### STATE-ACTION BALANCING IN CAUSAL INFERENCE

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(Please visit https://mgimm.github.io/presentation for additional information.)

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#### What we will talk about?

- Basic concepts of Causal Inference
  - Policy evaluation.
  - Unconfoundedness and Markov structure.
- Static Causal Inference
  - Inverse Probability Weighting (IPW) estimator.
  - G-computation estimator.
  - Doubly robust estimator.
  - Static state-action balancing (our methods).
- Dynamic Causal Inference (our new framework)
  - Measure flows in the change of policy.
  - Dynamical recursive balancing.
  - Error analysis of the policy evaluation estimators.

#### Notation and conventions

- $\xi(dx)$  (measure), f (test function),  $\xi(f) = \int f(x)\xi(dx)$ .
- M(x, dy) (transition kernel),  $M(f)(\cdot) = \int M(x, dy) f(y)$ , and  $\mu M(dy) = \int \mu(dx) M(x, dy)$ .
- A transition kernel is a family of state-indexed (probability) measures.
- For any random variables *X* and *Y*, there exists a Markov transition kernel *M* that connects their distributions.
- For a probability measure  $\xi(dx)$ , the empirical measure  $\xi_n$  is given by  $\frac{1}{n} \sum_{i=1}^n \delta_{X_i}$ , where  $X_i$  is the i.i.d. sample according to  $\xi(dx)$ .

#### Causal Inference (naive):

Statistics

+

Ability to intervene the data generation procedure (action)

Policy: Assignment of actions.

Policy evaluation: Predict the average causal effects of a given policy.

# Step 1: Static Causal Inference without personalized treatment

## Conceptual example of policy evaluation: Covid and Vaccination

Question: To vaccinate or not?

Model: Potential Outcomes framework (Rubin, 1974):

- *X*: Population covariate (age, sex, blood-type, etc).
- $A \in \{0, 1\}$ : Action assignment indicator (1:vaccinated vs. 0:not-vaccinated)
- (Y(0), Y(1)): Effects associated to vaccination (e.g., infection, side effects, etc).

Goal: Estimate the average potential outcomes  $\mathbb{E}[Y(1)]$  (and/or  $\mathbb{E}[Y(0)]$ ).  $\iff$  Policy evaluation (Everyone vaccinates (or not)).

Example: What is the average infection rate (on the whole population) after the vaccination?

 $\iff$  Estimation of  $\mathbb{E}[Y(1)]$ .

Why difficult?

Each individual has only one observation of two causal effects  $\implies$  missing value always exists.

## Three Classical methods: IPW, G-computation, DRE

#### Assumptions on the data collection:

Dataset:  $\mathcal{D}_n = \{(X^{(i)}, A^{(i)}, Y^{(i)}(A^{(i)})) : 1 \le i \le n\}.$ 

- Randomized study: Assume  $A \perp (Y(0), Y(1))$ .
- Observational study (unconfoundedness): Assume  $A \perp (Y(0), Y(1))$  given X.

#### 1. Inverse Probability Weighting (IPW):

$$\mathbb{E}\left[Y(A)\frac{\mathbf{1}_{\{A=1\}}}{\mathbb{P}(A=1\mid X)}\right] = \mathbb{E}\left[\mathbb{E}\left[Y(A)\frac{\mathbf{1}_{\{A=1\}}}{\mathbb{P}(A=1\mid X)}\mid X\right]\right] = \mathbb{E}\left[Y(1)\right].$$

Inverse Probability Weghting (IPW) estimator:

IPWE = 
$$\frac{1}{n} \sum_{i=1}^{n} Y^{(i)}(A^{(i)}) \frac{\mathbf{1}_{\{A^{(i)}=1\}}}{\hat{\mathbb{P}}(A=1 \mid X=X^{(i)})}.$$

The nuisance estimator  $\hat{\mathbb{P}}(A = 1 \mid X = X^{(i)})$  is estimated through a separated supervised learning (classification) problem.

#### 2. G-computation:

Denote by  $\mu_1(\cdot) = \mathbb{E}[Y(1) \mid X = \cdot]$ , then

$$\mathbb{E}\left[\mu_1(X)\right] = \mathbb{E}\left[Y(1)\right].$$

G-computation estimator

GE = 
$$\frac{1}{n} \sum_{i=1}^{n} \hat{\mu}_1(X^{(i)}),$$

where the nuisance estimator  $\hat{\mu}_1$  can also be obtained by a separate regression:

$${X^{(i)} \text{ to } Y^{(i)}(1) : 1 \le i \le n \text{ and } A^{(i)} = 1}$$

Can we combine these two ideas? yes!

#### 3. Doubly robust estimator:

$$DRE = \frac{1}{n} \sum_{i=1}^{n} (Y^{(i)}(A^{(i)}) - \hat{\mu}_1(X^{(i)})) \frac{\mathbf{1}_{\{A^{(i)}=1\}}}{\hat{\mathbb{P}}(A=1 \mid X=X^{(i)})} + \frac{1}{n} \sum_{i=1}^{n} \hat{\mu}_1(X^{(i)}).$$

Why interesting?

- Faster convergence rate (product of the two nuisance estimators).
- Semiparametric efficiency (optimal asymptotic variance over all parametric models) at optimal rate  $(\mathcal{O}_{\mathbb{P}}(1/\sqrt{n}))$ .

Q: What can we improve (i.e., our contributions) in this static setting?

A: 1. The IPW part, and 2. more complicated policy evaluation.

Q: Why the IPW part should be improved?

A: Numerical instability when the "inversed" probability is close to 0— a single poorly estimated probability in the whole data set may completely destroy the whole estimator! (This will be illustrated later!)

#### A closer look at IPW

Q: Why it works?

A: It balances two subpopulations, i.e.,

X(the whole population) and X(1) (people vaccinated),

through re-weighting. The associated weight function is

$$\mathring{\eta}(\cdot) = \frac{\mathbb{E}[A]}{\mathbb{P}(A=1 \mid X=\cdot)}.$$

#### Re-weighting transformation:

$$\Psi_{\eta}(\mu): \mu \mapsto \mu(\eta \times \cdot)$$

We have

$$\Psi_{\mathring{\eta}}(\xi_1) = \xi \quad and \quad \frac{\mathrm{d}\xi}{\mathrm{d}\xi_1} = \mathring{\eta}$$

where  $\xi_1$  (resp.  $\xi$ ) is the probability measure of X(1) (resp. X).

#### Reformulation of IPWE

We have

IPWE = 
$$\frac{1}{n} \sum_{i=1}^{n} Y^{(i)}(A^{(i)}) \frac{\mathbf{1}_{\{A^{(i)}=1\}}}{\hat{\mathbb{P}}(A=1 \mid X=X^{(i)})}$$
  
=  $\frac{1}{N_1} \sum_{i=1}^{N_1} \hat{\eta}(X(1)^{(i)}) Y^{(i)}(1),$ 

where  $\hat{\eta}(X(1)^{(i)}) = \frac{N_1/n}{\hat{\mathbb{P}}(A=1\mid X=\cdot)}$ , which is an empirical version of  $\eta$ .

Natural idea to improve IPW/get rid of the inverse manipulation:

Directly estimate the weight function that corrects the difference between two measures!

Idea (source measure:  $\xi_1$ ; target measure:  $\xi$ ):

$$\hat{\eta} = \arg\min_{\eta \in H} \text{ some-loss-between-measures}(\xi, \Psi_{\eta}(\xi_1)).$$

Are we able to generalize this simple idea to more general cases (e.g., with more complex policy/action assignment)? Yes! And this is our first contribution in the static setting!

# Step 2: Static Causal Inference with personalized treatment

## General policy evaluation

Policy is now modeled by a transition kernel  $\pi(x, da)$  from state space to action space.

- Sampling policy  $\pi(x, da)$ : policy that generates the data set  $\mathfrak{D}_n$ .
- Target policy  $\mathring{\pi}(x, da)$ : The policy to be evaluated.

Case 1: Finite-valued action (e.g., whether to vaccinate, Moderna or Pfizer?). Example: What is the average infection rate of the whole population if people with age> 60 get vaccinated?

No need to change the framework. For example, one may replace all the A=1 by  $A=\mathring{A}^{(i)}$  where  $\mathring{A}^{(i)}\sim\mathring{\pi}(X^{(i)},\cdot)$ .

Case 2: General cases (e.g., continuous-valued action when considering dosage, expenses, etc.)

Example: What is the average infection rate of the whole population if people with age> 60 get vaccinated with various dosage (from 50ml to 500ml)?

State-Action Markov reformulation.

## Markov structure of causal dynamics

One (tiny) step further from the Markov Decision Process.

- State-action variable:  $X^{\natural} = (X, A)$ .
- State-action space:  $X^{\natural} = X \times A$ .
- $\pi^{\natural} = \mathrm{id}_{\mathfrak{X}} \times \pi$ .
- Goal: estimate  $\mathcal{V}^{\dot{\pi}} = \mathbb{E}[\mathring{Y}] = \mathbb{E}[r(\mathring{Z})]$ .

Causal effects Y (resp.  $\mathring{Y}$ ) is now modeled by r(Z) (resp.  $r(\mathring{Z})$ ).

Why? Consistent with the dynamical setting.

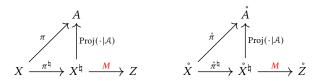


Figure: Markov structure of static causal model

When  $\#A < \infty$ , the dynamic is equivalent to the potential outcomes framework with unconfoundedness assumption.

#### Covariate shifts?

Denote by  $\xi$  the population distribution (X) of sampling policy. Denote by  $\dot{\xi}$  the population distribution  $(\mathring{X})$  of target policy. It is possible that  $\xi \neq \mathring{\xi}$ . (Lacking of external validation (Pearl et al., 2014).)

Example: The vaccination data set is collected in the US, how can we calibrate it so that it can be used to conduct causal inference in France?

What are we collecting?

- State-action variables under sampling policy (US):  $\{(X^{(i)}, A^{(i)}) : 1 \le i \le n\}$
- State variables of target policy (FR):  $\{\mathring{X}^{(i)}: 1 \leq i \leq m\}$ .
- Causal effects under sampling policy (US):  $\{r(Z^{(i)}): 1 \le i \le n\}$ .

What are we balancing (in order to get the weight function estimation)?

The (empirical) state-action distribution of  $X^{\sharp}$  and  $\mathring{X}^{\sharp}$ , denoted respectively by

re-weighted source measure:  $\Psi_{\eta^{\natural}}(\xi_n^{\pi^{\natural}})$  and target measure:  $\mathring{\xi}_m^{\dot{\pi}^{\natural}}$ .

#### Estimators: DE and DRE

Direct estimator:

$$\hat{\mathcal{V}}_{\scriptscriptstyle \mathrm{DE}}^{\mathring{\pi}} = \frac{1}{n} \sum_{i=1}^{n} \hat{\eta}^{\natural}(X^{\natural(i)}) r(Z^{(i)}),$$

Doubly robust estimator:

$$\hat{\mathcal{V}}_{\text{DRE}}^{\mathring{\pi}} = \frac{1}{n} \sum_{i=1}^{n} \hat{\eta}^{\natural}(X^{\natural(i)})(r(Z^{(i)}) - \hat{r}^{\natural(i)}(X^{\natural(i)})) + \frac{1}{m} \sum_{i=1}^{m} \mathring{\pi}^{\natural}(\hat{r}^{\natural(j)})(\mathring{X}^{(j)}),$$

where

- $\hat{\eta}^{\natural}$  is the estimated weight function  $\mathring{\eta}^{\natural}$  that corrects the difference between the two state-action distributions, i.e.,  $\Psi_{\mathring{\eta}^{\natural}}(\xi^{\pi^{\natural}}) = \mathring{\xi}^{\mathring{\pi}^{\natural}};$
- $\hat{r}^{\natural(j)}$  is the estimated conditional expectation function  $\mathbb{E}\left[r(Z)\mid X^{\natural}=\cdot\right]$  (or simply  $r^{\natural}=M(r)$ ) by a separated regression.

How to estimate the weight function?

Generalized IPW (through density ratio estimation, see, e.g., Sugiyama et al. (2012)). or Balancing (our method)!

## Teaser of balancing

#### Direct estimator and worst-case-error interpretation

Idea:  $r(Z^{(i)})$  can be regarded as a noisy version of  $r^{\natural}(X^{\natural(i)})$ . Hence, one considers to minimize the worst-case-error, i.e.,

$$\hat{H} = \underset{\eta^{\natural} \in H}{\operatorname{arg \, min}} \sup_{\gamma \in \Gamma} \left| \Psi_{\eta^{\natural}}(\xi_n^{\pi^{\natural}})(\gamma) - \mathring{\xi}_{mN}^{\mathring{\pi}^{\natural}}(\gamma) \right|,$$

Characterization of balancing:

- *H*: family of candidates of the weight function.
- Γ: family of test functions (integrable).

It is well-known that that sup-term is called Integral Probability Metric (IPM).

$$\hat{H} = \underset{\eta^{\natural} \in H}{\operatorname{arg \, min}} \ \left( \operatorname{IPM}_{\Gamma} \left( \Psi_{\eta^{\natural}}(\xi_{n}^{\pi^{\natural}}), \dot{\xi}_{mN}^{\dot{\pi}^{\natural}} \right)^{2} + \lambda \left\| \eta^{\natural} \right\|_{L^{2}(\xi_{n}^{\pi^{\natural}})}^{2} \right),$$

(Bias-Variance decomposition)

In this case, H is a  $L^2(\xi^{\pi^{\natural}})$ -ball.

Well-specifiedness:  $r^{\natural} \in \Gamma$ .

## Balancing for the DE

Example: Optimal Transport (OT) balancing without  $L^2$  penalty, see, e.g., Reygner and Touboul (2020).

#### Theorem (Informal)

When well-specified, the error of the DE is controlled by the sampling complexity of the chosen IPM.

Sampling complexity?

rate of convergence of  $\text{IPM}_{\Gamma}(\xi_n, \xi)$  for some empirical measure  $\xi_n$ , which is determined by the richness of  $\Gamma$ .

In the OT case, the sampling complexity is in general  $n^{-1/d}$  when d, the dimension of the state-action space, is large.

However, there is in general no reason that  $\hat{\eta}^{\natural}$  will converge to the ideal weight function  $\mathring{\eta}^{\natural}$  in an  $L^2$  sense, which is required by the DRE.

## Why $L^2$ convergence of weight function estimation matters?

Denote by  $\mathcal{V}^{\dot{\pi}}_{_{\text{ODRE}}}$  the oracle version of the DRE, namely, by replacing the nuisance estimatros  $\hat{\eta}^{\natural}$  and  $\hat{r}^{\natural}$  by their oracle/ideal counterparts  $\mathring{\eta}^{\natural}$  and  $r^{\natural}$ .

#### Theorem (Informal)

Under mild assumptions, we have

$$\left|\mathcal{V}_{\scriptscriptstyle \mathrm{ORE}}^{\mathring{\pi}} - \hat{\mathcal{V}}_{\scriptscriptstyle \mathrm{DRE}}^{\mathring{\pi}}\right| \leq C \left\|\hat{\eta}^{\natural} - \mathring{\eta}^{\natural}\right\|_{L^{2}(\xi_{n}^{\pi^{\natural}})} \left\|\hat{r}^{\natural} - r^{\natural}\right\|_{L^{2}(\xi_{n}^{\pi^{\natural}})} + o_{\mathbb{P}}\left(\sqrt{\frac{n+m}{nm}}\right).$$

In addition, when no covariate shifts are involved,  $\mathcal{V}_{\text{\tiny ODRE}}^{\mathring{\pi}}$  achieves semiparametric efficiency.

Error analysis of the DRE:

$$|DRE - REF| \leq \underbrace{|DRE - ODRE|}_{\mbox{Theorem above}} + \underbrace{|ODRE - REF|}_{\mbox{converges at parametric/optimal rate}}$$

## Riesz representable measure space: weight ← Riesz representer

- Source measure:  $\xi$ .
- Target measure:  $\mathring{\xi}$ .
- Riesz representable measure space:  $\Xi(\xi) := \{ \Psi_{\eta}(\xi) : \eta \in L^2(\xi) \}.$

Assume  $\mathring{\xi} \in \Xi(\xi)$ , then  $\Xi(\xi)$  serves as the candidate measure space of all the re-weighted source measure with an  $L^2$  weight.

#### Proposition

Let  $\xi$  be a positive finite measure on  $\mathfrak{X}$ . Denote by U the unit ball in  $L^2(\xi)$ . We have the following isometric isomorphism between the metric spaces  $L^2(\xi)$  and  $\Xi(\xi)$ :

$$(L^{2}(\xi), \|\cdot - \cdot\|_{L^{2}(\xi)}) \xrightarrow{\frac{\Psi \cdot (\xi)}{\frac{d\cdot}{d\xi}}} (\Xi(\xi), \mathrm{IPM}_{U}(\cdot, \cdot))$$

#### Heuristic:

On a compact state-action space, what if we use a RELU network to approximate the  $L^2$  unit ball?

## One step further to the $L^2$ convergence of weight estimation

Q: Do we really need an isometry in order to have an  $L^2$  convergence of  $\eta$  when conducting IPM-based optimization?

A: Not really!

Notation:  $\partial H = \{ \eta - \eta' : \eta, \eta' \in H \}.$ 

#### Lemma (Informal)

If  $\mathring{\eta}^{\natural} \in H$  and there exists  $\alpha > 0$  and  $\beta > 0$  such that  $\alpha(\partial H) \cap \beta U \subset \Gamma$ , then we have

$$\forall \eta^{\natural} \in L^{2}(\xi^{\pi^{\natural}}), \quad \left\| \eta^{\natural} - \mathring{\eta}^{\natural} \right\|_{L^{2}(\xi_{n}^{\pi^{\natural}})} \leq C_{\alpha,\beta} \mathrm{IPM}_{\Gamma} \left( \Psi_{\eta^{\natural}}(\xi_{n}^{\pi^{\natural}}), \Psi_{\mathring{\eta}^{\natural}}(\xi_{n}^{\pi^{\natural}}) \right)$$

The construction is similar to a dual version (in a Fenchel sense) of Chernozhukov et al. (2020).

#### Take home message:

when  $\Gamma$  is rich enough, the  $L^2$ -error of weight function estimation given by the IPM optimization is controlled by the sampling complexity of the chosen IPM.

#### Practical considerations

#### Pipeline:

- 1 Fix *H* to ensure that  $\mathring{\eta}^{\natural} \in H$ .
- 2 Construct Γ such that  $\alpha(\partial H)$  ∩  $\beta U$
- 3 Solve the adversarial optimization, i.e., arg min max-optimization.

#### Example (of our new method):

- H: Intersection of RKHS ball and  $L^2$ -ball.
- Γ: RKHS ball (which recovers MMD).
- Computation: Quadratic programming, explicitly solvable for small scale problem/ Gradient descend-based method for large scale problem.

## DE vs. DRE with our balancing method

#### DE:

- Requires that  $r^{\natural} \in \Gamma$ .
- Allows to optimized in  $H = L^2(\xi^{\pi^{\natural}})$ , i.e., *n*-value optimization.
- The error of the DE is controlled by the sampling complexity of the chosen IPM.

#### DRE:

- Requires that  $\mathring{\eta}^{\natural} \in H$ .
- Requires to model properly the candidate space *H*.
- The  $L^2$ -error of the weight function estimation is controlled by the sampling complexity of the chosen IPM.

Q: When the optimal (parametric) rate is achieved, the DRE is always better than the DE? A: No, their asymptotic variances are not comparable in general (see, e.g., Kallus and Uehara (2020)).

## Step 3: Dynamical Causal Inference

Offline Reinforcement Learning/Dynamical Treatment Regimes

## Dynamical Causal Inference under our new framework

Example: What is the average infection rate if we apply 3-vaccination policy with personalized treatment assignment (age<30 Pfizer, age>30 Moderna, with various dosage)?

- Infection may occurs after each injection.
- Infection will influence the future vaccination (infected  $\implies$  no vaccination).

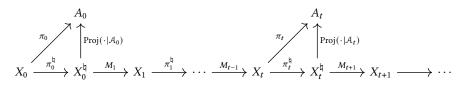


Figure: Markov structure of causal dynamics

Goal: Estimate 
$$\mathcal{V}^{\mathring{\pi}} = \mathbb{E}\left[\sum_{t=0}^{T} r_t(\mathring{X}_{t+1})\right]$$
.

#### Models

#### What is the data set?

- (US) State-Action trajectories under sampling policy  $\pi = (\pi_t; 0 \le t \le T)$  (a sequence of Markov kernels):  $\{(X_t^{(i)}, A_t^{(i)}; 0 \le t \le T) : 1 \le i \le n\}$ .
- (FR) Target initial state covariates:  $\{\mathring{X}_0^{(i)}: 1 \leq i \leq m\}$ .
- (US) Observed causal effects at each time step:  $\{r_t(X_{t+1}^{(i)}): 0 \le t \le T, 1 \le i \le n\}$ .

#### Terminal measures:

- $\xi_t^{\pi}$ : State terminal measure of  $X_t$  under sampling policy  $\pi$ .
- $\xi_t^{\pi^{\natural}}$ : State-action terminal measure of  $X_t^{\natural}$  under sampling policy  $\pi$ .
- $\mathring{\xi}_t^{\pi}$ : State terminal measure of  $\mathring{X}_t$  under target policy  $\mathring{\pi}$ .
- $\mathring{\xi}_t^{\pi^{\sharp}}$ : State-action terminal measure of  $\mathring{X}_t^{\sharp}$  under target policy  $\mathring{\pi}$ .

#### The objective re-writes

$$\mathcal{V}^{\dot{\pi}} = \sum_{t=0}^{T} \mathring{\xi}_{t+1}^{\dot{\pi}}(r_t) = \sum_{t=0}^{T} \mathring{\xi}_{t}^{\dot{\pi}^{\natural}}(r_t^{\natural}).$$

What happens if we change the policy?

## Measure flows in the change of policy

$$\xi_{0}^{\pi} \xrightarrow{\pi_{0}^{\natural}} \xi_{0}^{\pi^{\natural}} \xrightarrow{M_{1}} \xi_{1}^{\pi} \xrightarrow{\pi_{1}^{\natural}} \xi_{1}^{\pi^{\natural}} \xrightarrow{M_{2}} \cdots \xrightarrow{K_{t}^{\pi}} \xi_{t}^{\pi^{\natural}} \xrightarrow{\pi_{t}^{\natural}} \xi_{t}^{\pi^{\natural}} \xrightarrow{K_{t}^{\natural}} \cdots \xrightarrow{K_{t}^{\sharp}} \xi_{t}^{\pi^{\natural}} \xrightarrow{\Psi_{\hat{\eta}_{i}^{\natural}}} \underbrace{\psi_{\hat{\eta}_{i}^{\natural}}} \underbrace{\psi_{\hat{\eta}_{i}^{\flat}}} \underbrace{\psi_{\hat{\eta}_{i}^$$

Figure: Measure flows in the change of policy

What are these weight functions (when exist)?

$$\forall 1 \leq t \leq T, \ \forall x_t^{\natural} = (x_t, a_t) \in \mathcal{X}_t^{\natural}, \quad \mathring{e}_t^{\natural}(x_t^{\natural}) = \frac{\mathrm{d}\mathring{\pi}_t(x_t, \cdot)}{\mathrm{d}\pi_t(x_t, \cdot)}(a_t).$$

For t = 0, we let, taking into account the covariate shifts,

$$\forall x_0^{\natural} = (x_0, a_0) \in \mathcal{X}_0^{\natural}, \quad \mathring{e}_0^{\natural}(x_0^{\natural}) = \frac{\mathrm{d} \xi_0^{\check{\pi}}}{\mathrm{d} \xi_0^{\check{\pi}}}(x_0) \frac{\mathrm{d} \mathring{\pi}_0(x_0, \cdot)}{\mathrm{d} \pi_0(x_0, \cdot)}(a_0).$$

## Measure flows in the change of policy

$$(\text{US})\ \xi_{0}^{\pi} \xrightarrow{\pi_{0}^{\natural}} \xi_{0}^{\pi^{\natural}} \xrightarrow{M_{1}} \xi_{1}^{\pi^{\natural}} \xrightarrow{\pi_{1}^{\natural}} \xi_{1}^{\pi^{\natural}} \xrightarrow{M_{2}} \cdots \xrightarrow{K_{1}^{\sharp}} \xi_{t}^{\pi^{\natural}} \xrightarrow{\pi_{t}^{\natural}} \xi_{t}^{\pi^{\natural}} \xrightarrow{K_{1}^{\sharp}} \cdots \xrightarrow{K_{t}^{\sharp}} \xi_{t}^{\pi^{\natural}} \xrightarrow{\Psi_{\hat{\eta}_{1}^{\natural}}} \psi_{\hat{\eta}_{1}^{\natural}} \xrightarrow{\Psi_{\hat{\eta}_{1}^{\sharp}}} \psi_{\hat{\eta}_{1}^{\sharp}} \psi_{\hat{\eta}_{1}^{\sharp}} \psi_{\hat{\eta}_{1}^{\sharp}} \xrightarrow{\Psi_{\hat{\eta}_{1}^{\sharp}}} \psi_{\hat{\eta}_{1}^{\sharp}} \psi_$$

Figure: Measure flows in the change of policy

#### Proposition

Under mild assumptions, the weight functions  $\mathring{\eta}_t$  and  $\mathring{\eta}_t^{\natural}$  are well-defined respectively in  $L^1(\mathfrak{X}_t)$  and  $L^1(\mathfrak{X}_t^{\natural})$ . In addition, for any  $0 \le t \le T$ , we have

$$\mathring{\eta}_t^{\natural}(\cdot) = \mathbb{E}\left[\prod_{s=0}^t \mathring{e}_s^{\natural}(X_s^{\natural}) \mid X_t^{\natural} = \cdot\right] \quad and \quad \mathring{\eta}_{t+1}(\cdot) = \mathbb{E}\left[\mathring{\eta}_t^{\natural}(X_t^{\natural}) \mid X_{t+1} = \cdot\right].$$

So, possible to implement balancing? In a smart way, yes!

## New recursive balancing strategy

- Initial balancing: Compare  $\xi_n^{\pi^{\natural}}$  with  $\mathring{\xi}_{0,mN}^{\mathring{\pi}^{\natural}}$  to get the estimation of  $\{\hat{\eta}_0^{\natural}(X_0^{(i)}): 1 \leq i \leq n\}.$
- Weight smoothing: After getting  $\{\hat{\eta}_t^{\natural}(X_t^{\natural(i)}): 1 \leq i \leq n\}$  for  $t \geq 0$ , we run a separate regression (or do nothing, i.e., let  $\hat{\eta}_{t+1}(X_{t+1}^{(i)}) = \hat{\eta}_t^{\natural}(X_t^{\natural(i)})$ ) to get  $\{\hat{\eta}_{t+1}(X_{t+1}^{(i)}): 1 \leq i \leq n\}$ .
- Update balancing: Once we have  $\{\hat{\eta}_{t+1}(X_{t+1}^{(i)}): 1 \leq i \leq n\}$ , we compare  $\xi_{t+1,n}^{\pi^{\natural}}$  with  $\mathring{\xi}_{t+1,nN}^{\dagger^{\natural}}$  to get the estimation  $\{\hat{\eta}_{t+1}^{\natural}(X_{t+1}^{\natural(i)}): 1 \leq i \leq n\}$ .

#### PRO:

- Compatible with general Polish action space.
- No need to worry about covariate shifts (built-in solution).

#### CON:

• Can be computationally heavy in some setting.

Now that we have estimated the weight functions, what about the actual estimators?

## Our results on the error analysis of the DE and the DRE

Direct estimator:

$$\hat{\mathcal{V}}_{\scriptscriptstyle DE}^{\mathring{\pi}} = \sum_{t=0}^{T} \Psi_{\hat{\eta}_{t+1}}(\xi_{t+1,n}^{\pi})(r_t) = \frac{1}{n} \sum_{i=1}^{n} \sum_{t=0}^{T} \hat{\eta}_{t+1}^{(i)}(X_{t+1}^{(i)}) r_t(X_{t+1}^{(i)}).$$

Doubly robust estimator:

$$\hat{\mathcal{V}}_{\scriptscriptstyle \mathrm{DRE}}^{\mathring{\pi}} = \frac{1}{n} \sum_{i=1}^{n} \sum_{t=0}^{T} \left( \hat{\eta}_{t}^{\natural}(X_{t}^{\natural(i)}) \left( r_{t}(X_{t+1}^{(i)}) - \hat{r}_{t}^{\natural(i)}(X_{t}^{\natural(i)}) \right) + \hat{\eta}_{t-1}^{\natural}(X_{t-1}^{\natural(i)}) \mathring{\pi}_{t}^{\natural}(\hat{r}_{t}^{\natural(i)})(X_{t}^{(i)}) \right),$$

Sampling complexity of IPM:

$$\forall t \geq 1, \quad \sigma_t^{\text{\tiny{IPM}}}(n) = \text{IPM}_{\Gamma_t} \left( \Psi_{\mathring{\eta}_t^{\natural}}^{\natural}(\xi_{t,n}^{\pi^{\natural}}), \Psi_{\mathring{\eta}_t^{\natural}}^{\natural}(\xi_t^{\pi^{\natural}}) \right).$$

With a slight abuse of notation, we omit m and N at time 0, i.e.,

$$\sigma_0^{\text{\tiny IPM}}(n) = \sigma_0^{\text{\tiny IPM}}(n, m, N) = \text{IPM}_{\Gamma_0}\left(\Psi_{\mathring{\eta}_0^{\natural}}(\xi_{0,n}^{\pi^{\natural}}), \Psi_{\mathring{\eta}_0^{\natural}}(\xi_0^{\pi^{\natural}})\right) + \text{IPM}_{\Gamma_0}\left(\mathring{\xi}_0^{\mathring{\pi}^{\natural}}, \mathring{\xi}_{0,mN}^{\mathring{\pi}^{\natural}}\right).$$

#### Direct estimator

Well-specifiedness (dynamical version):

We say that the causal dynamics are well-specified by a sequence of collections of test functions  $\Gamma = (\Gamma_t; 0 \le t \le T)$  if

$$\forall 0 \le t \le T, \quad r_t^{\natural} = M_{t+1}(r_t) \in \Gamma_t,$$

and

$$\forall 1 \leq t \leq T, \ \forall \gamma_t \in \Gamma_t, \quad M_t^{\mathring{\pi}^{\natural}}(\gamma_t) \in \Gamma_{t-1}.$$

#### Theorem (Informal)

Under mild assumptions, if the causal dynamics are well-specified by  $\Gamma = (\Gamma_t; 0 \le t \le T)$ , then we have

$$\left|\hat{\mathcal{V}}_{\scriptscriptstyle DE}^{\mathring{\pi}} - \mathcal{V}^{\mathring{\pi}}\right| \leq C \left(\sum_{t=0}^{T} (T-t+1) \left(\sigma_t^{\scriptscriptstyle \mathrm{IPM}}(n) + \frac{1}{\sqrt{N}}\right)\right),\,$$

where C > 0 is a constant that is independent to n, m, N and T.

### Doubly robust estimator

For the error term given by weight smoothing, we denote

$$\sigma_t^{\text{ws}}(n) = \|\hat{\eta}_{t+1} - \mathring{\eta}_{t+1}\|_{L^2(\xi_{t+1}^{\pi}n)}.$$

we denote the error of the additional regression of the average reward function  $r^{\natural}$  by

$$\forall 0 \leq t \leq T, \quad \sigma_t^{\text{\tiny REG}}(n) = \left\| \hat{r}_t^{\natural} - r_t^{\natural} \right\|_{L^2(\xi_t^{\pi^{\natural}})}.$$

#### Theorem (Informal)

It the weight functions are well specified in  $H_t$  and if the implemented balancing satisfies

$$\forall 0 \le t \le T$$
,  $\exists \alpha_t, \beta_t > 0$ ,  $\alpha_t(\partial H_t) \cap \beta_t U_t \subset \Gamma_t$ ,

then we have

$$\left| \hat{\mathcal{V}}_{\text{DRE}}^{\mathring{\pi}} - \mathcal{V}^{\mathring{\pi}} \right| \leq C \left( \sum_{t=0}^{T} (T - t + 1) \left( \sigma_{t}^{\text{IPM}}(n) + \frac{1}{\sqrt{N}} + \sigma_{t}^{\text{WS}}(n) \right) \sigma_{t}^{\text{REG}}(n) \right)$$

where C > 0 is a constant that is independent from n, m, N, and T.

#### Conclusion

#### Our contributions:

- New state-action Markov reformulation of causal dynamics, that is capable of dealing with general action spaces and covariate shifts.
- New theoretical framework for balancing method through Riesz representable measure space arguments (connection between existing methods and inspiration of new methods).
- 3 Recursive balancing strategy, with transparent error analysis for the DE and the DRE.

#### More details:

State-Action Balancing in Multi-Stage Causal Inference. Q. Du, G. Biau, F. Petit, R. Porcher. (preprint, 2022).

## Perspectives

- 1 Balancing extracts features?
- 2 Connection with the Feynman-Kac formalism/Sequential Monte Carlo
  - How to efficiently interact with the environment with the collected offline data?
    - Variance Estimation in Adaptive Sequential Monte Carlo. Q. Du, A. Guyader. Annals of Applied Probability, 2021.
    - Asymmetric Sequential Monte Carlo. Q. Du. Under review, 2021.
  - What if we estimate directly the Markov kernel  $M_t$ ?
    - Wasserstein Random Forests and Applications in Heterogeneous Treatment Effects. Q. Du, G. Biau, F. Petit, R. Porcher. AISTATS 2021.
- 3 Transductive Transfer learning?

$$\arg\min_{f\in F} \mathrm{IPM}_{\Gamma}\left(\frac{1}{n}\sum_{i=1}^{n}\delta_{X_{i}}Y_{i}, \frac{1}{n}\sum_{i=1}^{n}\delta_{X_{i}}f(X_{i})\right)$$

## Thank you for your attention!

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