Structure learning ctd.
Identifiability
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References

CSC2541: Introduction to Causality Lecture 4 - Identification & Estimation

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Learning directed acyclic graphs

- There are several score based hill-climbing algorithms for structure learning of directed acyclic graphs.
- They learn via the following optimization problem:

$$\min_{\mathcal{G}} loss(\mathcal{G}) \text{ s.t. } \mathcal{G} \in DAG$$

- What constitutes a good score function?
 - ▶ Number should be low if the model *explains* the data and high if it does not.
 - When learning p(y|x) we maximize the log-likelihood of labels y given features x to learn parameters of the conditional distribution.
 - Posit a class of functions that generates the observations and use fit to data for learning structure.

Learning DAGs with linear structural causal models

- We can represent any d-dimensional graph of linear structural causal models in matrix notation as follows:
 - 1. Let $W \in \mathbb{R}^{d \times d}$ be a weight matrix representing the strength of edges and G(W) denote the graph,
 - 2. $B \in \{0,1\}^{d \times d}$ where $B[i,j] = 0 \iff w_{ij} = 0$ is the (binary) adjacency matrix,
 - 3. $x_j = w_j^{\top} X + \epsilon_j$ where $X = (X_1, \dots, X_d)$ are each dimensions of data (nodes in the graph) and $\epsilon = (\epsilon_1, \dots, \epsilon_d)$ are noise variables,
 - 4. For data matrix D, we can measure fit to data via a least-squares loss $l(W,D) = \frac{1}{2n}||D DW||_F^2$.
 - 5. We can regularize the loss function to learn a sparse DAG fits the data: $F(W, D) = l(W, D) + \lambda ||W||_1$.
 - 6. Finding DAGs then reduces to $\min_{W \in \mathbb{R}^{d \times d}} F(W, D)$ s.t. $G(W) \in DAGs$

Searching over DAGs

- ▶ Optimization problem is NP hard. Challenging due to the constraint in the optimization problem,
- ightharpoonup Acyclicity is a combinatorial constraint with the number of structures increasing super exponentially in d,
- ▶ DAGS with NO TEARS, Zheng et al., 2018, comes up with a creative solution to this problem!

Insight 1: Binary Adjacency Matrices and cycles

- Fact 1: $\operatorname{tr} B^k$ counts the number of length k closed paths (cycles) in a directed graph,
- ▶ Fact 2: DAG has no cycle iff $\sum_{k=1}^{\infty} \sum_{i=1}^{d} (B^k)_{ii} = 0$
- ► Consequence, B is a DAG iff $tr(\mathbb{I} B)^{-1} = d$

$$\operatorname{tr}(\mathbb{I} - B)^{-1} = \operatorname{tr} \sum_{k=0}^{\infty} B^{k}$$
 (Infinite geometric series)
$$= \operatorname{tr} \mathbb{I} + \operatorname{tr} \sum_{k=1}^{\infty} B^{k}$$

$$= d + \sum_{k=1}^{\infty} \sum_{i=1}^{d} (B^{k})_{ii}$$

$$= d$$

However B^k is difficult to compute and represent in computer memory.

Insight 2: Matrix exponents and weighted graphs

- ▶ We can use the matrix exponential $\exp X = \sum_{k=0}^{\infty} \frac{1}{k!} X^k$ which is well-defined.
- ▶ Consequence, B is a DAG iff trexp B = d, and its extension to the graph with weighted edges (Linear SCM) case yields:

Theorem - Characterizing DAGs with matrix exponents Zheng et al., $2018\,$

A matrix $W \in \mathbb{R}^{d \times d}$ is a DAG iff:

$$h(W) = \operatorname{tr} \exp(W \circ W) - d = 0$$

where o is the Hadamard product and

$$\nabla_W h(W) = \exp(W \circ W)^T \circ 2W$$

DAGS with NO TEARS

Smooth characterizations of acyclicity

- h(W) = 0 iff W is acyclic (i.e. G(W) represents a DAG),
- \blacktriangleright h(W) quantifies the DAGness of a graph,
- \triangleright h is smooth and has easy to compute derivatives.

Now, structure learning of a DAG (under a linear SCM) can be done via : $\min_{W \in \mathbb{R}^{d \times d}} F(W)$ s.t. h(W) = 0.

Extensions and future work

- ▶ There are non-linear extensions to this idea Lachapelle et al., 2019; Yu et al., 2021; may be interesting to explore for your projects!
- ▶ We learn structure and parameters jointly should we?

Questions?

Question

Any questions on structure learning?

Backdoor criterion and the adjustment formula

Backdoor criterion

A set of variables X satisfies the backdoor criterion relative to sets of variables T and Y in a DAG $\mathcal G$ if

- 1. no node in X is a descendant of a node in T, and
- 2. X blocks/d-separates **every** path between T and Y that contains an arrow to T (backdoor paths)

In the previous example, sets $\{C\}$ or $\{W\}$ or $\{C, W\}$ all satisfy the backdoor criterion relative to T, Y (but not $\{M\}$).

Theorem - Backdoor adjustment formula

If X satisfies the backdoor criterion relative to T, Y, then the interventional distribution P(Y|do(T)) is identifiable and is given by

$$P(Y = y|do(T = t)) = \sum_{x} P(Y = y|T = t, X = x)P(X = x)$$

Frontdoor criterion and adjustment formula

We were able to identify the causal effect even when the backdoor criterion was not satisfied

Frontdoor criterion

A set of variables M satisfies the frontdoor criterion relative to sets of variables T and Y in a DAG $\mathcal G$ if

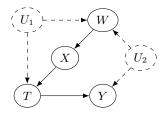
- 1. M blocks all directed paths from T to Y;
- 2. no unblocked backdoor path from T to M; and
- 3. all backdoor paths from M to Y are blocked by T.

Theorem - Frontdoor adjustment formula

If M satisfies the frontdoor criterion relative to T, Y, then the interventional distribution P(Y|do(T)) is identifiable and is given by

$$P(Y=y|do(T=t)) = \sum_{m} P(m|t) \sum_{t'} P(y|t',m) P(t')$$

What if backdoor and frontdoor criteria don't work?



We are interested in the causal effect of cardiac output (T) on the blood pressure (Y). X is the heart rate and W is catecholamine (a stress hormone). The levels of total peripheral resistance (U_1) and analgesia (U_2) are unobserved. ¹

- ▶ There is an unobserved backdoor path between T and Y, T, U₁, W, U₂, Y: Backdoor-criterion,
- \triangleright There is no mediator between T and Y: Frontdoor criterion,
- We can use do-calculus to decide if P(Y|do(T)) is identifiable.

¹Figure 1.a in Jung, Tian, and Bareinboim, 2021.

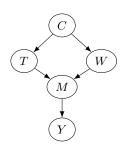
- do-calculus is a set of three inference rules that allows us to convert an interventional quantity into a probability expression involving observed quantities
- ▶ We'll consider general quantities P(Y|do(T=t), X=x) for arbitrary (sets of) variables T, X, Y

$$P(Y|do(T = t), X = x) := \frac{P(Y, X = x|do(T = t))}{P(X = x|do(T = t))}$$

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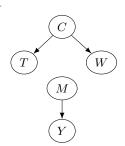
 \triangleright Notation. Graph \mathcal{G}



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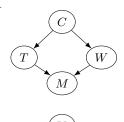
▶ Notation. Graph $\mathcal{G}_{\overline{M}}$



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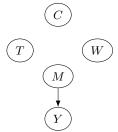
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▶ Notation. Graph $\mathcal{G}_{C,\overline{M}}$



$$P(Y|do(T=t), \textcolor{red}{X}, W) = P(Y|do(T=t), W) \quad \text{ if } \quad Y \perp \!\!\! \perp_{\mathcal{G}_{\overline{T}}} X|T, W$$

$$P(Y|do(T=t), \textcolor{red}{X}, W) = P(Y|do(T=t), W) \quad \text{ if } \quad Y \perp \!\!\! \perp_{\mathcal{G}_{\overline{T}}} X|T, W$$

Intuition:

▶ In the interventional/mutilated graph $\mathcal{G}_{\overline{T}}$, every path from T is causal. Therefore we can simplify the rule as:

$$P(Y|T=t,X,W) = P(Y|T=t,W) \text{ if } Y \perp \!\!\! \perp_{\mathcal{G}} X|T,W$$

Generalization of d-separation

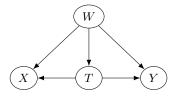
$$P(Y|do(T=t), X, W) = P(Y|do(T=t), W)$$
 if $Y \perp \!\!\! \perp_{\mathcal{G}_{\overline{T}}} X|T, W$

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Generalization of d-separation



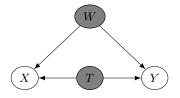
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Intuition:

▶ In the interventional/mutilated graph $\mathcal{G}_{\overline{T}}$, every path from T is causal. Therefore we can simplify the rule as:

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Generalization of d-separation



$$P(Y|do(T=t), \textcolor{red}{do(X=x)}, W) = P(Y|do(T=t), \textcolor{red}{X=x}, W) \quad \text{ if } \quad Y \perp \!\!\! \perp_{\mathcal{G}_{\overline{T},X}} X|T, W$$

$$P(Y|do(T=t), \underline{do(X=x)}, W) = P(Y|do(T=t), \underline{X=x}, W) \quad \text{if} \quad Y \perp \!\!\!\perp_{\mathcal{G}_{\overline{T}, X}} X|T, W$$

Intuition:

Removing all edges to T results in the interventional graph and:

$$P(Y|T=t, \frac{do(X=x)}{}), W) = P(Y|T=t, \frac{X=x}{}, W) \quad \text{if} \quad Y \perp \!\!\!\! \perp_{\mathcal{G}_{\underline{X}}} X|T, W$$

▶ If all backdoor paths from X to Y are blocked by T and W after removing the links between X and it's descendants, then conditioning on X = intervention on X

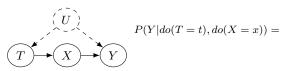
Generalization of backdoor criterion

$$P(Y|do(T=t), \frac{do(X=x)}{}, W) = P(Y|do(T=t), \frac{X=x}{}, W) \quad \text{if} \quad Y \perp \!\!\!\perp_{\mathcal{G}_{\overline{T},X}} X|T, W$$

Intuition:

- Removing all edges to T results in the interventional graph and: $P(Y|T=t, do(X=x)), W) = P(Y|T=t, X=x, W) \quad \text{if} \quad Y \perp \!\!\! \perp_{G_X} X|T, W$
- ▶ If all backdoor paths from X to Y are blocked by T and W after removing the links between X and it's descendants, then conditioning on X = intervention on X

Generalization of backdoor criterion

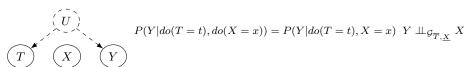


$$P(Y|do(T=t), \frac{do(X=x)}{}, W) = P(Y|do(T=t), \frac{X=x}{}, W) \quad \text{if} \quad Y \perp \!\!\!\perp_{\mathcal{G}_{\overline{T},X}} X|T, W$$

Intuition:

- Removing all edges to T results in the interventional graph and: $P(Y|T=t, do(X=x)), W) = P(Y|T=t, X=x, W) \quad \text{if} \quad Y \perp \!\!\! \perp_{G_X} X|T, W$
- ▶ If all backdoor paths from X to Y are blocked by T and W after removing the links between X and it's descendants, then conditioning on X = intervention on X

Generalization of backdoor criterion



Let
$$X = X_{\text{W-Anc}} \cup X_{\text{W-Rest}}$$
:

$$P(Y|do(T=t), \underline{do(X=x)}, W) = P(Y|do(T=t), W) \quad \text{ if } \quad Y \perp \!\!\! \perp_{\mathcal{G}_{\overline{T}, \overline{X_{\text{W.Rest}}}}} X|T, W$$

 $X_{\text{W-Rest}}$ is the set of nodes in X that not ancestors of any node (e.g. descendants of some nodes) in set W in $\mathcal{G}_{\overline{T}}$.

Let $X = X_{\text{W-Anc}} \cup X_{\text{W-Rest}}$:

$$P(Y|do(T=t), \underline{do(X=x)}, W) = P(Y|do(T=t), W) \quad \text{ if } \quad Y \perp \!\!\! \perp_{\mathcal{G}_{\overline{T}, \overline{X_{\text{W.Rest}}}}} X|T, W$$

 $X_{\text{W-Rest}}$ is the set of nodes in X that not ancestors of any node (e.g. descendants of some nodes) in set W in $\mathcal{G}_{\overline{T}}$.

▶ Removing all edges to T results in the interventional graph and:

$$P(Y|T=t, \frac{do(X=x)}{}, W) = P(Y|T=t, W)$$
 if $Y \perp \!\!\! \perp_{\mathcal{G}_{\overline{XW-Rest}}} X|T, W$

- We already know that $Y \perp \!\!\!\perp X_{W-Anc}|W$ (by definition),
- Now in $\mathcal{G}_{\overline{X_{\text{W-Rest}}}}$ we know that *if* there is a relationship between X and Y, it *must* be causal,
- ▶ Therefore the rule says that if $Y \perp \!\!\! \perp X|T,W$ in $\mathcal{G}_{\overline{X_{\text{W-Rest}}}}$ then interventions on $X_{\text{W-Rest}}$ can be freely inserted/deleted because we are guaranteed no causal paths and all non-causal paths are already blocked by W.

Rule 3 of do-calculus - Example

Figure: \mathcal{G}

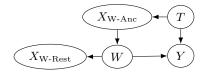
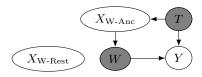


Figure: $\mathcal{G}_{\overline{T}, \overline{X_{\text{W-Rest}}}}$



do-calculus is complete¹

Theorem - Completeness of do-calculus

A causal effect P(Y=y|do(T=t)) is identifiable if and only if there exists a finite sequence of transformations, each conforming to one of the following inference rules that reduce P(Y=y|do(T=t)) into an expression involving observed quantities

1. Rule 1:

$$P(Y|do(T=t), \textcolor{red}{X}, W) = P(Y|do(T=t), W) \quad \text{ if } \ Y \perp \!\!\! \perp_{\mathcal{G}_{\overline{T}}} X|T, W$$

2. Rule 2:

$$\begin{split} P(Y|do(T=t), \frac{do(X=x)}{do(X=x)}, W) &= P(Y|do(T=t), \frac{X=x}{do(X=x)}, W) \\ \text{if } Y \perp \!\!\! \perp_{\mathcal{G}_{\overline{T},X}} X|T, W \end{split}$$

3. Rule 3:

$$\begin{split} &P(Y|do(T=t), \frac{do(X=x)}{do(X=t)}, W) = P(Y|do(T=t), W) \\ &\text{if } Y \perp \!\!\! \perp_{\mathcal{G}_{\overline{T}, \overline{XW}, \operatorname{Port}}} X|T, W \end{split}$$

¹Proof in Huang and Valtorta, 2012 and Shpitser and Pearl, 2012

Intuition for the rules of do-calculus

- ▶ Each rule first applies the intervention to the treatment resulting in $\mathcal{G}_{\overline{T}}$,
- Rule 1: Add/remove any variables that are d-separated in the interventional graph,
- ▶ Rule 2: We can replace conditioning with interventions whenever we are guaranteed that *T*, *W* block all backdoor paths,
- ▶ Rule 3: We can add/delete interventions over a set X as long as there are no direct causal paths between X and Y in the set of X that are non-ancestors of W (since W blocks the influence of the remaining set of X on Y).

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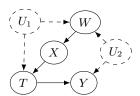
Backdoor and Frontdoor adjustment Do-calculus

Questions?

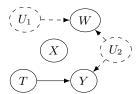
Question

Any questions on do-calculus?

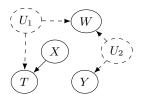
$$P(y|do(T=t))$$



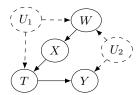
$$\begin{split} &P(y|do(T=t))\\ &=P(y|do(T=t), \textcolor{red}{do(X=x)}) \quad \text{(Rule 3: insertion of actions - } Y \perp \!\!\! \perp_{\mathcal{G}_{\overline{T},\overline{X}}} X|T) \end{split}$$



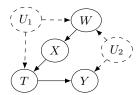
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$$\begin{split} &P(y|do(T=t))\\ &=P(y|do(T=t), do(X=x)) \quad \text{(Rule 3: insertion of actions - }Y \perp \!\!\! \perp_{\mathcal{G}_{\overline{T},\overline{X}}} X|T)\\ &=P(y|T=t, do(X=x)) \quad \text{(Rule 2: action/observation exchange - }Y \perp \!\!\! \perp_{\mathcal{G}_{\overline{X},\underline{T}}} T|X)\\ &=\frac{P(y,t|do(X=x))}{P(t|do(X=x))} \end{split}$$

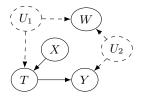


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Example - Identification with do-calculus

$$\begin{split} &P(y|do(T=t))\\ &=P(y|do(T=t), \textcolor{red}{do(X=x)}) \quad \text{(Rule 3: insertion of actions - } Y \perp \!\!\! \perp_{\mathcal{G}_{\overline{T},\overline{X}}} X|T)\\ &=P(y|T=t, \textcolor{red}{do(X=x)}) \quad \text{(Rule 2: action/observation exchange - } Y \perp \!\!\! \perp_{\mathcal{G}_{\overline{X},\overline{X}}} T|X)\\ &=\frac{P(y,t|do(X=x))}{P(t|do(X=x))}\\ &=\frac{\sum_{w}P(y,t|W=w,do(X=x))P(w|do(X=x))}{\sum_{w}P(t|W=w,do(X=x))P(w|do(X=x))} \quad \text{(Marginalization over } W)\\ &=\frac{\sum_{w}P(y,t|W=w,do(X=x))P(w)}{\sum_{w}P(t|W=w,do(X=x))P(w)} \quad \text{(Rule 3: deletion of actions - } W \perp \!\!\! \perp_{\mathcal{G}_{\overline{X}}} X) \end{split}$$



Example - Identification with do-calculus

$$P(y|do(T=t)) = P(y|do(T=t), do(X=x)) \quad \text{(Rule 3: insertion of actions - } Y \perp \downarrow_{\mathcal{G}_{\overline{T},\overline{X}}} X|T)$$

$$= P(y|T=t, do(X=x)) \quad \text{(Rule 2: action/observation exchange - } Y \perp \downarrow_{\mathcal{G}_{\overline{X},\underline{T}}} T|X)$$

$$= \frac{P(y,t|do(X=x))}{P(t|do(X=x))}$$

$$= \frac{\sum_{w} P(y,t|W=w, do(X=x))P(w|do(X=x))}{\sum_{w} P(t|W=w, do(X=x))P(w|do(X=x))} \quad \text{(Marginalization over } W)$$

$$= \frac{\sum_{w} P(y,t|W=w, do(X=x))P(w)}{\sum_{w} P(t|W=w, do(X=x))P(w)} \quad \text{(Rule 3: deletion of actions - } W \perp \downarrow_{\mathcal{G}_{\overline{X}}} X)$$

$$= \frac{\sum_{w} P(y,t|W=w, X=x)P(w)}{\sum_{w} P(t|W=w, X=x)P(w)} \quad \text{(Rule 2: action/observation exchange - } T, Y \perp \downarrow_{\mathcal{G}_{\underline{X}}} X|W)$$

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Backdoor and Frontdoor adjustment Do-calculus

Questions?

Question

Any questions on do-calculus?

The story thus far



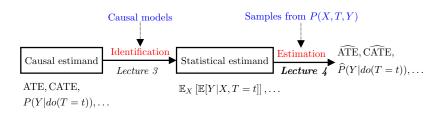
Marketing every machine learning model as being "causal".

Knowing the conditions and assumptions under which causal inference is feasible.

Figure: On the feasibility of causal inference

Estimation

- ▶ Thus far we have studied how to map from causal quantities onto statistical estimands.
- ▶ We'll turn to *estimation* how to map from *data* onto a statistical estimand.
- One of the areas where ideas from machine learning can play a big role in causal inference.



Estimation in supervised learning

Consider the following regression model:

- ▶ Data: $X \in \mathbb{R}^{N \times D}$; $Y \in \mathbb{R}^{N \times 1}$; x_i, y_i denote rows of each matrix.
- ▶ Model (trained): $f(x; \theta^*) = W^*x$, or $f(x; \theta^*) = W_2^*(\sigma(W_1^*x))$
- Estimating the risk of a regression model:
 - ▶ Estimand for risk: $\mathbb{E}[\mathcal{R}[(f(X,\theta^*),Y]]; \mathcal{R}(\hat{y},y) = \frac{1}{2}(y-\hat{y})^2$
 - Estimator: $\mathbb{E}[\mathcal{R}(f(X, \theta^*), Y)] = \frac{1}{N} \sum_{i=1}^{N} \mathcal{R}(f(x_i, \theta^*), y_i)$
- ► Conditional expectation of outcomes:
 - Estimand for conditional expectation: $\mathbb{E}[Y|X=x]$
 - Non-parameteric estimator: $\mathbb{E}[Y|X=x] = \frac{1}{\sum_{i=1}^{N} \mathbb{I}[x_j=x]} \sum_{i=1}^{N} y_i \mathbb{I}[x_i=x]$
 - Parametric estimator: $\mathbb{E}[Y|X=x] = f(x, \theta^*)$

We can use a predictive model to get an estimate of a conditional expectation!

Estimation of the G-formula/Backdoor adjustment

Focus on estimation in the backdoor setting today! Assuming positivity/unconfoundedness/graphical criteria for identifiability we obtain the following estimands for Average Treatment Effects:

- ► Let X be the adjustment set/backdoor path in the causal Bayesian network.
- ▶ Potential outcomes / Backdoor adjustment: $\mathbb{E}[Y_1 Y_0] = \mathbb{E}_X[\mathbb{E}[Y|T=1,X] \mathbb{E}[Y|T=0,X]]$

Strategy: Use predictive models to approximate Estimand 1 and 2.

$$\mathbb{E}_{W}[\underbrace{\mathbb{E}[Y|T=1,X]}_{Estimand\ 1} - \underbrace{\mathbb{E}[Y|T=0,X]}_{Estimand\ 2}]$$

Using models to estimate the G-formula

The use of parameteric methods to estimate the effect of interventions goes by many names:

- ▶ G-computation estimators
- ▶ Parametric G-formula
- ► Standardization
- ► S-learner

Conditional outcome modeling

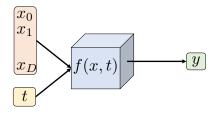


Figure: Using machine learning to fit conditional expectations

- $\mathcal{D} = \{(x_1, t_1, y_1), \dots, (x_N, t_N, y_N), \dots, (x_{N+\tilde{N}}, t_{N+\tilde{N}}, y_{N+\tilde{N}})\},$
- Fit $f(x,t) \approx \mathbb{E}[Y|X,T]$ using $\{(x_N,t_N,y_N),\ldots,(x_{N+\tilde{N}},t_{N+\tilde{N}},y_{N+\tilde{N}})\},$
- $ightharpoonup \widehat{CATE}(x) = f(x, 1) f(x, 0),$
- $ightharpoonup \widehat{ATE} = \frac{1}{N} \sum_{i=1}^{N} f(x_i, 1) f(x_i, 0)$

Grouped conditional outcome modeling

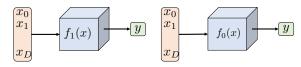


Figure: Using machine learning to fit grouped conditional expectations

- ▶ Let $\mathcal{D}_{tr} = \{(x_N, t_N, y_N), \dots, (x_{N+\tilde{N}}, t_{N+\tilde{N}}, y_{N+\tilde{N}})\} = \mathcal{D}_1 \cup \mathcal{D}_0,$
- $\mathcal{D}_1 = \{(x_1, 1, y_1), \dots, (x_k, 1, y_k)\} \& \mathcal{D}_0 = \{(x'_1, 0, y'_1), \dots, (x'_{k'}, 0, y'_{k'})\},$
- ▶ Fit $f_1(x) \approx \mathbb{E}[Y|X]$ using \mathcal{D}_1 and $f_0(x) \approx \mathbb{E}[Y|X]$ using \mathcal{D}_0 ,
- $\widehat{\text{CATE}}(x) = f_1(x) f_0(x),$
- $ightharpoonup \widehat{ATE} = \frac{1}{N} \sum_{i=1}^{N} f_1(x_i) f_0(x_i)$

Tradeoffs in the parametric G-formula

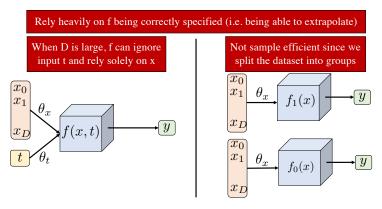


Figure: Tradeoffs in estimation

Covariate adjustment with linear models

- Lets assume that we model conditional expectations with linear models,
- ► Then $Y_t(x) = f(x,t) = \beta x + \gamma t + \epsilon_t$, $\mathbb{E}[\epsilon_t] = 0$,
- ▶ We can write out a closed form solution for CATE as follows:

$$\begin{aligned} \text{CATE}(x) &= \mathbb{E}[(\beta x + \gamma + \epsilon_1) - (\beta x + \epsilon_0)] \\ &= \mathbb{E}[\beta x + \gamma - \beta x] + \underbrace{\mathbb{E}[\epsilon_1] - \mathbb{E}[\epsilon_0]}_{0} \\ &= \gamma \end{aligned}$$

- 1. Takeaway 1: Goal in causal inference is to estimate γ well! f is a tool to get us there.
- 2. Takeaway 2: Often β (coefficients of adjustment set) are referred to as nuisance parameters.

Cost of model mis-specification

Consider the following *true* data generating process:

$$Y_t(x) = f^*(x,t) = \beta x + \gamma t + \delta x^2 + \epsilon_t, \ \mathbb{E}[\epsilon_t] = 0,$$

$$ightharpoonup ATE = \gamma$$

Now, lets say we estimate the following *hypothesized* predictive model:

$$\hat{Y}_t(x) = \hat{\beta}x + \hat{\gamma}t,$$

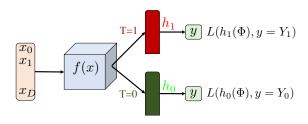
$$\hat{\gamma} = \gamma + \delta \frac{\mathbb{E}[xt]\mathbb{E}[x^2] - \mathbb{E}[t^2]\mathbb{E}[x^2t]}{\mathbb{E}[xt^2] - \mathbb{E}[x^2]\mathbb{E}[t^2]}$$

Mis-specification can result in bias: δ can result in an arbitrarily large bias in our causal estimate!

Non-linear functions

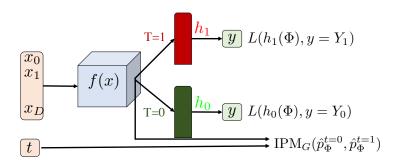
- ▶ Nonlinear functions have a rich history of being used in conditional outcome modeling in statistics and machine learning:
- Random forests and Bayesian Trees (J. L. Hill, 2011; J. Hill, Linero, and Murray, 2020),
- ► Gaussian processes (Alaa and Van Der Schaar, 2017; Schulam and Saria, 2017),
- ▶ Neural Networks (Johansson, Shalit, and Sontag, 2016),

TAR-Net (Johansson, Shalit, and Sontag, 2016)



- ▶ Grouped conditional outcome model is inefficient \rightarrow TAR-Net uses a neural network f(x) to learn a shared low-dimensional representation of high-dimensional data x for both treatment and control,
- ▶ Treatment head and control head are responsible for modeling outcomes under different treatment assignments.
- ▶ In finite samples, what happens when treatment assignment is predictive of outcome? \rightarrow Model's representation can rely solely on predicting treatment assignment i.e. it learns $f(x) = [f_1(x), f_0(x)]$.

TAR-Net (Johansson, Shalit, and Sontag, 2016)



Additional regularization penalty using an integral probability metric to ensure that the representation space h(x) is aligned for both treatment and control groups.

Questions?

Question

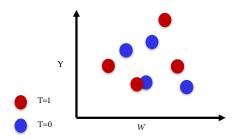
Any questions on parametric estimation?

Matching

- 1. For each observation in the treatment group, find "statistical twins" in the control group with similar covariates X (and vice versa), where X is a valid adjustment set
- 2. Use the Y values of the matched observations as the counterfactual outcomes for one at hand
- 3. Estimate average treatment effect as the difference between observed and imputed counterfactual values

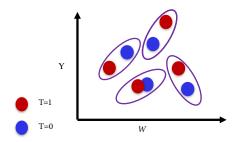
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Matching - Formal definition

Let the data $\mathcal{D} = \{(T^i, X^i, Y^i)\}_{i=1}^N$. To estimate the counterfactual Y_0^i for a sample i in the treatment group, we use (similar) samples from the control group (T=0):

$$\hat{Y}_0^i = \sum_{j \text{ s.t. } T^j = 0} w_{ij} Y^j$$

Similarly, to estimate the counterfactual Y_1^i for a sample i in the control group, we use samples from the treatment group:

$$\hat{Y}_1^i = \sum_{j \text{ s.t. } T^j = 1} w_{ij} Y^j$$

An estimation of ATE will be

$$\widehat{\text{ATE}} = \frac{1}{N} \sum_{i} Y_1^i - Y_0^i = \frac{1}{N} \left[\sum_{i; T^i = 1} \left(Y^i - \hat{Y}_0^i \right) + \sum_{i; T^i = 0} \left(\hat{Y}_1^i - Y^i \right) \right]$$

Different matching algorithms use different definitions of w_{ij}

Types of matching

- ▶ Exact matching: $w_{ij} = \begin{cases} \frac{1}{k_i} & \text{if } X^i = X^j \\ 0 & o.w. \end{cases}$ with k_i as the number of samples j with $X^i = X^j$
 - Problem: For high-dimensional X, it will be less likely to find an exact match
- ▶ Multivariate distance matching (MDM): Use (Euclidean) distance metric to find "close" observations as potential matches
 - \blacktriangleright We can use KNN algorithm to find the k closes observations in the control (treatment) group for each treated (controlled) sample, i.e.,

$$w_{ij} = \begin{cases} \frac{1}{k} & \text{if } X^j \in KNN(X^i) \\ 0 & o.w. \end{cases}$$

Matching - Pros and Cons

- + Interpretable, especially in small samples
- + Non-parametric
 - KNN-matching can be biased since $X^i \approx X^j \implies Y_0^i \approx Y_0^j, Y_1^i \approx Y_1^j$ (See Abadie and Imbens, 2011 for bias-correction for matching estimators)
 - Curse of dimensionality it gets harder to find good matches as dimension grows



Ozzy Osbourne

- Male
- Born in 1948
- Raised in the UK
- Married twice
- Lives in a castle
- Wealthy & famous



Prince Charles

- Male
- Born in 1948
- Raised in the UK
- Married twice
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Source: https://mobile.twitter.com/HallaMartin/status/1569311697717927937

Propensity scores

- ightharpoonup Matching can suffer from curse of dimensionality of X
- ightharpoonup Let's look at probability of treatment assignment given X

$$e(X) := P(T = 1|X)$$

Propensity scores

- ightharpoonup Matching can suffer from curse of dimensionality of X
- \triangleright Let's look at probability of treatment assignment given X

$$e(X) := P(T = 1|X)$$

 \triangleright e(X) summarizes high-dimensional variables X into one dimension!

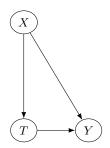
Theorem - Propensity Score

Assume X satisfies the backdoor criterion (conditional ignorability) w.r.t. T, Y. Given positivity, e(X) will also satisfy conditional ignorability, i.e.,

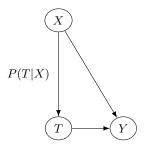
$$Y_0, Y_1 \perp \!\!\!\perp T|e(X)$$

► Helpful for matching!

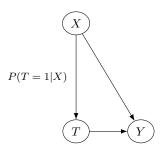
$$Y_0, Y_1 \perp \!\!\!\perp T | X \implies Y_0, Y_1 \perp \!\!\!\perp T | e(X)$$



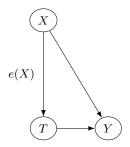
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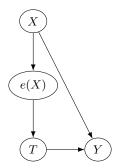
$$Y_0, Y_1 \perp \!\!\!\perp T | X \implies Y_0, Y_1 \perp \!\!\!\perp T | e(X)$$



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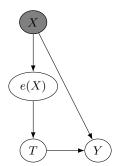


$$Y_0, Y_1 \perp \!\!\!\perp T | X \implies Y_0, Y_1 \perp \!\!\!\perp T | e(X)$$



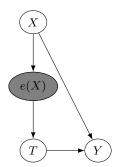
Slide credit to Brady Neal

$$Y_0, Y_1 \perp \!\!\!\perp T | X \implies Y_0, Y_1 \perp \!\!\!\perp T | e(X)$$



Slide credit to Brady Neal

$$Y_0, Y_1 \perp \!\!\!\perp T | X \implies Y_0, Y_1 \perp \!\!\!\perp T | e(X)$$



Slide credit to Brady Neal

Propensity score matching

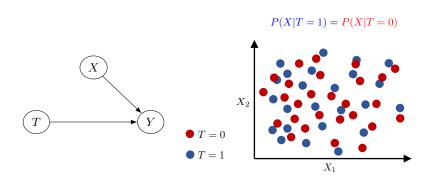
- ▶ Instead of computing multivariate distances, we can match the one-dimensional propensity score:
- ▶ Step 1: Estimate e(X) using a **parametric** method
- Step 2: Apply a matching algorithm (KNN) with distance $|e(X_i) e(X_j)|$

Propensity score matching

- ▶ Instead of computing multivariate distances, we can match the one-dimensional propensity score:
- ▶ Step 1: Estimate e(X) using a **parametric** method
- ▶ Step 2: Apply a matching algorithm (KNN) with distance $|e(X_i) e(X_j)|$
- ▶ This is not a magic, we still need to estimate P(T = 1|X)!
- ▶ A perfect predictor of *T* is not always good we can include more variables as *X* to get better treatment assignment predictions
 - ► Can increase variance,
 - See "Why Propensity Scores Should Not Be Used for Matching" by King and Nielsen, 2019.

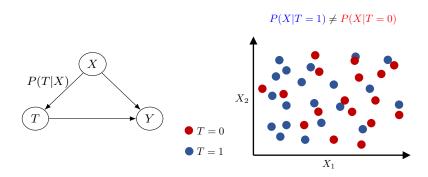
Inverse probability weighting (IPW)

► Causal estimation in RCTs is easier (control and treatment groups are similar)



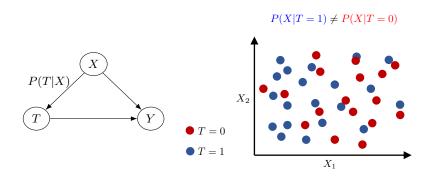
Inverse probability weighting (IPW)

▶ In observational studies, however, the treatment and control groups are not comparable.



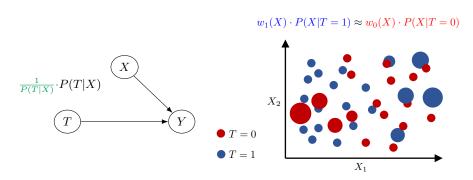
Inverse probability weighting (IPW)

▶ In observational studies, however, the treatment and control groups are not comparable. Can we make a pseudo-RCT by re-weighting samples?



Inverse probability weighting (IPW)

▶ In observational studies, however, the treatment and control groups are not comparable. Can we make a pseudo-RCT by re-weighting samples?



Samples re-weighted by the inverse propensity score of the treatment they received

$$\mathbb{E}[Y_t] = \mathbb{E}_X \left[\mathbb{E}[Y|X, T=t] \right]$$

(conditional ignorability)

$$\begin{split} \mathbb{E}[Y_t] &= \mathbb{E}_X \left[\mathbb{E}[Y|X,T=t] \right] & \text{(conditional ignorability)} \\ &= \sum_x \mathbb{E}[Y|X=x,T=t] P(X=x) \\ &= \sum_x \sum_y y P(y|x,t) P(x) \end{split}$$

$$\mathbb{E}[Y_t] = \mathbb{E}_X \left[\mathbb{E}[Y|X, T = t] \right] \qquad \text{(conditional ignorability)}$$

$$= \sum_x \mathbb{E}[Y|X = x, T = t] P(X = x)$$

$$= \sum_x \sum_y y P(y|x, t) P(x)$$

$$= \sum_x \sum_y y P(y|x, t) P(x) \frac{P(t|x)}{P(t|x)}$$

$$= \sum_x \sum_y y P(y|x, t) P(x) \frac{P(t|x)}{P(t|x)}$$

$$= \sum_{x,y} \frac{1}{P(t|x)} y P(x, y, t) \qquad (P(y|x, t) P(x) P(t|x) = P(x, y, t))$$

$$\mathbb{E}[Y_t] = \mathbb{E}_X \left[\mathbb{E}[Y|X, T = t] \right] \qquad \text{(conditional ignorability)}$$

$$= \sum_x \mathbb{E}[Y|X = x, T = t] P(X = x)$$

$$= \sum_x \sum_y y P(y|x, t) P(x)$$

$$= \sum_x \sum_y y P(y|x, t) P(x) \frac{P(t|x)}{P(t|x)}$$

$$= \sum_{x,y} \frac{1}{P(t|x)} y P(x, y, t) \qquad (P(y|x, t) P(x) P(t|x) = P(x, y, t))$$

$$= \sum_{x,y,t'} \underbrace{\frac{\mathbb{I}(t' = t)}{P(t|x)}}_{f(x,y,t')} y P(x, y, t')$$

$$= \sum_{x,y,t'} f(x, y, t') P(x, y, t')$$
(sum over T)

$$\mathbb{E}[Y_t] = \mathbb{E}_X \left[\mathbb{E}[Y|X, T = t] \right] \qquad \text{(conditional ignorability)}$$

$$= \sum_x \mathbb{E}[Y|X = x, T = t] P(X = x)$$

$$= \sum_x \sum_y y P(y|x, t) P(x)$$

$$= \sum_x \sum_y y P(y|x, t) P(x) \frac{P(t|x)}{P(t|x)}$$

$$= \sum_x \frac{1}{P(t|x)} y P(x, y, t) \qquad (P(y|x, t) P(x) P(t|x) = P(x, y, t))$$

$$= \sum_{x, y, t'} \frac{\mathbb{I}(t' = t)}{P(t|x)} y P(x, y, t')$$

$$= \sum_{x, y, t'} \frac{\mathbb{I}(t' = t)}{P(t|x)} y P(x, y, t')$$

$$= \sum_{x, y, t'} f(x, y, t') P(x, y, t')$$

$$= \mathbb{E}\left[f(X, Y, T)\right] = \mathbb{E}\left[\frac{\mathbb{I}(T = t)Y}{P(t|X)}\right]$$

► Hence,

$$ATE = \mathbb{E}\left[Y_1 - Y_0\right] = \mathbb{E}\left[\frac{\mathbb{I}(T=1)Y}{P(T=1|X)}\right] - \mathbb{E}\left[\frac{\mathbb{I}(T=0)Y}{P(T=0|X)}\right]$$
$$= \mathbb{E}\left[\frac{\mathbb{I}(T=1)Y}{e(X)}\right] - \mathbb{E}\left[\frac{\mathbb{I}(T=0)Y}{1 - e(X)}\right]$$

► Hence,

$$ATE = \mathbb{E}\left[Y_1 - Y_0\right] = \mathbb{E}\left[\frac{\mathbb{I}(T=1)Y}{P(T=1|X)}\right] - \mathbb{E}\left[\frac{\mathbb{I}(T=0)Y}{P(T=0|X)}\right]$$
$$= \mathbb{E}\left[\frac{\mathbb{I}(T=1)Y}{e(X)}\right] - \mathbb{E}\left[\frac{\mathbb{I}(T=0)Y}{1 - e(X)}\right]$$

• For a given dataset $\mathcal{D} = \{(x^i, t^i, y^i)\}_{i=1}^N$, an estimate of ATE will be

$$\widehat{\text{ATE}} = \frac{1}{N_1} \sum_{i; t^i = 1} \frac{y^i}{\hat{e}(x^i)} - \frac{1}{N_0} \sum_{i; t^i = 0} \frac{y^i}{1 - \hat{e}(x^i)}$$

for
$$N_1 = |\{i; t^i = 1\}|, N_0 = N - N_1.$$

► Hence.

$$\begin{split} \text{ATE} &= \mathbb{E}\left[Y_1 - Y_0\right] = \mathbb{E}\left[\frac{\mathbb{I}(T=1)Y}{P(T=1|X)}\right] - \mathbb{E}\left[\frac{\mathbb{I}(T=0)Y}{P(T=0|X)}\right] \\ &= \mathbb{E}\left[\frac{\mathbb{I}(T=1)Y}{e(X)}\right] - \mathbb{E}\left[\frac{\mathbb{I}(T=0)Y}{1 - e(X)}\right] \end{split}$$

▶ For a given dataset $\mathcal{D} = \{(x^i, t^i, y^i)\}_{i=1}^N$, an estimate of ATE will be

$$\widehat{ATE} = \frac{1}{N_1} \sum_{i;t^i=1} \frac{y^i}{\hat{e}(x^i)} - \frac{1}{N_0} \sum_{i;t^i=0} \frac{y^i}{1 - \hat{e}(x^i)}$$

for
$$N_1 = |\{i; t^i = 1\}|, N_0 = N - N_1.$$

- \triangleright Still we need to estimate e(X). If positivity is violated, propensity scores become non-informative and miscalibrated
- ► Small propensity scores can create large variance/errors

Questions?

Question

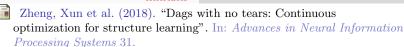
Any questions on weighting based estimators?

Recap - Lecture 4

- ► Identification
 - ▶ Backdoor criteria: Identical to adjustment via the G-formula,
 - Frontdoor criteria: Using mediators to identify causal effect on outcomes.
- ▶ Do-Calculus: Three rules to identify causal effects:
 - 1. Insertion or deletion of observations: Generalization of d-separation,
 - 2. Interchanging actions with observations : Generalization of the backdoor criteria.
 - 3. Insertion or delection of actions

Recap - Lecture 4

- ▶ Parametric Estimation:
 - ▶ Conditional outcome models
 - ► Grouped conditional outcome models
 - ► TAR-Net
- ▶ Weighting based estimators
 - ► Matching
 - Propensity scores and inverse propensity weighting



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