A/B Testing in Two-Sided Marketplaces: Data Integration, Designs and Reinforcement Learning

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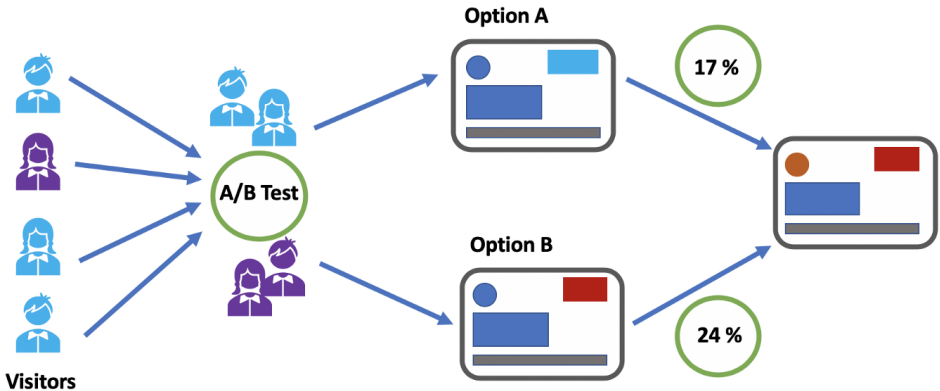
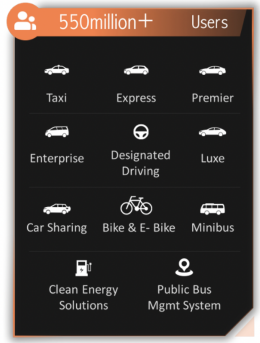
A/B Testing



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

Ridesharing



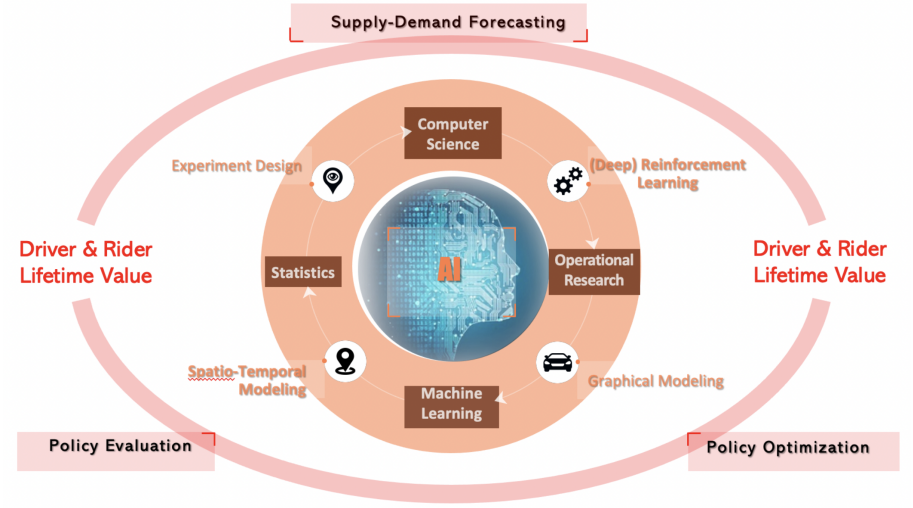
106TB+
vehicle trajectory data/day

4875TB+
data processed/day

40billion+
routing requests/day

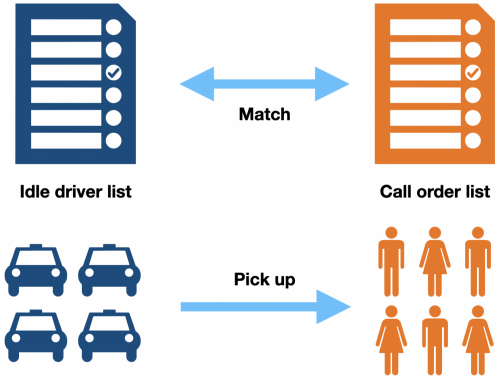
15billion+
location points/day

Ridesharing (Cont'd)



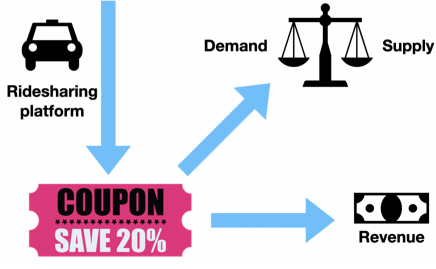
Policies of Interest

- **Order dispatching**



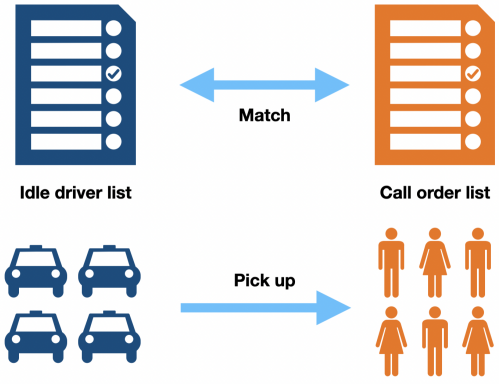
- **Subsidizing**

Passenger enters destination



Policies of Interest

- **Order dispatching**



- Subsidizing

Time Series Data

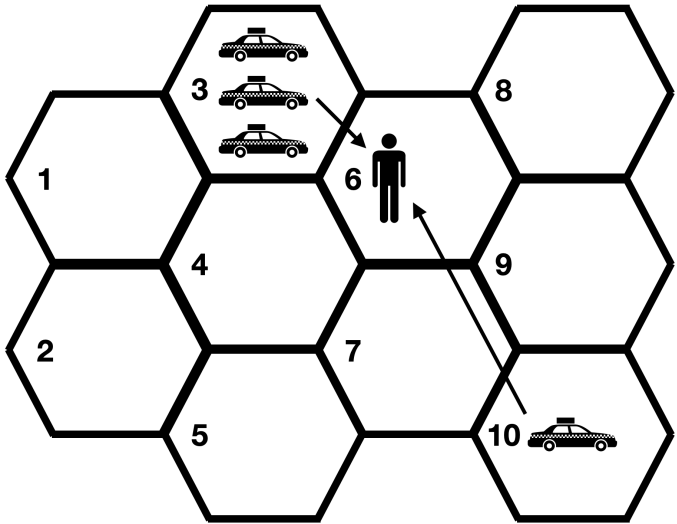
- Online experiment typically lasts for **two weeks**
- **30 minutes**/**1 hour** as one time unit
- Data forms a **time series** $\{(\boldsymbol{Y_t}, \boldsymbol{U_t}) : \mathbf{1} \leq \boldsymbol{t} \leq \boldsymbol{T}\}$
- **Observations** $\boldsymbol{Y_t} \in \mathbb{R}^{\mathbf{3}}$:
  1. **Outcome**: drivers' income or no. of completed orders
  2. **Supply**: no. of idle drivers
  3. **Demand**: no. of call orders
- **Treatment** $\boldsymbol{U_t} \in \{\mathbf{1}, -\mathbf{1}\}$:
  - **New** order dispatching policy $\boldsymbol{B}$
  - **Old** order dispatching policy $\boldsymbol{A}$

Challenges

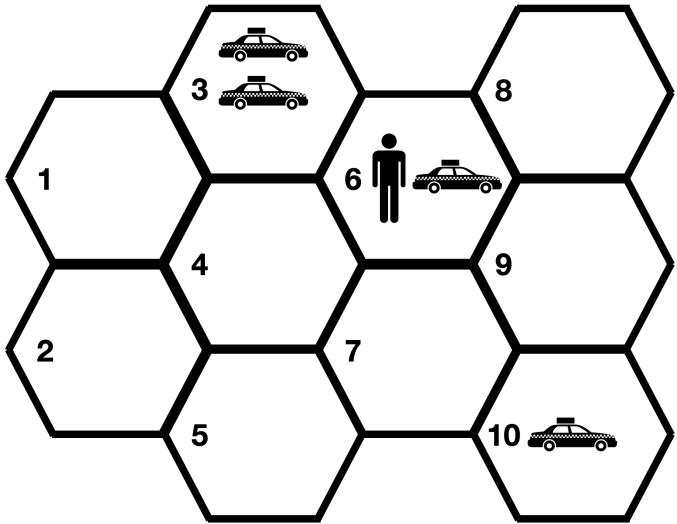
1. **Carryover Effects**:
   - Past treatments influence future observations [Li et al., 2024a, Figure 2] $\longrightarrow$
   - Invalidating many conventional A/B testing/causal inference methods [Shi et al., 2023].
2. **Partial Observability**:
   - The environmental state is not fully observable $\longrightarrow$
   - Leading to the violation of the Markov assumption.
3. **Small Sample Size**:
   - Online experiments typically last only two weeks [Xu et al., 2018] $\longrightarrow$
   - Increasing the variability of the average treatment effect (ATE) estimator.
4. **Weak Signal**:
   - Size of treatment effects ranges from 0.5% to 2% [Tang et al., 2019] $\longrightarrow$
   - Making it challenging to distinguish between new and old policies.

To our knowledge, **no** existing method has simultaneously addressed all four challenges.

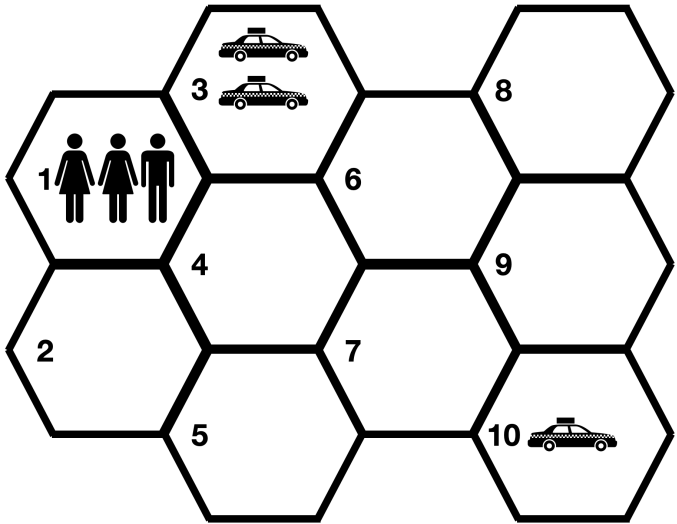
Challenge I: Carryover Effects



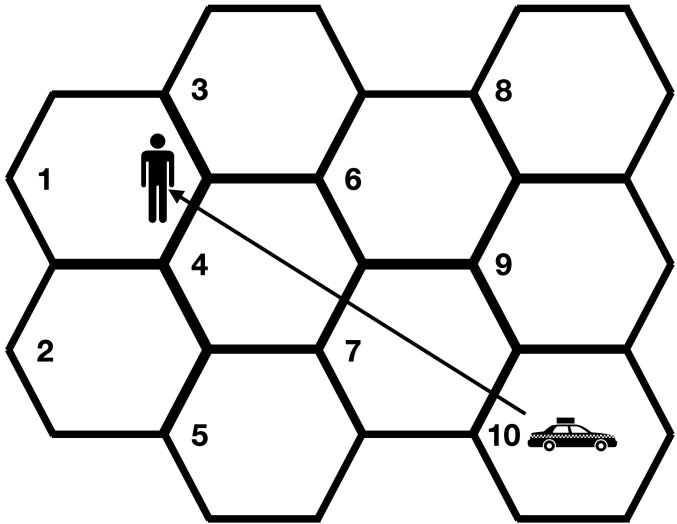
Adopting the Closest Driver Policy



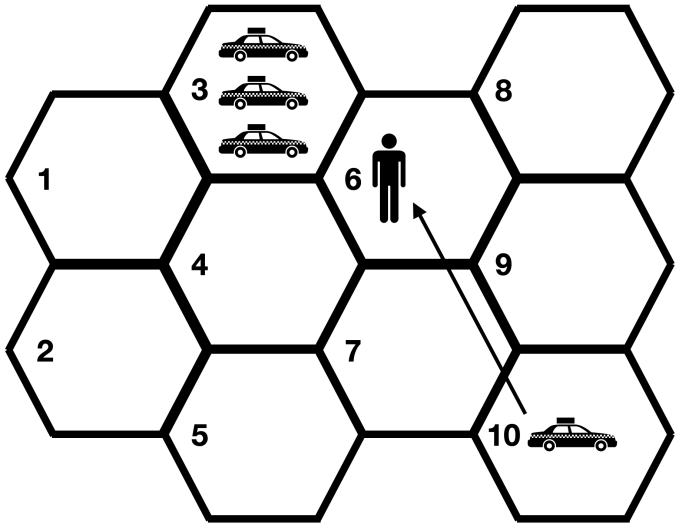
Some Time Later · · ·



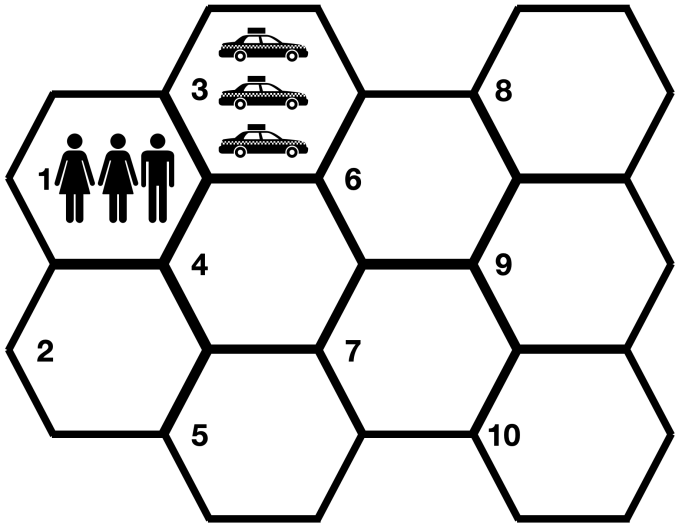
Miss One Order



Consider a Different Action



Able to Match All Orders

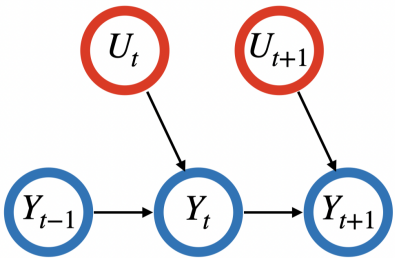


Challenge I: Carryover Effects (Cont'd)

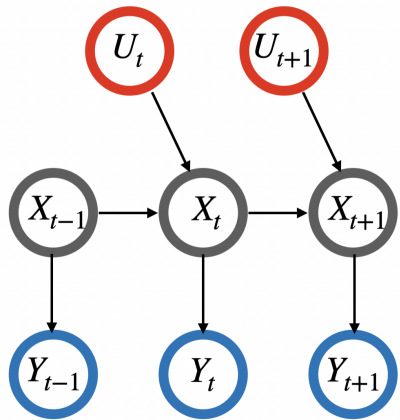
past treatments $\rightarrow$ distribution of drivers $\rightarrow$ future outcomes

Challenge II: Partial Observability

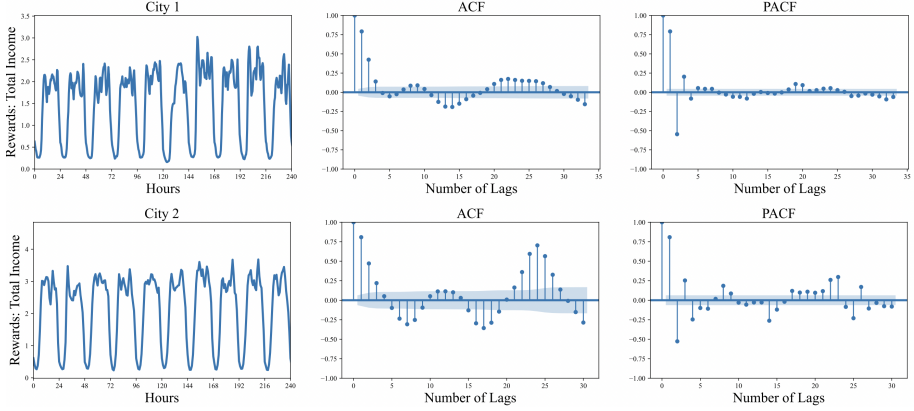
- **Fully Observable Markovian Environments**



- **Partially Observable non-Markovian Environments**

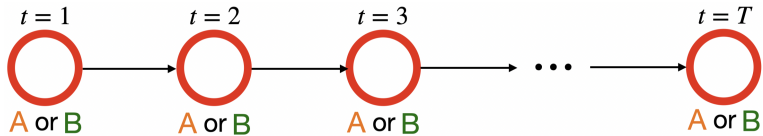


Challenge II: Partial Observability (Cont'd)

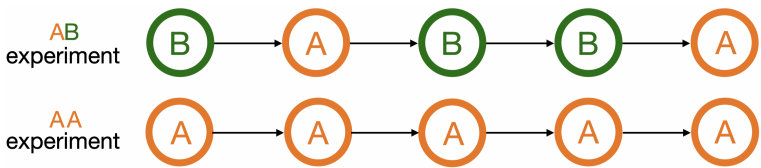


Challenge III & IV: Small sample & Weak Signal

- **Aim 1: Design**. Identify **optimal treatment allocation strategy** in online experiment that **minimizes MSE of ATE estimator**



- **Aim 2: Data Integration**. Combine **experimental data** (***A***/***B***) with **historical data** (***A***/***A***) to improve ATE estimation [Li et al., 2024b]



Project I

Optimal Treatment Allocation Strategies for A/B Testing in Partially Observable Environments

Joint work with Ke Sun, Linglong Kong & Hongtu Zhu

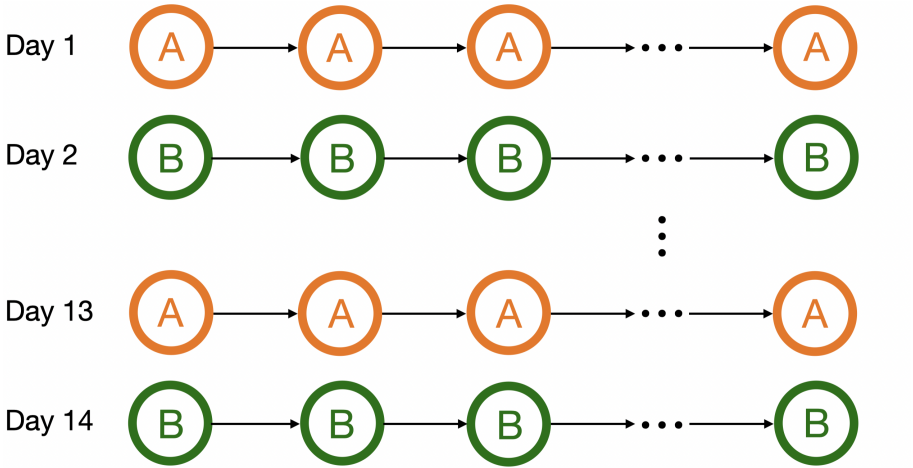
Average Treatment Effect

- Data summarized into a **time series** $\{(Y_t, U_t) : 1 \leq t \leq T\}$
- The first element of Y_t – denoted by R_t – represents the **outcome**
- **ATE** = **difference in average outcome** between the **new** and **old** policy

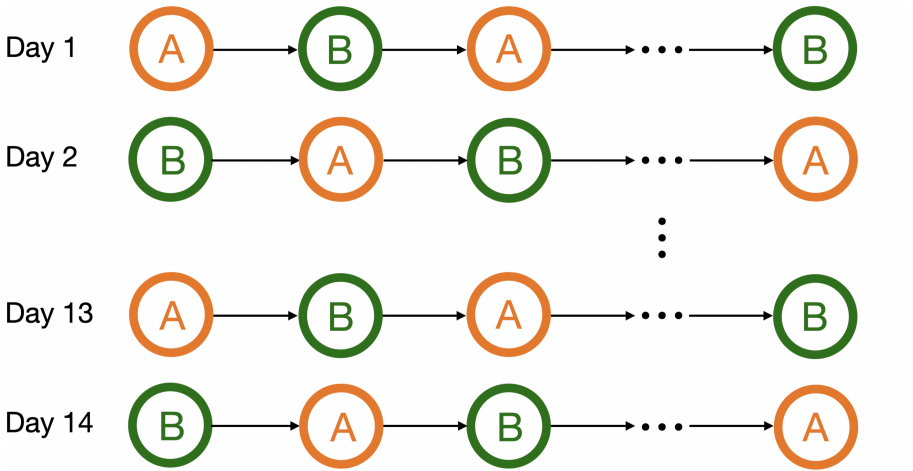
$$\lim_{T\to\infty}\left[\frac{1}{T}\sum_{t=1}^{T}\mathbb{E}R_t\right] - \lim_{T\to\infty}\left[\frac{1}{T}\sum_{t=1}^{T}\mathbb{E}R_t\right].$$

Letting $T \to \infty$ simplifies the analysis.

Alternating-day (AD) Design



Alternating-time (AT) Design



AD v.s. AT

Pros of **AD design**:

- Within each day, it is **on-policy** and avoids **distributional shift**, as opposed to **off-policy** designs (e.g., AT)
- On-policy designs are proven **optimal** in **fully observable Markovian** environments [Li et al., 2023a].

Pros of **AT design**:

- Widely employed in ridesharing companies like Lyft and Didi [Chamandy, 2016, Luo et al., 2024]
- According to my industrial collaborator, AT yields **less variable ATE estimators** than AD

AD v.s. AT (Cont'd)

- **Q: Why can off-policy designs, such as AT, be more efficient than AD?**
- **A: Due to partial observability...**

A Thought Experiment

- A simple setting **without carryover effects**:

$$R_t = \beta_{-1}\mathbb{I}(U_t = -1) + \beta_1\mathbb{I}(U_t = 1) + \varepsilon_t$$

- ATE equals $\beta_1 - \beta_{-1}$ and can be estimated by

$$\widehat{\text{ATE}} = \frac{\sum_{t=1}^{T} R_t\mathbb{I}(U_t = 1)}{\sum_{t=1}^{T}\mathbb{I}(U_t = 1)} - \frac{\sum_{t=1}^{T} R_t\mathbb{I}(U_t = -1)}{\sum_{t=1}^{T}\mathbb{I}(U_t = -1)}$$

A Thought Experiment (Cont'd)

The ATE estimator's asymptotic MSE under AD and AT is proportional to

$$\lim_{t\to\infty} \frac{1}{t}\mathrm{Var}(\varepsilon_1+\varepsilon_2+\varepsilon_3+\varepsilon_4+\cdots+\varepsilon_t) \quad \text{and} \quad \lim_{t\to\infty} \frac{1}{t}\mathrm{Var}(\varepsilon_1-\varepsilon_2+\varepsilon_3-\varepsilon_4+\cdots-\varepsilon_t)$$

which depends on the residual correlation:

- With **uncorrelated residuals**, both designs yield **same** MSEs
- With **positively correlated residuals**:
  - **AD assigns the same treatment** within each day, under which ATE estimator's variance inflates due to **accumulation** of these residuals
  - **AT alternates treatments** for adjacent observations, effectively **negating** these residuals, leading to more efficient ATE estimation
- With **negatively correlated residuals**, AD generally outperforms AT

When Can AT Be More Efficient than AD

Key Condition: Residuals are positively correlated

- **Rule out full observablity** (Markovianity) where residuals are uncorrelated.
- Can only be met under **partial observability**.
- Suggest partial observability is more realistic, aligning with my collaborator's finding.
- **Often satisfied** in practice:

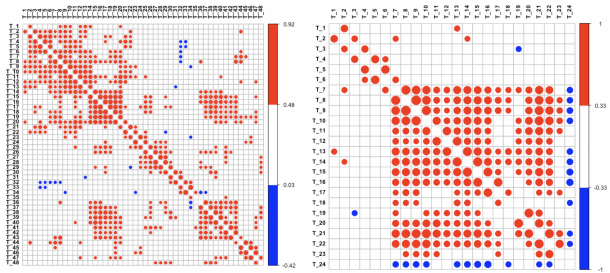


Figure: Estimated correlation coefficients between pairs of fitted outcome residuals from the two cities

Some Motivating Questions

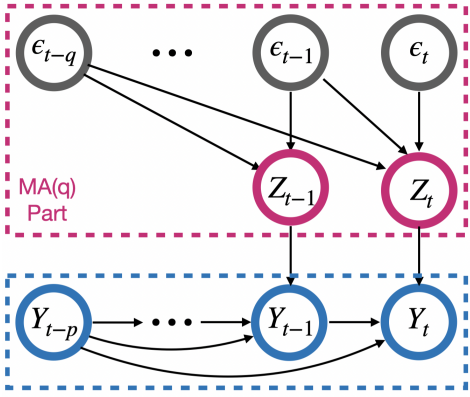
- **Q1: Previous analysis excludes carryover effects. Can we extend the results to accommodate carryover effects?**

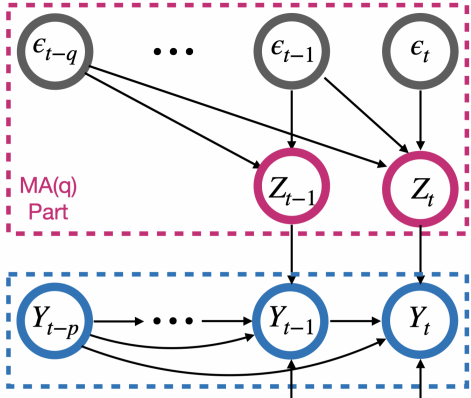
- **Q2: Previous analysis focuses on AD and AT. Can we consider more general designs?**

Our Contributions

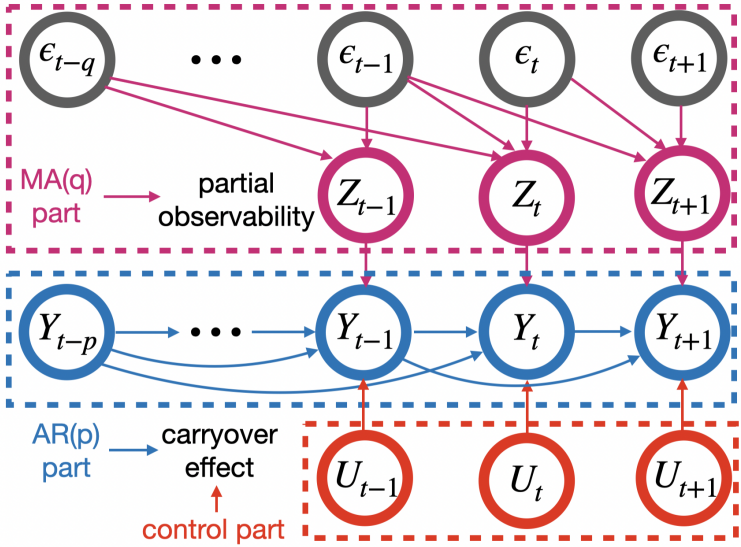
- **Methodologically**, we propose:
  1. A **controlled (V)ARMA** model $\rightarrow$ allow **carryover effects** & **partial observability**
  2. Two **efficiency indicators** $\rightarrow$ compare commonly used designs (AD, AT)
  3. A **reinforcement learning** (RL) algorithm $\rightarrow$ compute the **optimal design**
- **Theoretically**, we:
  1. Establish **asymptotic MSEs** of ATE estimators $\rightarrow$ compare different designs
  2. Introduce **weak signal condition** $\rightarrow$ simplify asymptotic analysis in sequential settings
  3. Prove the **optimal treatment allocation strategy** is $\boldsymbol{q}$-dependent $\rightarrow$ form the basis of our proposed RL algorithm
- **Empirically**, we demonstrate the advantages of our proposal using:
  1. A dispatch simulator (`https://github.com/callmespring/MDPOD`)
  2. Two real datasets from ridesharing companies.

Controlled VARMA Model: Introduction





Controlled VARMA Model: Introduction



Controlled VARMA Model: Connection

- Closely related to **state space models** or **linear quadratic regulator** (LQR)
  - The latter being a rich sub-class of **partially observable MDPs**
  - Using VARMA as opposed to LQR allows to leverage asymptotic theories developed in time series to derive optimal designs
- Compared to **MDPs**
  - Both controlled VARMA and MDP accommodate **carryover effects**
  - MDPs require full observability whereas controlled VARMA allows **partial observability**

Controlled VARMA Model: Estimation

Consider a univariate controlled ARMA

$$Y_t = \mu + \underbrace{\sum_{j=1}^{p} a_j Y_{t-j}}_{\text{AR Part}} + \underbrace{bU_t}_{\text{Control}} + e_t + \underbrace{\sum_{j=1}^{q} \theta_j e_{t-j}}_{\text{MA Part}}$$

- **AR parameters** $\{a_j\}_j$ & **control parameter** $b \to$ **ATE**, equal to $2b/\sum_j(1-a_j)$
  - Partial observability $\to$ standard OLS **fails** to consistently estimate b & $\{a_j\}_j$
  - Employ **Yule-Walker estimation** (method of moments) instead
  - Similar to **IV** estimation, utilize past observations as IVs
- **MA parameters** $\{\theta_j\}_j \to$ **residual correlation** $\to$ **optimal design**

Theory: Weak Signal Condition

- **Asymptotic framework**: large sample $T \to \infty$ & weak signal **ATE**$\to 0$
- **Empirical alignment**: size of ATE ranges from 0.5% to 2%
- **Theoretical simplification**: considerably simplifies the computation of ATE estimator's MSE in sequential settings. According to Taylor's expansion:

$$\widehat{\text{ATE}} - \text{ATE} = \frac{2\hat{b}}{1-\sum_j \hat{a}_j} - \frac{2b}{1-\sum_j a_j}$$

$$= \underbrace{\frac{2(\hat{b}-b)}{1-\sum_j a_j}}_{\text{Leading term. Easy to calculate its asymptotic variance under weak signal}} + \underbrace{\frac{2b}{(1-\sum_j a_j)^2}\sum_j(\hat{a}_j - a_j)}_{\text{Challenging to obtain the closed form of its asymptotic variance, but negligible under weak signal condition}} + \underbrace{o_p\left(\frac{1}{\sqrt{T}}\right)}_{\text{High-order reminder}}$$

Theory: Asymptotic MSE

We focus on the class of **observation-agnostic** designs:

- U_1 is randomly assigned
- The distribution of U_t depends on $(U_1, \cdots, U_{t-1})$, independent of $(Y_1, \cdots, Y_{t-1})$

It covers three commonly used designs:

1. Uniform random (UR) design: $\{U_t\}_t$ are uniformly independently generated
2. AD: $U_1 = U_2 = \cdots = U_D = -U_{D+1} = \cdots = -U_{2D} = U_{2D+1} = \cdots$
3. AT: $U_1 = -U_2 = U_3 = -U_4 = \cdots = (-1)^{T-1} U_T$

Theorem (Asymptotic MSE)

Given an **observation-agnostic** *design, let* $\xi = \lim_T \sum_{t=1}^T (\mathbb{E} U_t / T)$. *Under the* **weak signal** *condition, its ATE estimator's asymptotic MSE (after normalization) equals*

$$\lim_T \frac{4}{(1 - \sum_j a_j)^2 (1-\xi)^2 T} Var\Big[\sum_{t=1}^T (U_t - \xi)\varepsilon_t\Big].$$

Theory: Asymptotic MSE (Cont'd)

Corollary (Asymptotic MSE)

Under the **weak signal** *condition, the ATE estimator's asymptotic MSE (after normalization) under* **AD**, **UR** *and* **AT** *equals*

$$\begin{aligned}
\textbf{MSE(AD)} &= \frac{4\sigma^2}{(1-\sum_j a_j)^2}\Big[\sum_{j=0}^{q}\theta_j^2 + \sum_{j_1\neq j_2}\theta_{j_1}\theta_{j_2}\Big] \\
\textbf{MSE(UR)} &= \frac{4\sigma^2}{(1-\sum_j a_j)^2}\sum_{j=0}^{q}\theta_j^2 \\
\textbf{MSE(AT)} &= \frac{4\sigma^2}{(1-\sum_j a_j)^2}\Big[\sum_{j=0}^{q}\theta_j^2 + 2\sum_{j_1\neq j_2}(-1)^{|j_2-j_1|}\theta_{j_1}\theta_{j_2}\Big],
\end{aligned}$$

where σ^2 *denotes the variance of the white noise process.*

Design: Efficiency Indicator

Define two efficiency indicators

$$\mathbf{EI}_1 = \sum_{j_1 \neq j_2} \theta_{j_1}\theta_{j_2} \qquad \text{and} \qquad \mathbf{EI}_2 = \sum_{j_1 \neq j_2} (-1)^{|j_2 - j_1|}\theta_{j_1}\theta_{j_2}.$$

They measure **residual correlations** and can be used to compare the three designs:

- If both $\mathbf{EI}_1$ and $\mathbf{EI}_2 > \mathbf{0}$, **UR** outperforms **AD** & **AT**
- If $\mathbf{EI}_2 < \mathbf{0}$ and $\mathbf{EI}_1 > \mathbf{EI}_2$, **AT** outperforms the rest
- If $\mathbf{EI}_1 < \mathbf{0}$ and $\mathbf{EI}_2 > \mathbf{EI}_1$, **AD** outperforms the rest

MA parameters can be estimated using historical data (even without treatment data).

Design: Optimality

Theorem (Optimal Design)

The optimal design must satisfy $\lim_T \sum_{t=1}^{T}(\mathbb{E}\boldsymbol{U}_t/\boldsymbol{T}) = \mathbf{0}$. *Additionally, it must minimize*

$$\sum_{k=1}^{q}\Big[\lim_{T}\Big(\frac{1}{T}\sum_{t=1}^{T}\mathbb{E}\boldsymbol{U}_t\boldsymbol{U}_{t+k}\Big)\underbrace{\sum_{j=k}^{q}\theta_j\theta_{j-k}}_{c_k}\Big]$$

Objective: learn the optimal observation-agnostic design that:

(i) **Minimizes** the above criterion

(ii) **Maintains** a zero mean asymptotically, i.e., $\lim_T \sum_{t=1}^{T}(\mathbb{E}\boldsymbol{U}_t/\boldsymbol{T}) = \mathbf{0}$

Design: An RL Approach

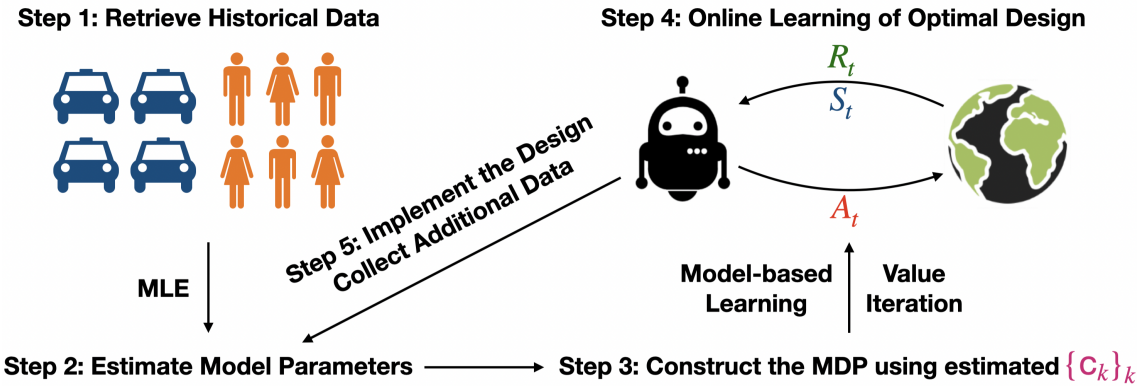
Solution: reformulate the minimization as an infinite-horizon average-reward RL problem

- **State S_t**: the collection of past q treatments $(U_{t-q}, U_{t-q+1}, \cdots, U_{t-1})$
- **Action A_t**: the current treatment $U_t \in \{-1, 1\}$
- **Reward R_t**: a deterministic function of state-action pair, $-\sum_{k=1}^{q} c_k(U_t U_{t-k})$

Easy to verify:

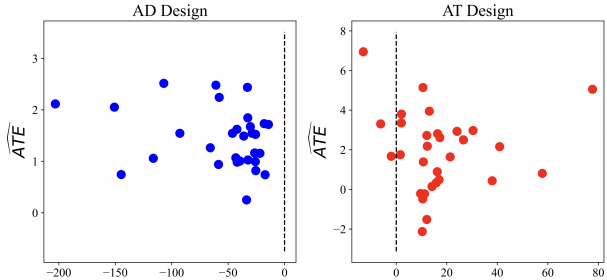
1. The minimization objective equals the negative average reward $\rightarrow$ equivalent to **maximizing the average reward**
2. The process is an **MDP** $\rightarrow$ there exists an optimal stationary policy maximizes the average reward $\rightarrow$ optimal design is q-**dependent**, i.e., U_t is a deterministic function of $(U_{t-q}, U_{t-q+1}, \cdots, U_{t-1})$ & this function is stationary in t
3. **Uniformly randomly** assign the first q treatments $\rightarrow$ the resulting design maintains a zero mean and is indeed optimal

Design: An RL Approach (Cont'd)



Empirical Study: Synthetic Environments

- A 9×9 dispatch simulator
- Available at `https://github.com/callmespring/MDPOD`
- Two efficiency indicators

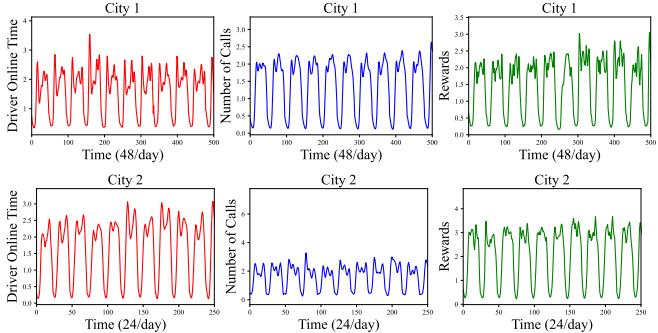


- ATE estimator's MSE under various designs

Design	AT	UR	Greedy	TMDP	NMDP	AD	Ours
MSE	8.33	2.23	1.10	0.56	0.42	**0.28**	**0.28**

Empirical Study: Real Datasets

- **Data**:



- We incorporate a **seasonal** term in our controlled VARMA model to account for seasonality. Below are MSEs of ATE estimators under different designs

City	$\mathbf{EI}_1$	$\mathbf{EI}_2$	AD	UR	AT	Ours
City 1	20.98	-21.11	11.98	11.63	9.72	**8.24**
City 2	-4.89	0.22	9.64	30.04	546.79	**8.38**

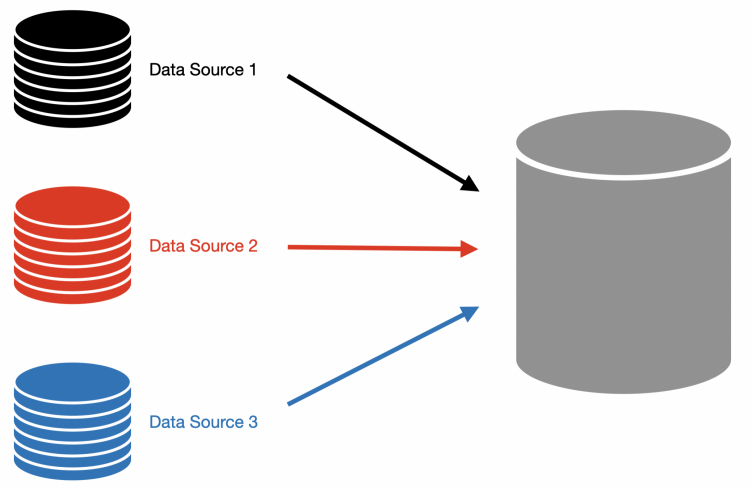
Project II

Combining Experimental and Historical Data for Policy Evaluation

— ICML (2024)

Joint work with Ting Li, Qianglin Wen, Yang Sui, Yongli Qin, Chunbo Lai & Hongtu Zhu

Data Integration



Example I: A/B Testing with Historical Data

Experiment data

Policy Control

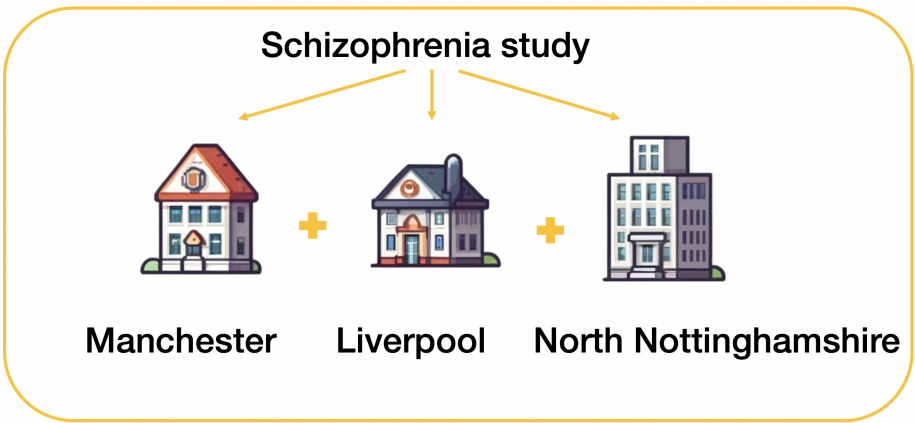
- limited duration
- weak treatment effect

Historical data

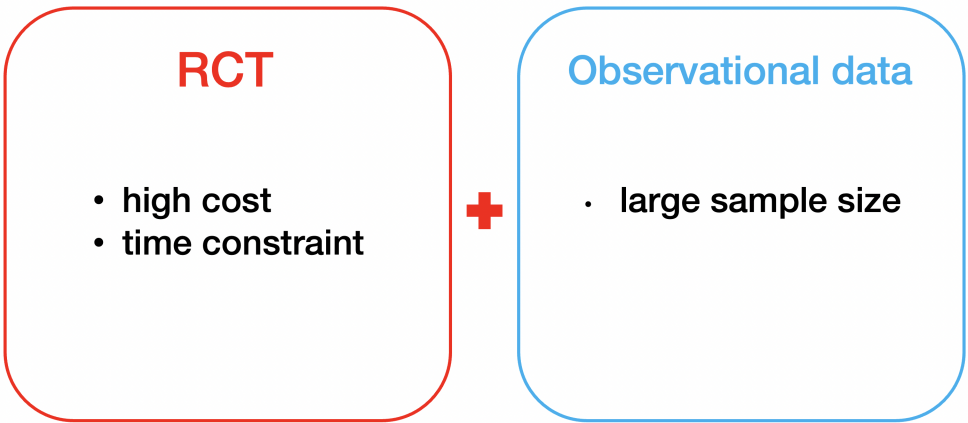
Control

- substantial volume

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

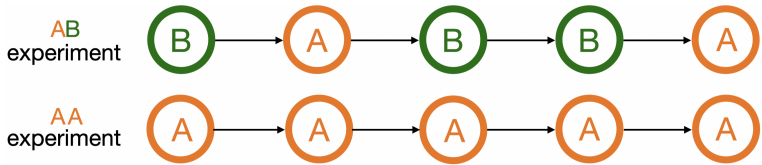


Example III: Combining Observational Data



A/B Testing with Historical Data

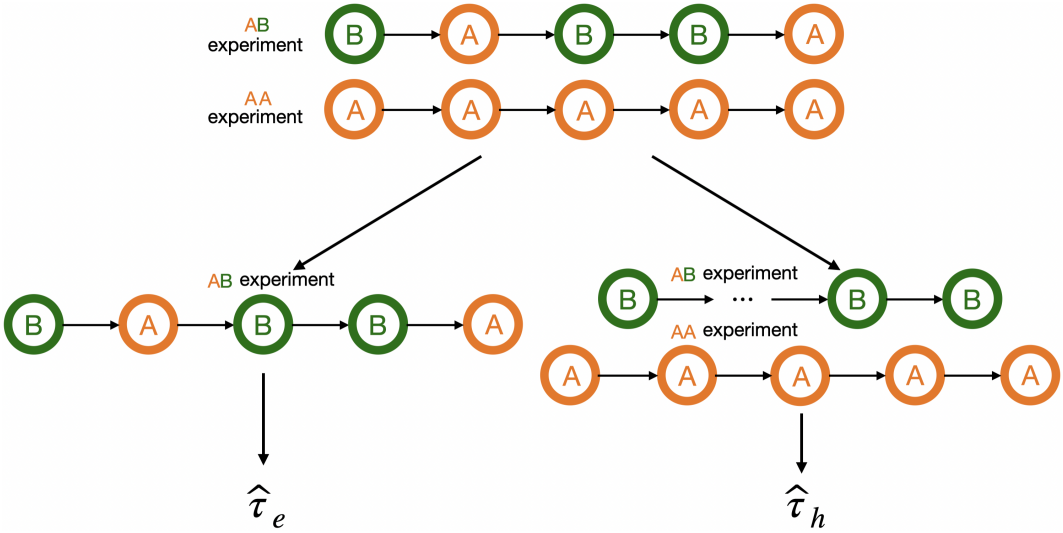
Objective: combine **experimental data** (***A***/***B***) with **historical data** (***A***/***A***) to improve ATE estimation



Challenge: **distributional shift** between experimental and historical data

- In **ridesharing**, the **nonstationary** of the environment → distributional shift [Wan et al., 2021]
- In **medicine**: the **heterogeneity** in characteristics of treatment setting → distributional shift [Shi et al., 2018]

Two Base Estimators



A Naive Weighted Estimator

- Consider the weighted estimator

$$\widehat{\boldsymbol{\tau}}_{\boldsymbol{w}} = \boldsymbol{w}\widehat{\boldsymbol{\tau}}_{\boldsymbol{e}} + (\mathbf{1} - \boldsymbol{w})\widehat{\boldsymbol{\tau}}_{\boldsymbol{h}},$$

  for some properly chosen weight $\boldsymbol{w} \in [0, 1]$ to minimize its $\mathrm{MSE}(\widehat{\boldsymbol{\tau}}_{\boldsymbol{w}})$.
- The weight $\boldsymbol{w}$ reflects a bias-variance tradeoff. A large $\boldsymbol{w}$ can:
  - Reduce **bias** of $\widehat{\boldsymbol{\tau}}_{\boldsymbol{w}}$ caused by the distributional shift between the datasets
  - Increase **variance** of $\widehat{\boldsymbol{\tau}}_{\boldsymbol{w}}$ as a result of not fully leveraging the historical data
- Natural to consider the following naive estimator that minimizes an estimated MSE:

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

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

Theoretical Analysis

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

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

Three competing estimators:

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

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 and the **efficiency bound** is the smallest achievable MSE among a broad class of regular estimators [Tsiatis, 2006].

Our Motivating Question

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

Our Proposal

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

- Each weight $\boldsymbol{w} \in [0, 1] \rightarrow$ an **arm** in bandit
- Negative MSE of $\widehat{\boldsymbol{\tau}}_{\boldsymbol{w}} \rightarrow$ **reward** of selecting an arm

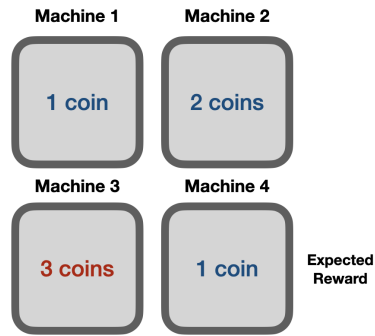
Objective in bandit: choose the **optimal** arm that maximizes its reward.

Multi-Armed Bandit Problem

- 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**

Offline Multi-Armed Bandit Problem

- k-armed bandit problem (k machines)
- $A_t \in \{1, \cdots, k\}$: 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**: Given $\{A_t, R_t\}_{0 \leq t < T}$, identify the best arm



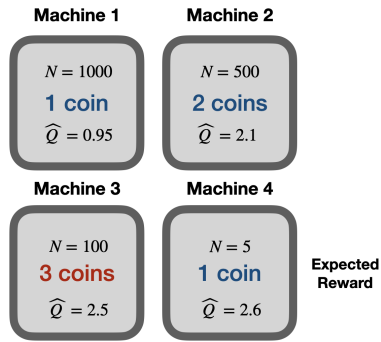
Greedy Action Selection (Non-pessimistic Estimator)

- **Action-value methods**:

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

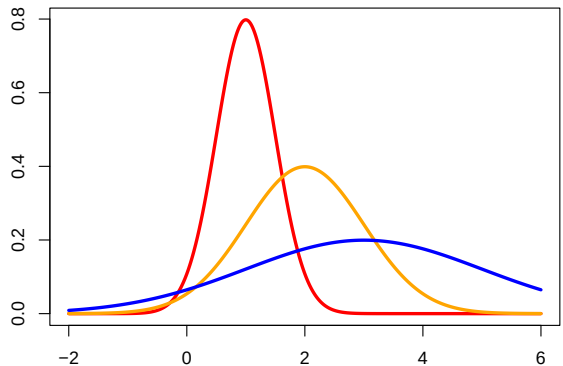
  where $N(a) = \sum_{t=0}^{T-1} \mathbb{I}(A_t = a)$ denotes the action counter

- **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 $N(a) \rightarrow$ small $L(a)$;
  - Small $N(a) \rightarrow$ large $L(a)$.
- Select actions maximizing lower confidence bound

$$a^* = \arg\max_a [\widehat{Q}(a) - L(a)].$$

Lower Confidence Bound (Cont'd)

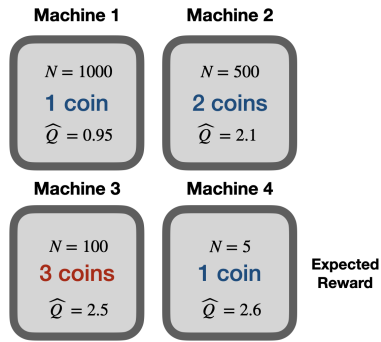
- Set $L(a) = \sqrt{c \log(T)/N(a)}$ for some positive constant c where T is the sample size of historical data
- According to **Hoeffding's inequality** (link), when rewards are bounded between 0 and 1, the event

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

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

Lower Confidence Bound (Cont'd)

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



Theory

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

- 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

Theory (Cont'd)

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

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

- 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

Back to Our Problem

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

- Each weight $\boldsymbol{w} \in [0, 1] \rightarrow$ an **arm** in bandit
- Negative MSE of $\widehat{\boldsymbol{\tau}}_{\boldsymbol{w}} \rightarrow$ **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 $\boldsymbol{b} \rightarrow$ low estimated MSE for small weights $\rightarrow$ estimated weight tends to be smaller than the ideal value $\rightarrow$ a significant bias in $\widehat{\boldsymbol{\tau}}_{\boldsymbol{w}}$
- This reveals the limitation of the nonpessimistic estimator when $\boldsymbol{b}$ is moderate or large.

Pessimistic Estimator

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 $\boldsymbol{U}$ for the estimated error such that $|\widehat{\boldsymbol{b}} - \boldsymbol{b}| \leq \boldsymbol{U}$ with large probability.
- **MSE estimation**: use $|\widehat{\boldsymbol{b}}| + \boldsymbol{U}$ 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 $\widehat{\mathrm{MSE}}_U(\widehat{\boldsymbol{\tau}}_{\boldsymbol{w}})$.
- **Weight selection**: select $\boldsymbol{w}$ that minimizes the upper bound $\widehat{\mathrm{MSE}}_U(\widehat{\boldsymbol{\tau}}_{\boldsymbol{w}})$.

Theoretical Analysis

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 and the **efficiency bound** is the smallest achievable MSE among a broad class of regular estimators [Tsiatis, 2006].

Simulation Study

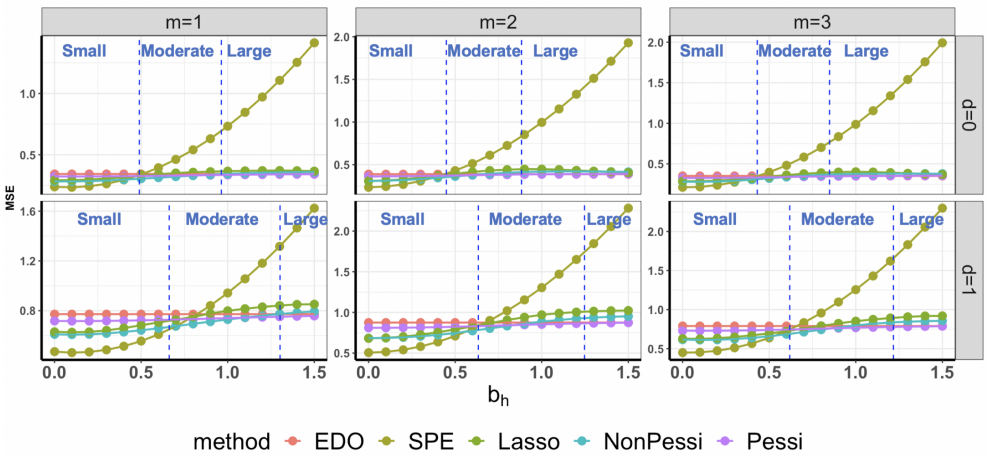
The effectiveness of different estimators is determined by the magnitude of the bias. To validate our theory, we further classify $\boldsymbol{b}$ into different regimes as follows

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

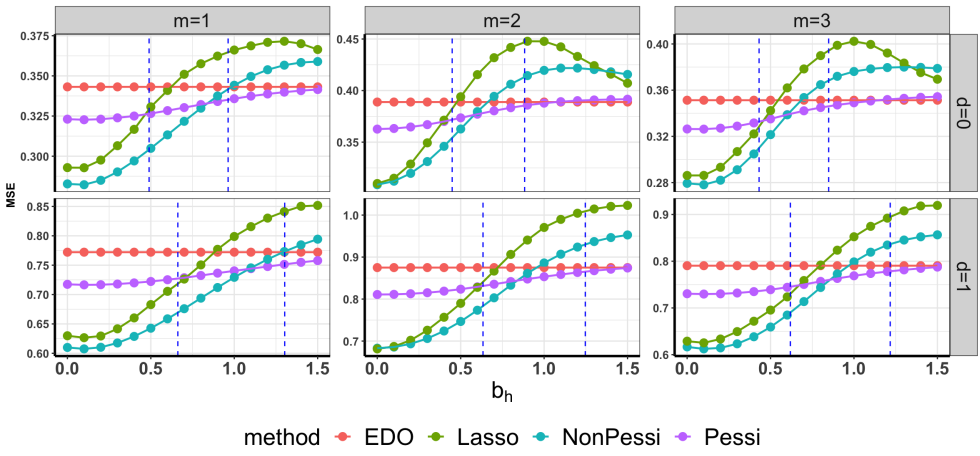
According to our theory, we set $c_1 = 1$ and $c_2 = \sqrt{\log(n)}$. This ensures:

- 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 (Cont'd)



Simulation Study (Cont'd)



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