STAT6061/STAT5008 – Causal Inference

Part 2-1. Treatment Assignment Mechanism and Experimental Design

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Treatment Assignment Mechanism

Definition (Treatment Assignment Mechanism) (Imbens and Rubin, 2015)
Given a population of N units, the assignment mechanism is a row-exchangeable function

$$\Pr\left(\widetilde{\boldsymbol{A}} \middle| \widetilde{\boldsymbol{X}}, \widetilde{\boldsymbol{Y}}(0), \widetilde{\boldsymbol{Y}}(1)\right)$$

taking on values in [0, 1], satisfying

$$\sum_{\widetilde{\boldsymbol{a}} \in \{0,1\}^N} \Pr\left(\widetilde{\boldsymbol{A}} = \widetilde{\boldsymbol{a}} \middle| \widetilde{\boldsymbol{X}}, \widetilde{\boldsymbol{Y}}(0), \widetilde{\boldsymbol{Y}}(1)\right) = 1$$

for all $\widetilde{\boldsymbol{X}}$, $\widetilde{\boldsymbol{Y}}(0)$, *and* $\widetilde{\boldsymbol{Y}}(1)$.

- The assignment mechanism is a probabilistic rule that determines the probabilities of all 2^N possible assignment vectors $\widetilde{\boldsymbol{A}} = (A_1, \dots, A_N)$ for N units, given potential outcomes ($\widetilde{\boldsymbol{Y}}(0), \widetilde{\boldsymbol{Y}}(1)$) and covariates ($\widetilde{\boldsymbol{X}}$).

Example 1 (clueless doctor)

Suppose $N = 2$. The $2^2 = 4$ possible assignment vectors $\widetilde{\boldsymbol{A}}$ are given by $\Omega = \{(0,0), (1,0), (0,1), (1,1)\}$

- Treatment assignment mechanism:

$$\Pr\left(\widetilde{\boldsymbol{A}} \middle| \widetilde{\boldsymbol{X}}, \widetilde{\boldsymbol{Y}}(0), \widetilde{\boldsymbol{Y}}(1)\right) = \frac{1}{4}, \qquad \widetilde{\boldsymbol{A}} \in \Omega$$

- Unit assignment probability:

$$\Pr\left(A_i = 1 \middle| \widetilde{\boldsymbol{X}}, \widetilde{\boldsymbol{Y}}(0), \widetilde{\boldsymbol{Y}}(1)\right) = \frac{1}{2}, \qquad i = 1, 2$$

Example 2 (perfect doctor)

Suppose $N=2$. The $2^2=4$ possible assignment vectors $\tilde{\boldsymbol{A}}$ are given by $\Omega=\{(0,0),(1,0),(0,1),(1,1)\}$

	$Y_2(1)-Y_2(0)>0$	$Y_2(1)-Y_2(0)\le 0$
$Y_1(1)-Y_1(0)>0$	- Treatment assignment mechanism: $\Pr\left(\tilde{\boldsymbol{A}}\middle\|\tilde{\boldsymbol{X}},\tilde{\boldsymbol{Y}}(0),\tilde{\boldsymbol{Y}}(1)\right)=\begin{cases}1 & ,\tilde{\boldsymbol{A}}=(1,1)\\ 0 & ,O.W.\end{cases}$ - Unit assignment probability: $\Pr\left(A_1=1\middle\|\tilde{\boldsymbol{X}},\tilde{\boldsymbol{Y}}(0),\tilde{\boldsymbol{Y}}(1)\right)=1$ $\Pr\left(A_2=1\middle\|\tilde{\boldsymbol{X}},\tilde{\boldsymbol{Y}}(0),\tilde{\boldsymbol{Y}}(1)\right)=1$	- Treatment assignment mechanism: $\Pr\left(\tilde{\boldsymbol{A}}\middle\|\tilde{\boldsymbol{X}},\tilde{\boldsymbol{Y}}(0),\tilde{\boldsymbol{Y}}(1)\right)=\begin{cases}1 & ,\tilde{\boldsymbol{A}}=(1,0)\\ 0 & ,O.W.\end{cases}$ - Unit assignment probability: $\Pr\left(A_1=1\middle\|\tilde{\boldsymbol{X}},\tilde{\boldsymbol{Y}}(0),\tilde{\boldsymbol{Y}}(1)\right)=1$ $\Pr\left(A_2=1\middle\|\tilde{\boldsymbol{X}},\tilde{\boldsymbol{Y}}(0),\tilde{\boldsymbol{Y}}(1)\right)=0$
$Y_1(1)-Y_1(0)\le 0$	- Treatment assignment mechanism: $\Pr\left(\tilde{\boldsymbol{A}}\middle\|\tilde{\boldsymbol{X}},\tilde{\boldsymbol{Y}}(0),\tilde{\boldsymbol{Y}}(1)\right)=\begin{cases}1 & ,\tilde{\boldsymbol{A}}=(0,1)\\ 0 & ,O.W.\end{cases}$ - Unit assignment probability: $\Pr\left(A_1=1\middle\|\tilde{\boldsymbol{X}},\tilde{\boldsymbol{Y}}(0),\tilde{\boldsymbol{Y}}(1)\right)=1$ $\Pr\left(A_2=1\middle\|\tilde{\boldsymbol{X}},\tilde{\boldsymbol{Y}}(0),\tilde{\boldsymbol{Y}}(1)\right)=1$	- Treatment assignment mechanism: $\Pr\left(\tilde{\boldsymbol{A}}\middle\|\tilde{\boldsymbol{X}},\tilde{\boldsymbol{Y}}(0),\tilde{\boldsymbol{Y}}(1)\right)=\begin{cases}1 & ,\tilde{\boldsymbol{A}}=(0,0)\\ 0 & ,O.W.\end{cases}$ - Unit assignment probability: $\Pr\left(A_1=1\middle\|\tilde{\boldsymbol{X}},\tilde{\boldsymbol{Y}}(0),\tilde{\boldsymbol{Y}}(1)\right)=0$ $\Pr\left(A_2=1\middle\|\tilde{\boldsymbol{X}},\tilde{\boldsymbol{Y}}(0),\tilde{\boldsymbol{Y}}(1)\right)=0$

Example 3 (sequential assignment)

Suppose $N = 3$. The $2^3 = 8$ possible assignment vectors $\widetilde{\boldsymbol{A}}$ are given by

$$\Omega = \{(0,0,0), (0,0,1), (0,1,0), (0,1,1), (1,0,0), (1,0,1), (1,1,0), (1,1,1)\}$$

- The rule for this sequential assignment of treatments to three units is described as follows:

1. First unit assignment: Assign treatment randomly using a fair coin toss.

2. Second unit assignment: Assign the second unit to the *alternative* treatment (opposite of the first unit).
   (Record the observed outcomes for the first and second units: Y_1^{obs} and Y_2^{obs})

3. Third unit assignment rule: Compare Y_1^{obs} and Y_2^{obs} to determine the better-performing treatment.
   - $Y_1^{obs} > Y_2^{obs} \rightarrow$ Assign third unit to first unit's treatment.
   - $Y_2^{obs} > Y_1^{obs} \rightarrow$ Assign third unit to second unit's treatment.
   - $Y_1^{obs} = Y_2^{obs} \rightarrow$ Assign third unit to control treatment

- Note that this strategy ensures that early experimental data influences treatment allocation for later units, incorporating an adaptive element in the sequential experiment.

Example 3 (sequential assignment)

Suppose $N = 3$. The $2^3 = 8$ possible assignment vectors $\tilde{\boldsymbol{A}}$ are given by

$$\Omega = \{(0,0,0),(0,0,1),(0,1,0),(0,1,1),(1,0,0),(1,0,1),(1,1,0),(1,1,1)\}$$

	$Y_2(1) - Y_1(0) > 0$	$Y_2(1) - Y_1(0) \le 0$
$Y_1(1) - Y_2(0) > 0$	- Treatment assignment mechanism: $\Pr(\tilde{\boldsymbol{A}} \mid \tilde{\boldsymbol{X}}, \tilde{\boldsymbol{Y}}(0), \tilde{\boldsymbol{Y}}(1)) = \begin{cases} 1/2 & , \tilde{\boldsymbol{A}} = (1,0,1),(0,1,1) \\ 0 & , O.W. \end{cases}$ - Unit assignment probability: $\Pr(A_1 = 1 \mid \tilde{\boldsymbol{X}}, \tilde{\boldsymbol{Y}}(0), \tilde{\boldsymbol{Y}}(1)) = 1/2$ $\Pr(A_2 = 1 \mid \tilde{\boldsymbol{X}}, \tilde{\boldsymbol{Y}}(0), \tilde{\boldsymbol{Y}}(1)) = 1/2$ $\Pr(A_3 = 1 \mid \tilde{\boldsymbol{X}}, \tilde{\boldsymbol{Y}}(0), \tilde{\boldsymbol{Y}}(1)) = 1$	- Treatment assignment mechanism: $\Pr(\tilde{\boldsymbol{A}} \mid \tilde{\boldsymbol{X}}, \tilde{\boldsymbol{Y}}(0), \tilde{\boldsymbol{Y}}(1)) = \begin{cases} 1/2 & , \tilde{\boldsymbol{A}} = (1,0,1),(0,1,0) \\ 0 & , O.W. \end{cases}$ - Unit assignment probability: $\Pr(A_1 = 1 \mid \tilde{\boldsymbol{X}}, \tilde{\boldsymbol{Y}}(0), \tilde{\boldsymbol{Y}}(1)) = 1/2$ $\Pr(A_2 = 1 \mid \tilde{\boldsymbol{X}}, \tilde{\boldsymbol{Y}}(0), \tilde{\boldsymbol{Y}}(1)) = 1/2$ $\Pr(A_3 = 1 \mid \tilde{\boldsymbol{X}}, \tilde{\boldsymbol{Y}}(0), \tilde{\boldsymbol{Y}}(1)) = 1/2$
$Y_1(1) - Y_2(0) \le 0$	- Treatment assignment mechanism: $\Pr(\tilde{\boldsymbol{A}} \mid \tilde{\boldsymbol{X}}, \tilde{\boldsymbol{Y}}(0), \tilde{\boldsymbol{Y}}(1)) = \begin{cases} 1/2 & , \tilde{\boldsymbol{A}} = (1,0,0),(0,1,1) \\ 0 & , O.W. \end{cases}$ - Unit assignment probability: $\Pr(A_1 = 1 \mid \tilde{\boldsymbol{X}}, \tilde{\boldsymbol{Y}}(0), \tilde{\boldsymbol{Y}}(1)) = 1/2$ $\Pr(A_2 = 1 \mid \tilde{\boldsymbol{X}}, \tilde{\boldsymbol{Y}}(0), \tilde{\boldsymbol{Y}}(1)) = 1/2$ $\Pr(A_3 = 1 \mid \tilde{\boldsymbol{X}}, \tilde{\boldsymbol{Y}}(0), \tilde{\boldsymbol{Y}}(1)) = 1/2$	- Treatment assignment mechanism: $\Pr(\tilde{\boldsymbol{A}} \mid \tilde{\boldsymbol{X}}, \tilde{\boldsymbol{Y}}(0), \tilde{\boldsymbol{Y}}(1)) = \begin{cases} 1/2 & , \tilde{\boldsymbol{A}} = (1,0,0),(0,1,0) \\ 0 & , O.W. \end{cases}$ - Unit assignment probability: $\Pr(A_1 = 1 \mid \tilde{\boldsymbol{X}}, \tilde{\boldsymbol{Y}}(0), \tilde{\boldsymbol{Y}}(1)) = 1/2$ $\Pr(A_2 = 1 \mid \tilde{\boldsymbol{X}}, \tilde{\boldsymbol{Y}}(0), \tilde{\boldsymbol{Y}}(1)) = 1/2$ $\Pr(A_3 = 1 \mid \tilde{\boldsymbol{X}}, \tilde{\boldsymbol{Y}}(0), \tilde{\boldsymbol{Y}}(1)) = 0$

Restrictions on the treatment assignment mechanism

Definition (Individualistic Assignment) (Imbens and Rubin, 2015)

A treatment assignment mechanism $\Pr\left(\widetilde{\boldsymbol{A}} \middle| \widetilde{\boldsymbol{X}}, \widetilde{\boldsymbol{Y}}(0), \widetilde{\boldsymbol{Y}}(1)\right)$ *is individualistic if, for some function* $q(\cdot) \in [0,1]$,

$$\Pr\left(A_i = 1 \middle| \widetilde{\boldsymbol{X}}, \widetilde{\boldsymbol{Y}}(0), \widetilde{\boldsymbol{Y}}(1)\right) = q(X_i, Y_i(0), Y_i(1))$$

for all i *= 1,. . . , N, and*

$$\Pr\left(\widetilde{\boldsymbol{A}} \middle| \widetilde{\boldsymbol{X}}, \widetilde{\boldsymbol{Y}}(0), \widetilde{\boldsymbol{Y}}(1)\right) = c \prod_{i=1}^{N} \left\{q\left(X_i, Y_i(0), Y_i(1)\right)\right\}^{A_i} \left\{1 - q\left(X_i, Y_i(0), Y_i(1)\right)\right\}^{1-A_i}$$

for $(\widetilde{\boldsymbol{X}}, \widetilde{\boldsymbol{Y}}(0), \widetilde{\boldsymbol{Y}}(1)) \in \Lambda$*, for some set* Λ*, and zero elsewhere.*

(c *is the constant that ensures that the probabilities sum to unity)*

- Individualistic assignment limits the dependence of a particular unit's assignment probability on the values of covariates and potential outcomes for other units.
- Individualistic assignment is violated in sequential experiments such as Example 3.

Restrictions on the treatment assignment mechanism

Definition (Individualistic Assignment) (Imbens and Rubin, 2015)
A treatment assignment mechanism $\Pr\left(\widetilde{\boldsymbol{A}}\middle|\widetilde{\boldsymbol{X}},\widetilde{\boldsymbol{Y}}(0),\widetilde{\boldsymbol{Y}}(1)\right)$ *is individualistic if, for some function* $q(\cdot)\in[0,1]$,

$$\Pr\left(A_i=1\middle|\widetilde{\boldsymbol{X}},\widetilde{\boldsymbol{Y}}(0),\widetilde{\boldsymbol{Y}}(1)\right)=q(X_i,Y_i(0),Y_i(1))$$

for all $i = 1,\ldots,N$, *and*

$$\Pr\left(\widetilde{\boldsymbol{A}}\middle|\widetilde{\boldsymbol{X}},\widetilde{\boldsymbol{Y}}(0),\widetilde{\boldsymbol{Y}}(1)\right)=c\prod_{i=1}^{N}\left\{q\left(X_i,Y_i(0),Y_i(1)\right)\right\}^{A_i}\left\{1-q\left(X_i,Y_i(0),Y_i(1)\right)\right\}^{1-A_i}$$

for $(\widetilde{\boldsymbol{X}},\widetilde{\boldsymbol{Y}}(0),\widetilde{\boldsymbol{Y}}(1))\in\Lambda$, *for some set* Λ, *and zero elsewhere.*
(c *is the constant that ensures that the probabilities sum to unity)*

- Propensity score:

$$e(x)=\frac{1}{N_x}\sum_{i\,\in\,\Omega_x}q\left(X_i,Y_i(0),Y_i(1)\right)$$

where $\Omega_x=\{j|X_j=x\}$ and N_x is the number of the elements in Ω_x

(The population-level propensity score is defined as $e(x)=\Pr(A=1|X=x,Y(0),Y(1))$)

Restrictions on the treatment assignment mechanism

Definition (Probabilistic Assignment) (Imbens and Rubin, 2015)

A treatment assignment mechanism $\Pr\left(\widetilde{\boldsymbol{A}}\middle|\widetilde{\boldsymbol{X}},\widetilde{\boldsymbol{Y}}(0),\widetilde{\boldsymbol{Y}}(1)\right)$ *is probabilistic if the probability of assignment to treatment for unit i is strictly between zero and one:*

$$0 < \Pr\left(A_i = 1\middle|\widetilde{\boldsymbol{X}},\widetilde{\boldsymbol{Y}}(0),\widetilde{\boldsymbol{Y}}(1)\right) < 1$$

for each possible $\widetilde{\boldsymbol{X}},\widetilde{\boldsymbol{Y}}(0),\widetilde{\boldsymbol{Y}}(1)$, *for all* i = *1,. . . , N.*

- Probabilistic assignment only requires that each unit has the potential to be assigned to either the active treatment or the control treatment.

Restrictions on the treatment assignment mechanism

Definition (Unconfounded Assignment) (Imbens and Rubin, 2015)

A treatment assignment mechanism $\Pr(\tilde{\boldsymbol{A}}|\tilde{\boldsymbol{X}},\tilde{\boldsymbol{Y}}(0),\tilde{\boldsymbol{Y}}(1))$ *is unconfounded if it does not depend on the potential outcomes:*

$$\Pr(\tilde{\boldsymbol{A}}|\tilde{\boldsymbol{X}},\tilde{\boldsymbol{Y}}(0),\tilde{\boldsymbol{Y}}(1)) = \Pr(\tilde{\boldsymbol{A}}|\tilde{\boldsymbol{X}})$$

for all $\tilde{\boldsymbol{A}}$, $\tilde{\boldsymbol{X}}$, $\tilde{\boldsymbol{Y}}(0)$, *and* $\tilde{\boldsymbol{Y}}(1)$.

- This disallows dependence of the assignment mechanism on the potential outcomes.

Remark 1: The combination of unconfoundedness and individualistic assignment is crucial, as it ensures that the assignment mechanism is **the product of the propensity scores**.

$$\Pr(\tilde{\boldsymbol{A}}|\tilde{\boldsymbol{X}},\tilde{\boldsymbol{Y}}(0),\tilde{\boldsymbol{Y}}(1)) = c\prod_{i=1}^{N}\{e(X_i)\}^{A_i}\{1-e(X_i)\}^{1-A_i}$$

Remark 2: Given individualistic assignment, the combination of probabilistic and unconfounded assignment is known as **strongly ignorable treatment assignment** (**strong ignorability**).

Randomized experiment

Definition (Randomized Experiment)

A randomized experiment is an assignment mechanism that
(i) is probabilistic, and
(ii) has a known functional form that is controlled by the researcher.

Definition (Classical Randomized Experiment)

A classical randomized experiment is a randomized experiment with an assignment mechanism that is
(i) individualistic, and
(ii) unconfounded.

- The definition of a classical randomized experiment excludes sequential experiments, such as the one in Example 3.
- A key example of a classical randomized experiment is a *completely randomized experiment*, which is discussed later.

Observational studies: regular assignment mechanisms

Definition (Observational Study)
An assignment mechanism corresponds to an observational study if the functional form of the assignment mechanism is unknown.

Definition (Regular Assignment Mechanism)
An assignment mechanism is regular if
(i) the assignment mechanism is individualistic,
(ii) the assignment mechanism is probabilistic, and
(iii) the assignment mechanism is unconfounded.

- An assignment mechanism is **irregular** when there is noncompliance in randomized experiments. (This occurs when the assigned treatment does not always correspond to the received treatment for some units.)

Classical randomized experiments

- Four types of classical randomized experiments
  - Bernoulli trials
  - Completely randomized experiment
  - Stratified (block) randomized experiment
  - Paired randomized experiments

- The key difference between the four types of classical randomized experiments is in the set of assignment vectors $\widetilde{\boldsymbol{A}}$ with positive probability.

Bernoulli trials

➢ Treatment assignment mechanism

$$\Pr\left(\widetilde{\boldsymbol{A}}\middle|\widetilde{\boldsymbol{X}},\widetilde{\boldsymbol{Y}}(0),\widetilde{\boldsymbol{Y}}(1)\right) = \Pr\left(\widetilde{\boldsymbol{A}}\middle|\widetilde{\boldsymbol{C}}\right) = \prod_{i=1}^{N}\{e(X_i)\}^{A_i}\{1 - e(X_i)\}^{1-A_i}$$

$\Rightarrow$ $A_1, \dots, A_N$ are *independent* and each $A_i \sim \text{Bernoulli}(p = e(X_i))$

- The simplest Bernoulli experiment is a fair coin experiment, where a unit is assigned to the treatment group if the coin lands heads and to the control group if it lands tails, meaning $e(X_i) = 1/2$ for all i.

$$\Pr\left(\widetilde{\boldsymbol{A}}\middle|\widetilde{\boldsymbol{X}},\widetilde{\boldsymbol{Y}}(0),\widetilde{\boldsymbol{Y}}(1)\right) = \left(\frac{1}{2}\right)^{N}$$

- A drawback of Bernoulli trials is the small but positive probability that all units receive the same treatment

Completely randomized experiment

➢ Treatment assignment mechanism

$$\Pr(\widetilde{\boldsymbol{A}}|\widetilde{\boldsymbol{X}},\widetilde{\boldsymbol{Y}}(0),\widetilde{\boldsymbol{Y}}(1)) = \Pr(\widetilde{\boldsymbol{A}}) = \begin{cases} \dfrac{1}{\binom{N}{N_1}} & \text{if } \sum_i A_i = N_1 \\ 0 & \text{otherwise} \end{cases}, \qquad \text{where } \binom{N}{N_1} = \frac{N!}{N_1!\,(N-N_1)!}$$

⇒ N_1 out of N units are randomly assigned to the treatment group, while the remaining $N_0 = N - N_1$ units are assigned to the control group.

- A completely randomized experiment ensures a fixed group size, but the assignments across units are not independent; in fact, $A_1,\ldots,A_N$ exhibit slight negative association.

- Complete randomization in finite samples CANNOT fully prevent covariate imbalance, especially for key covariates strongly linked to potential outcomes.

Stratified (block) randomized experiment

- Procedure:
  1. Blocking (Stratification): Group similar units based on pre-treatment covariates. Let $B_i \in \{1, \dots, J\}$ denote the block indicator.
  2. Stratified Randomization: Within each block, randomly assign treatments.

- Treatment assignment mechanism

$$\Pr\left(\widetilde{\boldsymbol{A}} \middle| \widetilde{\boldsymbol{X}}, \widetilde{\boldsymbol{Y}}(0), \widetilde{\boldsymbol{Y}}(1)\right) = \Pr\left(\widetilde{\boldsymbol{A}} \middle| \widetilde{\boldsymbol{X}}\right) = \begin{cases} \prod_j 1 \Big/ \binom{N(j)}{N_1(j)} & if \sum_{i \in \{s | B_s = j\}} A_i = N_1(j) \text{ for } j = 1, \dots, J \\ 0 & \text{otherwise} \end{cases}$$

$\Rightarrow$ $N_1(j)$ out of $N(j)$ units are randomly assigned to the treatment group in the *j*-th stratum/block, where $N(j)$ denotes the total number of units in the *j*-th stratum/block.

- Stratification reduces variance in potential outcomes within each stratum and enhances efficiency by balancing important covariates.

Paired randomized experiments

- Paired randomized experiment is the most extreme version of stratified randomized experiment with only one treated unit and one control unit.
  $\Rightarrow$ A paired randomized experiment is a stratified randomized experiment with
  $$N(j) = 2 \text{ and } N_1(j) = 1 \text{ for } j = 1, \dots, N/2$$

- Procedure:
  1. Pair units based the similarity of covariates.
  2. Randomize treatment assignment within each pair

- Treatment assignment mechanism

$$\Pr\left(\widetilde{\boldsymbol{A}} \middle| \widetilde{\boldsymbol{X}}, \widetilde{\boldsymbol{Y}}(0), \widetilde{\boldsymbol{Y}}(1)\right) = \Pr\left(\widetilde{\boldsymbol{A}} \middle| \widetilde{\boldsymbol{C}}\right) = \begin{cases} \left(\frac{1}{2}\right)^{N/2} & if \sum_{i \in \{s | B_s = j\}} A_i = N_1(j) \text{ for } j = 1, \dots, N/2 \\ 0 & \text{otherwise} \end{cases}$$

References

Imbens, G. W., & Rubin, D. B. (2015). *Causal inference in statistics, social, and biomedical sciences*. Cambridge university press.