### Counterfactual Evaluation for Offline Contextual Bandits

David S. Rosenberg

NYU: CDS

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Online vs offline in practice

# Online learning

- We briefly discussed online supervised learning in the bandit module.
- We discussed bandit methods more extensively,
  - have an online learning component.

#### Main advantage of online learning

New information about the environment can be used immediately.

## True online learning is pretty rare

- Consider a model recommending news stories on a webpage.
- Action: story recommendation.
- Reward: {0,1} indicating a click.
- With multiple users, this does not cleanly fit into "rounds" of a bandit problem:
  - Time 0: User 1 gets news story recommendation.
  - Time 1: User 1 goes for coffee.
  - Time 2: User 2 arrives and wants a news story recommendation.
  - Time 10: User 1 returns and clicks on story.
  - Time  $10+\varepsilon$ : Model updates with new feedback and gives User 2 recommendation.
- A pure bandit is too rigid for this setting.

# Online learning with delayed feedback

- We can let feedback be delayed.
- Handle all requests with policy that we have.
- Update policy as we get feedback.
- The impact of this delayed feedback is investigated in [CL11, Table 1].
- Issue is compounded if multiple servers are running model in parallel.
  - How often to synchronize data across models?
  - This is related to the problem of asynchronous distributed model training.

# Periodic batch retraining

- In practice, often sufficient and easier to periodically retrain the model.
  - e.g. daily, weekly, etc.
- In other words, use offline learning instead of online learning.
  - But refresh the model at regular intervals.

# Online vs offline learning for safety

- In many business contexts, models require extensive testing before deployment.
- e.g. Assessing the model on a test set with multiple performance metrics.
- But online learning introduces another level of complexity.
- The model is changing on the fly.
- Can a particular sequence of feedback (possibly adversarial)
  - make the model worse?
- Seems safer to deploy a static model that we've tested.

# Offline learning for bandits

- In the next couple modules,
   we'll discuss approaches to the bandit problem in the offline setting.
- This area goes by several names:
  - Counterfactual learning and evaluation
  - Offline bandit learning and evaluation
  - Batch learning with bandit feedback

Logged feedback

# Stationary / Static Policies

- In general, the policy  $\pi_t(\cdot | X_t, \mathcal{D}_t)$  at round t depends on the context  $X_t$  and the history  $\mathcal{D}_t$ :
- The dependence on the history  $\mathcal{D}_t$  allows the policy to learn over time.
- In our study of offline bandits, we will deal with static or "stationary" policies.

#### Definition

A stationary policy or static policy maps from a context  $x \in \mathcal{X}$  to a distribution over actions  $\mathcal{A}$ . We'll write  $\pi(a \mid x)$  for the probability of taking action  $a \in \mathcal{A}$  in context x under policy  $\pi$ .

Note that a stationary policy  $\pi(a|x)$  has no depedency on t or  $\mathcal{D}_t$ .

DS-GA 3001: Tools and Techniques for ML Logged feedback

Stationary / Static Policies

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Stationary / Static Policies

- In the offline contextual bandit literature, stationary policies are usually just referred to as "policies", since they're the only ones typically under consideration.
- policy is written as  $\pi(a \mid x)$ , we know it's stationary.

• As usual, the terminology isn't essential. The notation tells the story very clearly. If the

- "But wait!" you say. What if somebody tries to get clever and put the history into x?
- Good question. This is basically what happens in the reinforcement learning (RL) setting. In RL, however, the analogue of the context x is the "state", often denoted by s.
- Perhaps the key distinction between reinforcement learning and the bandit setting is that consecutive states in RL are assumed to be dependent. This allows the state to accumulate information over time.
- You'll remember that for the contextual bandit setting, we assumed that the contexts are generated i.i.d. That's the essential thing preventing us from putting the history  $\mathcal{D}_t$  into the context  $X_t$ .

# Stochastic contextual bandit with static policy

#### Stochastic k-armed contextual bandit with static policy $\pi_0$

1 Environment samples context and reward vector jointly, iid, for each round:

$$(X_1, R_1), \ldots, (X_n, R_n) \in \mathcal{X} \times \mathbb{R}^k$$
 i.i.d. from  $P$ ,

where 
$$R_i = (R_i(1), \ldots, R_i(k)) \in \mathbb{R}^k$$
.

- ② For i = 1, ..., n,
  - **1** Our algorithm **selects action**  $A_i \in \{1, ..., k\}$  according to  $A_i \sim \pi_0(\cdot \mid X_i)$ .
  - ② Our algorithm receives reward  $R_i(A_i)$ .
- Reminder:  $A_i \perp \!\!\!\perp R_i \mid X_i$ .

# Logged bandit feedback

- Suppose we run a static policy  $\pi_0(a \mid x)$  on a contextual bandit for n rounds.
- The logged bandit feedback (i.e. the "observed data") is given by

$$(X_1, A_1, R_1(A_1)), \ldots, (X_n, A_n, R_n(A_n)),$$

where  $R_i(A_i) \in \mathbb{R}$  is the reward received in round *i*.

- The policy  $\pi_0(a \mid x)$  is called the **logging policy**.
- Self-check: Are  $(X_1, A_1, R_1(A_1)), \dots, (X_n, A_n, R_n(A_n))$  i.i.d.?
  - Answer: Yes. (Because policy  $\pi_0$  is static .)

# Logged bands feedback • Suppose we re u a state goldy $m_0(u)$ a • Suppose we re u be substituted for u rough • The logged bands feedback (u, the 'charred data') is given by • (u, u, u, u) by • (u, u, u) by • (u, u) by • (u

■ Self-check: Are (X<sub>1</sub>, A<sub>1</sub>, R<sub>1</sub>(A<sub>1</sub>)),...,(X<sub>n</sub>, A<sub>n</sub>, R<sub>n</sub>(A<sub>n</sub>)) i.i.d.?
■ Answer: Yes. (Because policy no in static.)

- This is called **bandit** feedback specifically because in each round we only observe the reward corresponding to the action played.
- The analogous "full feedback" would be

$$(X_1, A_1, R_1), \ldots, (X_n, A_n, R_n),$$

where get the full rewards vector in each round.

- We could solve the full feedback case by training a multclass classifier to predict the action that has the highest reward in each round. This would be a straightforward supervised learning problem.
- With only the bandit feedback, however, we're in the explore/exploit setting, since we won't know for sure whether or not a particular action is the best without trying the other actions.
- If the policy  $\pi_0$  were not static, as in the online bandit setting, then logged bandit feedback from previous rounds,  $\sup_t = ((X_1, A_1, R_1(A_1)), \dots, (X_{n-1}, A_{n-1}, R_{n-1}(A_{n-1})))$

# Off-policy learning and evaluation

Suppose we have logged bandit feedback

$$\mathcal{D} = ((X_1, A_1, R_1(A_1)), \dots, (X_n, A_n, R_n(A_n))),$$

from a contextual bandit with logging policy  $\pi_0(a \mid x)$ .

• The two main problems for offline bandits:

#### Off-policy learning (counterfactual learning)

Use  $\mathcal{D}$  from policy  $\pi_0$  to learn a new policy  $\pi$  with better performance.

#### Off-policy evaluation (counterfactual evaluation)

Use  $\mathcal{D}$  from policy  $\pi_0$  to estimate the performance of a new policy  $\pi$ .

# Off-policy bandits vs supervised learning

- This module will be about off-policy evaluation.
- Next module will be about off-policy learning.
- In supervised learning, the empirical risk on a test set is a great performance estimate.
- Optimizing the same empirical risk on a training set is the main approach to ML.
- In a bandit setting, getting an unbiased performance estimate is nontrivial,
  - and the unbiased estimators can have high variance when  $\pi$  is very different from  $\pi_0$ .
- For off-policy learning, in addition to the overfitting concerns of supervised learning,
  - we have to deal with the different variances for our performance estimator and
  - there's a new type of overfitting called "propensity overfitting", which we'll discuss later.

The off-policy evaluation problem

#### The value function

#### **Definition**

The value of a static policy  $\pi(x \mid a)$  in a contextual bandit problem is given by

$$V(\pi) = \mathbb{E}[R(A)]$$
,

where  $(X,R) \sim P$  and  $A \mid X \sim \pi(\cdot \mid X)$ . The function  $V(\cdot)$  is called the **value function**.

- The value function is the analogue of the risk function in supervised learning.
- The risk of f is the expected loss of f for a random (X, Y).
- The value of  $\pi$  is the expected reward for selecting A according to  $\pi$ .

# Estimating value function from on-policy logs

Suppose we have logged bandit feedback

$$\mathcal{D} = ((X_1, A_1, R_1(A_1)), \dots, (X_n, A_n, R_n(A_n))),$$

from logging policy  $\pi_0(a \mid x)$ .

- Evaluating  $V(\pi_0)$  is called **on-policy evaluation**,
  - since logged data is generated by the policy we want to evaluate.
- A natural estimator is

$$\hat{V}(\pi_0) = \frac{1}{n} \sum_{i=1}^n R_i(A_i).$$

This is unbiased, since

$$\mathbb{E}\left[\hat{V}(\pi_0)\right] = \mathbb{E}\left[R_i(A_i)\right] = V(\pi_0).$$

# Estimating value function from off-policy logs

- Suppose we want to estimate  $V(\pi)$ , where  $\pi$  is different from the logging policy  $\pi_0$ .
- This is called **off-policy evaluation**.
- We can write

$$V(\pi) = \mathbb{E}_{(X,R)\sim P,A|X\sim\pi(\cdot|X)|}[R(A)].$$

- We want to estimate the expectation of R(A)
  - when  $A \mid X \sim \pi(\cdot \mid X)$ , but
  - we have  $A \mid X \sim \pi_0(\cdot \mid X)$  in our data  $\mathfrak{D}$ .
- We have a distribution mismatch.
- What can we do in this situation?

# Estimating value function from off-policy logs

- Just like the missing at random (MAR) setting, there are multiple methods for estimating  $V(\pi)$ .
- For each MAR estimator, there is an analogous policy value estimator:

MAR estimator	Off-policy value estimator
IPW mean	importance-weighted (IW) value estimator / "Model the bias"
self-normalized IPW mean	self-normalized IW value estimator [SJ15]
regression imputation	"Direct Method" / "Reward prediction"
augmented IPW	"doubly robust" estimator [DLL11]

Direct methods / "Model the world"

# The obvious thing?

• We want to estimate

$$V(\pi) = \mathbb{E}[R(A)]$$
  
=  $\mathbb{E}_X [\mathbb{E}_{R,A}[R(A) | X]],$ 

where  $A \sim \pi(\cdot \mid X)$ .

- We always have  $(X, R) \sim P$ , so won't mention that going forward.
- We have plenty of X's from the right distribution in our logs.
- So the outer expectation is easy to estimate using Monte Carlo.

If we knew the expected rewards...

- We want to calculate  $V(\pi) = \mathbb{E}\left[\mathbb{E}\left[R(A) \mid X\right]\right]$ .
- Let  $r(x, a) = \mathbb{E}[R(A) \mid X = x, A = a]$ .
- Then

$$\mathbb{E}[R(A) \mid X] = \mathbb{E}[\mathbb{E}[R(A) \mid X, A] \mid X]$$
$$= \mathbb{E}[r(X, A) \mid X]$$

Putting it together,

$$V(\pi) = \mathbb{E}_{X} \left[ \mathbb{E}_{A \sim \pi(\cdot \mid X)} \left[ r(X, A) \mid X \right] \right]$$
$$= \mathbb{E}_{X} \left[ \sum_{a=1}^{k} r(X, a) \pi(a \mid X) \right].$$

# Estimate with expected rewards

We have

$$V(\pi) = \mathbb{E}_X \left[ \sum_{a=1}^k r(X, a) \pi(a \mid X) \right]$$

• Create a Monte Carlo style estimator using our sample of contexts:

$$\hat{V}(\pi) = \sum_{i=1}^{n} \left[ \sum_{a=1}^{k} r(x_i, a) \pi(a \mid x_i) \right].$$

• But we don't know r(x, a) – what can we do?

# Estimating the rewards

- Can we estimate  $r(x, a) = \mathbb{E}[R(A) \mid X = x, A = a]$ ?
- (We discussed this in the contextual bandits module.)
- Our logs gives us data for this:  $(X_i, A_i, R_i(A_i))$ .
- This is a straightforward regression problem.
- Ok... there is a covariate shift here.
- We want to apply r(x, a) when  $A \sim \pi(\cdot \mid x)$ , but we have samples from  $A \sim \pi_0(\cdot \mid x)$ .
  - In this context, it's sometimes called a selection bias.
- Once we have an estimate  $\hat{r}(x, a)$ , we can plug it in.

#### Definition

The direct method of offline policy evaluation is

$$\hat{V}(\pi) = \sum_{i=1}^{n} \sum_{a=1}^{k} \hat{r}(x_i, a) \pi(a \mid x_i).$$

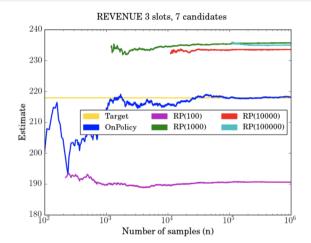
# DS-GA 3001: Tools and Techniques for ML —Direct methods / "Model the world"

Estimating the rewards

an we estimate $r(x, a) = \mathbb{E}[R(A) \mid X = x, A = a]$ ?
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nce we have an estimate $F(x,a)$ , we can plug it in.
ion
rect method of offline policy evaluation is
$\tilde{V}(\pi) = \sum_{i=1}^{n} \sum_{a=1}^{k} f(x_i, a) \pi(a \mid x_i).$

- In research papers, I haven't seen anybody fit  $\hat{r}(x,a)$  with importance weighting to correct for the covariate shift. This seems like an area worth pursuing. As we know from our study of regression imputation, importance weighting becomes importance when we have model misspecification and response bias / covariate shift.
- HOWEVER, in practice, we often don't want to evaluate just one policy. We often want to evaluate policies in a hyperparameter tuning setting, where we may want to evaluate 10-20 different policies. To use importance weighting, we'd have to train a different  $\hat{r}(x,a)$  for each policy we want to estimate.
- For learning, the situation is even worse as we traverse through policy space, the required importance weighting would be constantly changing.
- Perhaps these are the reasons that importance weighting doesn't show up much for policy evaluation.
- But also consider the misspecification part as we use more complicated models (e.g. deep neural networks), misspecification may become less of an issue.

# Experiment from Swaminathan and Joachims



• RP = Reward prediction / direct method with various training set sizes

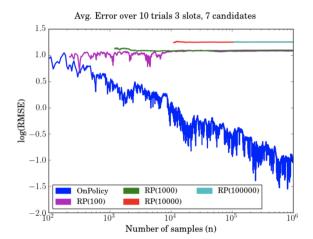
# DS-GA 3001: Tools and Techniques for ML L—Direct methods / "Model the world"

Experiment from Swaminathan and Joachims



- This was a simulated news recommender scenario. The reward function was a very complicated function of the context and the action.
- Because it's a simulation, we know the actual policy value that's the "target" yellow line.
- We can also actually run the policy we want to evaluate against the simulator and get an on-policy value estimate. That's the blue line. We can see that it converges fairly well to the target.
- The direct method (the RP(X) lines) don't bounce up and down much that's low variance. But they're quite a bit off from the target. My best guess for the poor performance is that it's a combination of model misspecification and covariate shift. It would be interesting to dig in more to this simulation to idenitfy what the issue is, including looking at the actual reward function. Are they using an hypothesis space that's very limited?

# Experiment from Swaminathan and Joachims



RP = Reward prediction / direct method with various training set sizes

From https://www.cs.cornell.edu/~adith/CfactSIGIR2016/Evaluation1.pdf page 21.

DS-GA 3001: Tools and Techniques for ML —Direct methods / "Model the world"

Experiment from Swaminathan and Joachims

• Same thing on a log scale, averaged over 10 trials.



# What's going on here?

- We've studied regression imputation before.
- We know we have problems when there's
  - model misspecification AND
  - sample bias
- Maybe we can do something about the sample bias with importance weighting?
- Maybe we can reduce model misspecification with a more complex model?
  - [possible project topics]

Importance-weighted value estimators

# Our approach

- For the IPW mean estimator, we argued heuristically and then showed  $\hat{\mu}_{ipw}$  was unbiased and consistent.
- For the value estimator, we'll directly leverage our knowledge of importance sampling.
- We'll just need to do some work to make it a clean application of our importance sampling theorem.

# Value function expansion

We have

$$V(\pi) = \mathbb{E}_{(X,R)\sim P,A\sim\pi|}[R(A)]$$
  
=  $\mathbb{E}_{(X,R)\sim P}[\mathbb{E}_{A\sim\pi}[R(A)\mid X,R]]$ 

- The challenge is the inner expectation it's w.r.t.  $\pi$  rather than  $\pi_0$ .
- Let's write the inner expectation as g(X, R), where

$$g(x,r) := \mathbb{E}_{A \sim \pi(\cdot|x)} [R(A) \mid X = x, R = r]$$
$$= \mathbb{E}_{A \sim \pi(\cdot|x)} [r(A)]$$

## Importance sampling

• By the Change of Measure Theorem (i.e. importance sampling), if  $\pi(a|x) > 0 \implies \pi_0(a|x) > 0$ , then

$$g(x,r) = \mathbb{E}_{A \sim \pi(\cdot|x)} \left[ r(A) \right] = \mathbb{E}_{A \sim \pi_0(\cdot|x)} \left[ r(A) \frac{\pi(A|x)}{\pi_0(A|x)} \right].$$

Plugging this in, we get

$$V(\pi) = \mathbb{E}_{(X,R)\sim P} \left[ \mathbb{E}_{A\sim \pi} \left[ R(A) \mid X, R \right] \right]$$

$$= \mathbb{E}_{(X,R)\sim P} \left[ g(X,R) \right]$$

$$= \mathbb{E}_{(X,R)\sim P} \left[ \mathbb{E}_{A\sim \pi_0} \left[ R(A) \frac{\pi(A \mid X)}{\pi_0(A \mid X)} \right] \right]$$

ullet So we can use  ${\mathcal D}$  to make an unbiased Monte Carlo estimate of the last expression.

## Importance-weighted value estimator

#### Definition

The **importance-weighted (IW) value estimator** for policy  $\pi$ , based on logged bandit feedback  $(X_1, A_1, R_1(A_1)), \ldots, (X_n, A_n, R_n(A_n))$  with actions chosen under a static logging policy  $\pi_0$  is

$$\hat{V}_{iw}(\pi) = \frac{1}{n} \sum_{i=1}^{n} R_i(A_i) \frac{\pi(A_i \mid X_i)}{\pi_0(A_i \mid X_i)}.$$

• The importance weights are defined as

$$W_i := \frac{\pi(A_i \mid X_i)}{\pi_0(A_i \mid X_i)}.$$

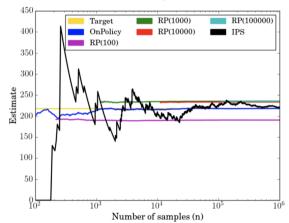
• The following follows immediately from the importance sampling formulation of  $V(\pi)$ :

## Theorem (The IW-estimator is unbiased.)

$$\textit{If } \pi(a \,|\, x) > 0 \implies \pi_0(a \,|\, x) > 0, \textit{ then } \mathbb{E}\left[\hat{V}_{\textit{ipw}}(\pi)\right] = V(\pi).$$

## Experiment from Swaminathan and Joachims

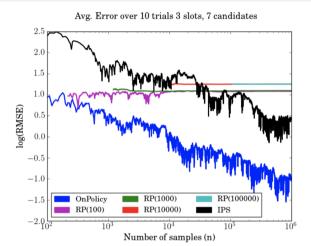




 $\bullet \ \mathsf{IPS} = \mathsf{inverse} \ \mathsf{propensity} \ \mathsf{scoring} = \mathsf{importance} \ \mathsf{weighted}$ 

 $\textbf{From } \texttt{https://www.cs.cornell.edu/} \texttt{`adith/CfactSIGIR2016/Evaluation1.pdf} \ \ \textbf{page 38}.$ 

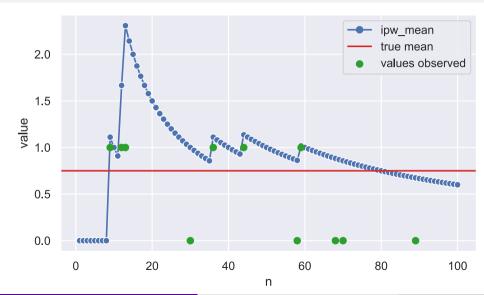
## Experiment from Swaminathan and Joachims



• IPS = inverse propensity scoring = importance weighted

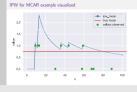
Self-normalized IW value estimators

# IPW for MCAR example visualized



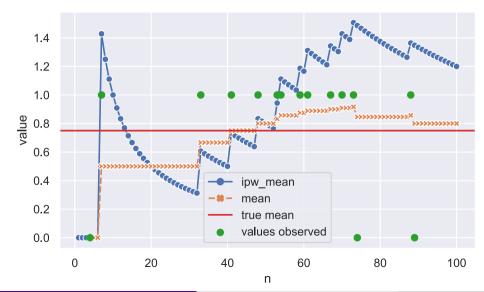
# DS-GA 3001: Tools and Techniques for ML Self-normalized IW value estimators

└─IPW for MCAR example visualized



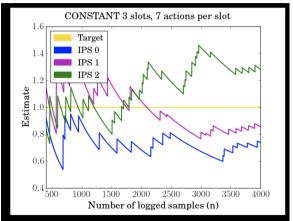
- The green dots represent observed values of  $Y_i$ .
- We can see that we had no observations of Y until  $Y_9 = 1$ .
- The horizontal red line shows the true mean of the  $Y_i$ 's.
- The blue dots show  $\hat{\mu}_{ipw}$  as n increases.
- Note the large jumps in  $\hat{\mu}_{ipw}$  whenever we get an observation with  $Y_i = 1$ . This is because each observed  $Y_i$  is scaled up by an inverse propensity weight of 10.
- Also note that between observations with  $Y_i = 1$ , ipw\_mean decays like 1/n towards 0.

# IPW mean for "too many" observations



# Simple experiment with $R_i \equiv 1.0$

• Swaminathan and Joachims try IW value estimator with  $R_i \equiv 1.0$ .



• 3 different sample paths

 $\textbf{From } \texttt{https://www.cs.cornell.edu/\~adith/CfactSIGIR2016/Evaluation2.pdf} \ \ \textbf{page 2}.$ 

#### Self-normalized IW value estimator

#### Definition

The self-normalized importance-weighted (IW) value estimator for policy  $\pi$ , based on logged bandit feedback  $(X_1, A_1, R_1(A_1)), \ldots, (X_n, A_n, R_n(A_n))$  with actions chosen under a static logging policy  $\pi_0$  is

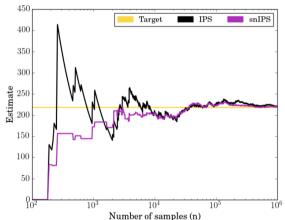
$$\hat{V}_{\mathsf{sn}_{-}\mathsf{iw}}(\pi) = \frac{\sum_{i=1}^{n} W_i R_i(A_i)}{\sum_{i=1}^{n} W_i},$$

where the importance weights are defined as

$$W_i := \frac{\pi(A_i \mid X_i)}{\pi_0(A_i \mid X_i)}.$$

### Self-normalized IW vs IW



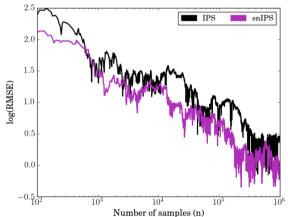


## • 3 different sample paths

 $\textbf{From } \texttt{https://www.cs.cornell.edu/} \\ \texttt{adith/CfactSIGIR2016/Evaluation2.pdf} \ \ \textbf{page} \ \ \textbf{6}.$ 

## Self-normalized IW vs IW





### • 3 different sample paths

## References

# Notation and Terminology

- A lot of our notation is based on [BWRB20], though we align with [SB18] and most probability textbooks in our use of capital letters to indicate random variables and lower case letters for the values they can take.
- Terminology-wise, what we call the importance weighted (IW) estimator is called the inverse propensity score (IPS) estimator in [JSdR18]. We call it the importance-weighted estimator to make the analogy to the importance-weighted empirical risk, which we defined in the module on covariate shift. Our terminology is also used in [BWRB20].

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