

# Off-policy Learning in Theory and in the Wild

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Based on joint works with

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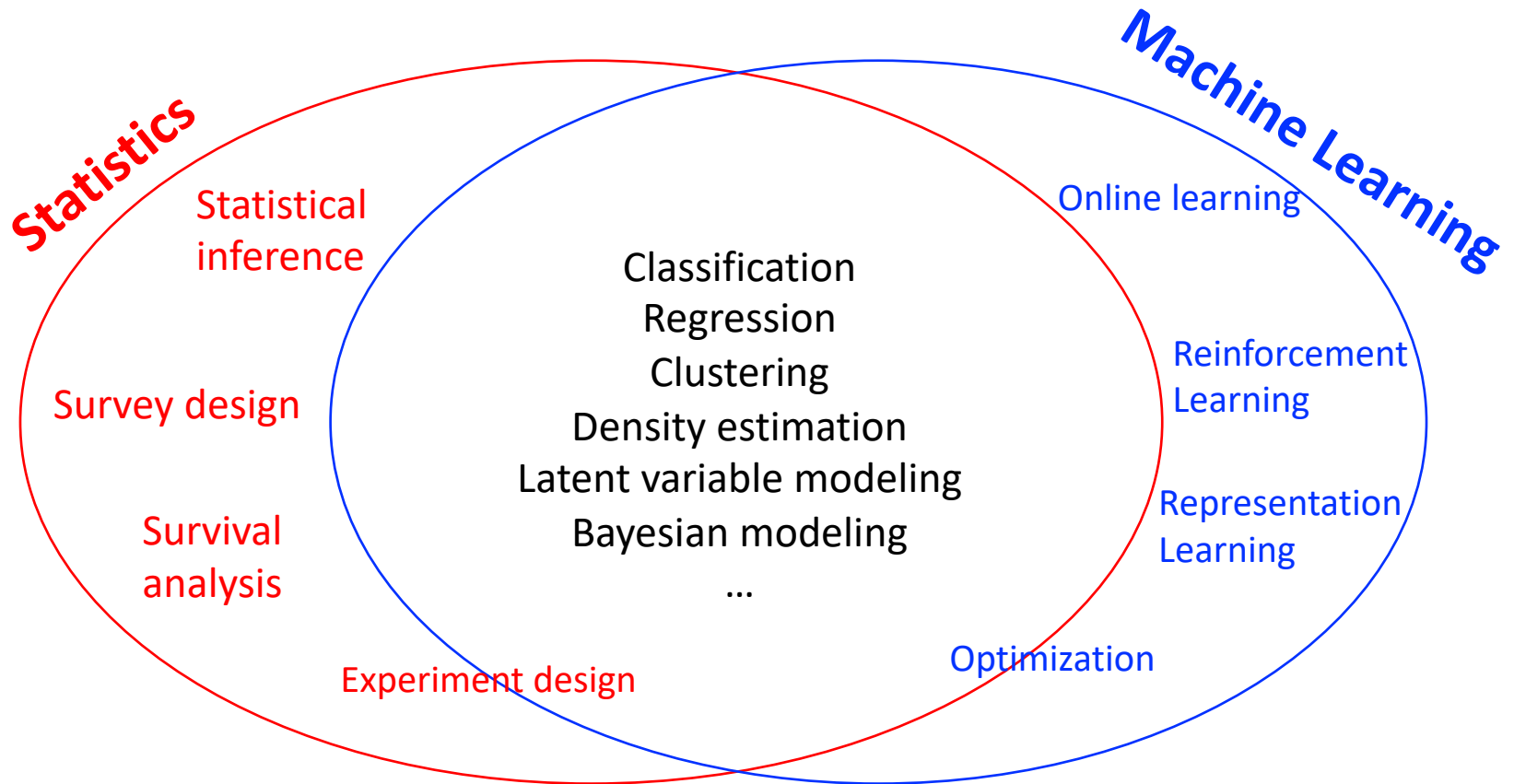
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# Statistics (since 1900s) vs ML (since 1950s)



# My (group's) research

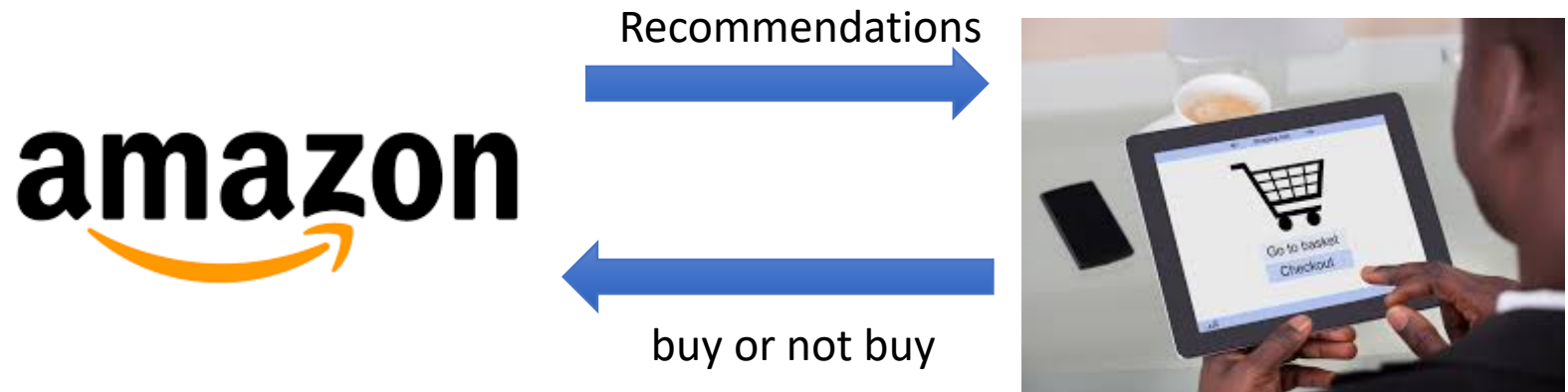
1. Trend filtering (locally adaptive methods)
  - making it online for time series forecasting.
2. Reinforcement learning
  - Learn from feedbacks. More efficient use of old data
3. Differential privacy
  - Do ML/Stats without risking identifying data points
4. Large scale optimization / deep learning
  - Compress time/space/energy in training.

# Outline today

- Off-policy evaluation and ATE estimation
  - A finite sample optimality theory
  - The SWITCH estimator
- Off-policy learning in the real world
  - Challenges: missing logging probabilities, confounders, model misspecification, complex action spaces
  - Solutions



# Off-Policy learning: an example



How to evaluate a new algorithm without actually running it live?

# Contextual bandits model

- Contexts:

- $x_1, \dots, x_n \sim \lambda$  drawn iid, possibly infinite domain

- Actions:

- $a_i \sim \mu(a|x_i)$  Taken by a randomized “Logging” policy

- Reward:

- $r_i \sim D(r|x_i, a_i)$  Revealed only for the action taken

- Value:

- $v^\mu = \mathbb{E}_{x \sim \lambda} \mathbb{E}_{a \sim \mu(\cdot|x)} \mathbb{E}_D [r|x, a]$

- We collect data  $(x_i, a_i, r_i)_{i=1}^n$  by the above processes.

# Off-policy Evaluation and Learning

## Off-policy evaluation

Estimate the value of a fixed target policy  $\pi$

$$v_\pi := \mathbb{E}_\pi [\text{Reward}]$$

## Off-policy learning

Find  $\pi \in \Pi$

that maximizes  $v_\pi$

- Using data  $(x_i, a_i, r_i)_{i=1}^n$
- often the policy  $\mu$  or logged propensities  $(\mu_i)_{i=1}^n$

# ATE estimation is a special case of off-policy evaluation

- a: Action  $\Leftrightarrow$  T: Treatment  $\{0,1\}$
  - r: Reward  $\Leftrightarrow$  Y: Response variable
  - x: Contexts  $\Leftrightarrow$  X: covariates
- 
- Take  $a = \{0,1\}$ ,  $\pi = [0.5,0.5]$
  - $r(x,a) = [2Y(X,T=1), -2Y(X,T=0)]$
- 
- Then, the value of  $\pi = \text{ATE}$

# Direct Method / Regression estimator

- Fit a regression model of the reward

$$\hat{r}(x, a) \approx \mathbb{E}(r|x, a) \quad \text{using the data}$$

- Then for any target policy

$$\hat{v}_{\text{DM}}^{\pi} = \frac{1}{n} \sum_{i=1}^n \sum_{a \in \mathcal{A}} \hat{r}(x_i, a) \pi(a|x_i)$$

## Pros:

- Low-variance.
- Can evaluate on unseen contexts

## Cons:

- Often high bias
- The model can be wrong/hard to learn

# Inverse propensity scoring / Importance sampling

(Horvitz & Thompson, 1952)

$$\hat{v}_{\text{IPS}}^{\pi} = \frac{1}{n} \sum_{i=1}^n \boxed{\frac{\pi(a_i | x_i)}{\mu(a_i | x_i)}} r_i \quad \text{Importance weights} \quad \text{=} \rho_i$$

## Pros:

- No assumption on rewards
- Unbiased
- Computationally efficient

## Cons:

- High variance when the weight is large

# Variants and combinations

- Modifying importance weights:
  - Trimmed IPS ([Bottou et. al. 2013](#))
  - Truncated/Reweighted IPS ([Bembom and van der Laan,2008](#))
- Doubly Robust estimators:
  - A systematic way of incorporating DM into IPS
  - Originated in statistics ([see e.g., Robins and Rotnitzky, 1995; Bang and Robins, 2005](#))
  - Used for off-policy evaluation ([Dudík et al., 2014](#))

Many estimators are out there.

**Are they optimal?** How good is good enough?

Our results in (W., Agarwal, Dudik, ICML-17):

1. **Minimax lower bound: IPS is optimal in the general case.**
2. **A new estimator --- SWITCH --- that can be even better than IPS in some cases.**



# What do we mean by optimal?

- A minimax formulation

$$\inf_{\hat{v}} \sup_{\text{a class of problems}} \mathbb{E}(\hat{v}(\text{Data}) - v^{\pi})^2$$

Taken over data  $\sim \mu$

- Fix context distribution and policies  $(\lambda, \mu, \pi)$
- A class of problems = a class of reward distributions.

# What do we mean by optimal?

- The class of problems: (generalizing [Li et. al. 2015](#))

$$\mathcal{R}(\sigma, R_{\max}) := \left\{ D(r|x, a) : 0 \leq \mathbb{E}_D[r|x, a] \leq R_{\max}(x, a) \text{ and} \right. \\ \left. \text{Var}_D[r|x, a] \leq \sigma^2(x, a) \text{ for all } x, a \right\}.$$

- The minimax risk

$$\inf_{\hat{v}} \sup_{D(r|a,x) \in \mathcal{R}(\sigma^2, R_{\max})} \mathbb{E}(\hat{v} - v^\pi)^2$$

# Lower bounding the minimax risk

- Our main theorem: assume  $\lambda$  is a probability density, then under mild moment conditions

$$\inf_{\hat{v}} \sup_{D(r|a,x) \in \mathcal{R}(\sigma^2, R_{\max})} \mathbb{E}(\hat{v} - v^\pi)^2$$
$$= \Omega \left[ \underbrace{\frac{1}{n} \left( \mathbb{E}_\mu[\rho^2 \sigma^2] \right)}_{\text{Randomness in reward}} + \underbrace{\mathbb{E}_\mu[\rho^2 R_{\max}^2]}_{\text{Randomness due to context distribution}} \right]$$

# This implies that **IPS is optimal!**

- The high variance is required.
  - In contextual bandits with **large context spaces** and **non-degenerate context distribution**.
- Previously, IPS is known to be **asymptotically inefficient**
  - for multi-arm bandit ([Li et. al., 2015](#))
  - for ATE. ([Hahn, Hirano, Imbens](#))

# Classical optimality theory (Hahn, 1998)

- $n^*$  Var[any LAN estimator] is greater than:

$$\mathbb{E}_{x \sim \mathcal{D}} \{ \mathbb{E}_{\mu} [\rho^2 \text{Var}(r|x, a)|x] \} + \text{Var}_{x \sim \mathcal{D}} \{ \mathbb{E}_{\mu} [\rho r|x] \} .$$

Take  supremum

$$\mathbb{E}_{\mu} [\rho^2 \sigma^2] + \mathbb{E}_{x \sim \mathcal{D}} [ \mathbb{E}_{\mu} [\rho R_{\max}|x]^2 ] .$$

- Our lower bound is bigger!

$$\mathbb{E}_{\mu} [\rho^2 \sigma^2] + \mathbb{E}_{\mu} [\rho^2 R_{\max}^2]$$

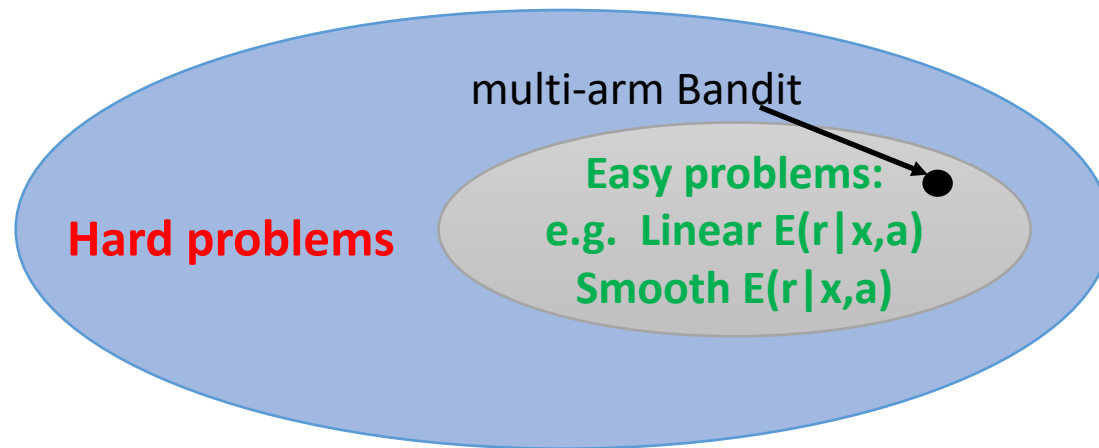
How could that be? There are estimators that achieve asymptotic efficiency.

- e.g., [Robins](#), [Hahn](#), [Hirano](#), [Imbens](#), and many others in the semiparametric efficiency industry!

<b>Assumption:</b>	<b>Realizable assumption:</b> $E[r x,a]$ is differentiable in $x$ for each $a$ .	<b>No assumption on <math>E[r x,a]</math> excepts boundedness.</b>
Consequences	Hirano et. al. is optimal. Imbens et. al. is optimal.  IPS is suboptimal!	IPS is optimal (up to a universal constant)
Caveat	Poor finite sample performance. Exponential dependence in $d$ .	Does NOT adapt to easier problems.

# The pursuit of adaptive estimators

The class of all contextual bandits problems



- Minimacity: perform optimally on **hard problems**.
- Adaptivity: perform better on **easier problems**.

Suppose we are given **an oracle**



- Could be very good, or completely off.
- How to **make the best use** of it?



# SWITCH estimator

- Recall that IPS is bad because:  $\hat{v}_{\text{IPS}}^{\pi} = \frac{1}{n} \sum_{i=1}^n \frac{\pi(a_i|x_i)}{\mu(a_i|x_i)} r_i$

- SWITCH estimator:

For each  $i = 1, \dots, n$ , for each action  $a \in \mathcal{A}$ :

if  $\pi(a|x_i)/\mu(a|x_i) \leq \tau$ :

Use IPS (or DR).

else:

Use the oracle estimator.

# Error bounds for SWITCH

$$\text{MSE}(\hat{v}_{\text{SWITCH}}) \leq$$

$$\frac{2}{n} \mathbb{E}_{\mu} \left[ \underbrace{(\sigma^2 + R_{\max}^2) \rho^2 \mathbf{1}(\rho \leq \tau)}_{(1)} \right]$$

$$+ \frac{2}{n} \mathbb{E}_{\pi} \left[ \underbrace{R_{\max}^2 \mathbf{1}(\rho > \tau)}_{(2)} \right]$$

$$+ \underbrace{\mathbb{E}_{\pi} \left[ \epsilon \mathbf{1}(\rho > \tau) \right]^2}_{(3)}$$

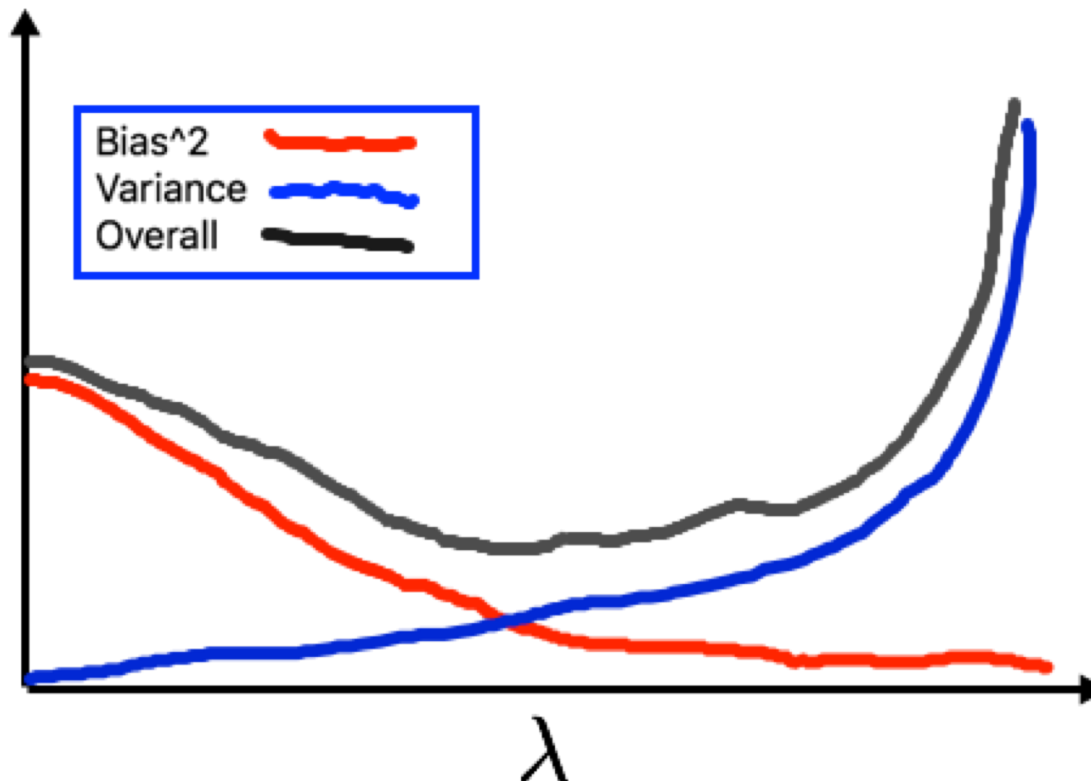
1) Variance from IPS (reduced by truncation)

2) Variance due to sampling  $x$ . Required even with perfect oracle

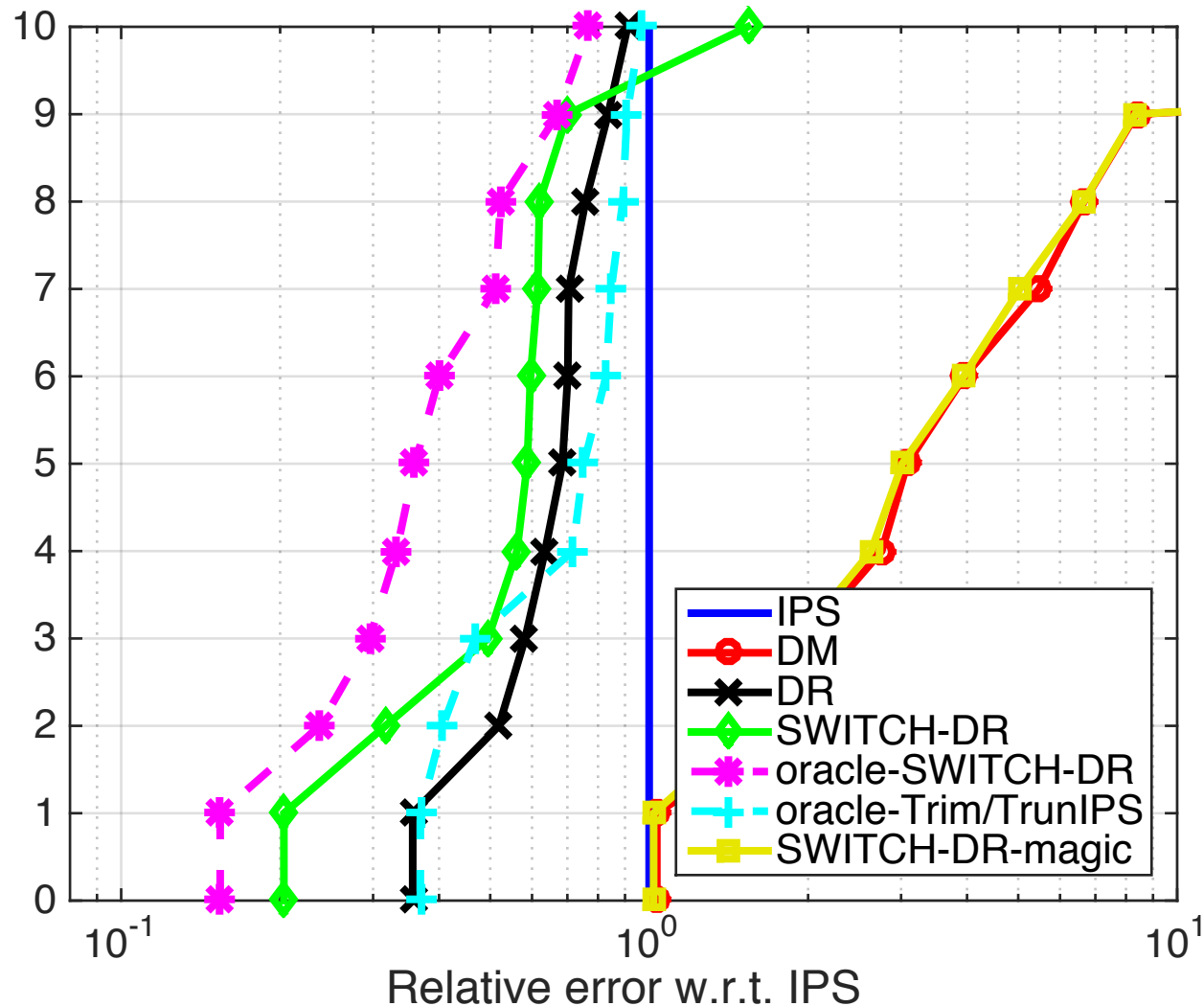
1) Bias from the oracle.

# How to choose the threshold?

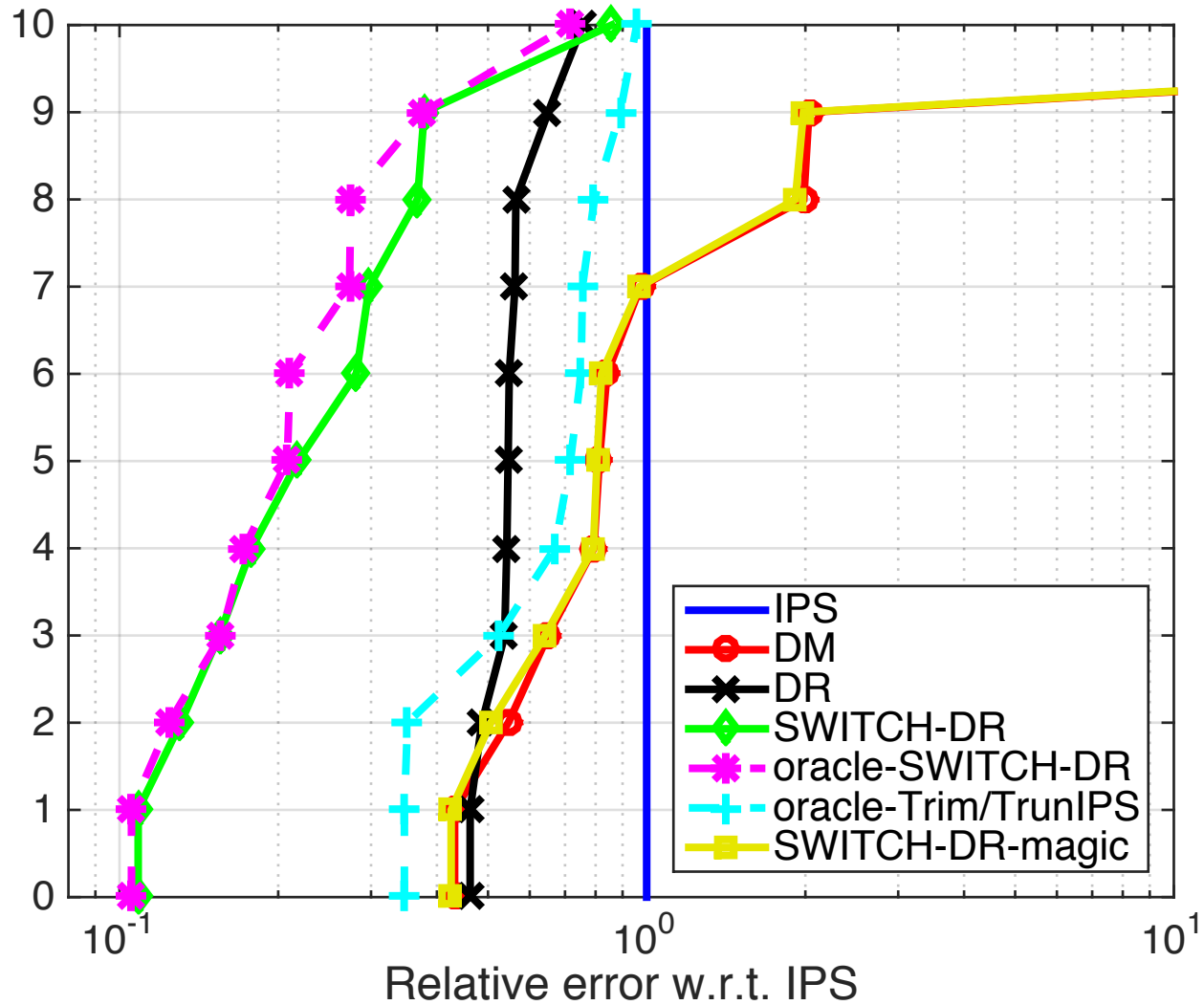
- Be conservative:
  - Minimize the variance + square bias upper bound.



# CDF of relative MSE over 10 UCI multiclass classification data sets.



# With additional label noise



# Quick summary of Part I

- Off-policy evaluation  $\Leftrightarrow$  a generalized ATE estimation
- Simple IPS cannot be improved except when having access to a realizable model.
- Best of both world: doubly robust and SWITCH

# Part 2: Off-Policy learning **in the Wild!**

## Off-policy evaluation

Estimate the value of a fixed target policy  $\pi$

$$v_\pi := \mathbb{E}_\pi[\text{Reward}]$$

## Off-policy learning

Find  $\pi \in \Pi$

that maximizes  $v_\pi$

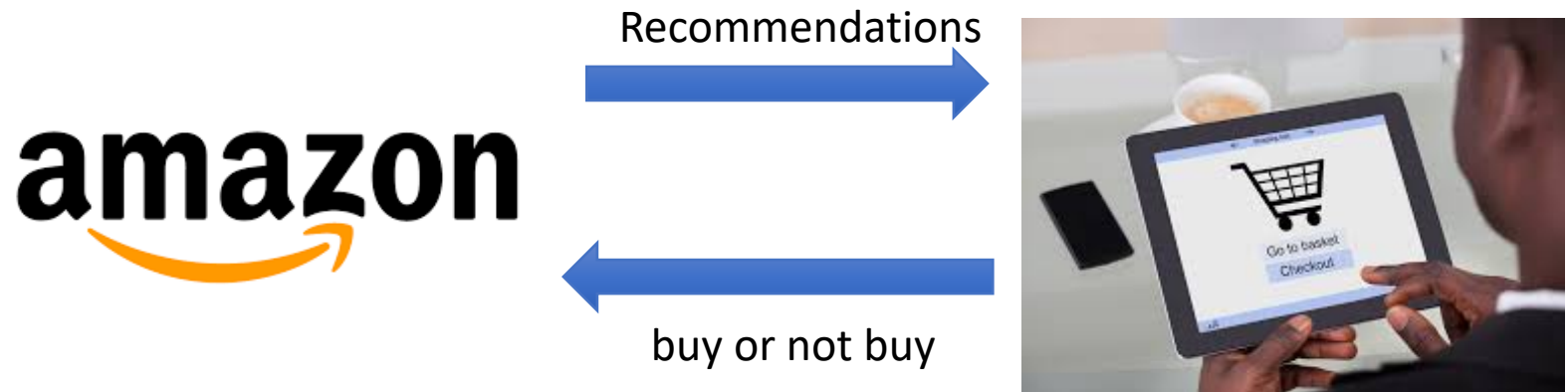
- Data set

$$(x_i, a_i, r_i)_{i=1}^n$$

- Logging policy

$$(\mu_i)_{i=1}^n$$

# Recommendation systems



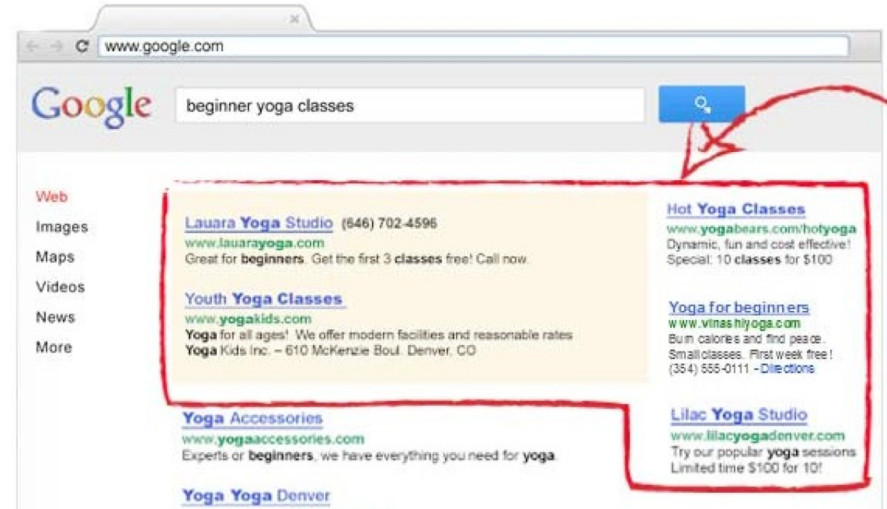
What's commonly being done in industry is collaborative filtering.

This is a **direct method**!



# Serving ads: Google/Criteo/Facebook

- $x$  = context/user features
- $a$  = ads features
- $r$  = click or not.



- Typical approach:
  - Some feature embedding of  $(x,a)$  into a really high-dimensional  $\phi(x,a)$
  - L1-regularized logistic regression to predict  $r$

This is again a **direct method!**

# Challenges of conducting offline learning in the wild

1. Reward models are always non-realizable
  - Direct methods are expected to have nontrivial bias.
2. Large action space, large importance weight
  - Think how many webpages are out there!
3. Missing logging probabilities
  - Even if randomized, we might not know the logging policy
4. Confounders: unrecorded common cause of action and reward!
  - Ad-hoc promotion, humans operator overruling the system.

Ma, W. and Narayanaswamy (2018) "Imitation-Regularized Offline Learning." under review.

# Two additional assumptions

- The expected reward obeys that

$$0 \leq \mathbb{E}[r|x, a] \leq R, \quad \forall x, a$$

- Not a strong assumption.
  - Satisfied in most applications, e.g., Click-Through-Rate optimization.
  - [Bottou et. al.](#) used this to construct lower bounds.
  - The reason why weight clipping / SWITCH works.

# Click-prediction by multiclass classification



$$\operatorname{argmin}_{\pi} \operatorname{CE}(\pi; r) = -\frac{1}{n} \sum_{i=1}^n r_i \log \pi(a_i | x_i).$$

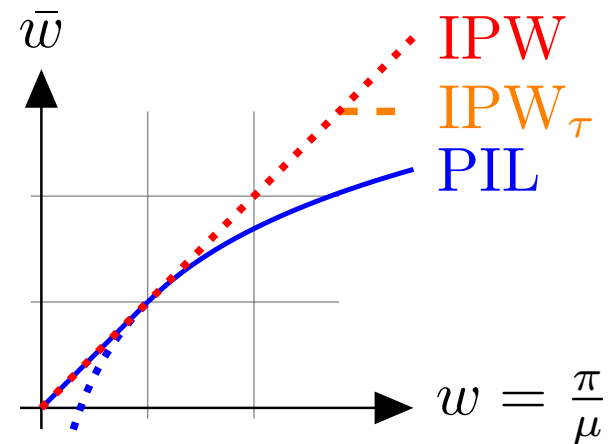
- Only when the user clicked, do we have a label.
- Train a multiclass classifier using the labeled examples.

# Causal interpretation of cross entropy-based direct click prediction

$$\frac{1}{n} \sum_{i=1}^n r_i \log \pi(a_i | x_i) - \log(\mu(a_i | x_i))$$

$$= \frac{1}{n} \sum_{i=1}^n r_i \log \left( \frac{\pi(a_i | x_i)}{\mu(a_i | x_i)} \right)$$

$$\approx \frac{1}{n} \sum_{i=1}^n r_i \left( \frac{\pi(a_i | x_i)}{\mu(a_i | x_i)} - 1 \right)$$



Policy Improvement Lower bound (PIL)

# Causal interpretation of cross entropy-based direct click prediction

$$\frac{1}{n} \sum_{i=1}^n r_i \log \pi(a_i | x_i) - \log(\mu(a_i | x_i))$$

- Implicitly maximize a lower bound of the counterfactual objective **without** having the logging probabilities!
- **Adaptive** to any unknown logging probabilities.
- We **can optimize but cannot evaluate** the lower bound!

# Our solution: Imitate the policy!

$$\text{KL}(\mu \parallel \pi) = \mathbb{E}_{\mu} \log \frac{\mu}{\pi} = -\mathbb{E}_{\mu} \log w.$$

Fully observed:

$$\text{IML}_{\text{full}}(\pi) = -\frac{1}{n} \sum_{i=1}^n \sum_{a \in \mathcal{A}(x_i)} \mu(a \mid x_i) \log w(a \mid x_i)$$

Partially observed:

$$\text{IML}_{\text{part}}(\pi) = -\frac{1}{n} \sum_{i=1}^n \log w_i;$$

Completely missing:

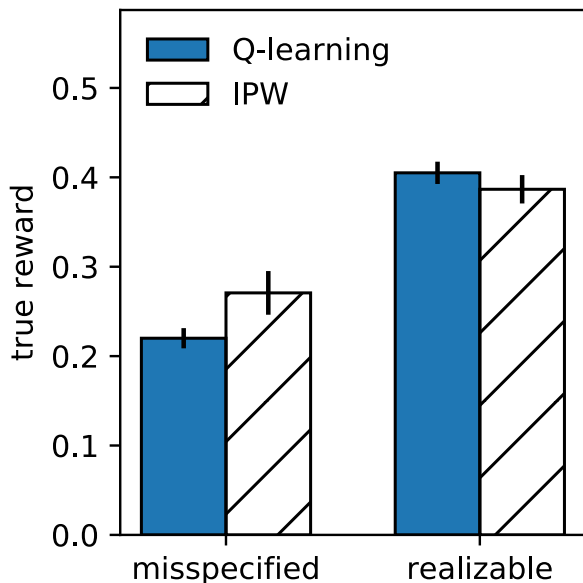
$$\text{IML}_{\text{miss}}(\pi) = -\frac{1}{n} \sum_{i=1}^n \log \pi(a_i \mid x_i) - \text{CE}(\mu; 1)$$

# Usage of IML

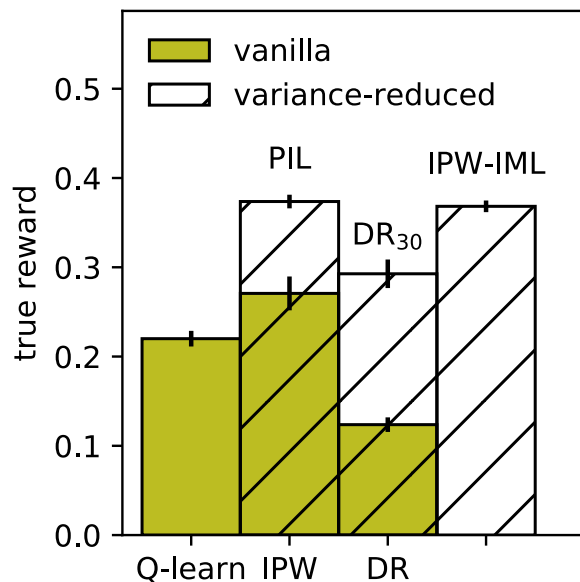
- To be use as a regularization
  - Closely related to safe-policy improvements.
  - Natural policy gradient
- To diagnose whether there is a confounder
  - If IML solution is nearly 0, then we have good evidence that there is no confounder
- To collect new data using IML policy



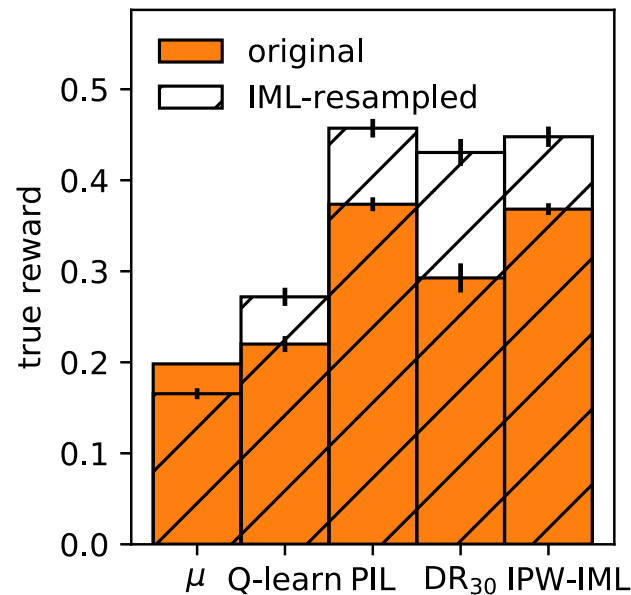
# Results on UCI Data Set: Optdigit



(a) Unbiased IPW is better than Q-learning with misspecified models.



(b) Variance reduction techniques further improve offline learning.



(c) Online application of IML improves future offline learning.

# The Criteo Counterfactual Dataset

- 1 million records on Ad impressions.
- 250 GB hosted on AWS



$$(x_i, a_i, r_i)_{i=1}^n$$

- They actually ran a randomized policy. And have logged  $(\mu_i)_{i=1}^n$



# Nothing gets better than their logging policy, but we are close...

Table 5: Criteo counterfactual analysis dataset [19].

Approach	Offline Est.	Gap (10)	Paired $\hat{\Delta}$
[ ]=greedy	( $\times 10^4$ )	(100%)	( $\times 10^4$ )
Logging	(53.3, 53.7)	( 0.0, 0.0)	( 0.1, 1.8)
IML	(51.5, 53.3)	(-0.3, 0.3)	( 0.0, 0.0)
Uniform	(41.8, 52.6)	( 7.0, 8.0)	(-10 , 0.1)
[Q-learn]	(49.3, 55.9)	( 3.0, 4.0)	(-2.8, 3.1)
POEM [31]	(51.4, 53.7)	( 0.1, 0.7)	(-1.0, 1.1)
IPWE <sub>100</sub>	(51.9, 54.5)	(-0.2, 0.5)	(-0.6, 1.9)
PIL-IML	(52.3, 53.7)	(-0.2, 0.2)	( 0.0, 0.8)
[IML]	(53.0, 55.1)	(-0.4, 0.2)	( 0.2, 2.4)
[PIL-IML]	(53.1, 55.2)	(-0.3, 0.3)	( 0.6, 2.9)

# Summary of Part II

1. Reward models are always non-realizable
  - Use a counterfactual objective!
2. Large action space, large importance weight
  - Optimize a low-variance lower bound instead!
3. Missing logging probabilities
  - You might not need them. If you do, use policy imitation!
4. Confounders
  - Can be detected using policy imitation!

# Take home messages

- Off-policy evaluation under the contextual bandits models is closely related to causal inference.
- Minimax optimality depends on assumptions, but ultimately we need estimators that are adaptive in finite sample.
- Offline policy learning is often an orthogonal problem. We can optimize a counterfactual lower bound without knowing the propensities.
- Policy imitation as a regularization and as a diagnosis tool.

# Thank you for your attention!

## Reference:

W., Agarwal, Dudik (2017) Optimal and adaptive off-policy evaluation in contextual bandits. ICML'17

Ma, W., Narayanaswamy (2018) Imitation-Regularized Offline Learning. AISTATS'19

