Causal Inference Methods in Data Science
Lecture 6: More on nontrivial inequality constraints, causal compatibility, and quantum-classical gap in causality; Outlook after this course

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July 14, 2022

Announcement

Turn in the paper review before next Wednesday on canvas!

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- Observational data, interventional data, background knowledge $\Rightarrow$ Causal graph/structure

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- Statistics and computation: estimators, confidence intervals

What causal inference is all about?

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- If a query is not identifiable, can we construct a nontrivial bound? Causal graph/structure implies (conditional) independences and nested (conditional) independences, which are **equality/algebraic constraints**, but how about **inequality/semi-algebraic constraints**?

IV inequality

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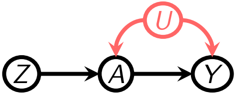

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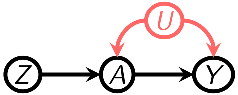
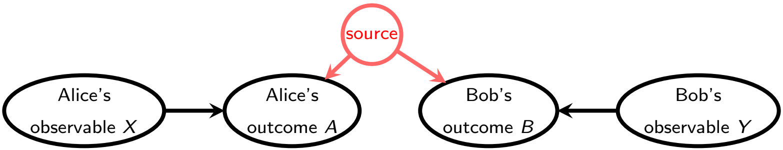


Bell-CHSH experiment:



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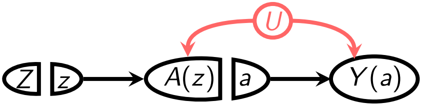
IV SWIG:



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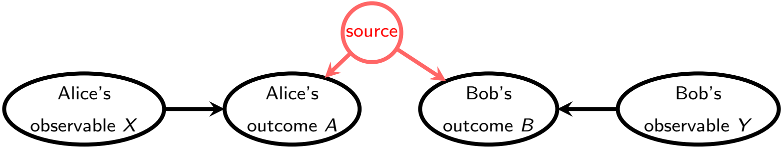

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- which suggests non-trivial inequalities imposed on the observed margin of IV DAG/SWIG:

Theorem 1 (Pearl UAI 1995)

When Z, A, Y have finite and discrete state spaces $\mathcal{Z}$, $\mathcal{A}$, $\mathcal{Y}$

$$\max_{a \in \mathcal{A}} \sum_{y \in \mathcal{Y}} \max_{z \in \mathcal{Z}} p(a, y|z) \leq 1$$

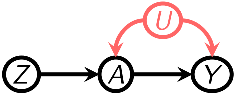
where $p(a, y|z) := \Pr(A = a, Y = y|Z = z)$

Implication: we can falsify IV assumptions by checking if IV inequality holds
But: Pearl's inequality is not sufficient except for binary IV models; see Bonet UAI 2001

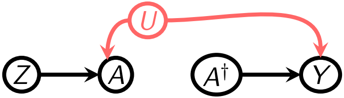
A "coupling" or "cloning" proof due to Robin Evans

Any discrete distribution $\mathbb{P}$ over (Z, A, Y) Markov to IV DAG $\Rightarrow$

For each $\mathfrak{a} \in \mathcal{A}$, able to construct a distribution $\mathbb{Q}_{\mathfrak{a}}$ such that $Y \perp\!\!\!\perp Z$ in $\mathbb{Q}_{\mathfrak{a}}$ and $q_{\mathfrak{a}}(\mathfrak{a}, y|z) = p(\mathfrak{a}, y|z)$ for every $y \in \mathcal{Y}$ and $z \in \mathcal{Z}$



$\mathbb{P}$



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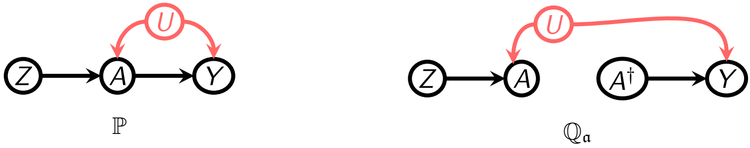

Under $\mathbb{Q}_{\mathfrak{a}}$, $Y \perp\!\!\!\perp Z$ so for $z \neq z'$

$$q_{\mathfrak{a}}(y|z) = q_{\mathfrak{a}}(y|z') \Rightarrow q_{\mathfrak{a}}(y|z) = q_{\mathfrak{a}}(\mathfrak{a}, y|z') + \sum_{a \neq \mathfrak{a}} q_{\mathfrak{a}}(a, y|z')$$

$$\Rightarrow q_{\mathfrak{a}}(y|z) = p(\mathfrak{a}, y|z') + \sum_{a \neq \mathfrak{a}} q_{\mathfrak{a}}(a, y|z')$$

$$\Rightarrow \max_{z \in \mathcal{Z}} p(\mathfrak{a}, y|z) \leq q_{\mathfrak{a}}(y|z) \Rightarrow \max_{\mathfrak{a} \in \mathcal{A}} \sum_{y \in \mathcal{Y}} \max_{z \in \mathcal{Z}} p(\mathfrak{a}, y|z) \leq 1$$

Generalizing IV inequality 1 – More general models

Theorem 2 (Theorem 4.2 of Evans IEEE MLSP 2012)

For any disjoint sets $\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C}, \boldsymbol{D}$ of observed vertices of a DAG $\mathcal{G}$, if $\boldsymbol{A}$ and $\boldsymbol{B}$ are d-separated by $\boldsymbol{C}$ in the corresponding SWIG by splitting node $\boldsymbol{D}$, then for any $\boldsymbol{D} = \mathfrak{d}$, there must exist a distribution $\mathbb{Q}_{\mathfrak{d}}$ under which $\boldsymbol{A} \perp\!\!\!\perp \boldsymbol{B} | \boldsymbol{C}$, compatible with $p(\boldsymbol{a}, \boldsymbol{b}, \mathfrak{d} | \boldsymbol{c})$.

Under $\mathbb{Q}_{\mathfrak{d}}$, we can use $\boldsymbol{A} \perp\!\!\!\perp \boldsymbol{B} | \boldsymbol{C}$ to derive non-trivial inequalities

Special case: $\boldsymbol{A} : Z, \boldsymbol{B} : Y, \boldsymbol{C} : \emptyset, \boldsymbol{D} : A$ in IV DAG

A sound criterion, but not necessarily complete (i.e. exhausting latent-variable DAGs with inequality constraints)

Generalizing IV inequality – Other related works

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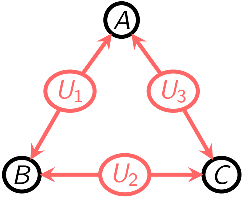
- Gunsilius 2020: impossibility results for continuous treatment
- $\cdots$

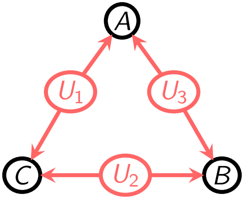
Beyond Bell-CHSH and IV models



"Triangle" model: possessing neither nontrivial (nested conditional) independences, nor inequality constraints using Evans' rule

But there are non-trivial inequality constraints!

Triangle model



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In fact, it induces the following constraints:

$$\{p(A = C) - p(A \neq C)\} + \{p(B = C) - p(B \neq C)\}$$
$$\leq 1 + \{p(A = 1) - p(A = 0)\}\{p(B = 1) - p(B = 0)\}$$

together with its symmetrized version (over permutations of A, B, C)

The inflation technique: Complete algorithm for finding inequality constraints

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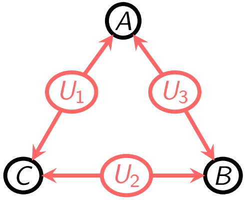
- Opposite to deriving equality (algebraic) constraints for latent-variable causal DAGs by latent projection to obtain ADMG, one can instead augment the graph by introducing copies of observables and latents, but also preserving ancestral relations!

Inflation graph for Triangle model: purely spurious correlation setting



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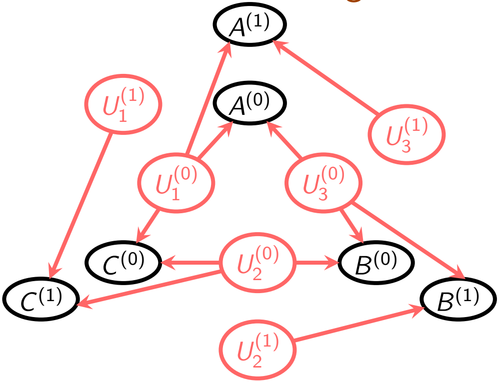

"Spiral" inflation of the "Triangle" model

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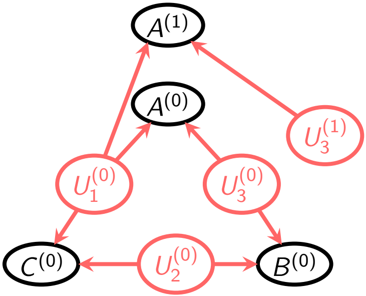

"Capped" inflation of the "Triangle" model

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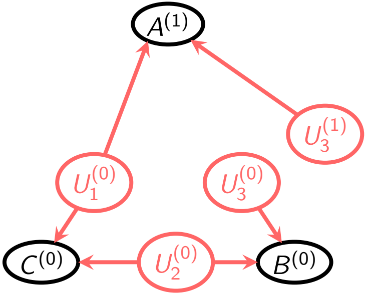

"Cut" inflation of the "Triangle" model

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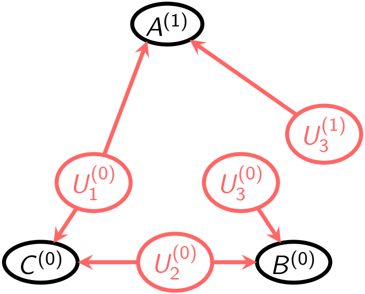

"Cut" inflation of the "Triangle" model

Finding "injectable sets": the subset C' of vertices in the inflated graph $\mathcal{H}$ such that their corresponding original vertex sets C in the original DAG $\mathcal{G}$ sat. $\mathcal{H}_{\text{an}_{\mathcal{H}}(C')} = \mathcal{G}_{\text{an}_{\mathcal{G}}(C)}$

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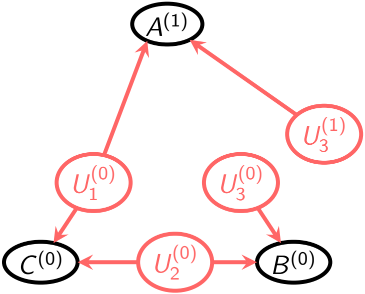

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If the subset C' of vertices in the inflated graph $\mathcal{H}$ is injectable, then $\mathbb{P}_{C'} = \mathbb{P}_C$

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- But importantly, $A^{(1)} \perp\!\!\!\perp B^{(0)}$ in $\mathcal{H}$, so

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- Since $\{A^{(1)}, C^{(0)}\}, \{B^{(0)}, C^{(0)}\}, \{A^{(1)}\}, \{B^{(0)}\}$ are injectable in Cut graph: non-trivial inequality

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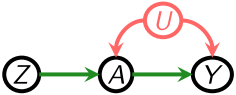
- Identify the "AI-expressible sets": sets that are disjoint union of d-separated injectable sets
- Find trivial inequalities satisfied by AI-expressible sets (often by LP) but leverage the d-separations
- Map back to the original graph as nontrivial inequality

IV model using inflation?

- There are non-spurious correlations among observed vertices for IV model



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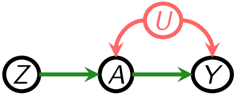

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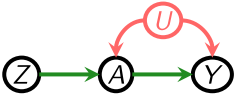

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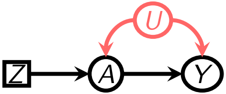

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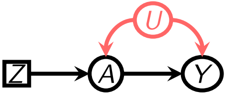

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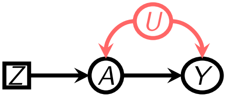

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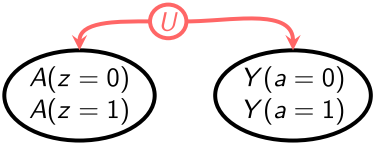

which becomes a purely-correlated scenario after **unpacking** satisfying

$$p(A = a, Y = y|Z = z) = p_{\text{unpacking}}(A(z) = a, Y(a) = y), a, z \in \{0, 1\}^2$$

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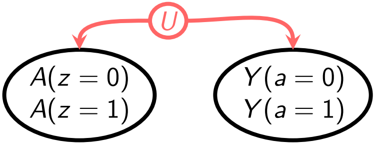

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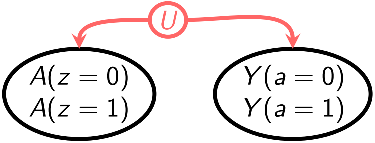

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- Deriving IV inequality? Now easy without even resorting to the inflation technique! See R code "bound.R"

$$\max_a \sum_y \max_z p(A = a, Y = y|Z = z)$$

$$\text{s.t.} \quad \sum_{a_0, a_1, y_0, y_1} p_{\text{unpack}}(A(z = 0) = a_0, A(z = 1) = a_1, Y(a = 0) = y_0, Y(a = 1) = y_1) = 1$$

$$\ldots$$

Completeness?

- The inflation technique is complete, but in the following weak sense: For arbitrary pure-spurious correlation models with L latent variables, there exists an inflation hierarchy indexed by an order m, when $m \to \infty$, if P is not compatible with the causal graph $\mathcal{G}$, then the m-th order inflation can witness it if

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- Overkill? Probably yes! For the following trivial case: $U \to A$ with $P(A=1)P(A=0) \leq \frac{1}{4}$, solving m-th order inflation gives us

$$\frac{1}{2}\frac{2m}{4m-2} > \frac{1}{4}$$

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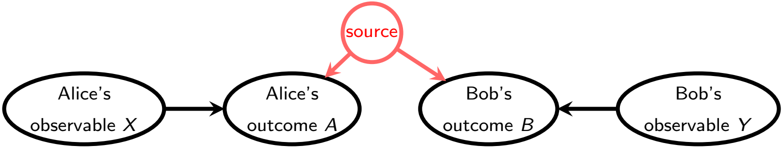
- Open problem: Could there be a short-cut?

classical-quantum gap?

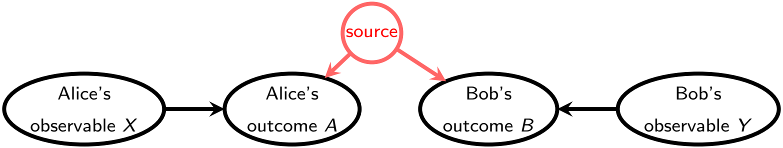
Earliest instance: Tsirelson bound



Bell-CHSH inequality falsifies the hidden-variable locality hypothesis predicted by classical physics; yet it relies on the "freedom of choice" hypothesis (exogeneity of Alice's and Bob's choice of observable); see Chaves et al. 2021

Quantum causal model (at least as formulated in the current literature): latent variables are quantum channels and observed variables are measuring quantum variables (so upon measurement, collapse)

Earliest instance: Tsirelson bound



Classical case: For simplicity assume both observable and outcome are $\{-1, +1\}$-valued then (immediate by unpacking, see R code "bound.R")

$$\mathbb{E}[AB|X = Y = 0] + \mathbb{E}[AB|X = 0, Y = 1] + \mathbb{E}[AB|X = 1, Y = 0] - \mathbb{E}[AB|X = Y = 1] \leq 2$$

This is the form of CHSH

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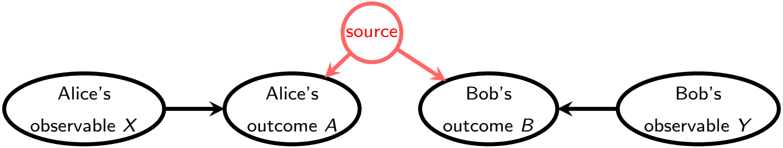

Quantum case: qubits are prepared in the following entangled states in the order of Alice and Bob

$$|\psi\rangle = \frac{1}{\sqrt{2}}\underbrace{|0\rangle\otimes|1\rangle}_{|\psi_1\rangle} - \frac{1}{\sqrt{2}}\underbrace{|1\rangle\otimes|0\rangle}_{|\psi_2\rangle} = \frac{1}{\sqrt{2}}\binom{0}{1}\otimes\binom{1}{0} - \frac{1}{\sqrt{2}}\binom{1}{0}\otimes\binom{0}{1}$$

Alice and Bob measure the outcome with different unitary matrices

$$\text{Alice: } \underbrace{\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}_{X=0} \text{ or } \underbrace{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}_{X=1} \text{ Bob: } \underbrace{\begin{pmatrix} -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}}_{Y=0} \text{ or } \underbrace{\begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}}_{Y=1}$$

Then $|\psi\rangle$ induces a density matrix (p.s.d.) $\varrho = \frac{1}{2}|\psi_1\rangle\langle\psi_1| + \frac{1}{2}|\psi_2\rangle\langle\psi_2|$, which further gives expectation of observable $C = A \otimes B$ to be $\mathrm{Tr}(\varrho C)$. Following commutativity of trace

$$\langle\psi|A_0\otimes B_0|\psi\rangle = \langle\psi|A_0\otimes B_1|\psi\rangle = \langle\psi|A_1\otimes B_0|\psi\rangle = \frac{1}{\sqrt{2}}, \langle\psi|A_1\otimes B_1|\psi\rangle = -\frac{1}{\sqrt{2}}$$

$$\Rightarrow \langle\psi|A_0\otimes B_0|\psi\rangle + \langle\psi|A_0\otimes B_1|\psi\rangle + \langle\psi|A_1\otimes B_0|\psi\rangle - \langle\psi|A_1\otimes B_1|\psi\rangle = 2\sqrt{2} > 2$$

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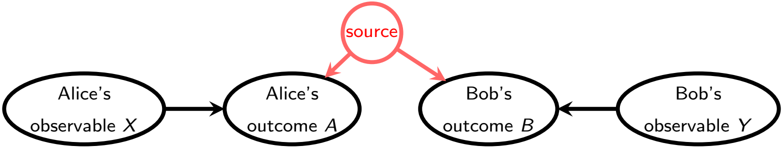

Any guess on how to prove the quantum CHSH bound $2\sqrt{2}$ in a more first-principled way like LP? See “bound.R”

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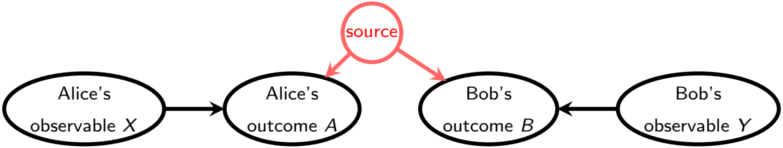

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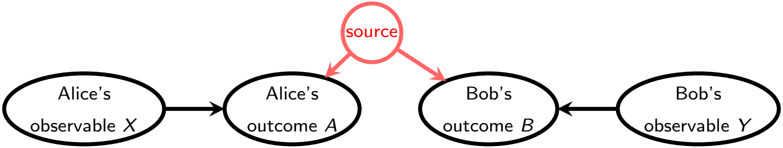

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But in general a polynomial programming problem so quantum causal compatibility is computationally hard! Exists SDP relaxation to solve it approximately

Looking ahead

What could be a good attitude towards causal inference?

I quote the following paragraph written by Ogburn, Shpitser, Tchetgen Tchetgen 2019 (a very angry rant because they were super annoyed by a paper written by famous machine learning researcher David Blei):

> *One of the most important roles of causal inference in statistics and data science is to be transparent about the strong, usually untestable assumptions under which causal inference is possible (Pearl, 2000; Robins, 2001). The burden for transparency about assumptions is arguably greater in causal inference than in other areas of statistics, because it is crucial that scientists and consumers of research, e.g. policy makers or doctors, have the tools to reason about whether an association is in fact causal...*
>
> *but unfortunately – we wish this were not the case! – it is impossible to identify causal effects in the presence of unmeasured confounding with nonparametric or empirically verifiable assumptions.*

What could be a good attitude towards causal inference?

Sounds hopeless? But before 1990's, causality is not even allowed to be studied in statistics

If you feel like having better ideas than what people have had, it could be a great thing! But do read a lot of papers before drawing the conclusion that some idea has not been done before (a lesson of David Blei and colleagues)

If you feel like the current methodology cannot solve your applied problem, it could be even a greater thing!

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- How to combine real world evidence with RCT evidence
- AI system with causality component (covered to some extent in Kun Kuang's guest lecture)

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- No modeling/distributional assumption on the data at all! All the randomness comes from the sampling process
- What is the estimand? What is the estimator? How to show the estimator is good without a reference true distribution $\mathbb{P}$?

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- Renew potential outcomes/counterfactuals by dropping SUTVA

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- What is the limit? How dense the network can be so that we can still learn something? What if the network is unknown?

RWE

- In exercises, we have seen a made-up scenario where trial might not be ideal for decision making but how do you optimally combine RWE with trial data?

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- In complex and dynamic scenario, how to combine RWE and trial?

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- Related to data combination (many different trials + many different observational studies, or more precisely many different interventions + many different passively observed data, e.g. large-scale CRISPR gene-knockdown experiments are a typical instance)

Causal invariance

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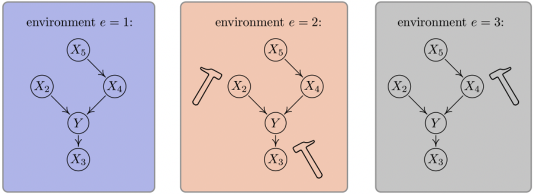
- Axiom: "causal relationship is invariant/stable across different environments"
- Math definition: If a subset $S \subseteq V$ is causal for a response Y, then for all different data distributions (environments) $e \in \mathcal{E}$ (a family of environments), $Y^e = g(V_S^e, u^e)$ with g invariant across different environments $\mathcal{E}$ and $u^e \sim F_u$ with F_u invariant across $\mathcal{E}$



The End! I covered quite a lot of grounds of causality. Hope Ya'll learnt something useful here and there!