Interactive learning via reductions

Daniel Hsu
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May 9, 2019
Simons Symposium on New Directions in Theoretical Machine Learning
Interactive learning via reductions
("How can we build on the recent success in supervised learning?")

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Interactive learning: Contextual bandits

Website operator
Interactive learning: Contextual bandits

Website operator
Loop:
1. User visits website with profile, browsing history...
2. Choose content to display on website.
3. Observe user reaction to content (e.g., click, “like”).
Interactive learning: Contextual bandits

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2. Choose content to display on website.
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Goal: choose content that yield desired user behavior.
Interactive learning: Active learning

E-mail service provider
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E-mail service provider
Loop:
1. Receive e-mail messages for users (spam or not).
2. Ask users to provide labels for some (borderline) messages.
3. Improve spam filter using newly labeled messages.
Interactive learning: Active learning

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Loop:
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3. Improve spam filter using newly labeled messages.

Goal: maximize accuracy of spam filter, minimize queries to users.
Interactive learning

1. Learning agent (a.k.a. "learner") interacts with the world (e.g., patients, users) to achieve goals and gather data.
2. Learner's performance based on chosen actions.
3. Data available to learner depends on chosen actions.
4. Efficient solutions to exploration/exploitation dilemma via reductions to supervised learning.
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Efficient solutions to exploration/exploitation dilemma via reductions to supervised learning

Rest of this talk:

1. Reductions for contextual bandits
2. Some challenges with this approach
   (an excuse to talk about generalization?)
1. Contextual bandit learning
Contextual bandit problem

For $t = 1, 2, \ldots, T$:

Nature draws $(x_t, r_t)$ from distribution $D$ over $X \times [0, 1]$.

1. Observe context $x_t \in X$. [e.g., user profile, search query]
2. Choose action $a_t \in A$. [e.g., ad to display]
3. Collect reward $r_t(a_t) \in [0, 1]$. [e.g., 1 if click, 0 otherwise]

Task: choose $a_t$'s that yield high expected reward (w.r.t. $D$).

Contextual: use features $x_t$ to choose good actions $a_t$.

Bandit: $r_t(a)$ for $a \neq a_t$ is not observed.

(Non-bandit setting: whole reward vector $r_t \in [0, 1]^A$ is observed.)
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Challenges

1. Exploration vs. exploitation
   ▶ Use what you've already learned (exploit), but also learn about actions that could be good (explore).
   ▶ Must balance to get good statistical performance.

2. Must use context
   ▶ Want to do as well as the best policy (i.e., decision rule) $\pi$: context $x \mapsto a$ from some policy class $\Pi$ (a set of decision rules).
   ▶ Computationally constrained with large $\Pi$.

3. Selection bias, especially while exploiting.
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3. **Selection bias**, especially while *exploiting*.
Learning objective

Regret (i.e., relative performance) to a policy class \( \Pi \):

\[
\max_{\pi \in \Pi} \frac{1}{T} \sum_{t=1}^{T} r_t(\pi(x_t)) - \frac{1}{T} \sum_{t=1}^{T} r_t(a_t)
\]

- average reward of best policy
- average reward of learner

Strong benchmark when \( \Pi \) has a policy w/ high expected reward.

**Goal:** regret \( \to 0 \) as fast as possible as \( T \to \infty \).
Contextual bandits via reduction to supervised learning

Let $K := |A|$ and $N := |\Pi|$.

Algorithm that operates via reduction to supervised learning (Agarwal, H., Kale, Langford, Li, & Schapire, 2014).

- Regret bound: $\tilde{O}\left(\sqrt{\frac{K \log N}{T}}\right)$.
- Near optimal statistical performance
- $\# \text{ calls to supervised learner for } \Pi$: $\tilde{O}\left(\sqrt{\frac{TK}{\log N}}\right)$.
- Uses supervised learner less than once per round
Hypothetical “full-information” setting

If we observed rewards for all actions \( r_t = (r_t(a) : a \in \mathcal{A}) \) ...
Hypothetical “full-information” setting

If we observed rewards for all actions \( r_t = (r_t(a) : a \in \mathcal{A}) \ldots \)

- Like supervised learning, have labeled data after \( t \) rounds:

\[
(x_1, r_1), \ldots, (x_t, r_t) \in \mathcal{X} \times \mathbb{R}^\mathcal{A}.
\]

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- Can often exploit structure of $\Pi$ to get tractable algorithms.

**Abstraction for supervised learning:** $\text{arg max oracle \ (AMO)}$

$$\text{AMO}\left( \{(x_i, r_i)\}_{i=1}^t \right) := \arg \max_{\pi \in \Pi} \sum_{i=1}^{t} r_i(\pi(x_i)).$$
Hypothetical “full-information” setting

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In bandit setting: use randomization + importance weighting.

Draw $a_t \sim P_t$ for some pre-specified prob. dist. $P_t$. 
Inverse propensity weighting (Horvitz & Thompson, 1952)

Importance-weighted estimate of reward from round $t$:

$$\forall a \in A. \quad \hat{r}_t(a) := \begin{cases} \frac{r_t(a_t)}{P_t(a)} & \text{if } a = a_t, \\ 0 & \text{otherwise}. \end{cases}$$

Estimate avg. reward of policy: $\hat{\text{Rew}}_t(\pi) := \frac{1}{t} \sum_{i=1}^{t} \hat{r}_i(\pi(x_i))$.

How should we choose action distribution $P_t$?
Hedging over policies

Get action distributions via policy distributions.

\[(Q, x) \rightarrow P\]

(policy distribution, context)  
action distribution
Hedging over policies

Get action distributions via policy distributions.

\[(Q, x) \mapsto P\]

(policy distribution, context) \quad \text{action distribution}

Policy distribution: \( Q = (Q(\pi) : \pi \in \Pi) \)

probability dist. over policies \( \pi \) in the policy class \( \Pi \)
Hedging over policies

Get action distributions via policy distributions.

\[(Q, x) \rightarrow P\]

(policy distribution, context) \hspace{1cm} action distribution

1: Pick initial distribution \(Q_1\) over policies \(\Pi\).
2: for round \(t = 1, 2, \ldots\) do
3: Nature draws \((x_t, r_t)\) from dist. \(D\) over \(X \times [0, 1]^A\).
4: Observe context \(x_t\).
5: Compute distribution \(P_t\) over \(A\) (using \(Q_t\) and \(x_t\)).
6: Pick action \(a_t \sim P_t\).
7: Collect reward \(r_t(a_t)\).
8: Compute new distribution \(Q_{t+1}\) over policies \(\Pi\).
9: end for
The “good policy distribution” problem

Convex feasibility problem for policy distribution $Q$

Theorem: Using feasible $Q_t$ in round $t$ $\Rightarrow$ near-optimal regret.

$\ast$ Can implement efficient “coordinate descent” solver via AMO.
The “good policy distribution” problem

**Convex feasibility problem for policy distribution $Q$**

\[
\sum_{\pi \in \Pi} Q(\pi) \cdot \hat{\text{Reg}}_t(\pi) \leq \sqrt{\frac{K \log N}{t}}
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(Low regret)
The “good policy distribution” problem

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$$\sum_{\pi \in \Pi} Q(\pi) \cdot \hat{\text{Reg}}_t(\pi) \leq \sqrt{\frac{K \log N}{t}}$$  \hspace{1cm} \text{(Low regret)}

$$\hat{\text{var}}_Q(\hat{\text{Rew}}_t(\pi)) \leq K \left(1 + \frac{\hat{\text{Reg}}_t(\pi)}{\sqrt{\frac{K \log N}{t}}} \right) \quad \forall \pi \in \Pi \hspace{1cm} \text{(Low variance)}$$
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★ Can implement efficient “coordinate descent” solver via AMO.
Implementation via AMO

Finding “low variance” constraint violation for $Q$:

$$\hat{\text{var}}_Q(\hat{\text{Rew}}_t(\pi)) \leq K \left( 1 + \frac{\hat{\text{Reg}}_t(\pi)}{\sqrt{K \log N}} \right) \quad \forall \pi \in \Pi \quad \text{(Low variance)}$$

1. Create fictitious rewards for each $i = 1, 2, \ldots, t$:

$$\tilde{r}_i(a) := K \cdot \frac{\hat{r}_i(a)}{\sqrt{K \log N}} + \frac{1}{Q(a|x_i)} \quad \forall a \in A.$$  

2. Obtain $\tilde{\pi} := \text{AMO}(\{(x_i, \tilde{r}_i)\}_{i=1}^t)$.

Fact: $\hat{\text{Rew}}_t(\tilde{\pi}) > \text{threshold}$ iff $\tilde{\pi}$’s constraint is violated.
Recap

Statistically optimal and efficient algorithm for contextual bandits by reduction to supervised learning.
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▶ Take advantage of advances in supervised learning technology (e.g., deep learning)!
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► Take advantage of advances in supervised learning technology (e.g., deep learning)!

► Similar algorithm design strategy works for active learning (Balcan, Beygelzimer, & Langford, 2006; Dasgupta, H., and Monteleoni, 2007; Beygelzimer, H., Langford, & Zhang, 2010; Zhang & Chaudhuri, 2014; Huang, Agarwal, H., Langford, and Schapire, 2015; Krishnamurthy, Agarwal, Huang, Daumé, & Langford, 2017; . . . )
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Statistically optimal and efficient algorithm for contextual bandits by reduction to supervised learning.

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So what is the catch?
2. Problems
Major impediments with current reductions

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Algorithm parameters depends critically on uniform generalization bound for policy class $\Pi$. 

▶ Used for balancing exploration & exploitation.

▶ Similar issue with active learning: generalization bounds are crucially used to measure prediction "confidence".
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Problems with uniform / \emph{a posteriori} generalization bounds

- **Uniform convergence bounds** (Vapnik & Chervonenkis, 1971): Never use (except maybe when $\log N = O(1)$).

- **Margin/norm-based generalization bounds** (e.g., Schapire, Freund, Bartlett, & Lee, 1998; Bartlett, Foster, & Telgarsky, 2017; ...): Useful for heavily-regularized models, or if observe large margin \emph{a posteriori}.

Unclear if appropriate for (say) large neural nets, at least as used in practice:

1. Find "overfitted" (interpolating) model with gradient descent.
2. **Inductive bias** (e.g., "gradient descent $\rightarrow$ least norm solution") is critical, but only part of the explanation for generalization. E.g., under what circumstances will the norm small?
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Some surprising behavior

(Belkin, H., Ma, & Mandal, 2018; Belkin, H., & Xu, 2019)

Fit two-layer neural network to training data with gradient descent.
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Mean squared error train/test on MNIST vs. # parameters

![Graph showing mean squared error for train and test data on MNIST vs. number of parameters, with a cusp indicating overfitting.](image-url)
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We prove this happens for certain “linearized” two-layer neural nets in some stylized settings. (Norm of predictor shows similar cusp.)
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Why do we observe good performance even when “overfitted”? 
Risk bounds for prediction rules that interpolate

- Most of existing theory doesn’t provide *a priori* guarantees for models that *interpolate* (noisy) training data.
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- Notable exception: **nearest neighbor** (Cover & Hart, 1967)

\[
\text{Err}(\text{NN}) \xrightarrow{n \to \infty} 2 \times \text{OPT} \quad \text{(sort of)}
\]
Risk bounds for prediction rules that interpolate

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- Notable exception: \textbf{nearest neighbor} (Cover & Hart, 1967)
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Would be great to have such results for interpolating neural nets, or even kernel machines.
Concluding remarks

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Thanks!

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3. Extra
(Sub-optimal) alternative

<table>
<thead>
<tr>
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<tbody>
<tr>
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Other alternatives: replace bounds with resampling methods (e.g., permutation tests, bootstrap). Can these be made optimal?
Simplicial interpolation

- IID training examples \((x_1, y_1), \ldots, (x_n, y_n)\) from \(\mathbb{R}^d \times [0, 1]\)
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- IID training examples \((x_1, y_1), \ldots, (x_n, y_n)\) from \(\mathbb{R}^d \times [0, 1]\)
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\[
\hat{\eta}(x) \text{ on each simplex by affine interp. of vertices' labels}
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For classification, let \(\hat{f}\) be plug-in classifier via \(\hat{\eta}\).
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Comparison to nearest neighbor

Restrict attention to a single simplex, with vertices $x_1, \ldots, x_{d+1}$.

- Suppose $\Pr(y = 1 \mid x) < 1/2$ for all points in the simplex.
- Suppose training data has $y_1 = \cdots = y_d = 0$ but $y_{d+1} = 1$ (due to noise, say).

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Nearest neighbor rule

Simplicial interpolation

$f(x) = 1$ here