# Minimax Off-Policy Evaluation for Multi-Armed Bandits





FODSI seminar, April 9th, 2021



#### Banghua Zhu EECS



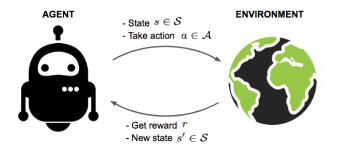
Jiantao Jiao EECS & Stat



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# Reinforcement learning (RL)



#### Goal: learn an optimal policy to maximize rewards









### on-policy evaluation

deploy policy in environment





#### on-policy evaluation

deploy policy in environment

- costly, dangerous, unethical





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### off-policy evaluation (OPE)

#### leverage historical data





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- distribution shift!

### Off-policy evaluation for multi-armed bandits

- how to optimally tackle distribution shift

# Off-policy evaluation for multi-armed bandits

- how to optimally tackle distribution shift

"Bridging Offline Reinforcement Learning and Imitation Learning: A Tale of Pessimism"

- with P. Rashidinejad, B. Zhu, J. Jiao, and S. Russell



### Background: multi-armed bandits and OPE

### **Multi-armed bandits**



- Action space:  $\mathcal{A} = [k] \coloneqq \{1, 2, \dots, k\}$
- Reward distributions:  $f \coloneqq \{f(\cdot \mid a)\}_{a \in \mathcal{A}}$

 $\mathcal{F}(r_{\max}) \coloneqq \{f \mid \operatorname{supp}(f(\,\cdot \mid a)) \subseteq [0, r_{\max}] \text{ for each } a \in [k]\}$ 

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- Policy  $\pi$ : a distribution over [k]
- Value function of a policy:  $V_f(\pi) \coloneqq \sum_{a \in [k]} \pi(a) r_f(a)$

—  $r_f(a)$ : mean reward of  $f(\cdot \mid a)$ 

Given

- observed data:  $\{(A_i, R_i)\}_{i=1}^n \stackrel{\text{i.i.d.}}{\sim} \pi_{\mathbf{b}} \otimes f$
- target policy  $\pi_t$

Goal: estimate value function of target policy

$$V_f(\pi_{\mathsf{t}}) = \sum_{a \in [k]} \pi_{\mathsf{t}}(a) r_f(a)$$

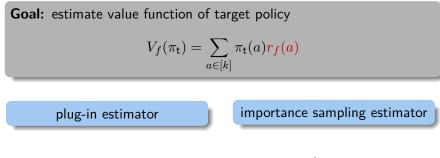
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$$V_f(\pi_{\mathsf{t}}) = \sum_{a \in [k]} \pi_{\mathsf{t}}(a) r_f(a)$$

plug-in estimator

$$\widehat{V}_{\mathsf{plug}} \coloneqq \sum_{a \in [k]} \pi_{\mathsf{t}}(a) \widehat{r}(a)$$

 $\widehat{r}(a) \coloneqq \mathsf{empirical} \ \mathsf{mean} \ \mathsf{reward}$ 



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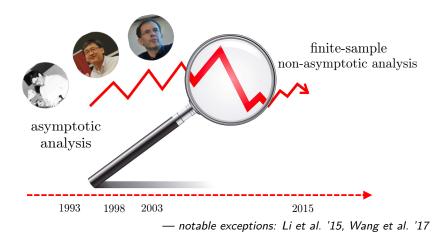
 $\widehat{V}_{\mathsf{IS}} \coloneqq \frac{1}{n} \sum_{i \in [n]} \rho(A_i) R_i$ 

$$\rho(a) \coloneqq \frac{\pi_{\mathsf{t}}(a)}{\pi_{\mathsf{b}}(a)}$$

### Gaps in statistical understanding of OPE

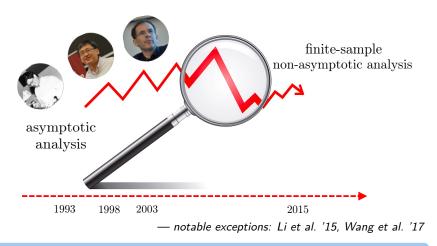
— a few motivating questions

### Non-asymptotic analysis of OPE



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### Non-asymptotic analysis of OPE



Can we develop procedures that are optimal for all sample sizes?

# Known vs. unknown behavior policies

Known behavior policy



Unknown behavior policy

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Known behavior policy



Unknown behavior policy

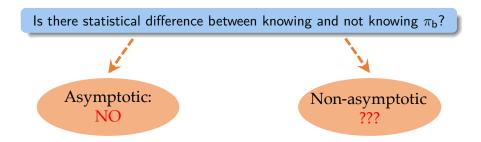
#### Is there statistical difference between knowing and not knowing $\pi_b$ ?

# Known vs. unknown behavior policies

Known behavior policy



### Unknown behavior policy







What if we have partial knowledge of behavior policy,



What if we have partial knowledge of behavior policy, say

• we know how close behavior policy is to target policy

$$\max_{a} \pi_{\mathsf{t}}(a) / \pi_{\mathsf{b}}(a) \le U$$



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• or how well behavior policy explores action space

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• or how well behavior policy explores action space

 $\min_{a} \pi_{\mathsf{b}}(a) \geq \nu$ 

Can we fully utilize such partial knowledge in OPE?

OPE with known behavior policy

# Plug-in and importance sampling estimators

Goal: estimate value function of target policy

$$V_f(\pi_t) = \sum_{a \in [k]} \pi_t(a) r_f(a)$$

plug-in estimator

importance sampling estimator

$$\widehat{V}_{\mathsf{plug}} \coloneqq \sum_{a \in [k]} \pi_{\mathsf{t}}(a) \widehat{r}(a)$$

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$$\rho(a) \coloneqq \frac{\pi_{\mathsf{t}}(a)}{\pi_{\mathsf{b}}(a)}$$

### Switch estimators

- inspired by Wang et al. '17

**Switch estimators:** for any subset  $S \subseteq [k]$ , we define

$$\widehat{V}_{\mathsf{switch}}(S) \coloneqq \sum_{a \in S} \pi_{\mathsf{t}}(a)\widehat{r}(a) + \frac{1}{n}\sum_{i=1}^{n} \rho(A_i)R_i\mathbb{1}\{A_i \notin S\}$$

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- when S = [k], recover plug-in estimator
- when  $S = \emptyset$ , recover importance sampling (IS) estimator
- $\bullet\,$  Intermediate choices of S lead to interpolation between plug-in and IS estimators

For any subset  $S \subseteq [k]$ , we have

$$\mathbb{E}_{\pi_{\mathsf{b}}\otimes f}[(\widehat{V}_{\mathsf{switch}}(S) - V_{f}(\pi_{\mathsf{t}}))^{2}] \leq 3r_{\max}^{2} \left\{ \pi_{\mathsf{t}}^{2}(S) + \frac{\sum_{a \notin S} \pi_{\mathsf{b}}(a)\rho^{2}(a)}{n} \right\}$$

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— How to choose subset S?

A simple idea:

$$\min_{S \subseteq [k]} \left\{ \pi_{\mathsf{t}}^2(S) + \frac{\sum_{a \notin S} \pi_{\mathsf{b}}(a) \rho^2(a)}{n} \right\}$$

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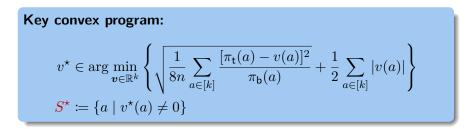
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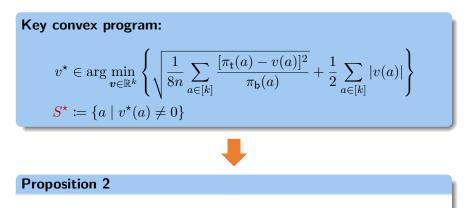
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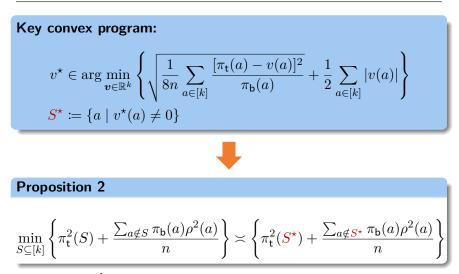
$$\min_{S \subseteq [k]} \left\{ \pi_{\mathsf{t}}^2(S) + \frac{\sum_{a \notin S} \pi_{\mathsf{b}}(a) \rho^2(a)}{n} \right\}$$

- combinatorial optimization problem!





$$\min_{S\subseteq[k]} \left\{ \pi_{\mathsf{t}}^2(S) + \frac{\sum_{a\notin S} \pi_{\mathsf{b}}(a)\rho^2(a)}{n} \right\} \asymp \left\{ \pi_{\mathsf{t}}^2(S^{\star}) + \frac{\sum_{a\notin S^{\star}} \pi_{\mathsf{b}}(a)\rho^2(a)}{n} \right\}$$



—  $\widehat{V}_{\rm switch}(S^{\star})$  is optimal among family of Switch estimators

# Is Switch estimator universally optimal?

Minimax risk of OPE:

$$\mathcal{R}_n^{\star}(\pi_{\mathsf{t}}; \pi_{\mathsf{b}}) \coloneqq \inf_{\widehat{V}} \sup_{f \in \mathcal{F}} \mathbb{E}_{\pi_{\mathsf{b}} \otimes f}[(\widehat{V} - V_f(\pi_{\mathsf{t}}))^2]$$

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### Theorem 1

For all pairs  $(\pi_{\rm b},\pi_{\rm t})$  and for all n, we have

$$\mathcal{R}_n^{\star}(\pi_{\mathsf{t}};\pi_{\mathsf{b}}) \gtrsim r_{\max}^2 \left\{ \pi_{\mathsf{t}}^2(\boldsymbol{S}^{\star}) + \frac{\sum_{a \notin \boldsymbol{S}^{\star}} \pi_{\mathsf{b}}(a)\rho^2(a)}{n} \right\}$$

- Switch estimator is minimax optimal for all sample sizes

• Degenerate case of on-policy evaluation, i.e.,  $\pi_t = \pi_b$ We know IS estimator (a.k.a. Monte Carlo estimator) is optimal

$$\widehat{V}_{\rm IS} = \frac{1}{n} \sum_{i=1}^{n} \rho(A_i) R_i = \frac{1}{n} \sum_{i=1}^{n} R_i$$

with optimal rate  $r_{
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It can be shown from our minimax theorem that  $S^{\star} = \emptyset$  in this case

• Large-sample regime: in general when  $\pi_{\rm t}\neq\pi_{\rm b},$  one can show that when

$$n \gg \frac{\max_{a \in [k]} \rho^2(a)}{\sum_{a \in [k]} \pi_{\mathsf{b}}(a) \rho^2(a)},$$

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- \* recover large-sample result in Li et al. '15 (bounded reward setting)
- \* our results accommodate any sample size, especially small sample size where IS could perform poorly

## Numerics

Setup:  $\pi_{t}(a) = 1/k$ ,  $f(\cdot \mid a) = \text{Bern}(0.5)$  for all  $a \in [k]$ , n = 1.5k  $\pi_{b}(1) = \pi_{b}(2) = \dots = \pi_{b}(\sqrt{k}) = \frac{1}{k^{2}}$ ,  $\pi_{b}(\sqrt{k}+1) = \pi_{b}(\sqrt{k}+2) = \dots = \pi_{b}(k) = \frac{1-\frac{1}{k^{3/2}}}{k-\sqrt{k}}$ 

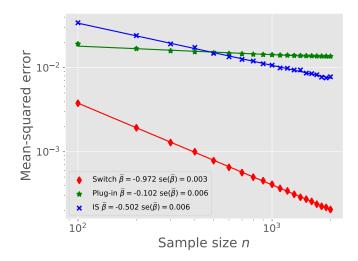
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### Theoretical predictions:

$$\begin{split} \mathbb{E}_{\pi_{\mathsf{b}}\otimes f}[(\widehat{V}_{\mathsf{plug}} - V_{f}(\pi_{\mathsf{t}}))^{2}] &\asymp 1, \\ \mathbb{E}_{\pi_{\mathsf{b}}\otimes f}[(\widehat{V}_{\mathsf{IS}} - V_{f}(\pi_{\mathsf{t}}))^{2}] &\asymp n^{-1/2}, \quad \text{and} \\ \mathbb{E}_{\pi_{\mathsf{b}}\otimes f}[(\widehat{V}_{\mathsf{switch}}(S^{\star}) - V_{f}(\pi_{\mathsf{t}}))^{2}] &\asymp n^{-1} \end{split}$$

# Numerics (cont.)



Switch estimator:  

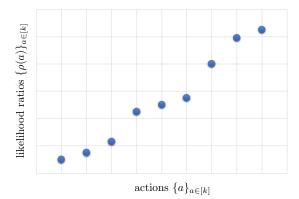
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### Key convex program:

$$v^{\star} \in \arg\min_{v \in \mathbb{R}^{k}} \left\{ \sqrt{\frac{1}{8n} \sum_{a \in [k]} \frac{[\pi_{t}(a) - v(a)]^{2}}{\pi_{b}(a)}} + \frac{1}{2} \sum_{a \in [k]} |v(a)| \right\}$$
$$S^{\star} \coloneqq \{a \mid v^{\star}(a) \neq 0\}$$

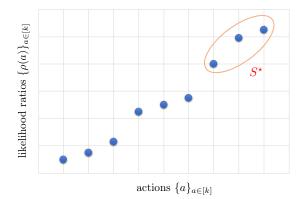
## A closer look at Switch estimator

### Without loss of generality, we assume



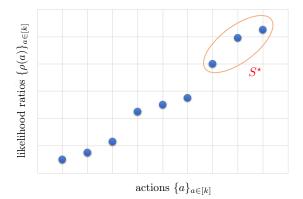
## A closer look at Switch estimator

 $S^{\star}$ —if nonempty—must contain actions with largest likelihood ratios



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Key message: Switch optimally truncates large likelihood ratios

variance reduction
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OPE with unknown behavior policy

# What's the right performance metric?

• First attempt: global worst-case risk of  $\widehat{V}$ 

$$\sup_{\pi_{\mathbf{b}}} \sup_{f \in \mathcal{F}} \mathbb{E}_{\pi_{\mathbf{b}} \otimes f}[(\widehat{V} - V_{f}(\pi_{\mathbf{t}}))^{2}]$$

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• Failure of attempt:

$$\inf_{\widehat{V}} \sup_{\pi_{\mathsf{b}}} \sup_{f \in \mathcal{F}} \mathbb{E}_{\pi_{\mathsf{b}} \otimes f}[(\widehat{V} - V_f(\pi_{\mathsf{t}}))^2] \asymp r_{\max}^2$$

in addition,  $\widehat{V}\equiv 0$  is minimax optimal...

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in addition,  $\widehat{V}\equiv 0$  is minimax optimal...

• Rationale for failure: adversary can choose bad behavior policy without paying price



## **Competitive ratio**

- inspired by online learning literature

Worst-case competitive ratio of  $\hat{V}$ :

$$\mathcal{C}(\widehat{V}; \pi_{\mathsf{t}}) \coloneqq \sup_{\pi_{\mathsf{b}}, f \in \mathcal{F}} \frac{\mathbb{E}_{\pi_{\mathsf{b}} \otimes f}[(\widehat{V} - V_{f}(\pi_{\mathsf{t}}))^{2}]}{\mathcal{R}_{n}^{\star}(\pi_{\mathsf{t}}; \pi_{\mathsf{b}})}$$

$$- \mathcal{R}_n^{\star}(\pi_{\mathsf{t}}; \pi_{\mathsf{b}}) = \inf_{\widehat{V}} \sup_{f \in \mathcal{F}} \mathbb{E}_{\pi_{\mathsf{b}} \otimes f}[(\widehat{V} - V_f(\pi_{\mathsf{t}}))^2]$$

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• Proof of concept: when  $\widehat{V}\equiv 0,$  we have

$$\mathcal{C}(\widehat{V}; \pi_{\mathsf{t}}) \geq \frac{\mathbb{E}_{\pi_{\mathsf{t}} \otimes f}[(\widehat{V} - V_{f}(\pi_{\mathsf{t}}))^{2}]}{\mathcal{R}_{n}^{\star}(\pi_{\mathsf{t}}; \pi_{\mathsf{t}})} \asymp \frac{(V_{f}(\pi))^{2}}{r_{\max}^{2}/n} \asymp n$$

## Competitive ratio of plug-in estimator

### Theorem 2

For any target policy  $\pi_t$ , plug-in estimator  $\hat{V}_{plug}$  satisfies

$$\sup_{\pi_{\mathsf{b}}, f \in \mathcal{F}} \frac{\mathbb{E}_{\pi_{\mathsf{b}} \otimes f}[(\widehat{V}_{\mathsf{plug}} - V_f(\pi_{\mathsf{t}}))^2]}{\mathcal{R}_n^{\star}(\pi_{\mathsf{t}}; \pi_{\mathsf{b}})} \lesssim |\operatorname{supp}(\pi_{\mathsf{t}})|$$

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Worst-case competitive ratio is at most k (since |supp(πt)| ≤ k)
 ⇒ plug-in estimator is strictly better than all-zeros estimator

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- Worst-case competitive ratio is at most k (since |supp(πt)| ≤ k)
   ⇒ plug-in estimator is strictly better than all-zeros estimator
- Adaptivity of plug-in estimator to target policy

Suppose that sample size obeys  $n \gg \frac{k}{\log k}$ . Then for each  $s \in \{1, 2, \ldots, k\}$ , there exists a target policy  $\pi_t$  supported on s actions and

$$\inf_{\widehat{V}} \sup_{\pi_{\mathsf{b}}, f \in \mathcal{F}} \frac{\mathbb{E}_{\pi_{\mathsf{b}} \otimes f}[(\widehat{V} - V_{f}(\pi_{\mathsf{t}}))^{2}]}{\mathcal{R}_{n}^{\star}(\pi_{\mathsf{t}}; \pi_{\mathsf{b}})} \gtrsim \max\left\{\frac{s}{\log k}, 1\right\}$$

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- Performance difference between knowing and not knowing behavior policy scales as  $|\operatorname{supp}(\pi_t)|$

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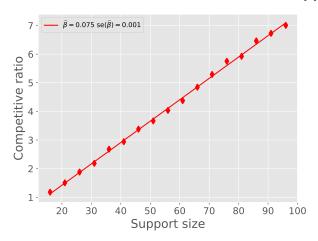
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- Performance difference between knowing and not knowing behavior policy scales as  $|\operatorname{supp}(\pi_t)|$

— in contrast to asymptotics

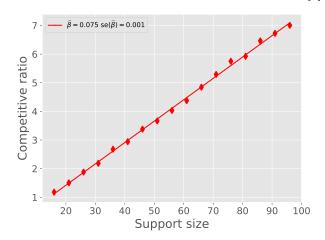
### Numerics

**Setup:** k = 100, n = 2k, fix  $\pi_b$  and vary  $\pi_t$  uniform over [s]



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Knowing behavior policy helps in non-asymptotics!

## OPE with partial knowledge of behavior policy

# OPE with partial knowledge of behavior policy



What if we have partial knowledge of behavior policy?

Our focus: minimum exploration probability

$$\pi_{\mathsf{b}} \in \Pi(\boldsymbol{\nu}) \coloneqq \{\pi \mid \min_{a \in [k]} \pi(a) \ge \boldsymbol{\nu}\}$$

 $-\nu \in [0,1/k]$ 

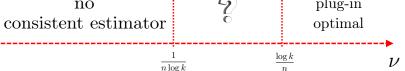
## **Optimal estimators**

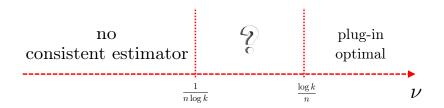
Goal: develop estimators that can achieve

$$\inf_{\widehat{V}} \sup_{(\pi_{\mathbf{b}}, f) \in \Pi(\nu) \times \mathcal{F}} \mathbb{E}_{\pi_{\mathbf{b}} \otimes f}[(\widehat{V} - V_{f}(\pi_{\mathbf{t}}))^{2}]$$

## **Optimal estimators**

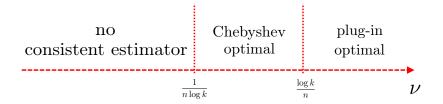
**Goal:** develop estimators that can achieve  $\inf_{\widehat{V}} \sup_{(\pi_{b},f)\in\Pi(\nu)\times\mathcal{F}} \mathbb{E}_{\pi_{b}\otimes f}[(\widehat{V}-V_{f}(\pi_{t}))^{2}]$ no
plug-in





• Why plug-in fails when  $\pi_{b}$  is less exploratory?

- large bias due to insufficient observations



• Why plug-in fails when  $\pi_b$  is less exploratory?

- large bias due to insufficient observations

• How to reduce bias?

draw connection to support size estimation (cf. Wu and Yang '16)
 best polynomial approximation

plug-in estimator

Chebyshev estimator

$$\widehat{V}_{\mathsf{plug}} \coloneqq \sum_{a \in [k]} \pi_{\mathsf{t}}(a) \widehat{r}(a)$$

$$\widehat{V}_{\mathsf{C}} \coloneqq \sum_{a \in [k]} \pi_{\mathsf{t}}(a) \widehat{r}(a) g_L(n(a))$$

 $\widehat{r}(a) \coloneqq \mathsf{empirical} \ \mathsf{mean} \ \mathsf{reward}$ 

 $g_L(n(a)) \coloneqq \mathsf{Chebyshev} \ \mathsf{poly}$ 

- Known  $\pi_b$ : Switch is minimax optimal for all sample sizes
- Unknown  $\pi_b$ : fundamentally different, plug-in is near-optimal
- Partial knowledge: improvement is possible, bias reduction is needed

# **Concluding remarks**

- Known  $\pi_b$ : Switch is minimax optimal for all sample sizes
- Unknown  $\pi_{\rm b}$ : fundamentally different, plug-in is near-optimal
- Partial knowledge: improvement is possible, bias reduction is needed

• Extension to other reward families



- Smooth characterization of gap between knowing and not knowing  $\pi_{\rm b}$
- Adaptivity to  $\min_a \pi_{\mathsf{b}}(a)$

#### Paper:

"Minimax Off-Policy Evaluation for Multi-Armed Bandits,"

C. Ma, B. Zhu, J. Jiao, M. J. Wainwright, arXiv:2101.07781, 2021