

# Non-Parametric Instrumental Variable Models for Categorical Data

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Joint work with James Robins (Harvard)

# Outline

- Randomized experiments
- Observational studies
- Combining observational studies
- Instrumental variables
- Testing instrumental variable models
- Bayesian inference

# Potential outcomes with binary treatment and outcome

For binary treatment  $X$ , we define two potential outcome variables:

- $Y(x = 0)$ : the value of  $Y$  that *would* be observed for a given unit *if* assigned  $X = 0$ ;
- $Y(x = 1)$ : the value of  $Y$  that *would* be observed for a given unit *if* assigned  $X = 1$ ;

*Notation:* We will use  $Y(x_i)$  as an abbreviation for  $Y(x = i)$

## Drug Response Types:

In the simplest case where  $Y$  is a binary outcome we can think of patients as belonging to one of 4 'types':

| $Y(x_0)$ | $Y(x_1)$ | Name                       |
|----------|----------|----------------------------|
| 0        | 0        | <i>Never Recover (NR)</i>  |
| 0        | 1        | <i>Helped (HE)</i>         |
| 1        | 0        | <i>Hurt (HU)</i>           |
| 1        | 1        | <i>Always Recover (AR)</i> |

# Identification Problem

**Want:**  $P(Y(x_0), Y(x_1))$ ;      **Given:**  $P(Y | X=0), P(Y | X=1)$

Under randomization:  $X \perp\!\!\!\perp Y(x_i)$  implies:

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Thus the observed joint  $P(Y|X)$  puts two restrictions on  $P(Y(x_0), Y(x_1))$ :

$$\begin{aligned} P(Y=1 | X=0) &= P(Y(x_0)=1, Y(x_1)=0) + P(Y(x_0)=1, Y(x_1)=1) \\ P(Y=1 | X=1) &= P(Y(x_0)=0, Y(x_1)=1) + P(Y(x_0)=1, Y(x_1)=1). \end{aligned}$$

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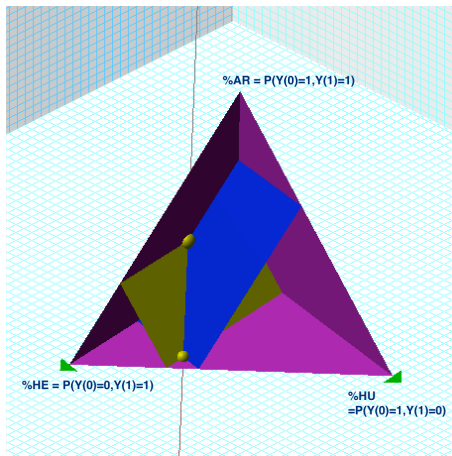
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Each restriction implies a 2-d subset in  $\Delta_3$ .  
Intersection forms a 1-d subset on which ACE is constant.

# 3-d Plot



In this plot:

$$P(Y=1 \mid X=0) = P(Y(x_0) = 1) = \%HU + \%AR = 0.3, \text{ (yellow)}$$

$$P(Y=1 \mid X=1) = P(Y(x_1) = 1) = \%HE + \%AR = 0.6, \text{ (blue)}$$



## Two-way Table

Under randomization, the relationship between the counterfactual distribution  $P(Y(x_0), Y(x_1))$  and the observed distributions  $\{P(Y | x_0), P(Y | x_1)\}$  is:

|      |                | col sums                |                         |
|------|----------------|-------------------------|-------------------------|
|      |                | $P(Y=0   X=0)$          | $P(Y=1   X=0)$          |
| row  | $P(Y=0   X=1)$ | $P(Y(x_0)=0, Y(x_1)=0)$ | $P(Y(x_0)=1, Y(x_1)=0)$ |
| sums | $P(Y=1   X=1)$ | $P(Y(x_0)=0, Y(x_1)=1)$ | $P(Y(x_0)=1, Y(x_1)=1)$ |

Here  $P(Y=i | X=j) = P(Y(x_j)=i)$  due to randomization.

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Equivalently we may write this in terms of types

|                | $P(Y=0   X=0)$ | $P(Y=1   X=0)$ |
|----------------|----------------|----------------|
| $P(Y=0   X=1)$ | $P(NR)$        | $P(HU)$        |
| $P(Y=1   X=1)$ | $P(HE)$        | $P(AR)$        |

# Observational study: one-way table!

| Observed      | Counterfactual            |
|---------------|---------------------------|
| $p(X=0, Y=0)$ | $p(X=0, NR) + p(X=0, HE)$ |
| $p(X=0, Y=1)$ | $p(X=0, HU) + p(X=0, AR)$ |
| $p(X=1, Y=0)$ | $p(X=1, NR) + p(X=1, HU)$ |
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# Bounds on joints $P(Y(x_0), Y(x_1))$

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$$0 \leq \%HE \leq P(X=0, Y=0) + P(X=1, Y=1)$$

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$$0 \leq \%HE \leq P(X=0, Y=0) + P(X=1, Y=1)$$

$$0 \leq \%HU \leq P(X=0, Y=1) + P(X=1, Y=0)$$

$$0 \leq \%NR \leq P(X=0, Y=0) + P(X=1, Y=0) = P(Y=0)$$

$$0 \leq \%AR \leq P(X=0, Y=1) + P(X=1, Y=1) = P(Y=1)$$

# Bounds on margins $P(Y(x_i))$

| Observed      | Counterfactual            |
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| $p(X=0, Y=0)$ | $p(X=0, NR) + p(X=0, HE)$ |
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We also have the following inequalities on the marginals:

$$\{ P(Y(x_0) = 1) = P(HU) + P(AR)$$

$$\{ P(Y(x_1) = 1) = P(HE) + P(AR)$$

$$P(X=0, Y=1) \leq P(Y(x_0)=1) \leq 1 - P(X=0, Y=0)$$

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$$P(Y(x_0) = 1) = P(HU) + P(AR)$$

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$$P(Y(x_0)=0) = P(HU) + P(NR)$$

$$P(Y(x_1)=0) = P(NR) + P(HU)$$

$$P(HU) + P(AR)$$

$$P(X=0, Y=1) \leq P(Y(x_0)=1) \leq 1 - P(X=0, Y=0)$$

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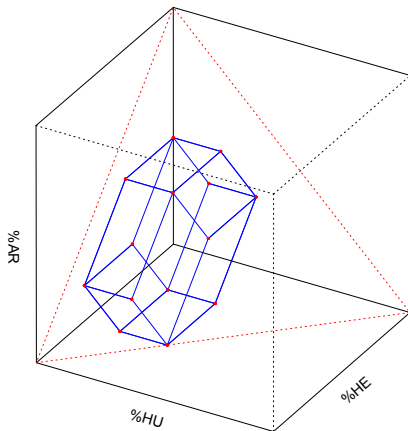
$$P(X=1, Y=0) \leq P(Y(x_0)=0) \leq 1 - P(X=1, Y=1)$$

Thus we have 6 pairs of parallel planes.

$$\therefore P(Y(x_0)=0) = 1 - P(Y(x_0)=1) - P(Y(x_1)=0) - P(X=0)$$

# Polytope for observational study

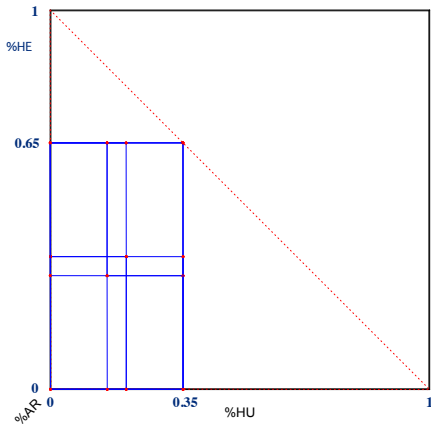
Set of margins  $P(Y(x_0), Y(x_1))$  compatible with the Obs. Study.





# ACE bounds

$$ACE = \% HE - \% HU$$



(But why is this helpful!?)

# Inference for the ACE without randomization

(Robins-Manski bounds)

Suppose that we do **not** know that  $X \perp\!\!\!\perp Y(x_0)$  and  $X \perp\!\!\!\perp Y(x_1)$ .

What can be inferred from the observed distribution  $P(X, Y)$ ?

General case:

$$\begin{aligned} & -(P(X=0, Y=1) + P(X=1, Y=0)) \\ & \leqslant \text{ACE}(X \rightarrow Y) \\ & \leqslant P(X=0, Y=0) + P(X=1, Y=1) \end{aligned}$$

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$\Rightarrow$  Bounds are of length 1 and will always include zero.

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Z: assignment to treatment or control arm (randomized);

X: whether patient takes (more than certain amount of) drug;

Y: patient's health outcome.

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|---|---|---|-------|
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| 0 | 0 | 1 | 14    |
| 0 | 1 | 0 | 0     |
| 0 | 1 | 1 | 0     |
| 1 | 0 | 0 | 52    |
| 1 | 0 | 1 | 12    |
| 1 | 1 | 0 | 23    |
| 1 | 1 | 1 | 78    |

(Data originally considered by Efron and Feldman (1991); dichotomized by Pearl.)

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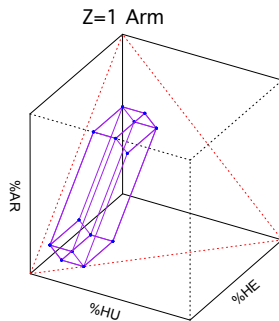
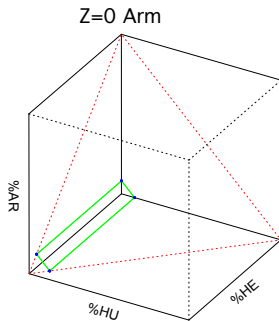
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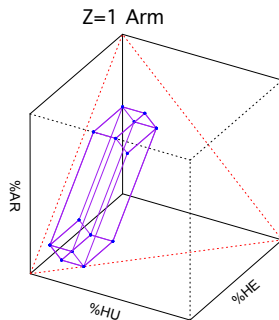
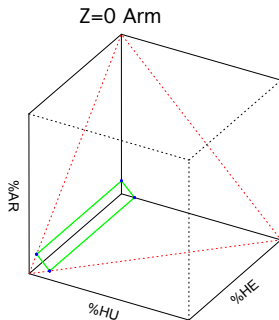
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**Idea:** Analyze each Z arm as an observational study.

# Each Z Arm



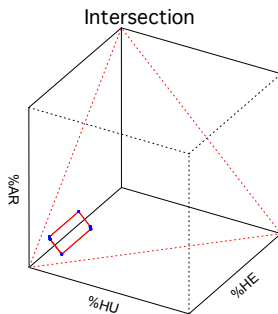
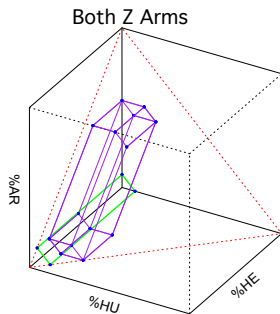
# Each Z Arm



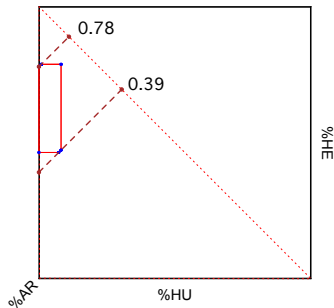
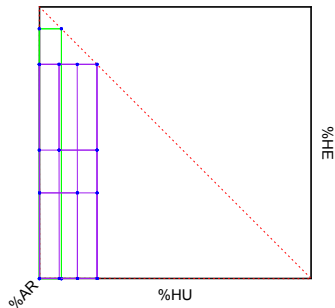
$Z = 0$  arm polytope is 2-d since  $Z = 0 \Rightarrow X = 0$



# Combining the Arms



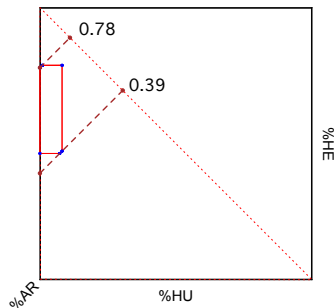
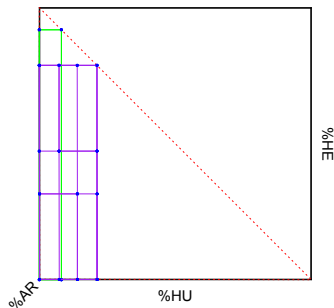
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Upper bound is: 0.78; lower bound is 0.39

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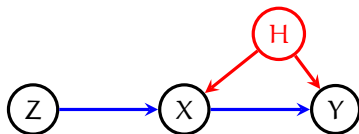
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These are the [Balke and Pearl \(1993\)](#) bounds, obtained via principal strata and computational algebra;

# Instrumental Variable Model

We assume that assignment  $Z$  has no direct effect on the outcome  $Y$  except through  $X$ , so  $Y(x, z_0) = Y(x, z_1) \equiv Y(x)$ ;



$Z$  is said to be an ‘instrument’ for the effect of  $X$  on  $Y$ .

Potential outcomes:

$$X(z_0), X(z_1), Y(x_0), Y(x_1)$$

Randomization becomes: for all  $x, z$ ,  $Z \perp\!\!\!\perp \{X(z), Y(x)\}$

The assumptions: (i) No direct effect of  $Z$  on  $Y$ , and (ii)  $Z$  randomized are sufficient to justify the intersecting polytope analysis.

## Bounds on ACE: Previous results

- Robins (1989) and Manski (1990) derived the ‘natural’ bounds:

$$\begin{aligned} & p(y_1 | z_1) - p(y_1 | z_0) - p(y_1, x_0 | z_1) - p(y_0, x_1 | z_0) \\ & \leq \text{ACE}(X \rightarrow Y) \leq \\ & p(y_1 | z_1) - p(y_1 | z_0) + p(y_0, x_0 | z_1) + p(y_1, x_1 | z_0) \end{aligned}$$

These are not sharp if there are Defiers;

they follow from (and are sharp) under  $Z \perp\!\!\!\perp Y(x_0)$ ,  $Z \perp\!\!\!\perp Y(x_1)$ .

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- Balke and Pearl (1993) derived closed form expression for ACE bounds via computational algebra;  
Resulting expressions are maxima and minima over 8 different expressions.
- Dawid (2002) re-derived these bounds without (explicitly!) using potential outcomes, again using computational algebra.

An advantage of the approach taken here is that it extends to  $Z$  with finitely many levels.

## Extending to $p$ levels of $Z$ : Identification

Solving the identification problem requires no further work:

Intersect  $p$  polytopes.



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Intersect  $p$  polytopes.

The set of distributions  $P(Y(x_0), Y(x_1))$  that are compatible with  $P(X, Y|Z)$  is **still** given by the following **six pairs of parallel planes**:

$$0 \leq \%NR \leq \min_i p(y_0 | z_i)$$

$$0 \leq \%AR \leq \min_i p(y_1 | z_i)$$

$$0 \leq \%HE \leq \min_i \{p(x_1, y_1 | z_i) + p(x_0, y_0 | z_i)\}$$

$$0 \leq \%HU \leq \min_i \{p(x_0, y_1 | z_i) + p(x_1, y_0 | z_i)\}$$

$$\max_i p(x_0, y_1 | z_i) \leq P(Y(x_0)=1) \leq \min_i \{1 - p(x_0, y_0 | z_i)\}$$

$$\max_i p(x_1, y_1 | z_i) \leq P(Y(x_1)=1) \leq \min_i \{1 - p(x_1, y_0 | z_i)\}$$

# Generalizing to more levels of $Z$

## Theorem (R+Robins 2014)

If  $X, Y$  binary and  $Z$  with  $p$  levels then under the IV model:

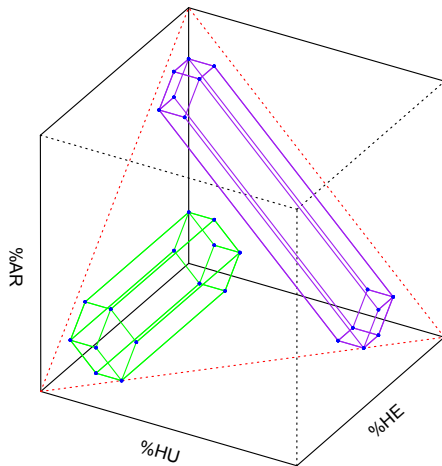
$$1 - g(1, 0) - g(0, 1) \leq \text{ACE}(X \rightarrow Y) \leq g(0, 0) + g(1, 1) - 1,$$

where

$$g(i, j) \equiv \min \left\{ \min_z [P(X=i, Y=j | Z=z) + P(X=1-i | Z=z)], \right. \\ \left. \min_{z, \tilde{z}: z \neq \tilde{z}} [P(X=i, Y=j | Z=z) + P(X=1-i, Y=0 | Z=z) \right. \\ \left. + P(X=i, Y=j | Z=\tilde{z}) + P(X=1-i, Y=1 | Z=\tilde{z})] \right\}.$$

This exploits the fact that  $P(Y(x_0) = 1)$  and  $P(Y(x_1) = 1)$  are variation independent.

# Polytopes may not intersect



$\Rightarrow$  Model places testable constraints on  $P(X, Y \mid Z)$ .

## Model for $P(X, Y \mid Z)$ ( $Z$ binary)

*Counterfactual*

*Observed*



$$\Delta_{15}$$

$\rightarrow$

$$\Delta_3 \times \Delta_3$$

$$P(\{X(z), Y(x)\})$$

$\mapsto$

$$(P(X, Y \mid Z=0), P(X, Y \mid Z=1))$$

# Model for observables

For  $Z$  binary requiring that the polytopes intersect leads to the following:  
If  $p(X, Y \mid Z)$  is compatible with the binary IV model iff

$$p(Y=0, X=0 \mid Z=0) + p(Y=1, X=0 \mid Z=1) \leq 1,$$

$$p(Y=0, X=0 \mid Z=1) + p(Y=1, X=0 \mid Z=0) \leq 1,$$

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they provide a test of the binary IV model.

Can be interpreted as bounding away from zero  $E[Y(z_1, x) - Y(z_0, x)]$ ,  
the average direct effect of  $Z$  on  $Y$ , holding  $X$  fixed at  $x$ .

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These are the IV inequalities of Pearl (1995) and Bonet (2001);  
they provide a test of the binary IV model.

Can be interpreted as bounding away from zero  $E[Y(z_1, x) - Y(z_0, x)]$ ,  
the average direct effect of  $Z$  on  $Y$ , holding  $X$  fixed at  $x$ . Leads to smooth  
variation independent parametrization of model (R, Evans & Robins, 2011).

# Model for observables

Hard to visualize this subset of  $\Delta_3 \times \Delta_3$ .

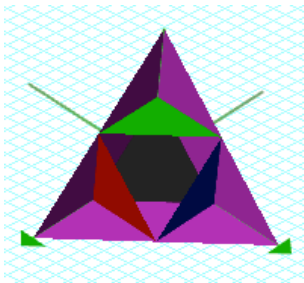
Can project onto the co-ordinates given by the LHS of the inequalities:

$$u_1 \equiv \sum_j p(y_j, x_0 | z_j) \quad u_2 \equiv \sum_k p(y_k, x_0 | z_{1-k})$$

$$u_3 \equiv \sum_j p(y_j, x_1 | z_j) \quad u_4 \equiv \sum_k p(y_k, x_1 | z_{1-k})$$

then since  $\sum_i u_i = 2$ ,  $(u_1, u_2, u_3, u_4)$  lies in a 3-d simplex with sum 2.

The IV inequalities are  $u_i \leq 1$  for  $i = 1, \dots, 4$ . This gives an octahedron:





# Model for observables

Hard to visualize this subset of  $\Delta_3 \times \Delta_3$ .

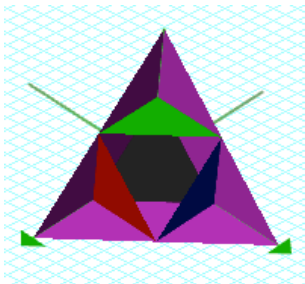
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**Corollary:** At most one inequality is ever violated. (see also Cai, Kuroki, Pearl, Tian, 2008)

## Extending to $p$ levels of $Z$ : Observable model

Explicitly characterizing the set of observed distributions  $P(X, Y|Z)$  does require more work. Three known types of constraint:

$2p(p - 1)$  IV inequalities, these involve 2 levels of  $Z$ ;

$4p(p - 1)(p - 2)$  inequalities found by Bonet (2001), these involve 3 levels of  $Z$

$p!/(p - 4)!$  inequalities found by R, which involve 4 levels of  $Z$ .

**Conjecture:** These are the only constraints.

Confirmed by direct computation for  $p \leq 7$ .

(Note: Implicit solution given by seeing if the set of distributions  $P(Y(x_0), Y(x_1))$  is non-empty.)

# Bayesian Inference

What about sampling variability?

The true population distribution  $p(x, y \mid z)$  is not equal to the empirical distribution observed in the sample.

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# Bayesian Inference

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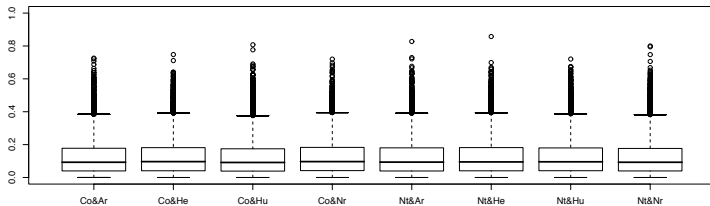
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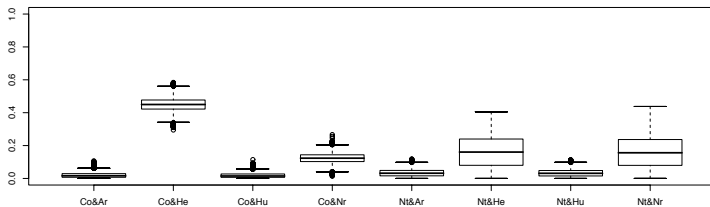
$$\{P(X(z_0), X(z_1), Y(x_0), Y(x_1))\}.$$

⇒ Use MCMC to sample from posterior distribution.

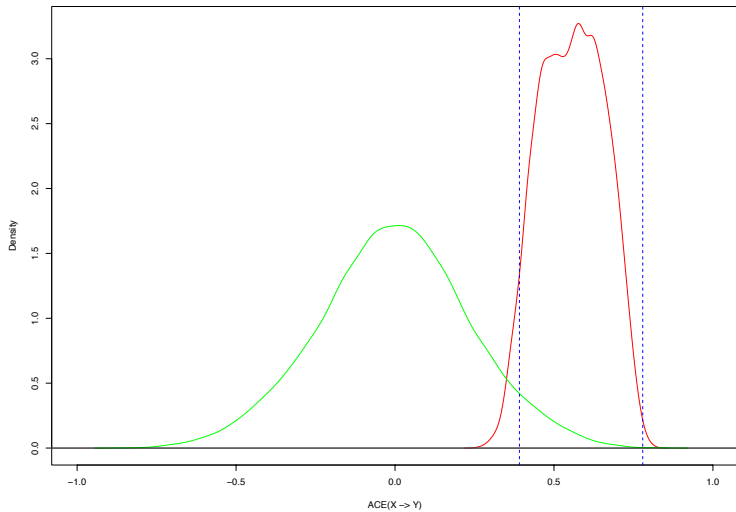
Marginal Prior distributions; Dir(1,...,1)

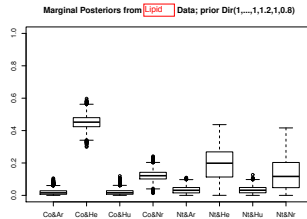
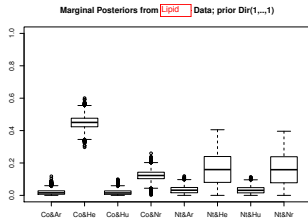
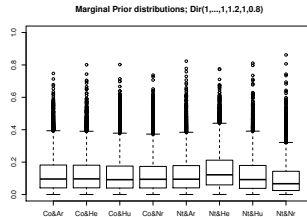
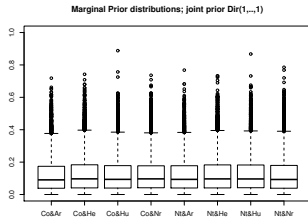


Marginal Posterior distributions from Lipid Data; Prior Dir(1,...,1)



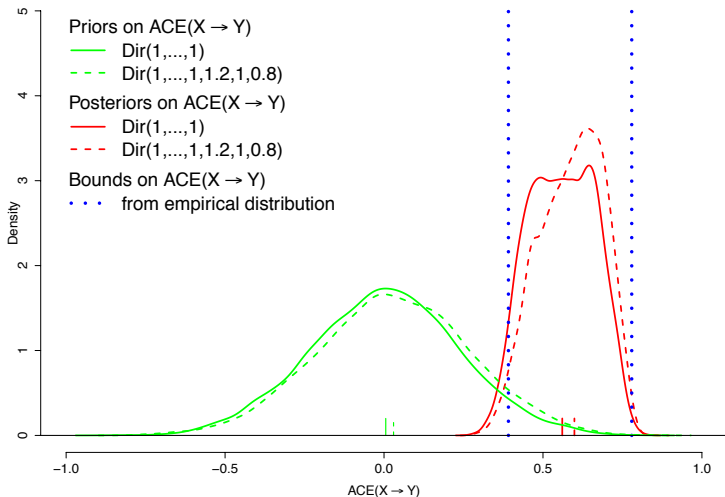
Prior  $\text{Dir}(1, \dots, 1)$  and Posterior for  $\text{ACE}(X \rightarrow Y)$  from Lipid Data







Prior and posterior on  $ACE(X \rightarrow Y)$  for Lipid data  
Uniform & perturbed uniform priors on potential outcomes



# Is the problem caused by the priors?

Try a 'unit' information prior:

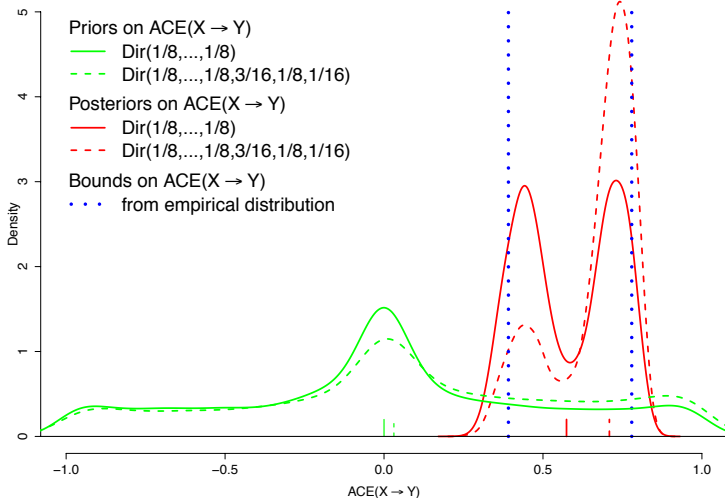
$$p(\{X(z), Y(x)\}) \sim \text{Dir}(1/8, \dots, 1/8)$$

vs.

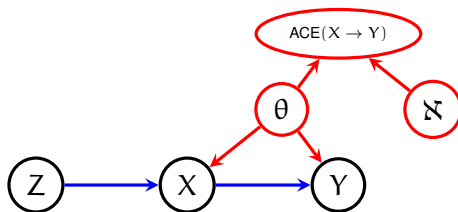
$$p(\{X(z), Y(x)\}) \sim \text{Dir}(1/8, \dots, 1/8, 3/16, 1/8, 1/16)$$

(?Though 'unit' of whose information?)

# Prior and posterior on $ACE(X \rightarrow Y)$ for Lipid data Unit & perturbed unit priors on potential outcomes



# Big picture: How to formulate priors transparently



We will re-parameterize:

$$\{P(X(z_0), X(z_1), Y(x_0), Y(x_1))\} \leftrightarrow (\theta, \aleph)$$

$\theta$  is a 6 dim. parameter, (completely!) identifiable from  $P(X, Y | Z)$ .

$\aleph$  is a 9 dim. parameter, (completely!) non-identifiable.

$$P(\theta, \aleph) = P(\theta)P(\aleph)$$

$$P(\theta, \aleph | Z, X, Y) = P(\theta | Z, X, Y)p(\aleph)$$

Note that  $\aleph \perp\!\!\!\perp Z, X, Y$

# Simple implementation (I)

Recall that the binary IV model is defined by the inequalities:

$$\begin{aligned}P(Y=0, X=0 \mid Z=0) + P(Y=1, X=0 \mid Z=1) &\leq 1, \\P(Y=0, X=0 \mid Z=1) + P(Y=1, X=0 \mid Z=0) &\leq 1, \\P(Y=0, X=1 \mid Z=0) + P(Y=1, X=1 \mid Z=1) &\leq 1, \\P(Y=0, X=1 \mid Z=1) + P(Y=1, X=1 \mid Z=0) &\leq 1.\end{aligned}\tag{1}$$

*Prior:* Dirichlet on  $P(X, Y \mid Z)$  restricted (and re-normalized) to those distributions obeying (1).

*Posterior:* The usual Dirichlet posterior, again restricted to those distributions obeying (1).

Inference may be performed by ‘straight’ Monte-Carlo.

# Simple Implementation (II)

To obtain the posterior distribution on the ACE bounds, perform the following steps:

- 1 Specify Dirichlet  $(\alpha_{00z}, \alpha_{01z}, \alpha_{10z}, \alpha_{11z})$  priors on  $p(x, y|z)$  for  $z = 0, 1$ .
- 2 Compute the posteriors in the usual way:  
Dirichlet  $(\alpha_{00z} + n_{00z}, \alpha_{01z} + n_{01z}, \alpha_{10z} + n_{10z}, \alpha_{11z} + n_{11z})$   
where  $n_{ijz}$  is the number of observations with  $X = i, Y = j, Z = z$ .
- 3 Simulate  $p^{(1)}(x, y|z), \dots, p^{(N)}(x, y|z)$  from this posterior.
- 4 Throw out any  $p^{(i)}(x, y|z)$  violating the inequalities (1).
- 5 Compute upper and lower bounds on the ACE from each distribution  $p^{(i)}(x, y|z)$  remaining after step 4.

## Back to Lipid Data

Parametrize IV model as:

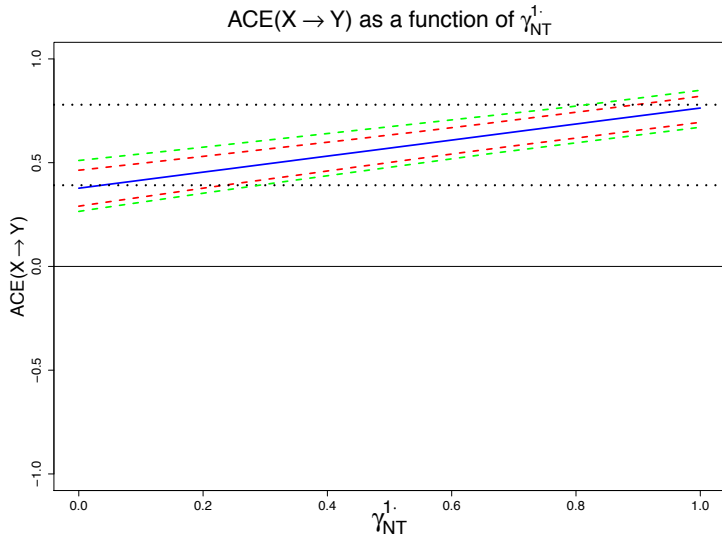
$p(X, Y | Z)$  obeying IV inequalities

Use  $\text{Dir}(1, 1)$  for  $p(x = 0, y | z = 0)$  (since  $p(x = 1, y | z = 0) = 0$ )

and  $\text{Dir}(1, 1, 1, 1)$  for  $p(x, y | z = 1)$ .

(Posterior probability that IV model holds: 0.368; prior probability was 0.5.)

We then truncate and renormalize using the IV inequalities.



Here  $\gamma_{NT}^1 \equiv P(Y(x_1) = 1 \mid NT)$ , the probability of a good outcome for Never Takers, if they were to get the drug; this is completely unidentified.



# Summary

- Potential outcome models provide a way to formulate causal models in terms of missing data
- Geometric analysis of randomized and observational studies
- Instrumental variable design may be seen as combining observational studies
- Non-parametric IV models impose testable constraints
- These constraints lead to a *transparent* method of Bayesian analysis.

**Thank you!**

# What if I don't believe (deterministic) potential outcomes exist?

- Dawid (2003), Cai *et al.* (2008) show that IV inequalities may be derived without assuming existence of deterministic potential outcomes, likewise for ACE bounds  
⇒ multivariate link functions for GLMs are also useful even under probabilistic potential outcome models.

Similar 'coupling' arguments may also be given for the generalizations to more states for  $X$  and  $Z$ .

## Extending to $p$ levels of $Z$ , $q$ levels of $X$ : identification

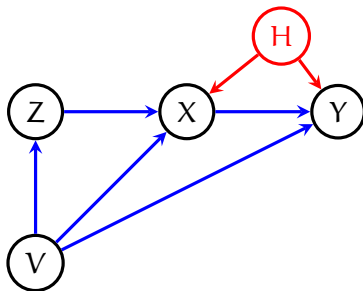
**Conjecture:** The set of distributions  $P(Y(x_1), \dots, Y(x_q))$  compatible with  $P(X, Y|Z)$  is given by the following constraints:  
For every non-empty subset  $A \subseteq \{1, \dots, q\}$ , every assignment  $(y^i, i \in A)$ , with  $y^i \in \{0, 1\}^{|A|}$  and every  $z \in \{1, \dots, p\}$ :

$$0 \leq P(\{Y(x_i) = y^i, i \in A\}) \leq \sum_{j \in A} p(Y=y^j, X=j \mid z) + \sum_{k \notin A} p(X=k \mid z) \quad (2)$$

*Necessity is established. Sufficiency has been proved up to  $p \leq 7$ ; sketch of proof in general.*

# Incorporating baseline covariates

May wish to model  $ACE(X \rightarrow Y)$  as a function of possibly continuous baseline covariates.

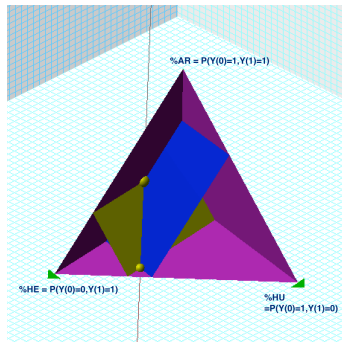


# Generalized Linear Models

Need: a multivariate link function (aka diffeomorphism) from  $\mathbb{R}^6$  into subset of  $\Delta_3 \times \Delta_3$  given by the inequalities defining the IV model

$\Rightarrow$  incorporate covariates as in a multivariate GLM.

# Fréchet inequalities



Equation for line segment in simplex:

$$\left\{ \begin{array}{lcl} P(1, 1) & = & t \\ P(1, 0) & = & c_0 - t \\ P(0, 1) & = & c_1 - t \\ P(0, 0) & = & 1 - c_0 - c_1 + t \end{array} \quad t \in [\max\{0, (c_0 + c_1) - 1\}, \min\{c_0, c_1\}] \right\} \quad \left. \begin{array}{l} c_0 \equiv P(Y=1 \mid x_0) \\ c_1 \equiv P(Y=1 \mid x_1) \end{array} \right\}$$

Extreme points are given by 'Fréchet inequalities'.