Learning with Instrumental and Proxy Variables

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Joint work with

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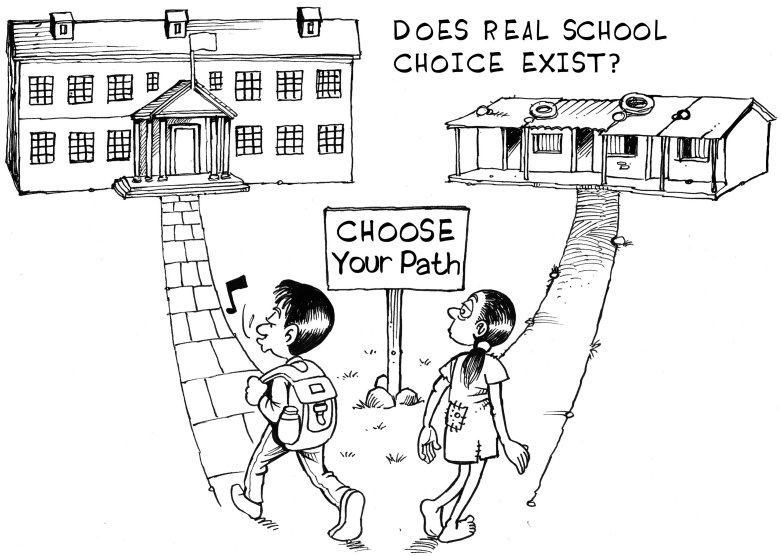
Hi! PARIS Summer School 2022

July 7, 2022

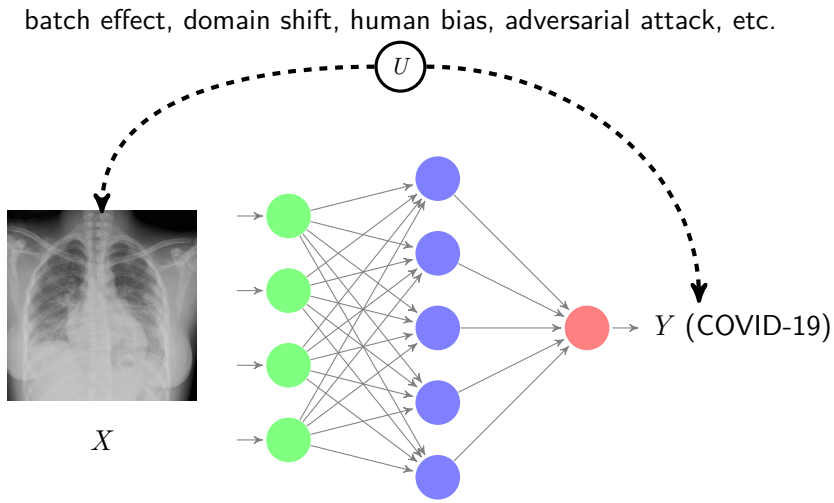
Unobserved Confounder / Spurious Correlation

Causal Inference



$\texttt{Education}\ (X) \rightarrow \texttt{Income}\ (Y)$

Machine Learning



$Y = f(X) + \varepsilon_u$

[**UAI** 2020; **NeurIPS** 2020; **ICML** 2021; Zhang et al. **Under Review**]

Spurious Correlation

- An **interventional distribution** $P(\,Y \,|\, \mathsf{do}(X = x))$.

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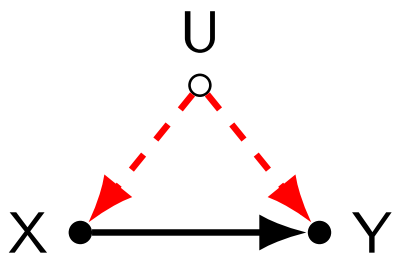
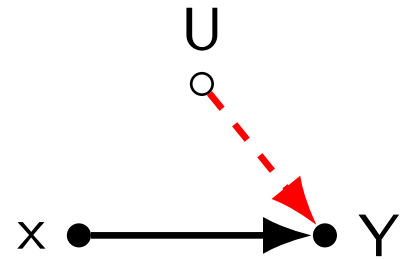
- An **interventional distribution** $P(Y \mid \text{do}(X = x))$.
- $P(Y \mid \text{do}(X = x)) \neq P(Y \mid X = x)$ **observational distribution**



$P(Y \mid X = x)$



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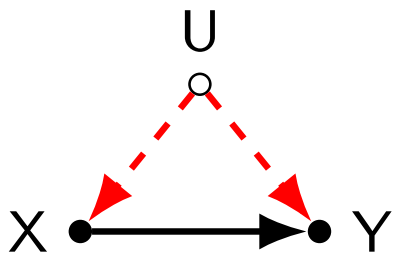

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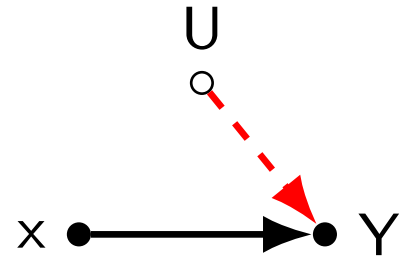
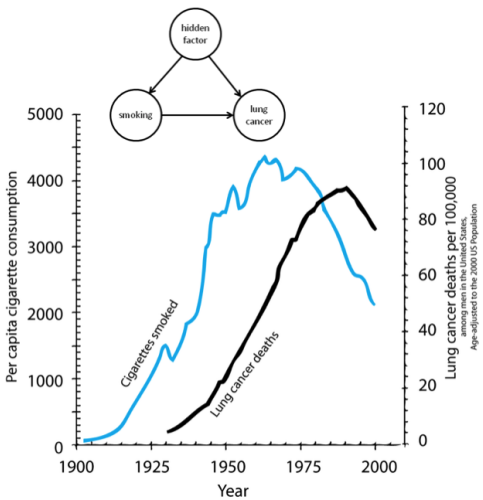


$P(Y \mid \text{do}(X = x))$

- The confounder U creates a **spurious correlation** between X and Y.



$X =$ `smoking (cigarettes smoked)`

$Y =$ `lung cancer deaths`

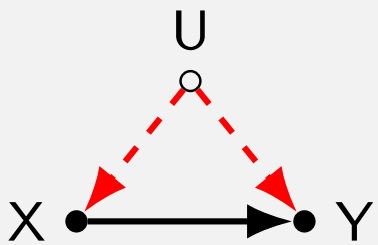
$P(Y \mid X = x) =$ `observed dealths from data`

$\text{do}(X = 0) =$ `smoking banned`

$P(Y \mid \text{do}(X = 0)) =$ `dealths after the ban`

Additive Noise Model

Newey and Powell (2003); Hoyer et al. (2008); Peters et al. (2014)



Structural Equations

$$Y \leftarrow f(X) + \varepsilon(U), \qquad \mathbb{E}[\varepsilon] = 0$$
$$X \leftarrow g(U) + \nu, \qquad \mathbb{E}[\nu] = 0$$

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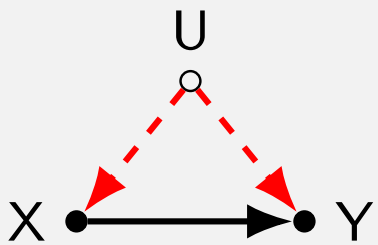

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- **CI**: $\mathbb{E}[\,Y \,|\, \mathsf{do}(X = x)] = f(x)$ **ML**: $\mathbb{E}[\,Y \,|\, X = x] = f(x)$

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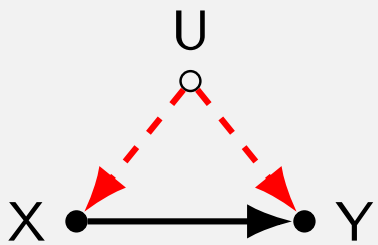

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$$\mathbb{E}[\,Y \,|\, X = x] = f(x) + \mathbb{E}[\varepsilon \,|\, x]$$

- Estimate $\widehat{\mathbb{E}}[\,Y \,|\, X = x]$ from the sample $(x_1, y_1), \ldots, (x_n, y_n) \sim P(X, Y)$
  - A biased estimate of $\mathbb{E}[\,Y \,|\, \mathrm{do}(X = x)]$.
  - The estimate $\widehat{\mathbb{E}}[\,Y \,|\, X = x]$ can be **unstable** because of $\mathbb{E}[\varepsilon \,|\, x]$.

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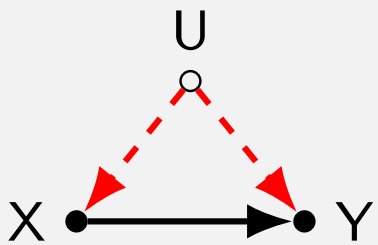

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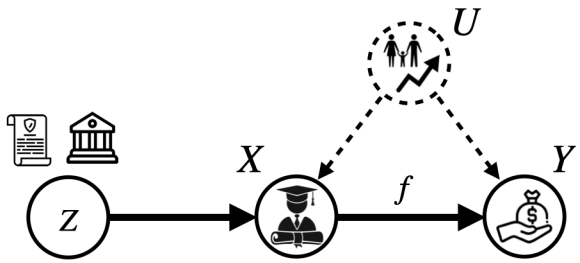
  - A biased estimate of $\mathbb{E}[\,Y \,|\, \mathrm{do}(X = x)]$.
  - The estimate $\widehat{\mathbb{E}}[\,Y \,|\, X = x]$ can be **unstable** because of $\mathbb{E}[\varepsilon \,|\, x]$.
- Impossible to recover $f(x)$ without further assumptions.

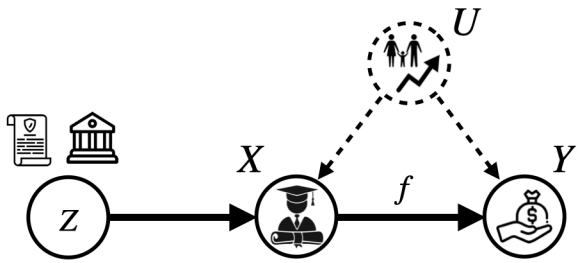
Instrumental Variables



Assumptions

1. **Relevance**: $P(X|Z)$ is not constant in Z.
2. **Exclusion restriction**: Z affects Y only through X.
3. **Unconfoundedness**: Z is independent from U.

Instrumental Variables



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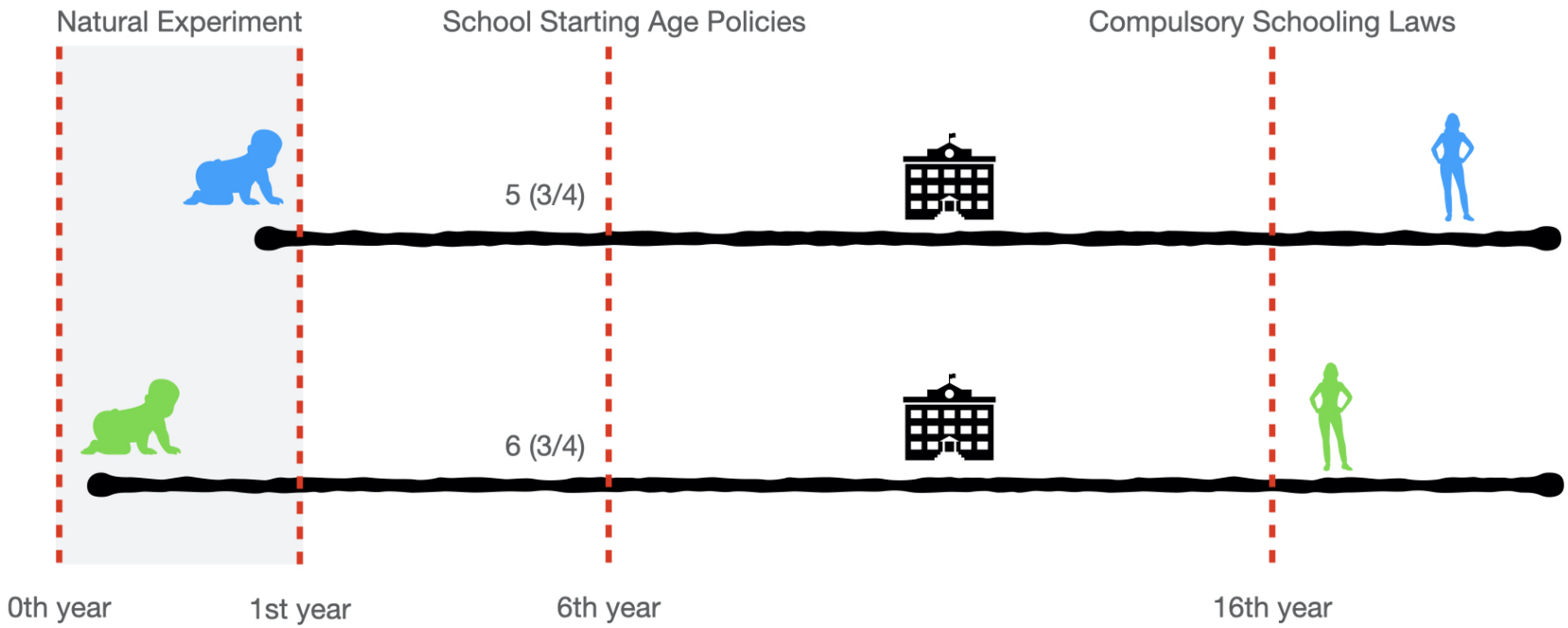
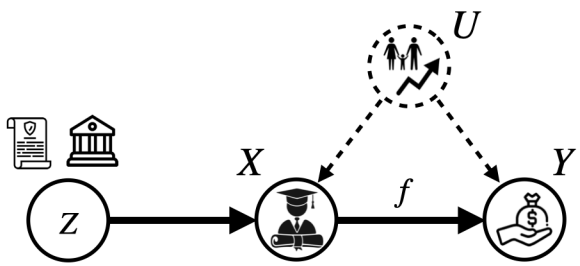


[Angrist and Krueger (1991); Angrist and Krueger (2001)]

Nobel Prize 2021

Nonparametric Instrumental Variable Regression

Newey and Powell (2003, **Econometrica**)



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- Taking the conditional expectation wrt Z on both sides

$$\begin{aligned} Y &= f(X) + \varepsilon \\ \mathbb{E}[Y \mid Z] &= \mathbb{E}[f(X) \mid Z] + \underbrace{\mathbb{E}[\varepsilon \mid Z]}_{=\mathbb{E}[\varepsilon]=0} \end{aligned}$$

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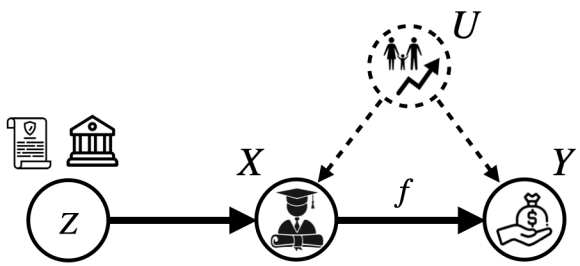

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- A **Fredholm integral equation** of the first kind

$$\mathbb{E}[Y \mid Z] = \int f(x)\, dP(x \mid Z)$$

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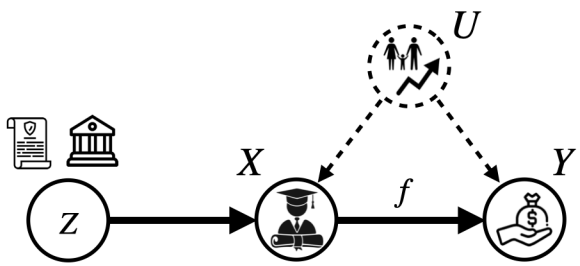

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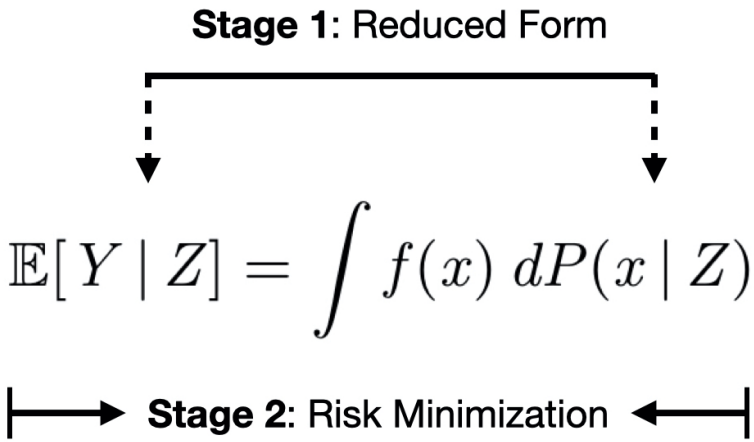
- **Completeness condition** [D'Haultfoeuille (2011, **Econ Theory**)]

For all measurable functions g, $\mathbb{E}[g(X) \mid Z] = 0$ a.s. $\Rightarrow g(X) = 0$ a.s.

Fredholm Integral Equation: Two-Stage Estimation



Population risk

$$\min_{f \in \mathcal{F}} \mathbb{E}_Z \left[\left(\mathbb{E}[Y \mid Z] - \mathbb{E}_{X|Z}[f(X)] \right)^2 \right]$$

Empirical risk: $(x_i, y_i, z_i) \sim P(X, Y, Z)$

$$\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \left[\left(\widehat{\mathbb{E}}[Y \mid z_i] - \widehat{\mathbb{E}}_{X|z_i}[f(X)] \right)^2 \right]$$

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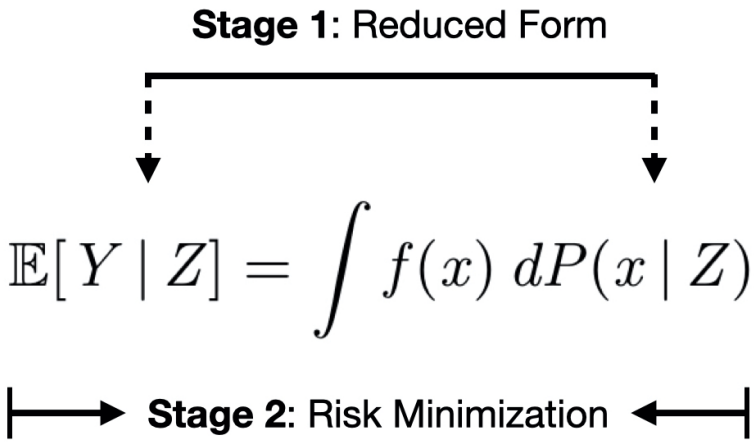

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Previous work

- **2SLS** [Angrist and Imbens (1996)]
- **SieveIV** [Newey and Powell (2003)]
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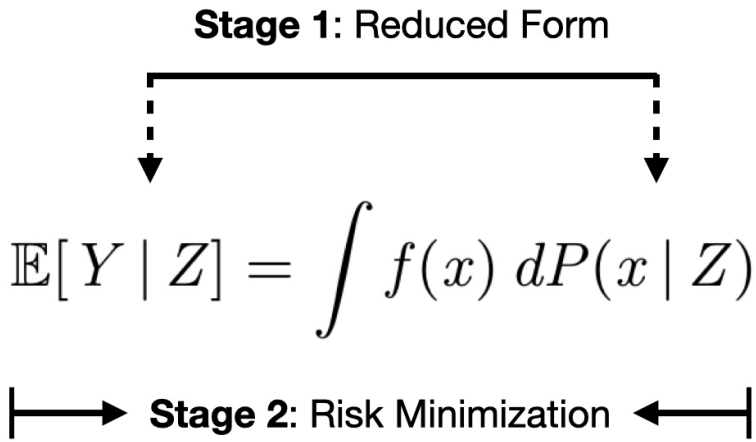
Fredholm Integral Equation: Two-Stage Estimation



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Challenges

- Require **data splitting** for two-stage estimation.
- Estimate $P(X \mid Z)$ using **one observation** from $P(X \mid Z = z)$.
- The first stage is known as "**forbidden regression**" in econometrics.
- It violates **Vapnik's principle** [Vapnik 1998].

DualIV: From Two-Stage Estimation to Two-Player Game

Muandet, Mehrjou, Lee, Raj. (2020, **NeurIPS**); Liao et al (2020, **NeurIPS**)

$$
\begin{aligned}
\min_{f\in\mathcal{F}} R(f) &= \min_{f\in\mathcal{F}} \mathbb{E}_Z[(\mathbb{E}[Y\mid Z]-\mathbb{E}_{X|Z}[f(X)])^2] \\
&\overset{(a)}{=} \min_{f\in\mathcal{F}} \mathbb{E}_Z[\max_{u\in\mathbb{R}}\{\mathbb{E}_{X|Z}[f(X)]u-\mathbb{E}[Y|Z]u-\frac{1}{2}u^2\}] \\
&\overset{(b)}{=} \min_{f\in\mathcal{F}}\max_{u\in\mathcal{U}} \mathbb{E}_Z[\mathbb{E}_{X|Z}[f(X)]u(Z)-\mathbb{E}[Y|Z]u(Z)-\frac{1}{2}u^2(Z)] \\
&= \min_{f\in\mathcal{F}}\max_{u\in\mathcal{U}} \mathbb{E}_Z[(\mathbb{E}_{X|Z}[f(X)]-\mathbb{E}[Y|Z])u(Z)-\frac{1}{2}u^2(Z)] \\
&= \boldsymbol{\min_{f\in\mathcal{F}}\max_{u\in\mathcal{U}} \mathbb{E}_{XYZ}[(f(X)-Y)u(Z)-\frac{1}{2}u^2(Z)]}
\end{aligned}
$$

(a) **Fenchel duality**: Let $\ell_y(\cdot)=\ell(y,\cdot)$ be a convex loss. For $\ell(y,y')=(y-y')^2$,

$$\ell_y(v)=\max_u\{uv-\ell_y^\star(u)\},\quad \ell_y^\star(u)=uy+\frac{1}{2}u^2.$$

(b) **Interchangeability**: $\mathbb{E}_\omega[\max_{u\in\mathbb{R}} f(u,\omega)]=\max_{u(\cdot)\in\mathcal{U}}\mathbb{E}_\omega[f(u(\omega),\omega)]$.

Dai et al. (2017; Lemma 1), Rockafellar and Wets (1998; Ch. 14), and Shapiro et al. (2014; Ch. 7)

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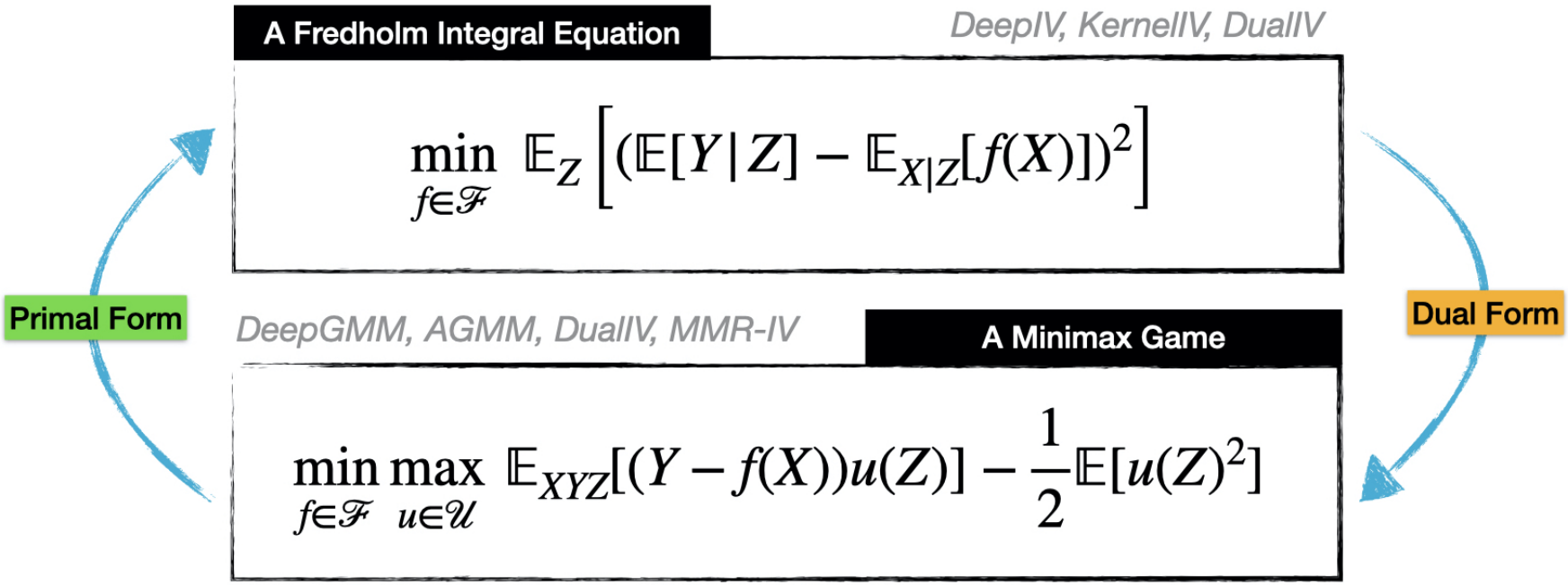

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Data: $(x_1, y_1, z_1), \ldots, (x_n, y_n, z_n) \sim P(X, Y, Z)$

- **Adversarial learning** ($\mathcal{F} = \{f_{\boldsymbol{\psi}} : \boldsymbol{\psi} \in \mathbb{R}^q\}$ and $\mathcal{U} = \{u_{\boldsymbol{\theta}} : \boldsymbol{\theta} \in \mathbb{R}^p\}$)

$$\min_{\boldsymbol{\psi} \in \mathbb{R}^q} \max_{\boldsymbol{\theta} \in \mathbb{R}^p} \frac{1}{n} \sum_{i=1}^{n} [(y_i - f_{\boldsymbol{\psi}}(x_i)) u_{\boldsymbol{\theta}}(z_i)] - \frac{\gamma}{2} \|u_{\boldsymbol{\theta}}\|^2 + \frac{\lambda}{2} \|f_{\boldsymbol{\psi}}\|^2$$

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- **M-estimators** (A unit ball within an RKHS, i.e., $\mathcal{U} = \{u : \mathcal{H}_{k_{\mathcal{Z}}}, \|u\| \leq 1\}$)

$$\min_{f \in \mathcal{F}} R_V(f) = \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} (y_i - f(x_i)) k_{\mathcal{Z}}(z_i, z_j) (y_j - f(x_j)) + \frac{\lambda}{2} \|f\|^2$$

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- **Kernel machines** ($\mathcal{F} \in \mathcal{H}_{k_{\mathcal{X}}}$ and $\mathcal{U} = \{u : \mathcal{H}_{k_{\mathcal{Z}}}, \|u\| \leq 1\}$)

$$f(x) = \sum_{i=1}^{n}\alpha_i k_{\mathcal{X}}(x_i, x), \quad \boldsymbol{\alpha} = (\mathbf{KLK} + \lambda\mathbf{K})^{-1}\mathbf{KL}\boldsymbol{y}$$

where $\mathbf{K}_{ij} = k_{\mathcal{X}}(x_i, x_j)$, $\mathbf{L}_{ij} = k_{\mathcal{Z}}(z_i, z_j)/n^2$, and $\boldsymbol{y} = (y_1, \ldots, y_n)^\top$.

[Bennett et al. (2019, **NeurIPS**); Muandet et al. (2020, **UAI**); Dikkala et al. (2020, **NeurIPS**); Zhang et al. (2022, **UR**)]

DualIV: From Two-Stage Estimation to Two-Player Game

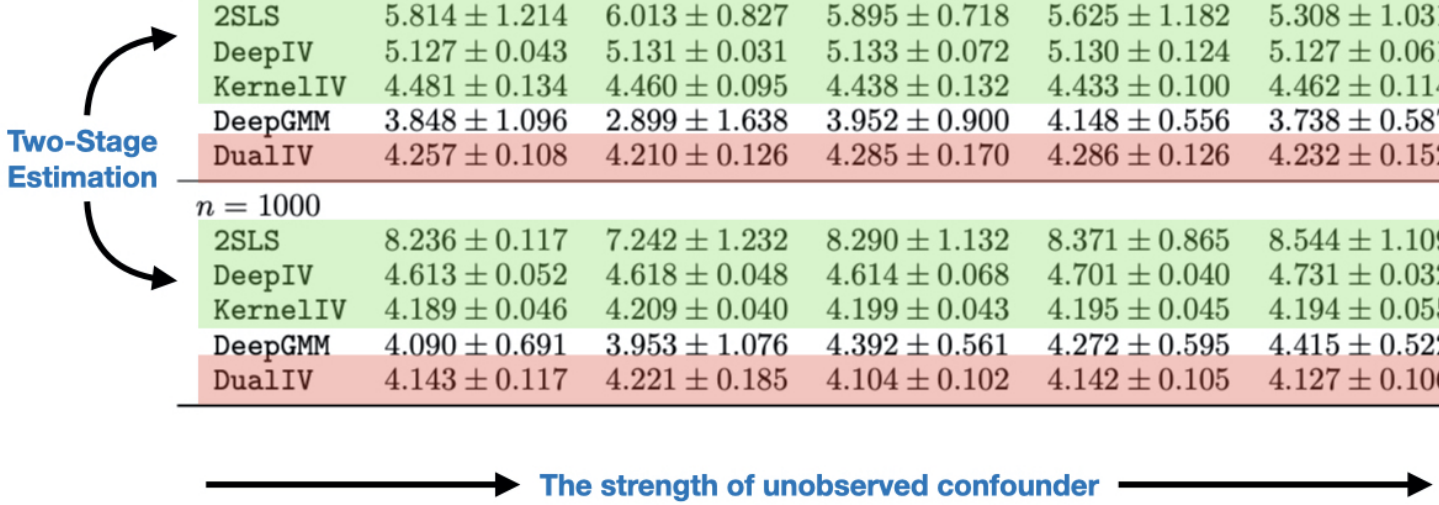
Muandet, Mehrjou, Lee, Raj. (2020, **NeurIPS**)

Demand design: $Y = f(X) + \varepsilon$ where $X = (P, T, S)$ and $Z = (C, T, S)$

- Y: sale, P: price, (T, S): time of year and customer sentiment
- Sale Y and price P are confounded by supply-side market forces
- C: supply cost shifter (instrument)

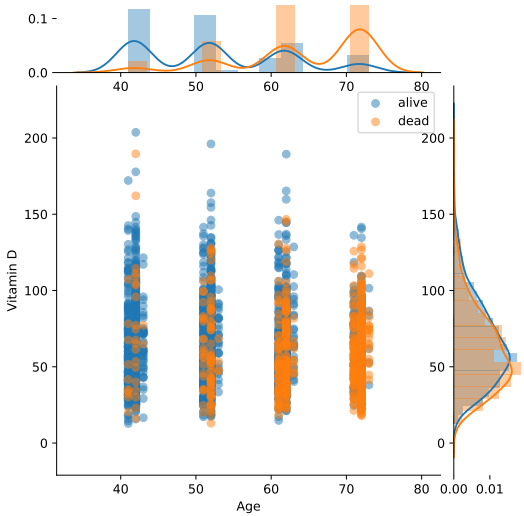
Table 1: Comparisons of IV regression methods in small (top) and medium (bottom) sample size regimes. We report the $\log_{10}$ mean squared error (MSE) and its standard deviations over 20 trials.

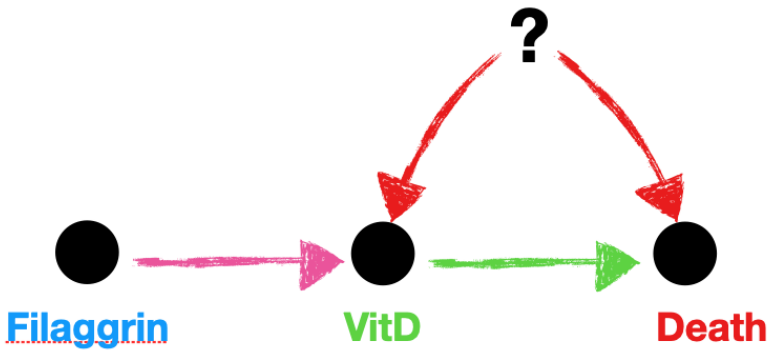
$n = 50$	$\log_{10}$ **Mean Squared Error (MSE)**				
	$\rho = 0.1$	$\rho = 0.25$	$\rho = 0.5$	$\rho = 0.75$	$\rho = 0.9$
2SLS	5.814 ± 1.214	6.013 ± 0.827	5.895 ± 0.718	5.625 ± 1.182	5.308 ± 1.031
DeepIV	5.127 ± 0.043	5.131 ± 0.031	5.133 ± 0.072	5.130 ± 0.124	5.127 ± 0.061
KernelIV	4.481 ± 0.134	4.460 ± 0.095	4.438 ± 0.132	4.433 ± 0.100	4.462 ± 0.114
DeepGMM	3.848 ± 1.096	2.899 ± 1.638	3.952 ± 0.900	4.148 ± 0.556	3.738 ± 0.587
DualIV	4.257 ± 0.108	4.210 ± 0.126	4.285 ± 0.170	4.286 ± 0.126	4.232 ± 0.152
$n = 1000$					
2SLS	8.236 ± 0.117	7.242 ± 1.232	8.290 ± 1.132	8.371 ± 0.865	8.544 ± 1.109
DeepIV	4.613 ± 0.052	4.618 ± 0.048	4.614 ± 0.068	4.701 ± 0.040	4.731 ± 0.032
KernelIV	4.189 ± 0.046	4.209 ± 0.040	4.199 ± 0.043	4.195 ± 0.045	4.194 ± 0.055
DeepGMM	4.090 ± 0.691	3.953 ± 1.076	4.392 ± 0.561	4.272 ± 0.595	4.415 ± 0.522
DualIV	4.143 ± 0.117	4.221 ± 0.185	4.104 ± 0.102	4.142 ± 0.105	4.127 ± 0.106



Improvement over two-stage methods: $\sim$20% ($n = 50$) and $\sim$9% ($n = 1000$)

Vitamin D Data



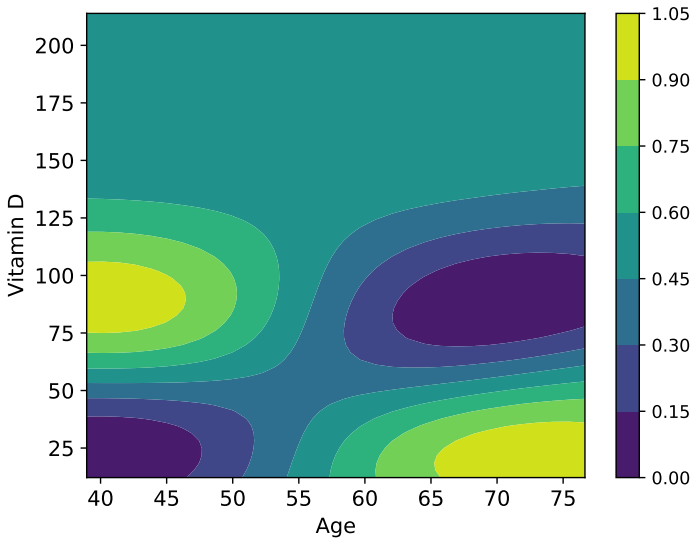


- A 10-year study on 2571 individuals aged 40–71.
- There are 4 variables:
  1. **Age** (at baseline)
  2. **Filaggrin** (binary indicator of filaggrin mutations)
  3. **VitD** (vitamin D level at baseline)
  4. **Death** (binary indicator of death during study)
- The goal is to evaluate the potential effect of VitD on Death.

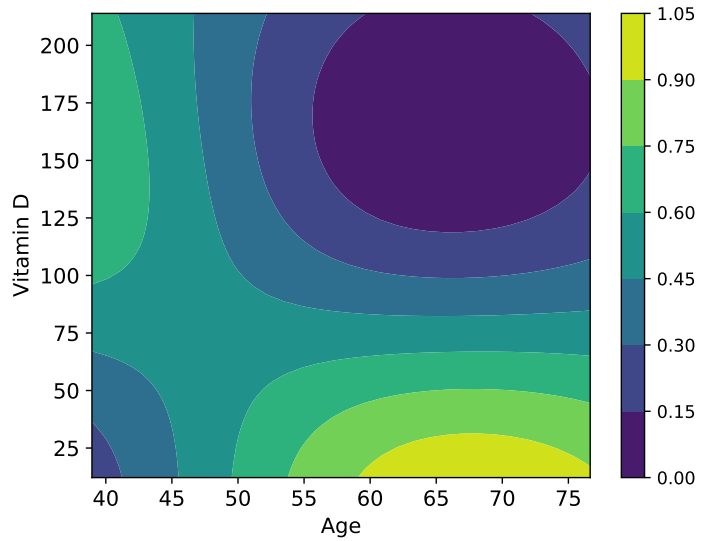
$$X = \text{VitD}, \quad Y = \text{Death}, \quad Z = \text{Filaggrin}$$

Vitamin D Data

$$\text{Death} = f(\text{VitD}, \text{Age})$$



(a) Kernel Ridge Regression (IV: None)

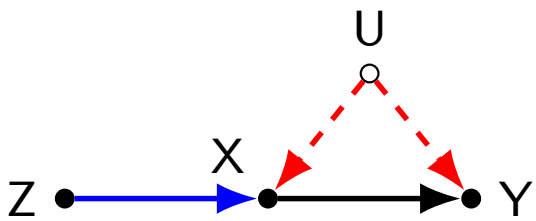


(b) Our Method (IV: Filaggrin Mutation)

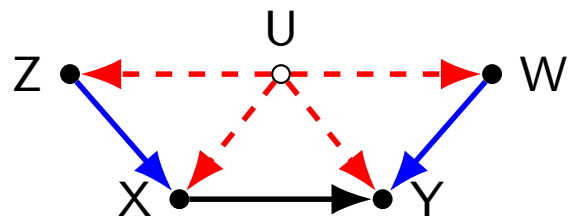
Proximal Causal Learning with Kernels

Mastouri, Zhu, Gultchin, Korba, Silva, Kusner, Gretton, Muandet (2021, **ICML**)

Instrumental Variable



Proxy Variables



- Treatment-inducing proxy Z and outcome-inducing proxy W

[Miao et al. (2018, **Biometrika**)]

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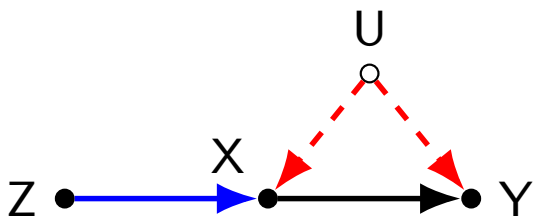

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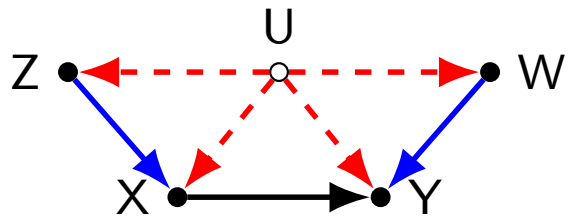

- Treatment-inducing proxy Z and outcome-inducing proxy W
- The **causal effect** estimation

$$\mathbb{E}[\,Y \,|\, \mathrm{do}(X = x)] = \mathbb{E}_W[h(x, W)]$$

where h is a **confounding bridge** function satisfying an integral equation

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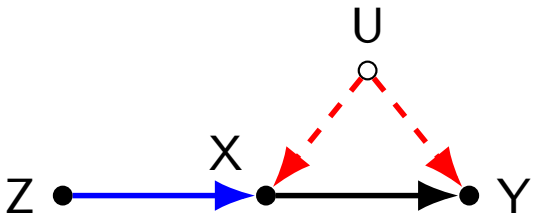

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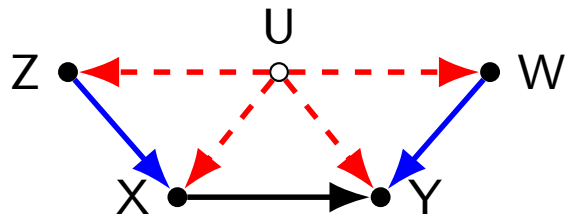

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- The impact of **legalized abortion** (X) on **crime** (Y) [Donohue and Levitt (2001)]
  (Supreme Court's 1973 decision in *Roe* v. *Wade*)

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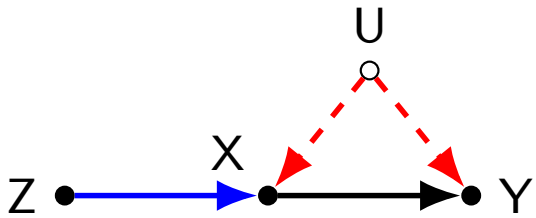

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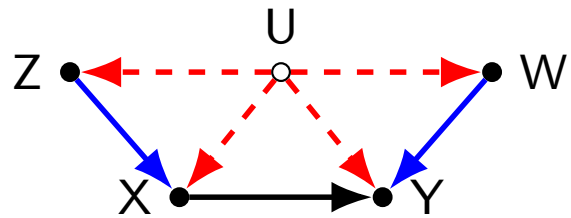

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- The impact of **grade retention** (X) on **cognitive outcome** (Y) [Deaner (2018)]

[Miao et al. (2018, **Biometrika**)]

Fantastic "Instruments" and Where to Find Them

Mendelian Randomization

[Adam (2019, **Nature**)]

Issue: weak instruments

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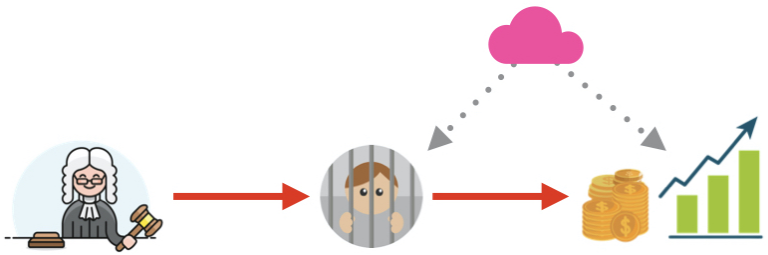
[Adam (2019, **Nature**)]

Issue: weak instruments

Judge Leniency Design

[Kling (2006, **AER**)]



Issue: algorithmic decision making

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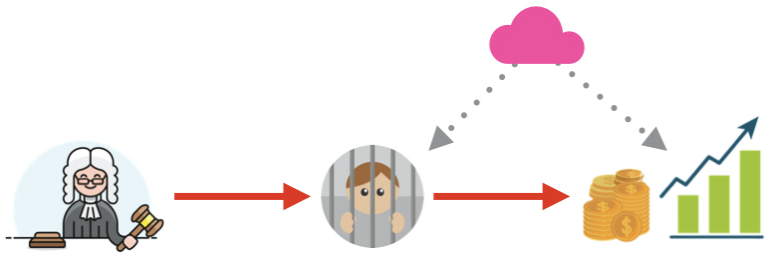
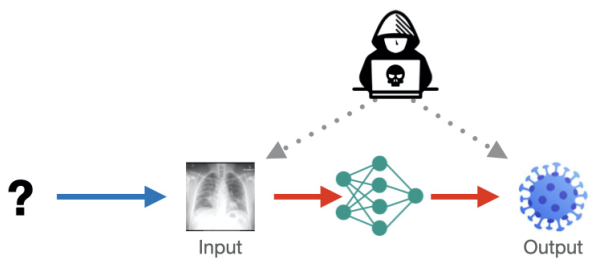


Issue: algorithmic decision making

Adversarial Examples

[N.A.]



Issue: prone to adversarial attack

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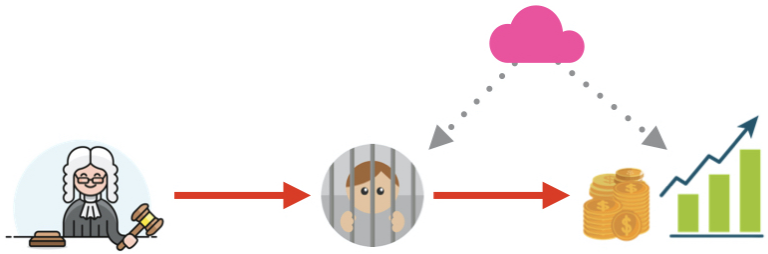

Issue: algorithmic decision making

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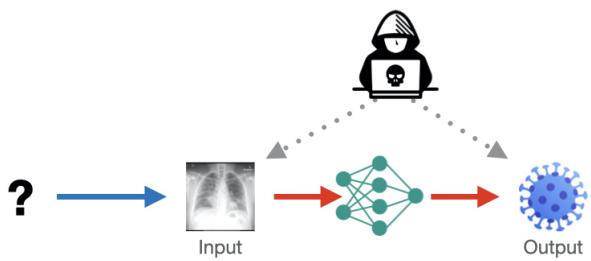
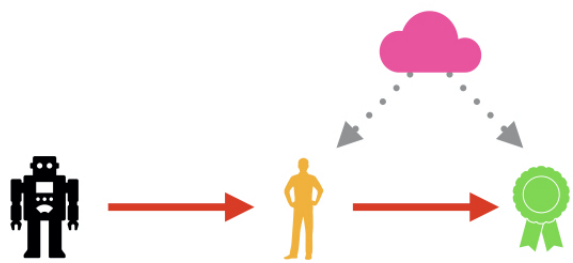


Issue: prone to adversarial attack

Algorithmic Instruments
[Ngo et al. (2021, **ICML**)]



Issue: non-compliance