}, U_{1,i} \perp\!\!\!\perp Z_i$. Thus, the reduced form regression $Z \to Y$ also leads to unbiased estimates.

The same cannot be said of the regression that estimates direct and indirect effects, without further assumptions.

$$\begin{aligned}
Y_i &= Z_i Y_i(1, D_i(1)) + (1 - Z_i) Y_i(0, D_i(0)) \\
&= Z_i D_i Y_i(1,1) \\
&\quad + (1 - Z_i) D_i Y_i(0,1) \\
&\quad + Z_i (1 - D_i) Y_i(1,0) \\
&\quad + (1 - Z_i)(1 - D_i) Y_i(0,0) \\
&= Y_i(0,0) \\
&\quad + Z_i \left[Y_i(1,0) - Y_i(0,0) \right] \\
&\quad + D_i \left[Y_i(0,1) - Y_i(0,0) \right] \\
&\quad + Z_i D_i \left[Y_i(1,1) - Y_i(1,0) - (Y_i(0,1) - Y_i(0,0)) \right]
\end{aligned}$$

And so Y_i can be written as a regression equation in terms of the observed factors and error terms.

$$\begin{aligned}
Y_i = &\ \mu_0(0; \boldsymbol{X}_i) \\
&+ D_i \left[\mu_1(0; \boldsymbol{X}_i) - \mu_0(0; \boldsymbol{X}_i) \right] \\
&+ Z_i \left[\mu_0(1; \boldsymbol{X}_i) - \mu_0(0; \boldsymbol{X}_i) \right] \\
&+ Z_i D_i \left[\mu_1(1; \boldsymbol{X}_i) - \mu_0(1; \boldsymbol{X}_i) - (\mu_1(0; \boldsymbol{X}_i) - \mu_0(0; \boldsymbol{X}_i)) \right] \\
&+ U_{0,i} + D_i \left(U_{1,i} - U_{0,i} \right) \\
=: &\ \alpha + \beta D_i + \gamma Z_i + \delta Z_i D_i + \zeta(\boldsymbol{X}_i) + (1 - D_i) U_{0,i} + D_i U_{1,i}
\end{aligned}$$

With the following definitions:

(a) $\alpha = \mathbb{E}\left[\mu_0(0; \boldsymbol{X}_i) \right]$ and $\zeta(\boldsymbol{X}_i) = \mu_0(0; \boldsymbol{X}_i) - \alpha$ are the intercept terms.

(b) $\beta = \mu_1(0; \boldsymbol{X}_i) - \mu_0(0; \boldsymbol{X}_i)$ is the indirect effect under $Z_i = 0$

(c) $\gamma = \mu_0(1; \boldsymbol{X}_i) - \mu_0(0; \boldsymbol{X}_i)$ is the direct effect under $D_i = 0$.

(d) $\delta = \mu_1(1; \boldsymbol{X}_i) - \mu_0(1; \boldsymbol{X}_i) - (\mu_1(0; \boldsymbol{X}_i) - \mu_0(0; \boldsymbol{X}_i))$ is the interaction effect.

(e) $(1 - D_i) U_{0,i} + D_i U_{1,i}$ is the remaining error term.

This sequence gives us the resulting regression equation:

$$\begin{aligned}
\mathbb{E}\left[Y_i \,|\, Z_i, D_i, \boldsymbol{X}_i \right] \;=\; & \alpha + \beta D_i + \gamma Z_i + \delta Z_i D_i + \zeta(\boldsymbol{X}_i) \\
& + (1 - D_i) \mathbb{E}\left[U_{0,i} \,|\, D_i = 0, \boldsymbol{X}_i \right] + D_i \mathbb{E}\left[U_{1,i} \,|\, D_i = 1, \boldsymbol{X}_i \right]
\end{aligned}$$

Taking the conditional expectation, and collecting for the expressions of the direct and indirect effects:[18]

$$\begin{aligned}
\mathbb{E}\left[Y_i(Z_i, D_i(1)) - Y_i(Z_i, D_i(0))\right] &= \mathbb{E}\left[\pi\left(\beta + Z_i\delta\right)\right] \\
\mathbb{E}\left[Y_i(1, D_i(Z_i)) - Y_i(0, D_i(Z_i))\right] &= \mathbb{E}\left[\gamma + \delta D_i\right]
\end{aligned}$$

These terms are conventionally estimated in a simultaneous regression (Imai, Keele & Yamamoto 2010).

If sequential ignorability does not hold, then the regression estimates from estimating the mediation equations (without adjusting for the contaminated bias term) suffer from omitted variables bias.

$$\begin{aligned}
\mathbb{E}_{\boldsymbol{X}_i}\left[\mathbb{E}\left[Y_i \mid Z_i = D_i = 0, \boldsymbol{X}_i\right]\right] &= \mathbb{E}\left[\alpha\right] + \mathbb{E}\left[U_{0,i} \mid D_i = 0\right] \\
\mathbb{E}_{\boldsymbol{X}_i}\left[\mathbb{E}\left[Y_i \mid Z_i = 0, D_i = 1, \boldsymbol{X}_i\right] - \mathbb{E}\left[Y_i \mid Z_i = 0, D_i = 0, \boldsymbol{X}_i\right]\right] &= \mathbb{E}\left[\beta\right] + \left(\mathbb{E}\left[U_{1,i} \mid D_i = 1\right] - \mathbb{E}\left[U_{0,i} \mid D_i = 0\right]\right) \\
\mathbb{E}_{\boldsymbol{X}_i}\left[\mathbb{E}\left[Y_i \mid Z_i = 1, D_i = 0, \boldsymbol{X}_i\right] - \mathbb{E}\left[Y_i \mid Z_i = 0, D_i = 0, \boldsymbol{X}_i\right]\right] &= \mathbb{E}\left[\gamma\right] + \mathbb{E}\left[U_{0,i} \mid D_i = 0\right] \\
\mathbb{E}_{\boldsymbol{X}_i}\begin{bmatrix}\mathbb{E}\left[Y_i \mid Z_i = 1, D_i = 1, \boldsymbol{X}_i\right] - \mathbb{E}\left[Y_i \mid Z_i = 1, D_i = 0, \boldsymbol{X}_i\right] \\ -\left(\mathbb{E}\left[Y_i \mid Z_i = 0, D_i = 1, \boldsymbol{X}_i\right] - \mathbb{E}\left[Y_i \mid Z_i = 0, D_i = 0, \boldsymbol{X}_i\right]\right)\end{bmatrix} &= \mathbb{E}\left[\delta\right]
\end{aligned}$$

And so the ADE and AIE estimates are contaminated by these bias terms. Additionally, the AIE estimates refers to gains from the mediator among $D(z)$ compliers (not the entire average), so will be biased when not accounting for this, too.

A.4 Control Function Identification

Write the proof in here, following Vytlacil (2002) construction in the forward direction. Note that the notation needs updating for no exclusion restriction.

A.5 Control Function Simulation

A number of statistical packages, for the R language (R Core Team 2023), made the simulation analysis for this paper possible.

- *Tidyverse* (Wickham, Averick, Bryan, Chang, McGowan, François, Grolemund, Hayes, Henry, Hester, Kuhn, Pedersen, Miller, Bache, Müller, Ooms, Robinson, Seidel, Spinu, Takahashi, Vaughan, Wilke, Woo & Yutani 2019) collected tools for data analysis in the R language.
- *Splines* (Wang & Yan 2021) allows semi-parametric estimation, using splines, in the R language.

[18]These equations have simpler expressions after assuming constant treatment effects in a linear framework; I have avoided this as having compliers, and controlling for observed factors $\boldsymbol{X}_i$ only makes sense in the case of heterogeneous treatment effects.

- *Mediate* (Imai, Keele, Tingley & Yamamoto 2010) automates the sequential-ignorability estimates of CM effects (Imai, Keele & Yamamoto 2010) in the R language.