Simulation: Causal Mediation with Selection 1 September 2024
Senan Hogan-Hennessy, seh325@cornell.edu Cornell University

This document investigates a system where a randomised measure Z affects an outcome Y via two channels: directly $Z \to Y$, and indirectly via a mediator $D(Z) \to Y$.

Causal mediation methods decompose the effect of Z into indirect effects, the proportion of effect going through the $D(Z) \to Y$ channel, and direct effects, the $Z \to Y$ channel. Conventional methods assume that D is randomly assigned, conditional on Z and other observed covariates $\boldsymbol{X}_i$; this assumption is unlikely to hold in observation settings, such as relying on quasi-experimental variation in Z.

This document simulates a system where D is not randomly assigned, but is the result of Roy-style selection (based on treatment gains) involving observed selection factors $\boldsymbol{X}_i$ and unobserved U_i. It shows how conventional estimators, controlling only for observed $\boldsymbol{X}_i$ behave under different assumptions about the distribution of U_i.

1 Notation

Write Y_i for the observed outcome value e.g., long-run income, for individuals $i = 1, \dots, N$. Suppose Y_i is the outcome of two binary variables, $Z_i = 0, 1$ which is assigned randomly, and $D_i = 0, 1$ which individuals **select into** based on which Z value they receive. The researcher observes D_i, Y_i, but not their respective potential outcomes:

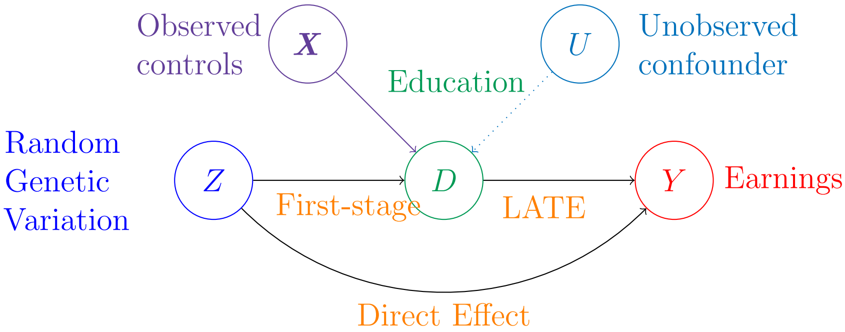
$$\begin{aligned}
D_i &= Z_i D_i(1) + (1 - Z_i) D_i(0), \\
&= \begin{cases} D_i(1), & \text{if } Z_i = 1 \\ D_i(0), & \text{if } Z_i = 0 \end{cases} \\
Y_i &= Z_i Y_i(1, D_i(1)) + (1 - Z_i) Y_i(0, D_i(0)) \\
&= \begin{cases} Y_i(1,1), & \text{if } Z_i = 1, D_i(1) = 1 \\ Y_i(1,0), & \text{if } Z_i = 1,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

In my empirical work, Z is a binary version of the gene score for education (differenced from parents' values, EA score), $D_i(Z_i)$ is a choice to complete higher education, and Y_i a measure of long-run income. $\boldsymbol{X}_i$ is demographic information, gender, age, and every measure of socio-economic standing available; U_i is covariates the **researcher wants to control for, but does not observe** in the data they have.

1.1 Direct and Indirect Effects

Causal mediation aims to decompose the reduced form effect of $Z \to Y$ into two separate pathways: indirectly through D, and directly absent D.

Figure 1: Structural Causal Graph of the Triangular System, $Z \to D \to Y$.



$$
\begin{aligned}
\text{Reduced Form:} \quad & \mathbb{E}\left[Y_i(1, D_i(1)) - Y_i(0, D_i(0))\right] = \mathbb{E}\left[Y_i \mid Z_i = 1\right] - \mathbb{E}\left[Y_i \mid Z_i = 0\right] \\
\text{Indirect Effect, } D(Z) \to Y: \quad & \mathbb{E}\left[Y_i(Z_i, D_i(1)) - Y_i(Z_i, D_i(0))\right] \\
\text{Direct Effect, } Z \to Y: \quad & \mathbb{E}\left[Y_i(1, D_i(Z_i)) - Y_i(0, D_i(Z_i))\right]
\end{aligned}
$$

The reduced form is the average effect of EA score on later-life earnings; the indirect effect is the effect of EA score operating purely through increased education; the direct effect is the effect of EA score operating absent education.

2 A Regression Framework for Direct and Indirect Effects

Inference for direct and direct effects can be written in a regression framework, showing how correlation between the error term and the mediator persistently biases estimates.

To motivate a regression framework, write $Y_i(Z, D)$ as a sum of observed factors Z_i, $\boldsymbol{X}_i$ and unobserved factors.

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

μ_0, μ_1 are unknown functions, $U_{0,i}, U_{1,i}$ are mean zero error terms with unknown distributions, independent of $Z_i, \boldsymbol{X}_i$ — but possibly correlated with D_i.

$$
\begin{aligned}
Y_i &= Z_i Y_i(1, D_i(1)) + (1 - Z_i) Y_i(0, D_i(0)) \\
&= Y_i(0, D_i(0)) + Z_i \left[Y_i(1, D_i(1)) - Y_i(0, D_i(0))\right] \\
&= \underbrace{\mu_{D_i(0;\boldsymbol{X}_i)}(0)}_{\text{Intercept}} + \underbrace{Z_i \left[\mu_{D_i(1)}(1; \boldsymbol{X}_i) - \mu_{D_i(0)}(0; \boldsymbol{X}_i)\right]}_{\text{Regressor}} \\
&\quad + \underbrace{U_{D_i(0),i} + Z_i \left(U_{D_i(1),i} - U_{D_i(0),i}\right)}_{\text{Error term, mean zero}} \\
&=: \phi_i + \varphi_i Z_i + \epsilon_i
\end{aligned}
$$

$$
\implies \mathbb{E}\left[Y_i \mid Z_i\right] = \mathbb{E}\left[\phi_i\right] + \mathbb{E}\left[\varphi_i\right] Z_i + \mathbb{E}\left[\epsilon_i\right], \text{ and thus unbiased estimates since } Z_i \perp\!\!\!\perp \varphi_i, \epsilon_i.
$$

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

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

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

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

$$\begin{aligned}
Y_i = &\ \mu_0(0; \boldsymbol{X}_i) \\
&+ Z_i \left[\mu_0(1; \boldsymbol{X}_i) - \mu_0(0; \boldsymbol{X}_i) \right] \\
&+ D_i \left[\mu_1(0; \boldsymbol{X}_i) - \mu_0(0; \boldsymbol{X}_i) \right] \\
&+ Z_i D_i \left[\mu_1(1; \boldsymbol{X}_i) - \mu_0(1; \boldsymbol{X}_i) - (\mu_1(0; \boldsymbol{X}_i) - \mu_0(0; \boldsymbol{X}_i)) \right] \\
&+ U_{0,i} + D_i \left(U_{1,i} - U_{0,i} \right) \\
=: &\ \alpha_i + \beta_i D_i + \gamma_i Z_i + \delta_i Z_i D_i + \varepsilon_i
\end{aligned}$$

$\alpha_i, \beta_i, \delta_i$ are the relevant direct effect under $D_i = 1$, indirect effect under $Z_i = 1$, δ_i the interaction effect, and ε_i the remaining error term. Collecting for the expressions of the direct and indirect effects:[1]

$$\begin{aligned}
\mathbb{E}\left[Y_i(Z_i, D_i(1)) - Y_i(Z_i, D_i(0)) \right] &= \mathbb{E}\left[(\beta_i + Z_i \delta_i) \times (D_i(1) - D_i(0)) \right] \\
\mathbb{E}\left[Y_i(1, D_i(Z_i)) - Y_i(0, D_i(Z_i)) \right] &= \mathbb{E}\left[\gamma_i + \delta_i D_i \right]
\end{aligned}$$

By assumption $Z_i \perp\!\!\!\perp \gamma_i, \varepsilon_i$, so that the regression only gives unbiased estimates if D_i is also conditionally random: $D_i(z) \perp\!\!\!\perp \varepsilon_i \mid \boldsymbol{X}_i$.

2.1 Selection into Education

Conventional causal mediation work point identifies the indirect and direct effects by additionally **assuming that D_i is randomly assigned**, conditional on $\{\boldsymbol{X}_i, Z_i\}$ — known as sequential ignorability (Imai et al., 2010).

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

[1] These equations have simpler expressions after assuming constant treatment effects; 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.

In the education context, point identifying direct and indirect effects requires the **researcher controls for all sources of selection-into-education**.

While this assumption may hold true in two-way randomised experiments (e.g., in a laboratory or two-way RCT), it is unlikely to hold in the case of quasi-experimental variation in Z, or when modelling education as a mediator — absent a separate identification strategy for education D. To expand this point in an econometric selection-into-treatment framework, suppose selection follows a Roy model, where individual i weighs the costs and benefits of completing education.

$$D_i(Z_i) = \mathbb{1}\left\{ \underbrace{C_i(Z_i)}_{\text{Costs}} \leq \underbrace{Y_i(Z_i, 1) - Y_i(Z_i, 0)}_{\text{Gains}} \right\}$$

Education choice $D_i(z)$ is clearly related to $Y_i(z, d)$ in this model, so let's see what the equation looks like in terms of sequential ignorability. As above, decompose costs into observed and unobserved factors.

$$C_i(Z_i) = \mu_C(Z_i; \boldsymbol{X}_i) + U_{C,i}$$

And so we can write the first-stage selection equation in full.

$$D_i(Z_i) = \mathbb{1}\left\{ \underbrace{U_{C,i} + U_{0,i} - U_{1,i}}_{\text{Unobserved}} \leq \underbrace{\mu_1(Z_i; \boldsymbol{X}_i) - \mu_0(Z_i; \boldsymbol{X}_i) - \mu_C(Z_i; \boldsymbol{X}_i)}_{\text{Observed}} \right\}$$

Sequential ignorability, where $Y_i(z, d) \perp\!\!\!\perp D_i(z') \mid \boldsymbol{X}_i$, would then require that $\mathbb{E}\left[U_{0,i} - U_{1,i} \mid D_i\right] = 0$ — no unobserved selection! This is unlikely to hold true, unless there is another identification strategy for D_i — in addition to the one used for Z_i.

3 Simulation

This simulation assumes that

1. $\Pr(Z_i = 1) = \frac{1}{2}$ for every individual, so that Z_i is randomly assigned.
2. $U_{0,i}, U_{1,i} \sim \text{BivarNormal}(\rho, 0, 0, \sigma_0, \sigma_1)$, and $U_C = 0$ for simplicity.
3. $N = 1,000$
4. Observed covariates $\boldsymbol{X}_i = [X_i^1]$ is composed of $X_i^1 \sim \text{N}(0, 1)$.

The observed part of potential outcomes, $\mu_D(Z; \boldsymbol{X}_i)$, are simulated in a linear system, with $\boldsymbol{X}_i \sim N(5, 1)$ and the following definitions.

$$\begin{aligned}
\mu_0(0; \boldsymbol{X}_i) &= \beta_0 \boldsymbol{X}_i && = \boldsymbol{X}_i \\
\mu_1(0; \boldsymbol{X}_i) &= \beta_1 \boldsymbol{X}_i && = 2\boldsymbol{X}_i \\
\mu_0(1; \boldsymbol{X}_i) &= \beta_0 \boldsymbol{X}_i + \gamma_0 && = \boldsymbol{X}_i + 0.5 \\
\mu_1(1; \boldsymbol{X}_i) &= \beta_1 \boldsymbol{X}_i + \gamma_1 && = 2\boldsymbol{X}_i + 1 \\
\mu_C(0; \boldsymbol{X}_i) &= 5 \\
\mu_C(1; \boldsymbol{X}_i) &= 3.75
\end{aligned}$$

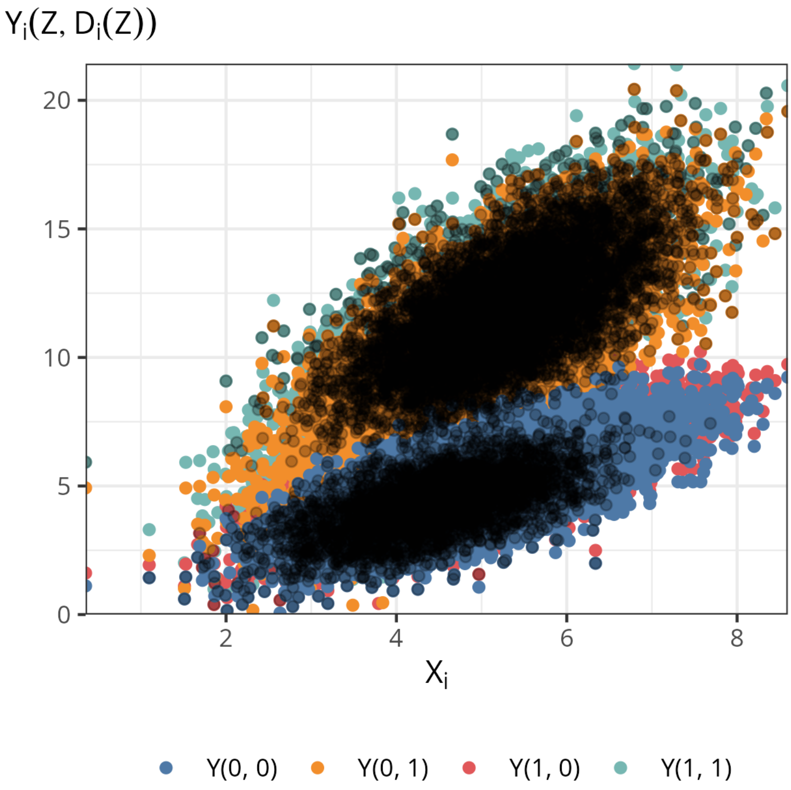
These values have the following properties, relevant to this system:

- There are compliers i.e., $0 < \Pr(D_i(0) < D_i(1))$ since gains to education do not always outweigh costs
- There are no defiers i.e., $0 = \Pr(D_i(0) > D_i(1))$ since opportunity costs of education are higher in $Z_i = 1$
- $\text{Corr}(U_{i,0}, U_{i,1}) = \rho > 0$ indicates positive selection into education, where those with higher incomes more often take education (independently of gains)
- $\sigma_1 \neq \sigma_0$ indicates heteoskedasicity in D_i, where error term variance is correlated with D_i.

What does this system look like?

$$\begin{aligned}
Y_i(Z_i, 0) = \beta_0 \boldsymbol{X}_i + \gamma_0 Z_i + U_{0,i}, \quad Y_i(Z_i, 1) = \beta_1 \boldsymbol{X}_i + \gamma_1 Z_i + U_{1,i} \\
D_i(Z_i) = \mathbb{1}\left\{\mu_C(Z_i; \boldsymbol{X}_i) + U_{C,i} \leq Y_i(Z_i, 1) - Y_i(Z_i, 0)\right\} \\
\implies Y_i = \beta_0 \boldsymbol{X}_i + \gamma_0 Z_i + \left[(\beta_0 - \beta_1)\boldsymbol{X}_i\right] D_i + (\gamma_1 - \gamma_0) Z_i D_i + U_{0,i} + D_i\left(U_{1,i} - U_{0,i}\right) \\
= \boldsymbol{X}_i + 0.5 Z_i + \boldsymbol{X}_i D_i + 0.5 Z_i D_i + \underbrace{U_{0,i} + D_i\left(U_{1,i} - U_{0,i}\right)}_{\text{Correlated error term}} \\
\mathbb{E}\left[Y_i(Z_i, 1) - Y_i(Z_i, 0)\right] = (\beta_1 - \beta_0)\mathbb{E}\left[\boldsymbol{X}_i\right] + (\gamma_1 - \gamma_0)\mathbb{E}\left[Z_i\right] + \mathbb{E}\left[U_{1,i} - U_{0,i}\right] = 5.25 \\
\mathbb{E}\left[Y_i(1, D_i(Z_i)) - Y_i(0, D_i(Z_i))\right] = \gamma_0 + (\gamma_1 - \gamma_0)\mathbb{E}\left[D_i\right] = 0.8313
\end{aligned}$$

Figure 2: Simulated Outcomes, with $\rho, \sigma_0, \sigma_1 = 3/4, 1, 2$.



Note: The transparent black dots are overlaid realised Y_i values. See the first equation for an explanation of how $Y_i(0,1)$ is only realised for always-takers, $D_i(0) = 1$.

3.1 Varying the Parameter Values

There are three values that define the system, mimicking the famous sample selection model of Heckman (1974, 1979):

Parameter	Equation	Explanation
ρ	$\mathrm{Corr}(U_{i,0}, U_{i,1})$	Correlation between $D_i = 1$ and $D_i = 0$ error terms
σ_0	$\mathrm{Var}(U_{i,0})^{\frac{1}{2}}$	Standard deviation of $D_i = 0$ error terms
σ_1	$\mathrm{Var}(U_{i,1})^{\frac{1}{2}}$	Standard deviation of $D_i = 1$ error terms

This simulation file varies the values of ρ, σ_0, σ_1 to investigate how the bias in conventional mediation estimates behaves under different assumptions of the unobserved error values U_0, U_1.

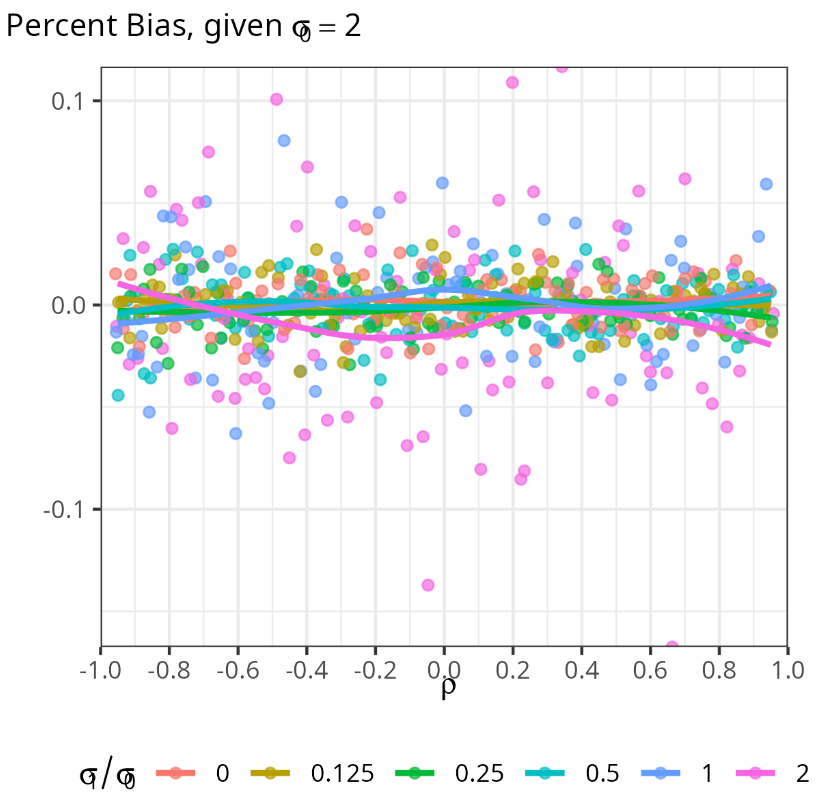
3.2 Bias in the Reduced Form Estimate

I expected the following relationship between these parameter values, and the bias in estimating the **reduced form effect**, $\mathbb{E}[Y_i \mid Z_i = 1] - \mathbb{E}[Y_i \mid Z_i = 0]$.

- Increasing both σ_0, σ_1 reduces precision
- $\sigma_1/\sigma_0 \neq 1$ indicates heteroskedasticity along D_i (not bias)
- Changing ρ has no effect on bias (may affect precision).

This is generally confirmed by the simulation, in Figure 3.

Figure 3: Bias in Reduced Form Estimates in Simulated Data, across different ρ, σ_0, σ_1 values.



Note: This figure shows the percent bias in the regression $Y_i = \phi + \theta Z_i + \boldsymbol{\zeta}_i' \boldsymbol{X}_i + \eta_i$, where the y-axis is $(\widehat{\theta}_{\text{OLS}} - \theta)/\theta$, given θ the true value of the reduced form effect.

3.3 Bias in the Direct and Indirect Effect Estimates

I expected the following relationship between these parameter values, and the bias in estimating the **Direct Effect** $Z \to Y: \quad \mathbb{E}[Y_i(1, D_i(Z_i)) - Y_i(0, D_i(Z_i))]$

- This estimate relies on estimating $D \to Y$ by selection-on-observables, so $\rho > 0$ indicates unobserved selection into treatment and downwards biases estimates

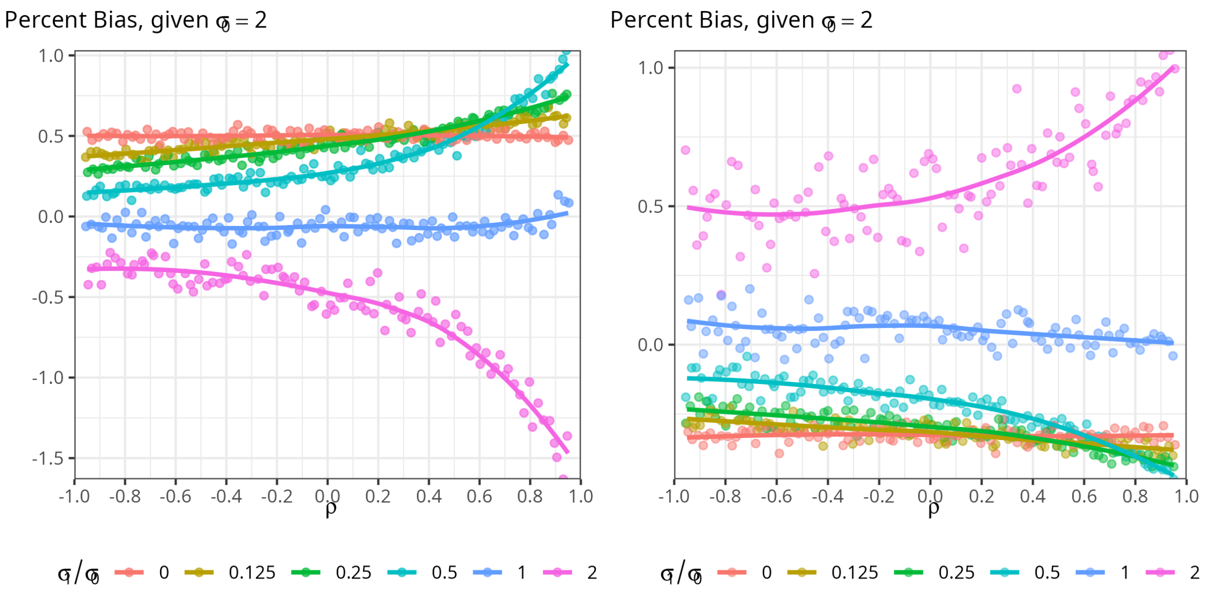
- σ_0, σ_1 have ambiguous effects on bias, beyond heteroskedasticity for inference.

I expected the following relationship between these parameter values, and the bias in estimating the **Indirect Effect** $D(Z) \to Y: \ \mathbb{E}\left[Y_i(Z_i, D_i(1)) - Y_i(Z_i, D_i(0))\right]$.

- This estimate relies on estimating $D \to Y$ by selection-on-observables, so $\rho > 0$ indicates unobserved selection into treatment and upwards biases estimates
- σ_0, σ_1 have ambiguous effects on bias, beyond heteroskedasticity for inference.

Figure 4: Bias of Point Estimates in Simulated Data, across different ρ, σ_0, σ_1 values.

(a) Direct Effect Estimates. **(b)** Indirect Effect Estimates.



Note: This figure shows the percent bias in the regression $Y_i = \alpha + \beta D_i + \gamma Z_i + \delta Z_i D_i + \boldsymbol{\zeta}_i' \boldsymbol{X}_i + \varepsilon_i$, where the y-axis is the corresponding OLS estimate for direct or indirect minus then divided by the true value of the reduced form effect.

4 A Control Function Solution(?)

I have shown above that the mediation equations without sequential ignorability take the following form, with first-stage error term $U_i = -(U_{1,i} - U_{0,i} - U_{C,i})$ and non-parametric regressor $\mu = \mu_1 - \mu_0 - \mu_C$.

$$D_i(Z_i) = \mathbb{1}\left\{U_i \leq \mu(Z_i; \boldsymbol{X}_i)\right\}$$
$$Y_i = \alpha_i + \gamma_i Z_i + \beta_i D_i + \delta_i Z_i D_i + U_{0,i} + D_i\left(U_{1,i} - U_{0,i}\right)$$

The control function approach solves identification in this exact problem. The classic Heckman (1979) approach does so by maximum likelihood with errors $U_{1,i}, U_{0,i}$ assumed normal. **This approach works exactly in the simulation above, i.e. with simulated normal errors (and even heterogeneous treatment effects).**

Newer semi-parametric approaches use a two-step approach to avoid assuming the distribution of the error terms (Newey et al., 1999; Imbens and Newey, 2009). The identifying assumption is that error terms in the first and second-stages are correlated, so that first-stage predicted residuals control for endogeneity in the second-stage.

$$\widehat{U}_i = D_i - \widehat{\mathbb{E}\left[D_i \mid \boldsymbol{X}_i, Z_i\right]} = \widehat{f_D}(\mu(Z_i\ \boldsymbol{X}_i))$$
$$Y_i = \alpha_i + \beta_i D_i + \gamma_i Z_i + \delta_i Z_i D_i + \widehat{U}_i D_i + \varepsilon_i$$

This assumption holds exactly in the Roy model, with perfectly correlated errors (minus costs variation).

4.1 Discussion:

I don't see any modern applied work using control function estimators. . . .

The control function approach assumes the error terms in the first-stage selection equation are informative for the errors in the second-stage outcome equation; this is trivial in the Roy model, though not the only first-stage selection consistent with the approach. It may make sense for me to write exclusively in a structural setting using the Roy model, and hold off on considering this approach more generally.

I have concerns:

- I only see highly technical econometric theory papers taking the control function approach
- The control function approach here replaces one assumption (D_i randomised) for another (correlated error terms).
- The second assumption is consistent (inspired by) the Roy model; the first assumption is inconsistent with a general labour/natural experiment setting
- Is this approach straying too far into the "structural world" for an applied project?

A Appendix

A.1 Things to look into

Newest thought: Use a semi-parametric two-step control function estimator to get estimates of the direct and indirect effects.

A.1.1 Thought on Sensitivity Analysis

If the above two-step control function works, then controlling for $\boldsymbol{X}_i$ in the second stage is irrelevant, except for precision (i.e., magnitude of standard errors). So estimates with varying inclusion of controls in $\boldsymbol{X}_i$ should be unbiased, even if less precise.

This should be investigated, showing the two-step control function estimates sequentially adding controls in $\boldsymbol{X}_i$ and that there is no general trend (other than more precise estimates).

A.1.2 Explaining Compliance

Sequential ignorability assumes that all levers of selection are controlled for in observed factors $\boldsymbol{X}_i$. The next step is getting a measure of how much compliance is unexplained, which is equivalent to how large U_i is in the outcome equation in the Roy model.

The first option is to measure how much compliance is explained by $\boldsymbol{X}_i$.

$$\text{Var}\left(D_i(1) - D_i(0)\right) = \underbrace{\text{Var}\left(\mathbb{E}\left[D_i(1) - D_i(0) \,|\, X_i\right]\right)}_{\text{Compliance explained by } \boldsymbol{X}_i} + \underbrace{\mathbb{E}\left[\text{Var}\left(D_i(1) - D_i(0) \,|\, |\boldsymbol{X}_i\right)\right]}_{\text{Compliance unexplained}}$$

$$\implies R_U^2 = 1 - \frac{\text{Var}\left(\mathbb{E}\left[D_i(1) - D_i(0) \,|\, X_i\right]\right)}{\text{Var}\left(D_i(1) - D_i(0)\right)}$$

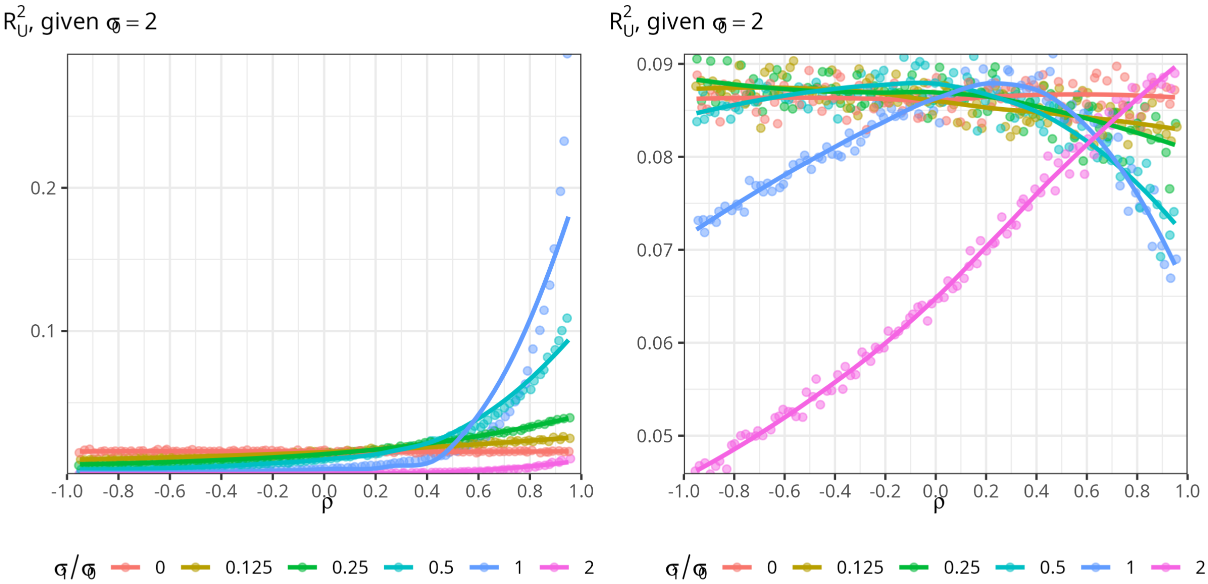
The second option is to measure how much variation in observed D_i is explained by $\boldsymbol{X}_i$, in the spirit of Altonji et al. (2005).

$$\text{Var}\left(D_i\right) = \underbrace{\text{Var}\left(\mathbb{E}\left[D_i \,|\, X_i\right]\right)}_{\text{Var}(D_i) \text{ explained by } \boldsymbol{X}_i} + \underbrace{\mathbb{E}\left[\text{Var}\left(D_i \,|\, |\boldsymbol{X}_i\right)\right]}_{\text{Var}(D_i) \text{ unexplained}}$$

$$\implies R_U^2 = 1 - \frac{\text{Var}\left(\mathbb{E}\left[D_i \,|\, X_i\right]\right)}{\text{Var}\left(D_i\right)}$$

Figure A1: Simulated R_U^2 Values.

(a) $R_U^2 = 1 - \frac{\mathrm{Var}(\mathbb{E}[D_i(1) - D_i(0) \,|\, X_i])}{\mathrm{Var}(D_i(1) - D_i(0))}$. (b) $R_U^2 = 1 - \frac{\mathrm{Var}(\mathbb{E}[D_i \,|\, X_i])}{\mathrm{Var}(D_i)}$.



Note: This figure shows the true values of R_U^2 in each simulation, based on bivariate normal error terms

Current thoughts: The idea of using R_U^2 seems not useful, given recent thoughts on using a two-step control function estimator Propose a hypothesis test, based on an estimated R_U^2 values, which (if violated) tests sequential ignorability (maybe only if selection is a Roy model). If $H_0 : R_U^2 = 0$ is rejected, then motivates the use of a control function estimator of the direct and indirect effects, instead of sequential ignorability estimates.

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