Off-policy Learning in Theory and in the Wild

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Based on joint works with

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

**Statistics**
- Statistical inference
- Survey design
- Survival analysis
- Experiment design

**Machine Learning**
- Online learning
- Reinforcement Learning
- Representation Learning
- Optimization

**Common Areas**
- Classification
- Regression
- Clustering
- Density estimation
- Latent variable modeling
- Bayesian modeling
- ...
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:**
  - \( x_1, \ldots, x_n \sim \lambda \) drawn iid, possibly infinite domain

- **Actions:**
  - \( a_i \sim \mu(a \mid x_i) \) Taken by a randomized “Logging” policy

- **Reward:**
  - \( r_i \sim D(r \mid x_i, a_i) \) Revealed only for the action taken

- **Value:**
  - \( V^\mu = \mathbb{E}_{x \sim \lambda} \mathbb{E}_{a \sim \mu(\cdot \mid x)} \mathbb{E}_{D} [r \mid x, a] \)

- 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 $a = \{0,1\}, \pi = [0.5,0.5]$ $\pi$ = [0.5,0.5] $\pi$ = [0.5,0.5]
- $r(\mathbf{x},a) = [2Y(\mathbf{X},T=1), -2Y(\mathbf{X},T=0)]$

- Then, the value of $\pi = ATE$
Direct Method / Regression estimator

• Fit a regression model of the reward

\[ \hat{r}(x, a) \approx \mathbb{E}(r | x, a) \] using the data

• Then for any target policy

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

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)

\[
\hat{\psi}^{\pi}_{\text{IPS}} = \frac{1}{n} \sum_{i=1}^{n} \frac{\pi(a_i | x_i)}{\mu(a_i | x_i)} r_i \]

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/Reweightd 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

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

• 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)

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

- The minimax risk

\[
\inf_{\hat{\nu}} \sup_{D(r,a|x) \in \mathcal{R}(\sigma^2, R_{\max})} \mathbb{E}(\hat{\nu} - \nu^\pi)^2
\]
Lower bounding the minimax risk

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

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

$$= \Omega \left[ \frac{1}{n} \left( \mathbb{E}_\mu [\rho^2 \sigma^2] + \mathbb{E}_\mu [\rho^2 R_{\text{max}}^2] \right) \right]$$

- Randomness in reward
- Randomness due to context distribution

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

• $n^* \text{Var}[\text{any LAN estimator}]$ is greater than:

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

Take supremum

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

• Our lower bound is bigger!

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

| Assumption: | Realizable assumption: $E[r|x,a]$ is differentiable in $x$ for each $a$. | No assumption on $E[r|x,a]$ excepts boundedness. |
|-------------|-------------------------------------------------|-------------------------------------------------|
| 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**

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

**Easy problems**: e.g., Linear $E(r|x,a)$, Smooth $E(r|x,a)$

**Hard problems**:

The class of all contextual bandits 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:

\[ \hat{\pi}_{\text{IPS}} = \frac{1}{n} \sum_{i=1}^{n} \frac{\pi(a_i | x_i)}{\mu(a_i | x_i)} r_i \]

• SWITCH estimator:

For each \( i = 1, \ldots, n \), for each action \( a \in A \):

if \( \frac{\pi(a | x_i)}{\mu(a | x_i)} \leq \tau \):

Use IPS (or DR).

else:

Use the oracle estimator.
Error bounds for SWITCH

\[
\text{MSE}(\hat{v}_{\text{SWITCH}}) \leq \frac{2}{n} \mathbb{E}_\mu \left[ (\sigma^2 + R_{\text{max}}^2) \rho^2 \mathbf{1}(\rho \leq \tau) \right] + \frac{2}{n} \mathbb{E}_\pi \left[ R_{\text{max}}^2 \mathbf{1}(\rho > \tau) \right] + \mathbb{E}_\pi \left[ \epsilon \mathbf{1}(\rho > \tau) \right]^2
\]

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

![Graph showing relative error with additional label noise](image)
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 \( \pi \)

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

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.

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

\[
\arg\min_\pi \text{CE}(\pi; r) = -\frac{1}{n} \sum_{i=1}^{n} r_i \log \pi(a_i | x_i).
\]

- 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

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

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

\[
\approx \frac{1}{n} \sum_{i=1}^{n} r_i \left( \frac{\pi(a_i | x_i)}{\mu(a_i | x_i)} - 1 \right)
\]
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 \textbf{without} having the logging probabilities!

- \textbf{Adaptive} to any unknown logging probabilities.

- We can optimize \textbf{but cannot evaluate} the lower bound!
Our solution: Imitate the policy!

\[
\text{KL}(\mu \| \pi) = \mathbb{E}_\mu \log \frac{\mu}{\pi} = -\mathbb{E}_\mu \log w. \\
\]

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 used 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
We compare three methods: PIL, PIL with DR extensions, and the original policy itself. We observed that IPW policy learning behaved similarly for realizable and misspecified models, where the solid boxes are carried over from Figure 3a, with the addition of the logging models misspecified and full-rank models realizable. As discussed earlier, Q-learning studies the biased correlation between the actions given the contexts. Therefore, IPW leads to better actions. On the other hand, Q-learning and IPW could only realize full-rank model, i.e., using a second-order model, better data for future online applications.

Figure 3a shows that Q-learning and IPW policy learning improved multiclass accuracy when trained with full knowledge of the original multiclass labels, we can further improve offline learning. (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].

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