# Parameterizing and Simulating from Causal Models by Robin Evans and Vanessa Didelez

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This discussion of Evans and Didelez (2021) is based on a Online Causal Conference Seminar, this Recording and this Recording.

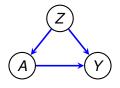
#### **Outline**

- Introduction
  - Notations
  - g-null paradox
- Proposed Method
  - General setting
  - Cognate Probabilities
  - Frugal parameterization
  - Variation Independence
- Main result
- Model fitting
- Simulation study
- Discussion



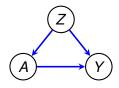
#### Example

Consider *X*: diet, *Y*: BMI, *Z*: indicator of education level.



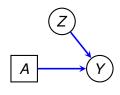
#### Example

Consider *X*: diet, *Y*: BMI, *Z*: indicator of education level.



If we performed an experiment where A = a is set by external intervention,

- the randomized A removes confounding effect from Z, i.e.  $A \perp \!\!\! \perp Z$ .
- marginal dist [Z], conditional dist [Y|A,Z] are preserved.



#### The Problem

As in Marginal Structural Models (MSM) by Robins et al. (2000), we consider the potential outcome of Y given X = x, i.e., the marginal effect of X on Y. Under SUTVA, SRA, and Positivity:

$$P^*(Y = y | A = a) = \sum_{z} P(Z = z) P(Y = y | Z = z, A = a),$$
 (1)

which is also denoted as P(Y = y | do(A = a)).

- [·]\*: distribution/parameter from causal or interventional distribution
- [-]: distribution/parameter from observational regime

#### Example R1

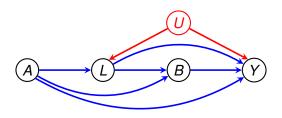


Figure 1: The causal model from Havercroft and Didelez (2012).

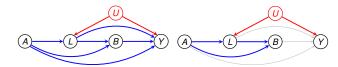
- The second treatment B depends on both the first treatment A and an intermediate outcome L
- The variable *U* is 'hidden' or latent
- Identifiable quantities are functions of P<sub>ALBY</sub>
- ullet Quantity of interest: conditional distribution  $P_{Y|A,B}$

#### g-formula and g-null

**g-formula (Robins, 1986)**: Under the assumption of positivity and the causal structure implied by the graph ( $p_{L|AB} = p_{L|A}$ ),  $p_{Y|AB}$  is identified by the g-formula

$$p_{Y|AB}(y \mid do(a,b)) := \int p_{Y|ALB}(y \mid a, \ell, b) \cdot p_{L|A}(\ell \mid a) d\ell.$$
 (2)

**g-null:**  $H_0: A, B$  has no effect on Y, i.e. there are no arrows from A to Y, nor B to Y.



#### g-null Paradox

**g-null Paradox (Robins and Wasserman, 2013)**:  $p_{Y|AB}$  would depend on A even if g-null is true, i.e. A, B has no causal effect on Y. **Example:** Suppose

$$Z|A \sim Ber(expit(\alpha A)), \ \mathbb{E}[Y|A, Z, B] = A\beta_a + Z\beta_z + B\beta_b,$$

then

$$\mathbb{E}[Y|do(A,B)] = A\beta_a + B\beta_b + expit(\alpha A)\beta_z.$$

For  $\mathbb{E}[Y|do(A,B)]$  to be independent from A, we need

$$\beta_a = 0$$
 and  $\alpha \beta_z = 0$ ,

which is equivalent to

either 
$$Y \perp \!\!\!\perp A, Z | B$$
 or  $\begin{cases} Y \perp \!\!\!\perp A | B \\ A \perp \!\!\!\perp Z \end{cases}$ 



#### Models avoiding g-null Paradox

J.Robins invented many causal models such as marginal structural models (MSM) and structural nested models (SNM) to make it easier to estimate causal effects. These models

- they lead to tractable estimators
- they are semiparametric
- they avoid the g-null paradox

## Marginal Structural Models (MSM)

MSM was proposed to work on longitudinal data, where there are time-dependent confounders, and treatments depend on historical data. Given a time series of covariates  $Z_t$ , treatments  $A_t$ , and responses  $Y_t$ :

$$\{(Z_t, A_t, Y_t)\}_{t=1}^T.$$

An MSM:

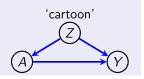
$$g(a_1,\ldots,a_T)=\mathbb{E}(Y(a_1,\ldots,a_T))=\beta_0+\beta_1\sum_t a_t,$$

where  $\beta_0, \beta_1$  can be easily estimated without invoking the g-null paradox.

## Setup

#### In general, consider the following setting

- A treatments and effect modifiers
- Y outcome(s) of interest
- Z other variables to be marginalized

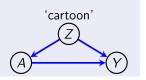


Objective: find  $p_{Y|do(A)} \equiv P^*(Y|A)$ .

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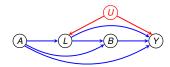
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There is no strict causal order on A, Z, Y. In Example R1,

A' = (A, B), Z' = L, Y' = Y. Confounder U is unobserved.



## Cognate Probabilities

We say  $P^*(y|a)$  is cognate to P(y|a) (within P(z, a, y)) if  $\exists w(z|a)$  s.t.,

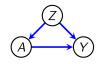
$$P^*(y|a) = \int \underbrace{P(y|a,z)w(z|a)}_{P^*(y|a,z)} dz,$$

where w(z|a) is a kernel function such that

$$w(z|a) \geq 0, \quad \int w(z|a)dz = 1, \forall a.$$

## Cognate Probabilities: Examples

Y: diabetes, A: treatment, Z: genetic information



$$P(y|a) = \int P(y|a,z)P(z|a)dz$$

$$P^*(y|a) = P(y|do(a)) = \int P(y|a,z)P(z)dz$$

Thus,  $P^*(y|a)$  is cognate to P(y|a) by treating P(z) as kernel function.

## Cognate Probabilities: Examples

Y: diabetes, A: treatment, C: gene, Z: associated economics data.



$$P_c^*(y|a) = P(y|c, do(a)) = \int P(y|a, z, c)P(z|c)dz$$

Therefore,  $P_c^*(y|a)$  is cognate to P(y|a,c) by treating P(z|c) as the kernel function.

## Cognate Probabilities: Examples

We can calculate the probability of **potential outcome** of Y when A is set to a, given observed A = a',

$$P^*(Y(a)|a') = \int P_{Y|ZA}(y|z,a)P_{Z|A}(z|a')dz$$

where  $P^*(Y(a)|a')$  is cognate to P(Y(a)|a').

**Effect of Treatment on the Treated (ETT):** 

$$\mathsf{ETT} = \mathbb{E}[\,Y(1)\mid A=1] - \mathbb{E}[\,Y(0)\mid A=1],\,\mathsf{where}$$

$$\mathbb{E}(Y(a)|a') = \int \int y P_{Y|ZA}(y|z,a) P_{Z|A}(z|a') \, dy \, dz$$

$$= \int y \underbrace{\int P_{Y|ZA}(y|z,a) P_{Z|A}(z|a') \, dz}_{\text{Cognate to } P_{Y|ZA}} \, dy$$

## Reformulate Cognate Probabilities

$$P_{Y|A}^*(y|a) = \int P_{Y|ZA}(y|z,a)w(z|a)dz$$

$$= \int \frac{P_{ZAY}(z,a,y)}{P_{ZA}(z,a)}w(z|a)dz$$

$$= \int \frac{P_{ZAY}^*(z,a,y)}{P_{ZA}^*(z,a,y)}w(z|a)dz,$$

where

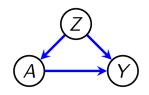
$$P_{ZAY}^{*}(z, a, y) = P_{ZAY}(z, a, y) \frac{P_{ZA}^{*}(z, a)}{P_{ZA}(z, a)}$$

$$= P_{ZAY}(z, a, y) \frac{P_{A}^{*}(a)w(z|a)}{P_{ZA}(z, a)}$$

$$= P_{Y|ZA}(y|z, a)P_{A}^{*}(a)w(z|a)$$

Therefore  $P_{Y|A}^*$  can be seen as taken from  $P_{ZAY}^*$ .

## Frugal Parameterization



To identify observational distribution  $p_{XYZ}$ , decompose it into 3 parts

- $P_{ZA}$ : the past
- $P_{Y|A}^*$ : the *causal* distribution of interest
- $\phi_{YZ|A}^*$ : a dependence measure

#### Variation Independence

Given  $\phi$  and  $\psi$  are two functions defined on  $\Theta$ . We say  $\phi$  and  $\psi$  are **Variation Independent** if

$$(\phi \times \psi)(\Theta) = \phi(\Theta) \times \psi(\Theta)$$

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(A1) Given a frugal parameterization

$$\theta = (\underbrace{\theta_{ZA}}_{past}, \underbrace{\theta_{Y|A}}_{causal}, \underbrace{\phi_{YZ|A}}_{association}),$$

the parameter  $\phi_{YZ|A}$  is jointly variation independent of  $\theta_{ZA}$  and  $\theta_{Y|A}$ .

- Ensures the space of joint distribution can be separated
- Not necessary for main result, but makes interpretation easier

## Association parameterizations satisfying (A1)

If A, Y, Z are finite categorical variables,

• conditional odds ratio:  $\phi_{YZ|A} := \frac{\rho(1,1|a)\rho(0,0|a)}{\rho(1,0|a)\rho(0,1|a)}$ .

If A, Y, Z are multivariate Gaussian random variables/ distributions defined by first two moments,

- partial correlation:  $\rho_{YZ|A} := Cor(Y, Z|A)$
- If A, Y, Z are general continuous variables,
  - conditional copula:

$$C_{YZ|A}(u, v|a) := \Pr(F_Y(Y) \le u, F_Z(Z) \le v|A = a), u, v \in [0, 1].$$

- If A, Y, Z involve continuous and binary variables,
  - use Gaussian conditional copula that is dichotomized for binary components Fan et al. (2017)

*Remark:*  $\phi_{YZ|A}$  is parametric to specify the family of copulas of interest.



#### Main Result I

Given a parameterization of  $P_{ZAY}$ 

$$\theta = (\underbrace{\theta_{ZA}}_{P_{ZA}}, \underbrace{\theta_{Y|A}}_{P_{Y|A}}, \underbrace{\phi_{YZ|A}}_{P_{YZ|A}}),$$

we can choose any parametric model for any **cognate** distribution  $P_{Y|A}^*$  to construct a smooth frugal parameterization of  $P_{ZAY}$ ,

$$\theta^* = (\underbrace{\theta_{\mathsf{ZA}}}_{P_{\mathsf{ZA}}}, \underbrace{\theta_{\mathsf{Y|A}}^*}_{P_{\mathsf{Y|A}}^*}, \underbrace{\phi_{\mathsf{YZ|A}}^*}_{P_{\mathsf{YZ|A}}^*}).$$

- ullet  $P_{Y|A}^*$  is determined by the analyst based on subject matter
- ullet  $\theta$  and  $\theta^*$  are not generally the same
- ullet and  $\theta^*$  correspond to different interpretations

#### Main Result II

**(A2)** The product  $P_{ZA}^* = w \cdot P_A^*$  has a smooth and regular parameterization  $\eta_{ZA} := \eta_{ZA}(\theta_{ZA})$ , where  $\eta_{ZA}$  is a twice differentiable function with a Jacobian of constant rank.

**(A3)** (Positivity)  $P_{ZA}$  is absolutely continuous w.r.t.  $P_{ZA}^*$  at true distribution  $P_{ZAY}$ ,

$$P_{ZA}^*(z,a) = 0 \implies P_{ZA}(z,a) = 0, \ \forall z,a$$

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**Theorem 3.1:** Under (A2) - (A3), We can smoothly parameterize the joint distribution P with a frugal parameterization of

$$P_{ZA}, P_{Y|A}^*, \phi_{YZ|A}^*$$

if and only if *P* can be smoothly parameterized by the same models applied to

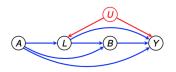
$$P_{ZA}$$
,  $P_{Y|A}$ ,  $\phi_{YZ|A}$ .

One-line proof:  $P_{ZAY}^* = P_{ZAY} \frac{P_{ZA}^*}{P_{ZA}} = P_{ZAY} \frac{w \cdot P_A^*}{P_{ZA}}$ 

## **Example R1: Parameterizing**

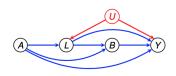
Take Z = L, X = (A, B), then we can parameterize  $P_{ALBY}$  using

$$P_{ALB}(a, \ell, b)$$
  $P_{Y|AB}^*(y|a, b)$   $\phi_{LY|AB}^*(\ell, y|a, b)$ 



- $A \sim Ber(\theta_a)$ ,  $L|A = a \sim Exp(exp(-(\alpha_0 + \alpha_a a)))$
- $B|A = a, L = \ell \sim Ber(expit(\gamma_0 + \gamma_a a + \gamma_\ell \ell + \gamma_{a\ell} a \ell))$
- $LY|do(A=a,B=b)\sim BiGaussian$  with correlation parameter  $ho_{ab}$
- $Y|do(A = a, B = b) \sim N(\beta_0 + \beta_a a + \beta_b b + \beta_{ab} ab, \sigma^2)$

#### Example R1: Sampling



[Step 1]  $A \sim Ber(\theta_a)$ ,  $B \sim Ber(\theta_b)$ 

[Step 2] Generate correlated quantiles for L, Y from copula

 $LY|do(A=a,B=b) \sim BiGaussian$  with correlation parameter  $\rho_{ab}$ .

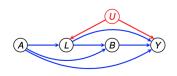
[Step 3] Generate Y and L using Inverse CDF (using quantiles from Step 2) from

$$Y|do(A = a, B = b) \sim N(\beta_0 + \beta_a a + \beta_b b + \beta_{ab} ab, \sigma^2),$$

$$L|A = a \sim Exp(exp(-(\alpha_0 + \alpha_a a)))$$

 $\implies$  Intervened Distribution of Y

#### Example R1: Sampling



[Step 1]  $A \sim Ber(\theta_a)$ ,  $B \sim Ber(\theta_b)$ 

**[Step 2]** Generate correlated quantiles for L, Y from copula

 $LY|do(A=a,B=b) \sim BiGaussian$  with correlation parameter  $\rho_{ab}$ .

[Step 3] Generate Y and L using Inverse CDF (using quantiles from Step 2) from

$$Y|do(A = a, B = b) \sim N(\beta_0 + \beta_a a + \beta_b b + \beta_{ab} ab, \sigma^2),$$

$$L|A = a \sim \textit{Exp}(\exp(-(\alpha_0 + \alpha_a a)))$$

 $\implies$  Intervened Distribution of Y

[Step 4] Generate *B* using rejection sampling such that

$$B|A = a, L = \ell \sim Ber(expit(\gamma_0 + \gamma_a a + \gamma_\ell \ell + \gamma_{a\ell} a\ell)).$$

→ Observational Distribution of Y



#### Maximum Likelihood Estimation (MLE)

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(A5) 
$$\mathsf{KL}(P_{ZA}||P_{ZA}^*) := \mathbb{E}_{P_{ZA}}\{\log \frac{P_{ZA}(z,a)}{P_{ZA}^*(z,a)}\} < \infty.$$

**Theorem 5.1** Suppose  $\theta^*$  is a frugal parameterization with weight function  $w(z) = p_Z(z)$  (i.e. the MSM model); and (A5) holds. Then MLE  $\hat{\eta}$  of  $\eta(\theta^*)$  obtained with the observed data (i.e. data generated using distribtion  $P_{ZAY}$  with parameters  $\theta^* = (\theta_{ZA}, \theta^*_{Y|A}, \phi^*_{YZ|A})$ ) will be consistent for the distribution in the causal model with parameters  $\eta = (\eta_{ZA}(\theta_{ZA}), \theta^*_{Y|A}, \phi^*_{YZ|A})$ ,

$$\sqrt{n} \left\{ \begin{pmatrix} \hat{\theta}_{Y|A}^* \\ \hat{\phi}_{YZ|A}^* \end{pmatrix} - \begin{pmatrix} \theta_{Y|A}^* \\ \phi_{YZ|A}^* \end{pmatrix} \right\} \implies N(0, I(\theta^*)_{\theta_{Y|A}^*, \phi_{YZ|A}^*}^{-1})$$

#### Maximum Likelihood Estimation (MLE)

MLE for  $P_{Y|A}^*$  is obtained by maximizing the likelihood for the causal model w.r.t observational joint distribution  $P_{ZAY}$ .

(A5) 
$$\mathsf{KL}(P_{Z\!A}||P_{Z\!A}^*) := \mathbb{E}_{P_{Z\!A}}\{\log \frac{P_{Z\!A}(z,a)}{P_{Z\!A}^*(z,a)}\} < \infty.$$

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**Remark:** When the models are correctly specified, MLE is the most efficient. Otherwise, IPW and AIPW(Doubly Robust) are recommended in practice.

#### **Estimators**

Naïve:

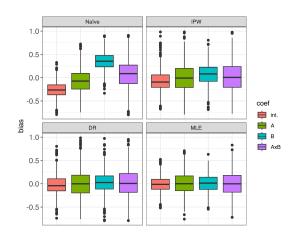
$$\mathbb{E}[Y \mid A = a, B = b] = \beta_0 + \beta_A a + \beta_B b + \beta_{AB} ab$$

• IPW:

logit
$$P(B = 1|A = a, L = \ell) = \alpha_0 + \alpha_A a + \alpha_L \ell$$
,

$$\widehat{Y}_{\text{IPW}}(A = a, B = b) = \frac{1}{n} \sum_{i=1}^{n} \frac{\delta_i(a_i = a, b_i = b) Y_i}{\widehat{P}_{B|AL}(b|a, \ell_i))}$$

#### Simulation Results



- Naïve outcome regressor does not work
- IPW, DR, MLE work well when the model is correctly specified
- MLE is more efficient when model correctly specified

#### **Discussion**

We've seen that there is generally a tension between:

- simple specification of the joint distribution P, in order to facilitate simulation and likelihood-based inference;
- simple specification of the target of inference  $P^*(y \mid a, b)$  (i.e. some interventional marginal quantity) in order that it is interpretable;
- enforcing marginal constraints implied by the causal model. (In our case this was  $Z \perp\!\!\!\perp B \mid A$  under  $P^*$ .)

The frugal parameterization resolves these as best one can.

## Thank you!

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## Takeaway and Discussion I

Traditional problem of interest: Given a joint distribution P, we can apply the g-formula to get the causal distribution P\* for the counterfactual Y\*,

$$P \stackrel{g}{\Longrightarrow} P^*$$

The reverse problem

$$P^* \stackrel{?}{\Longrightarrow} P.$$

g-formula

$$P^*(y|a) = \int P(y|x,a)dP(x)$$

where

$$P_a(y) = P^*(y|a) = P(y|do(A=a))$$

## Another Perspective of he Frugal Construction

$$p(x, a, y) = p(x, a)p(y|x, a) \stackrel{\text{do(a)}}{=} p(x, a)p_a(y|x) = p(x, a)\frac{p_a(x, y)}{p_a(x)}$$
$$= p(x, a)\frac{p_a(x)p_a(y)c_a(x, y)}{p_a(x)} = p(x, a)p_a(y)c_a(x, y).$$

where  $p_a(y)$  can be parameterized using MSM,  $p_a(y; \beta)$ . This construction avoids the specification of both  $p_a(x), p_a(y)$ .