Combining Experimental and Historical Data for Policy Evaluation

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Data Integration



Example I: A/B Testing



Taken from https://towardsdatascience.com/how-to-conduct-a-b-testing-3076074a8458

Example I: A/B Testing with Historical Data



Example II: Meta Analysis [Shi et al., 2018]



Example III: Combining Observational Data



Challenge: Distributional Shift

- **Example I**: In ridesharing, the **nonstationarity** of the environment → distributional shift between experimental and historical datasets [Wan et al., 2021]
- Example II: In medicine, the heterogeneity in characteristics of treatment setting → distributional shift among different data sources [Shi et al., 2018]
- Example III: The observational data is subject to unmeasured confounding \rightarrow distributional shift between RCT and observational data



- Data integration for causal inference
 - Example I: Leverage historical datasets under control [Li et al., 2023]
 - Example II: Federated causal inference [Han et al., 2021, 2023]
 - Example III: Combining RCT and observational data [Kallus et al., 2018, Yang and Ding, 2020]
- Other related works
 - Meta analysis & meta learning [DerSimonian and Laird, 1986]
 - Transfer & federated learning [Li et al., 2022]
 - Heterogeneous RL [Shi et al., 2018, Chen et al., 2024]
 - Off-policy evaluation [Jung and Bellot, 2024]

A/B Testing with Historical Data

Objective: combine experimental data with historical data to improve ATE estimation



Challenge: distributional shift between experimental and historical data

Two Base Estimators



A Naive Weighted Estimator

• Consider the weighted estimator

$$\widehat{ au}_{m{w}}=m{w}\widehat{ au}_{m{e}}+(m{1}-m{w})\widehat{ au}_{m{h}},$$

for some properly chosen weight $\boldsymbol{w} \in [0,1]$ to minimize its $\mathrm{MSE}(\widehat{\boldsymbol{\tau}}_{\boldsymbol{w}})$.

- The weight *w* reflects a bias-variance tradeoff. A large *w* can:
 - Reduce **bias** of $\hat{\tau}_w$ caused by the distributional shift between the datasets
 - Increase variance of $\widehat{ au}_{m{w}}$ as a result of not fully leveraging the historical data
- Natural to consider the following naive estimator that minimizes an estimated MSE:

$$\widehat{\mathrm{MSE}}(\widehat{\boldsymbol{\tau}}_{\boldsymbol{w}}) = \widehat{\mathrm{Bias}}^2(\widehat{\boldsymbol{\tau}}_{\boldsymbol{w}}) + \widehat{\mathsf{Var}}(\widehat{\boldsymbol{\tau}}_{\boldsymbol{w}}).$$

We refer to this estimator as the **non-pessimistic** estimator.

Three scenarios, depending on the bias $m{b} = \mathbb{E}(\widehat{m{b}}) = \mathbb{E}(\widehat{m{ au}}_{m{h}} - \widehat{m{ au}}_{m{e}})$

- 1. **Small bias**: *b* is much smaller than the standard deviation of its estimator;
- Moderate bias: b is comparable to or larger than the standard deviation, yet falls within the high confidence bounds of b;
- 3. Large bias: *b* is much larger than the estimation error.

Three competing estimators:

- 1. **EDO** (experimental-data-only) estimator which sets w = 1;
- 2. **SPE** (semi-parametrically efficient) estimator [Li et al., 2023] developed under the assumption of no bias;
- 3. Oracle estimator which optimizes \boldsymbol{w} to minimize $MSE(\hat{\boldsymbol{\tau}}_{\boldsymbol{w}})$;

| SPE | Oracle | EDO |
|-----|--------|--------|
| 0 | b | → bias |
| 0 | υ | 100 |

Theoretical Analysis (Cont'd)

| Bias | Non-pessimistic estimator | Optimal estimator |
|----------|----------------------------|-------------------|
| Zero | Close to efficiency bound | SPE/Oracle |
| Small | Close to oracle MSE | SPE/Oracle |
| Moderate | May suffer a large MSE | Oracle |
| Large | Oracle property | EDO/Oracle |

- The oracle MSE denotes MSE of the oracle estimator
- The efficiency bound is the smallest achievable MSE among a broad class of regular estimators [Tsiatis, 2006].

Can we develop an estimator that works well with moderate bias?

Main idea: reformulate the weight selection as an offline bandit problem

- Each weight $\pmb{w} \in [0,1] \rightarrow$ an $\pmb{\operatorname{arm}}$ in bandit
- Negative MSE of $\widehat{ au}_{m{w}}
 ightarrow {m{reward}}$ of selecting an arm

Objective in bandit: choose the optimal arm that maximizes its reward.

Multi-Armed Bandit



- The simplest RL problem
- A casino with **multiple** slot machines
- Playing each machine yields an independent **reward**.
- Limited knowledge (unknown reward distribution for each machine) and resources (time)
- **Objective**: determine which machine to pick at each time to maximize the expected **cumulative rewards**

Multi-Armed Bandit (Con't)

- *k*-armed bandit problem (*k* machines)
- *A_t* ∈ {1, · · · , *k*}: arm (machine) pulled (experimented) at time *t*
- $R_t \in \mathbb{R}$: reward at time t
- $Q(a) = \mathbb{E}(R_t | A_t = a)$ expected reward for each arm a (unknown)
- **Objective**: maximize $\sum_{t=1}^{T} \mathbb{E}\mathbf{R}_{t}$.



Greedy Action Selection

• Action-value methods:

$$\widehat{Q}(a) = N^{-1}(a) \sum_{t=0}^{T-1} R_t \mathbb{I}(A_t = a)$$

where
$$N(a) = \sum_{t=0}^{T-1} \mathbb{I}(A_t = a)$$
 denotes the action counter

- Greedy policy: $\arg \max_{a} \widehat{Q}(a)$
- Less-explored action $\rightarrow N(a)$ is small \rightarrow inaccurate $\widehat{Q}(a) \rightarrow$ suboptimal policy (see the plot on the right)



The Optimistic Principle

- Used in **online** settings to balance exploration-exploitation tradeoff
- The more **uncertain** we are about an action-value
- The more **important** it is to explore that action
- It could be the **best** action
- Likely to pick blue action
- Forms the basis for **upper confidence bound** (UCB)



Upper Confidence Bound

• Estimate an upper confidence $U_t(a)$ for each action value such that

 $Q(a) \leq \widehat{Q}_t(a) + U_t(a),$

with high probability.

- $U_t(a)$ quantifies the uncertainty and depends on $N_t(a)$ (number of times arm a has been selected up to time t)
 - Large $N_t(a) \rightarrow \text{small } U_t(a)$;
 - Small $N_t(a) \rightarrow \text{large } U_t(a)$.
- Select actions maximizing upper confidence bound

$$\mathbf{a}^* = \arg\max_{\mathbf{a}} [\widehat{\mathbf{Q}}_t(\mathbf{a}) + \mathbf{U}_t(\mathbf{a})].$$

• Combines exploration $(U_t(a))$ and exploitation $(\widehat{Q}_t(a))$.

Offline Multi-Armed Bandit Problem

- *k*-armed bandit problem (*k* machines)
- *A_t* ∈ {1, · · · , *k*}: arm (machine) pulled (experimented) at time *t*
- $R_t \in \mathbb{R}$: reward at time t
- Q(a) = E(R_t | A_t = a) expected reward for each arm a (unknown)
- Objective: Given {A_t, R_t}_{0≤t<T}, identify the best arm



Greedy Action Selection (Non-pessimistic Estimator)

• Action-value methods:

$$\widehat{Q}(a) = N^{-1}(a) \sum_{t=0}^{T-1} R_t \mathbb{I}(A_t = a)$$

where $N(a) = \sum_{t=0}^{T-1} \mathbb{I}(A_t = a)$ denotes the action counter

- Greedy policy: $\arg \max_{a} \widehat{Q}(a)$
- Less-explored action $\rightarrow N(a)$ is small \rightarrow inaccurate $\widehat{Q}(a) \rightarrow$ suboptimal policy (see the plot on the right)



The Pessimistic Principle

- In offline settings
- The less **uncertain** we are about an action-value
- The more **important** it is to use that action
- It could be the **best** action
- Likely to pick red action
- Yields the **lower confidence bound** (LCB) algorithm



Lower Confidence Bound

• Estimate an lower confidence L(a) for each action value such that

$$Q(a) \geq \widehat{Q}(a) - L(a),$$

with high probability.

- L(a) quantifies the **uncertainty** and depends on N(a) (number of times arm a has been selected in the historical data)
 - Large $N(a) \rightarrow \text{small } L(a)$;
 - Small $N(a) \rightarrow \text{large } L(a)$.
- Select actions maximizing lower confidence bound

$$oldsymbol{a}^* = rg\max_{oldsymbol{a}} [\widehat{oldsymbol{Q}}(oldsymbol{a}) - oldsymbol{L}(oldsymbol{a})].$$

- Set $L(a) = \sqrt{c \log(T)/N(a)}$ for some positive constant c where T is the sample size of historical data
- According to Hoeffding's inequality (<u>link</u>), when rewards are bounded between 0 and 1, the event

$$|\boldsymbol{Q}(\boldsymbol{a}) - \widehat{\boldsymbol{Q}}(\boldsymbol{a})| \leq \boldsymbol{L}(\boldsymbol{a}),$$

holds with probability at least $1-2\mathcal{T}^{-2c}$ (converges to 1 as $\mathcal{T} \to \infty$).

Lower Confidence Bound (Cont'd)

- $\widehat{Q}(4) > \widehat{Q}(3)$
- T = 1605. Set c = 1.
- $L(3) = \sqrt{\log(T)/N(3)} = 0.272$
- $L(4) = \sqrt{\log(T)/N(4)} = 1.215$
- $\hat{Q}(3) L(3) > \hat{Q}(4) L(4)$
- $\widehat{Q}(3) L(3) > \max(\widehat{Q}(1), \widehat{Q}(2))$
- Correctly identify optimal action





Define the regret, as the difference between the expected reward under the **best arm** and that under the **selected arm**.

Theorem (Greedy Action Selection)

Regret of greedy action selection is upper bounded by $2 \max_{a} |\widehat{Q}(a) - Q(a)|$, whose value is bounded by $2\sqrt{c \log(T) / \min_{a} N(a)}$ (according to Hoeffding's inequality) with probability approaching 1

- The upper bound depends on the estimation error of each Q-estimator
- The regret is small when each arm has sufficiently many observations
- However, it would yield a large regret when one arm is less-explored
- This reveals the **limitation** of greedy action selection

Theorem (LCB; see also Jin et al. [2021])

Regret of the LCB algorithm is upper bounded by $2\sqrt{c \log(T)/N(a^{opt})}$ where a^{opt} denotes the best arm with probability approaching 1

- The upper bound depends on the estimation error of best arm's Q-estimator only
- The regret is small when the **best** arm has sufficiently many observations
- This is much weaker than requiring each arm to have sufficiently many observations
- This reveals the **advantage** of LCB algorithm

Main idea: reformulate the weight selection as an offline bandit problem

- Each weight $\textbf{\textit{w}} \in [0,1] \rightarrow$ an arm in bandit
- Negative MSE of $\widehat{ au}_{m{w}}
 ightarrow {m{reward}}$ of selecting an arm

Nonpessimistic estimator chooses the arm that maximizes an estimated negative MSE

- It requires a **uniform consistency** condition: the estimated MSE converges to its oracle value uniformly across all weights
- Underestimate the bias $b \to \text{low}$ estimated MSE for small weights \to estimated weight tends to be smaller than the ideal value \to a significant bias in $\hat{\tau}_w$
- This reveals the limitation of the nonpessimistic estimator when **b** is moderate or large.

 $\mbox{Main idea}:$ select the arm that maximizes a lower bound of the negative MSE, or equivalently, an upper bound of the MSE

- Uncertainty quantification: compute an uncertainty quantifier U for the estimated error such that $|\hat{b} b| \le U$ with large probability.
- MSE estimation: use $|\hat{\boldsymbol{b}}| + \boldsymbol{U}$ as a pessimistic estimator for the bias \boldsymbol{b} and plug this estimator into the MSE formula to construct an upper bound of the MSE $\widehat{\text{MSE}}_{U}(\hat{\boldsymbol{\tau}}_{\boldsymbol{w}})$.
- Weight selection: select w that minimizes the upper bound $\widehat{MSE}_U(\widehat{\tau}_w)$.

| Bias | Non-pessimistic estimator | Pessimistic estimator | Optimal estimator |
|----------|----------------------------|---------------------------------|-------------------|
| Zero | Close to efficiency bound | Same order to oracle MSE | SPE/Oracle |
| Small | Close to oracle MSE | Same order to oracle MSE | SPE/Oracle |
| Moderate | May suffer a large MSE | Oracle property | Oracle |
| Large | Oracle property | Oracle property | EDO/Oracle |

- The oracle MSE denotes MSE of the oracle estimator.
- The efficiency bound is the smallest achievable MSE among a broad class of regular estimators [Tsiatis, 2006].

Simulation Study

The effectiveness of different estimators is determined by the magnitude of the bias. To validate our theory, we further classify \boldsymbol{b} into different regimes as follows

- Small bias regime (SPE estimator is expected to be optimal): $|m{b}| \le c_1 \sqrt{\mathsf{Var}(\widehat{m{b}})};$
- Moderatel bias regime (the proposed pessimistic estimator is expected to be optimal): $c_1 < \frac{|\mathbf{b}|}{\sqrt{\operatorname{Var}(\hat{\mathbf{b}})}} \leq c_2$;
- Large bias regime (EDO estimator is expected to be optimal): $|\boldsymbol{b}| > c_2 \sqrt{\text{Var}(\widehat{\boldsymbol{b}})}$.

According to our theory, we set $c_1 = 1$ and $c_2 = \sqrt{\log(n)}$. This ensures:

- Scenarios where variance dominates the bias are categorized within the small bias region.
- When the bias exceeds the established high confidence bound, it is classified under the large bias regime.

Simulation Study: Bandit Simulation

- NonPessi: the proposed non-pessimistic estimator.
- Pessi: the proposed pessimistic estimator.
- **EDO**: the doubly robust estimator $\hat{\tau}_e$ constructed based on the experimental data only (see (1)).
- Lasso: a weighted estimator $\hat{\tau}_{Lasso} = w\hat{\tau}_e + (1-w)\hat{\tau}_h$ that linearly combines the ATE estimator $\hat{\tau}_e$ based on experimental data and $\hat{\tau}_h$ based on historical data, where the weight w is chosen to minimize the estimated variance of the final ATE estimator with the Lasso penalty (Cheng & Cai, 2021),
- SPE: the semi-parametrically efficient estimator proposed by Li et al. (2023) developed under the assumption of no reward shift between the experimental and historical data, i.e., $r_e(0, s) = r_h(s)$ for any *s*.



Ridesharing Data-based Sequential Simulation



Pessimistic estimator shows robustness in dealing with distributional shift

Simulation Study: Confidence Intervals



- While maintaining nominal coverage, the pessimistic estimator yields narrower confidence intervals compared to the EDO estimator
- Improvement in efficiency by incorporating historical data.



- Policy evaluation using both **experimental** and **historical** datasets, allowing distributional shifts between the two datasets.
- Two weighted estimators that leverage both data sources.
- The proposed **non-pessimistic estimator** chooses the weight by minimizing an estimated MSE.
- The proposed **pessimistic estimator** further employs the pessimistic principle to boost its robustness.
- Our theoretical and empirical analyses identify the most effective estimator within each regime.

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