Adaptive Experimental Design with Temporal Interference

Mohammad Rasouli — Peter Glynn — *Ramesh Johari*
Stanford University
rjohari@stanford.edu

3 June 2019

Motivation: Testing algorithms

Suppose you are one of these:

You have two algorithms A and B that you want to compare (e.g., matching algorithms).

Each algorithm changes the *state* of the system.

How do you design an experiment (A/B test) and an estimator to compare them?

Naive solution: Randomize over time

Suppose at each decision epoch, we randomly flip a coin and run either A (heads) or B (tails).

Why is this not a good idea?

Naive solution: Randomize over time

Suppose at each decision epoch, we randomly flip a coin and run either A (heads) or B (tails).

Why is this not a good idea?

Temporal interference: Each algorithm's action changes the *state* as seen by the other algorithm.

Therefore experimental units (time steps) *interfere* with each other, introducing *bias*.

Industry practice: Switchback designs

Many platforms (ridesharing, delivery marketplaces, etc.) use *switchback designs* to run A/B tests of algorithms:

1. Divide time into *fixed length non-overlapping intervals*.
2. In each successive interval, assign one of algorithm A or B.
3. Compute sample average estimate $\widehat{\text{SAE}}_A$ and $\widehat{\text{SAE}}_B$ of reward of A and B respectively.
4. Compute $\widehat{\text{SAE}}_A - \widehat{\text{SAE}}_B$ as *treatment effect estimate* $\widehat{\text{TE}}$.

Note: Doesn't eliminate temporal interference.

Overview of our contributions

We cast the problem of testing two algorithms as a theoretical problem of *testing two Markov chains*.

We focus on *consistent* estimation of TE.

- We develop a *Markov policy* for allocation, that together with a MLE for $\hat{TE}$, is *consistent* and *sample efficient*.
- We develop a *regenerative policy* for allocation that is *consistent* when used with the SAE for $\hat{TE}$ (but not sample efficient).

Related work

- *Mitigating network interference*

  Sobel (2006); Hudgens and Halloran (2008); Manski (2013); Ugander et al. (2013); Manski (2013); Eckles et al. (2017); Choi (2017); Baird et al. (2018); Athey et al. (2018); Basse et al. (2019)

- *Mitigating marketplace interference*

  Kohavi et al. (2009); Ostrovsky and Schwarz (2011); Bottou et al. (2013); Blake and Coey (2014); Basse et al. (2016); Wager and Xu (2019)

Related work (continued)

- *Estimation of a single Markov chain*

  Billingsley (1961); Kutoyants (2013)

- *Markov decision processes with minimum variance objectives*: Generally computationally intractable

  Sobel (1982, 1994); Di Castroet et al. (2012); Filar et al. (1989); Iancu et al. (2015); Mannor and Tsitsiklis (2011); Yu et al. (2018)

- *Pure exploration in reinforcement learning*: Focus on finding the best policy

  Brunskill et al. (2017); Putta and Tulabandhula (2017)

- *Offline policy evaluation in reinforcement learning*

  Precup et al. (2000), Dudik et al. (2015), Theocharous et al. (2015), Thomas and Brunskill (2016), etc.

Preliminaries

Nonparametric model

- Discrete time $n = 0, 1, 2, \ldots$
- Finite state space S (x, y denote states)

Nonparametric model

- Discrete time $n = 0, 1, 2, \ldots$
- Finite state space S (x, y denote states)
- Two algorithms (actions) 1 and 2 (ℓ denotes algorithm)
- Unknown irreducible transition matrices $\boldsymbol{P}(\ell) = (P(\ell, x, y), x, y \in S)$
- Invariant distributions $\boldsymbol{\pi}(\ell) = (\pi(\ell, x), x \in S)$ (row vector)

Nonparametric model

- Discrete time $n = 0, 1, 2, \ldots$
- Finite state space S (x, y denote states)
- Two algorithms (actions) 1 and 2 (ℓ denotes algorithm)
- Unknown irreducible transition matrices $\boldsymbol{P}(\ell) = (P(\ell, x, y), x, y \in S)$
- Invariant distributions $\boldsymbol{\pi}(\ell) = (\pi(\ell, x), x \in S)$ (row vector)
- Unknown reward distribution $R \sim f(\cdot|\ell, x, y)$ (finite mean and variance)
- $r(\ell, x) = \mathbb{E}[R|\ell, x]$; $\boldsymbol{r}(\ell) = (r(\ell, x), x \in S)$ (column vector)

Nonparametric model

- Discrete time $n = 0, 1, 2, \ldots$
- Finite state space S (x, y denote states)
- Two algorithms (actions) 1 and 2 (ℓ denotes algorithm)
- Unknown irreducible transition matrices $\boldsymbol{P}(\ell) = (P(\ell, x, y), x, y \in S)$
- Invariant distributions $\boldsymbol{\pi}(\ell) = (\pi(\ell, x), x \in S)$ (row vector)
- Unknown reward distribution $R \sim f(\cdot|\ell, x, y)$ (finite mean and variance)
- $r(\ell, x) = \mathbb{E}[R|\ell, x]$; $\boldsymbol{r}(\ell) = (r(\ell, x), x \in S)$ (column vector)

At time n: State X_n, action A_n, reward R_n

The estimation problem

Treatment effect of interest is the *steady state reward difference*:

$$\begin{aligned}\alpha = \alpha(2) - \alpha(1) &= \sum_x \pi(2,x) r(2,x) - \sum_x \pi(1,x) r(1,x) \\ &= \boldsymbol{\pi}(2)\boldsymbol{r}(2) - \boldsymbol{\pi}(1)\boldsymbol{r}(1).\end{aligned}$$

The estimation problem

Treatment effect of interest is the *steady state reward difference*:

$$\alpha = \alpha(2) - \alpha(1) = \sum_x \pi(2,x)r(2,x) - \sum_x \pi(1,x)r(1,x)$$
$$= \boldsymbol{\pi}(2)\boldsymbol{r}(2) - \boldsymbol{\pi}(1)\boldsymbol{r}(1).$$

We get to choose an estimator and a policy:

- Estimator: $\alpha = (\alpha_n : n \geq 0)$, $\alpha_n \in \mathbb{R}$
- Policy: $A = (A_n : n \geq 0)$, $A_n \in \{1, 2\}$

Estimator and policy are adapted to history, and policy can be randomized.

Maximum likelihood estimation

The maximum likelihood estimator

Definitions:

$$\Gamma_n(\ell, x) := \#\text{ of plays of } \ell \text{ in first } n \text{ steps} = \sum_{j=0}^{n-1} I(X_j = x, A_j = \ell)$$

$$r_n(\ell, x) := \text{SAE of } r(\ell, x) = \frac{\sum_{j=0}^{n-1} I(X_j = x, A_j = \ell) R_{j+1}}{\max\{\Gamma_n(\ell, x), 1\}}$$

$$P_n(\ell, x, y) := \text{SAE of } P(\ell, x, y) = \frac{\sum_{j=0}^{n-1} I(X_j = x, A_j = \ell, X_{j+1} = y)}{\max\{\Gamma_n(\ell, x), 1\}}$$

Let $\boldsymbol{\pi}_n(\ell)$ be invariant distribution of $\boldsymbol{P}_n(\ell)$ (exists a.s. as $n \to \infty$). Then:

$$\alpha_n^{\text{MLE}} = \boldsymbol{\pi}_n(2)\boldsymbol{r}_n(2) - \boldsymbol{\pi}_n(1)\boldsymbol{r}_n(1).$$

Time-average regular policies

We optimize over time-average regular policies.

Definition

Policy A is *time-average regular* if

$$\frac{1}{n}\Gamma_n(\ell, x) \xrightarrow{p} \gamma(\ell, x)$$

as $n \to \infty$ for each $x \in S, \ell = 1, 2$, and (possibly random) $\gamma(\ell, x)$.

We call $\gamma = (\gamma(\ell, x) : x \in S, \ell = 1, 2)$ the *policy limit*.

(For our theory we will require $\gamma(\ell, x) > 0$ a.s.)

Central limit theorem for MLE

Theorem

For any time-average regular policy A with strictly positive policy limits:

$$n^{1/2}(\alpha_n^{MLE} - \alpha) \Rightarrow \sum_x \frac{\pi(2,x)\sigma(2,x)}{\gamma(2,x)^{1/2}} G(2,x) - \sum_x \frac{\pi(1,x)\sigma(1,x)}{\gamma(1,x)^{1/2}} G(1,x).$$

where:

- $G(\ell, x)$ are i.i.d. $N(0,1)$;
- $\sigma^2(\ell, x) = \mathrm{Var}\left(R_j + \tilde{g}(\ell, X_j) \mid X_{j-1} = x, A_{j-1} = \ell\right)$ (assume positive);
- $\tilde{\boldsymbol{g}}(\ell)$ solves the following *Poisson equation*:

$$\tilde{\boldsymbol{g}}(\ell) = (\boldsymbol{I} - \boldsymbol{P}(\ell) + \boldsymbol{\Pi}(\ell))^{-1} \boldsymbol{r}(\ell)$$

- $\boldsymbol{\Pi}(\ell)$ is the matrix where each row is $\boldsymbol{\pi}(\ell)$.

Central limit theorem for MLE: Single chain

Key idea:

$$\begin{aligned}\alpha_n(\ell) - \alpha(\ell) &= \sum_x \pi_n(\ell, x) r_n(\ell, x) - \sum_x \pi(\ell, x) r(\ell, x) \\ &= \boldsymbol{\pi}_n(\ell)\big(\boldsymbol{r}_n(\ell) - \boldsymbol{r}(\ell)\big) + \big(\boldsymbol{\pi}_n(\ell) - \boldsymbol{\pi}(\ell)\big)\boldsymbol{r}(\ell) \\ &= \boldsymbol{\pi}_n(\ell)\big(\boldsymbol{r}_n(\ell) - \boldsymbol{r}(\ell)\big) + \boldsymbol{\pi}_n(\ell)\big(\boldsymbol{P}_n(\ell) - \boldsymbol{P}(\ell)\big)\tilde{\boldsymbol{g}}(\ell)\end{aligned}$$

We combine the preceding idea with martingale arguments to handle adaptive sampling.

Optimal oracle policy for MLE

Let $\mathcal{K}$ be the (convex, compact) set of all $\big(\kappa(\ell, x) : x \in S, \ell = 1, 2\big)$ such that:

$$\begin{aligned}
\kappa(1, y) + \kappa(2, y) &= \sum_{\ell} \sum_{x} \kappa(\ell, x) P(\ell, x, y), \quad y \in S; \\
\sum_{\ell} \sum_{x} \kappa(\ell, x) &= 1; \\
\kappa(\ell, x) &\geq 0.
\end{aligned}$$

Lemma: The law of any time-average regular policy limit γ is a probability measure over $\mathcal{K}$.

Optimal oracle policy for MLE

Let κ^* be the solution to the following convex optimization problem:

$$\begin{aligned} \text{minimize} \quad & \sum_{\ell} \sum_{x} \frac{\pi^2(\ell, x)\sigma^2(\ell, x)}{\kappa(\ell, x)} \\ \text{subject to} \quad & \kappa \in \mathcal{K}. \end{aligned}$$

Then κ^* can be realized as the policy limit of the following *stationary, Markov* policy:

Run algorithm ℓ in state x with probability:

$$p^*(\ell, x) = \frac{\kappa^*(\ell, x)}{\kappa^*(1, x) + \kappa^*(2, x)}.$$

Optimal oracle policy for MLE

Theorem

The policy p^* minimizes the asymptotic variance of $n^{1/2}(\alpha_n^{\mathit{MLE}} - \alpha)$ over time-average regular policies.

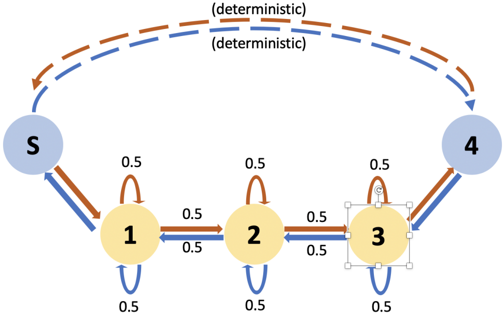
Proof idea: Use Jensen's inequality on asymptotic variance of $n^{1/2}\big(\alpha_n^{\mathsf{MLE}} - \alpha\big)$:

$$\mathbb{E}\Big[\sum_{\ell}\sum_{x}\frac{\pi^2(\ell,x)\sigma^2(\ell,x)}{\gamma(\ell,x)}\Big]$$

The value of cooperative exploration

Cooperative exploration: Two chains can yield much more efficient estimation than either chain alone.

Example: Deterministic reward $r = 1$ in states $1, 2, 3$, and zero reward elsewhere. Estimating red or blue chain alone has asymptotic variance $\Theta(S)$ higher than using both together!



Optimal online policy for MLE

Without knowledge of the primitives, we can compute $\kappa_n(\ell, x)$ as the optimal solution given $\boldsymbol{P}_n(\ell)$, and set:

$$p_n(\ell, x) = (1 - \epsilon_n)\left(\frac{\kappa_n(\ell, x)}{\kappa_n(1, x) + \kappa_n(2, x)}\right) + \frac{1}{2}\epsilon_n,$$

with $\epsilon_n = n^{-1/2}$ (forced exploration).

This yields the asymptotically optimal policy limits in an online fashion.

Sample average estimation

Sample average estimation

Given a policy A, the sample average estimator is:

$$\alpha_n^{\mathsf{SAE}} = \frac{\sum_{j=0}^{n-1} I(A_j = 2) R_{j+1}}{\sum_{j=0}^{n-1} I(A_j = 2)} - \frac{\sum_{j=0}^{n-1} I(A_j = 1) R_{j+1}}{\sum_{j=0}^{n-1} I(A_j = 1)}$$

This estimator is computationally much less intensive.

However, it suffers from *temporal interference* every time the policy switches chains.

Regenerative policies

Fix a state x^r (the *regeneration* state).

Only change chains at visits to x^r; at each visit, choose ℓ with probability $p(\ell)$.

Regenerative policies

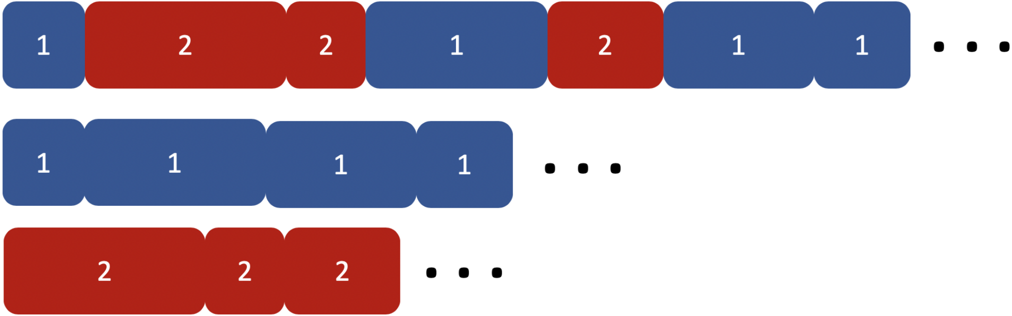
Fix a state x^r (the *regeneration* state).

Only change chains at visits to x^r; at each visit, choose ℓ with probability $p(\ell)$.

Regenerative policies

Fix a state x^r (the *regeneration* state).

Only change chains at visits to x^r; at each visit, choose ℓ with probability $p(\ell)$.



Consistency and central limit theorem

SAE of regenerative policy is *consistent*
(no temporal interference asymptotically by design).

Can show: There exists $q(\ell)$ (depending on x^r and p) such that $q(1) + q(2) = 1$ and $\gamma(\ell, x) = q(\ell)\pi(\ell, x)$ for all ℓ, x.

$q(\ell)$ gives the fraction of time spent with chain ℓ.
(Can choose any q we want by varying p.)

Since *as if* we have two parallel runs of each chain,
convergence is at rate $n^{1/2}$ and CLT holds.

Optimal oracle regenerative policy

Easy to show that optimal oracle regenerative policy has:

$$q^*(\ell) = \frac{\overline{\sigma}(\ell)}{\overline{\sigma}(1) + \overline{\sigma}(2)},$$

where $\overline{\sigma}^2(\ell) = \sum_x \pi(\ell, x)\sigma^2(\ell, x)$.

Scaled asymptotic variance of this policy is $(\overline{\sigma}(1) + \overline{\sigma}(2))^2$ (achievable with *any* choice of x^r).

Can similarly construct an asymptotically equivalent online algorithm.

Optimal oracle regenerative policy

Easy to show that optimal oracle regenerative policy has:

$$q^*(\ell) = \frac{\overline{\sigma}(\ell)}{\overline{\sigma}(1) + \overline{\sigma}(2)},$$

where $\overline{\sigma}^2(\ell) = \sum_x \pi(\ell, x)\sigma^2(\ell, x)$.

Scaled asymptotic variance of this policy is $(\overline{\sigma}(1) + \overline{\sigma}(2))^2$ (achievable with *any* choice of x^r).

Can similarly construct an asymptotically equivalent online algorithm.

Unboundedly *suboptimal* in general relative to MLE with Markov optimal policy: There we had $|S|$ degrees of freedom vs. only one degree of freedom here.

Concluding thoughts

Summary and looking ahead

We proposed a benchmark model with which to evaluate sampling efficiency of consistent estimator-design pairs for switchback experimentation.

There are several considerations we have not addressed:

- Finite horizon analysis
- Multiple treatments
- Nonstationarity
- Heterogeneous treatment effects