Towards a Theory of Generalization in Reinforcement Learning

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Hello Harvard (and MIT)!
Progress of RL in Practice

[AlphaZero, Silver et.al, 17]

[OpenAI Five, 18]
Markov Decision Processes: a framework for RL
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• A policy: 
  \( \pi : \text{States} \rightarrow \text{Actions} \)
Markov Decision Processes: a framework for RL

- A policy: \( \pi : \text{States} \rightarrow \text{Actions} \)
- Execute \( \pi \) to obtain a trajectory:
  \[ s_0, a_0, r_0, s_1, a_1, r_1 \ldots s_{H-1}, a_{H-1}, r_{H-1} \]
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  \( s_0, a_0, r_0, s_1, a_1, r_1 \ldots s_{H-1}, a_{H-1}, r_{H-1} \)
- Cumulative \( H \)-step reward:
  \[
  \begin{align*}
  V^\pi_H(s) &= \mathbb{E}_\pi \left[ \sum_{t=0}^{H-1} r_t \mid s_0 = s \right], \\
  Q^\pi_H(s, a) &= \mathbb{E}_\pi \left[ \sum_{t=0}^{H-1} r_t \mid s_0 = s, a_0 = a \right]
  \end{align*}
  \]
Markov Decision Processes: a framework for RL

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• Cumulative \( H \)-step reward:
  \[
  V^\pi_H(s) = \mathbb{E}_\pi \left[ \sum_{t=0}^{H-1} r_t \middle| s_0 = s \right], \quad Q^\pi_H(s, a) = \mathbb{E}_\pi \left[ \sum_{t=0}^{H-1} r_t \middle| s_0 = s, a_0 = a \right]
  \]

• Goal: Find a policy \( \pi \) that maximizes our value \( V^\pi(s_0) \) from \( s_0 \).

  Episodic setting: We start at \( s_0 \); act for \( H \) steps; repeat…
Challenges in RL

![Grid with challenges in RL](image-url)
Challenges in RL

1. Exploration
   (the environment may be unknown)
Challenges in RL

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2. Credit assignment problem
   (due to delayed rewards)
Challenges in RL

1. Exploration (the environment may be unknown)

2. Credit assignment problem (due to delayed rewards)

3. Large state/action spaces:
   - hand state: joint angles/velocities
   - cube state: configuration
   - actions: forces applied to actuators
Part-0:
A Whirlwind Tour of Generalization
from Supervised Learning to RL
Provable Generalization in Supervised Learning (SL)

Generalization is possible in the IID supervised learning setting!

To get $\epsilon$-close to best in hypothesis class $\mathcal{F}$, we need # of samples that is:
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- “Occam’s Razor” Bound (finite hypothesis class): need $O(\log |\mathcal{F}|/\epsilon^2)$
Provable Generalization in Supervised Learning (SL)

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To get $\epsilon$-close to best in hypothesis class $\mathcal{F}$, we need # of samples that is:

- “Occam’s Razor” Bound (finite hypothesis class): need $O(\log |\mathcal{F}|/\epsilon^2)$
- Various Improvements:
  - VC dim $O(\text{VC}(\mathcal{F})/\epsilon^2)$; Classification (margin bounds): $O(\text{margin}/\epsilon^2)$;
    Linear regression: $O(\text{dimension}/\epsilon^2)$
  - Deep Learning: the algorithm also determines the complexity control

The key idea in SL: data reuse
With a training set, we can simultaneously evaluate the loss of all hypotheses in our class!
Sample Efficient RL in the Tabular Case (no generalization here)
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- \( S = \# \text{states}, A = \# \text{actions}, H = \# \text{horizon} \)
- We have an (unknown) MDP.

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- Thm: [Kearns & Singh ‘98] In the episodic setting, $\text{poly}(S, A, H, 1/\epsilon)$ samples suffice to find an $\epsilon$-opt policy.
  Key idea: optimism + dynamic programming
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- Lots improvements on the rate:
  [Brafman & Tennenholtz ’02][K. ’03][Auer+, ’09][Agrawal, Jia ’17][Azar+, ’13],[Dann & Brunskill ’15]

- Provable Q-learning (+bonus):
  [Strehl+ (2006)], [Szita & Szepesvari ‘10],[Jin+ ‘18]
I: Provable Generalization in RL

Q1: Can we find an $\epsilon$-opt policy with no $S$ dependence?

- How can we reuse data to estimate the value of all policies in a policy class $\mathcal{F}$?
  
  Idea: Trajectory tree algo
  
  dataset collection: uniformly at random choose actions for all $H$ steps in an episode.
  
  estimation: uses importance sampling to evaluate every $f \in \mathcal{F}$
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- Thm: [Kearns, Mansour, & Ng ’00]
  
  To find an $\epsilon$-best in class policy, the trajectory tree algo uses $O(A^H \log(|\mathcal{F}|/\epsilon^2))$ samples

"classic

pen" because

MDP is

stock."
I: Provable Generalization in RL

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  To find an $\epsilon$-best in class policy, the trajectory tree algo uses $O(A^H \log(|\mathcal{F}|)/\epsilon^2)$ samples
  
  - Only $\log(|\mathcal{F}|)$ dependence on hypothesis class size.
  
  - There are VC analogues as well.

- Can we avoid the $2^H$ dependence to find an an $\epsilon$-best-in-class policy?
  
  Agnostically, NO!

  Proof: Consider a binary tree with $2^H$-policies and a sparse reward at a leaf node.
II: Provable Generalization in RL
Q2: Can we find an $\epsilon$-opt policy with no $S, A$ dependence and $\text{poly}(H,1/\epsilon, "complexity measure")$ samples?
II: Provable Generalization in RL

- **Q2**: Can we find an $\epsilon$-opt policy with no $S, A$ dependence and $\text{poly}(H, 1/\epsilon, "complexity measure")$ samples?
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• **Q2**: Can we find an $\epsilon$-opt policy with no $S, A$ dependence and $\text{poly}(H,1/\epsilon, "complexity measure")$ samples?
  • Agnostically/best-in-class? NO.
  • With various stronger assumptions, of course.
II: Provable Generalization in RL

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What is the nature of the assumptions under which generalization in RL is possible?
(what is necessary? what is sufficient?)
Today’s Lecture

What are necessary representational and distributional conditions that permit provably sample-efficient offline reinforcement learning?
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• Part I: bandits & linear bandits
  (let’s start with horizon $H = 1$ case)
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• Part II: Lower bounds:
  Linear realizability: natural conditions to impose
  Is RL possible?
Today’s Lecture

What are **necessary representational and distributional conditions** that permit provably sample-efficient offline reinforcement learning?

- **Part I**: bandits & **linear bandits**
  (let’s start with horizon \( H = 1 \) case)

- **Part II**: **Lower bounds**:
  *Linear realizability*: natural conditions to impose
  Is RL possible?

- **Part III**: **Upper bounds**:
  Are there unifying conditions that are sufficient?
Part-1: Bandits (the $H = 1$ case)

(Let’s set the stage for RL!)
Multi-armed bandits

How should we allocate $T$ tokens to $A$ “arms” to maximize our return?

[Robins ’52, Gittins’79, Lai & Robbins ‘85 ...]
Multi-armed bandits

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• Very successful algo when $A$ is small.
• What can we do when the number of arms $A$ is large?
Dealing with the large action case

Bandits
• decision: pull an arm

Linear (RKHS) Bandits
• decision: choose some $x \in \mathcal{X}$
• e.g. $x \in R$
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• widely used generalization: The “linear bandit” model [Abe & Long+ ’99]
successful in many applications: scheduling, ads…
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• widely used generalization: The “linear bandit” model [Abe & Long+ ’99]
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• decision: $x_t$, reward: $r_t$, reward model:

\[ r_t = f(x_t) + \text{noise}, \quad f(x) = w^* \cdot \phi(x) \]
Dealing with the large action case

**Bandits**

- decision: pull an arm

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$$ r_t = f(x_t) + \text{noise}, \quad f(x) = w^* \cdot \phi(x) $$

- Hypothesis class $\mathcal{F}$ is set of linear/RKHS functions
Linear-UCB/GP-UCB:
Algorithmic Principle: Optimism in the face of uncertainty

Pick input that maximizes upper confidence bound:

$$x_t = \arg \max_{x \in D} \mu_{t-1}(x) + \beta_t \sigma_{t-1}(x)$$
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How should we choose \( \beta_t \)?
Theorem: [Dani, Hayes, & K. ’08], [Srinivas, Krause, K. & Seeger '10]
Assuming $\mathcal{F}$ is an RKHS (with bounded norm), if we choose $\beta_t$ “correctly”,

$$
\frac{1}{T} \sum_{t=1}^{T} [f(x^*) - f(x_t)] = O^* \left( \sqrt{\frac{\gamma_T}{T}} \right)
$$

where $\gamma_T := \max_{x_0 \ldots x_{T-1} \in \mathcal{X}} \log \det \left( I + \sum_{t=0}^{T-1} \phi(x_t)\phi(x_t)^T \right)$
Regret of Lin-UCB/GP-UCB

(Generalization in action space)

**Theorem:** [Dani, Hayes, & K. ’08], [Srinivas, Krause, K. & Seeger '10]

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\frac{1}{T} \sum_{t=1}^{T} \left[ f(x^*) - f(x_t) \right] = \mathcal{O}^* \left( \sqrt{\frac{\gamma_T}{T}} \right) \leq \sqrt{\frac{d}{T}}
$$

where $\gamma_T := \max_{x_0, \ldots, x_{T-1} \in \mathcal{X}} \log \det \left( I + \sum_{t=0}^{T-1} \phi(x_t)\phi(x_t)^T \right)$

- **Key complexity concept:** “**maximum information gain**” $\gamma_T$ determines the regret
  - $\gamma_T \approx d \log T$ for $\phi$ in $d$-dimensions
  - Think of $\gamma_T$ as the “effective dimension”
- **Easy to incorporate context**
- Also: [Auer+ ’02; Abbasi-Yadkori+ ’11]
Switch
(LinUCB analysis)
Part-2: RL
What are necessary conditions?
Let’s look at the most natural assumptions.
Approx. Dynamic Programming with Linear Function Approximation
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Basic idea: approximate the $Q(s, a)$ values with linear basis functions $\phi_1(s, a), \ldots, \phi_d(s, a)$. (where $d \ll \#\text{states, \#actions}$)
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- Lots of work on this approach, e.g. [Tesauro, '95], [de Farias & Van Roy '03], [Wen & Van Roy '13]
Approx. Dynamic Programming

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$$E[r_t | a_t] = \sum_{i=1}^{d} \phi_i(s_t, a_t)$$

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What conditions must our basis functions (our representations) satisfy in order for his approach to work?
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What conditions must our basis functions (our representations) satisfy in order for his approach to work?

- Let’s look at the most basic question with “linearly realizable $Q^*$”
RL with Linearly Realizable $Q^*$-Function Approximation
(Does there exist a sample efficient algo?)
RL with Linearly Realizable Q*-Function Approximation
(Does there exist a sample efficient algo?)

• Suppose we have a feature map: $\vec{\phi}(s, a) \in \mathbb{R}^d$. 
RL with Linearly Realizable Q*-Function Approximation
(Does there exist a sample efficient algo?)

• Suppose we have a feature map: \( \vec{\phi}(s, a) \in R^d \).

• (A1: Linearly Realizable Q*): Assume for all \( s, a, h \in [H] \), there exists \( w_1^*, \ldots w_H^* \in R^d \) s.t.

\[
Q_h^*(s, a) = w_h^* \cdot \phi(s, a)
\]

\[
\hat{Q}_h^*(s) = \arg \max_a Q_h^*(s, a)
\]
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• Aside: the linear programing viewpoint.
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• Aside: the linear programming viewpoint.
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  • The LP is not general because it encodes the Bellman optimality constraints.
  • We have sampling access (in the episodic setting).
Linearly Realizability is Not Sufficient for RL
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Theorem:
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• [Weisz, Amortila, Szepesvári ‘21]:

There exists an MDP and a \( \phi \) satisfying A1 s.t any online RL algorithm (with knowledge of \( \phi \)) requires \( \Omega(\min(2^d,2^H)) \) samples to output the value \( V^*(s_0) \) up to constant additive error (with prob. \( \geq 0.9 \)).
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• [Wang, Wang, K. ‘21]:
  Let’s make the problem even easier, where we also assume:
  A2 (Large Suboptimality Gap): for all $a \neq \pi^*(s)$, $V^*_h(s) - Q^*_h(s, a) \geq 1/16$.
  The lower bound holds even with both A1 and A2.
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Comments: An exponential separation between online RL vs simulation access.

[Du, K., Wang, Yang ‘20]: A1+A2+simulator access (input: any $s, a$; output: $s' \sim P(\cdot | s, a), r(s,a)$)
$\implies$ there is sample efficient approach to find an $\epsilon$-opt policy.
Construction Sketch: a Hard MDP Family
(A “leaking complete graph”)

\[ h = 1 \quad 2 \quad 3 \]

\[ H \]
Construction Sketch: a Hard MDP Family

(A "leaking complete graph")

- \( m \) is an integer (we will set \( m \approx 2^d \))
Construction Sketch: a Hard MDP Family

(A "leaking complete graph")

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- the state space: \{\overline{1}, \ldots, \overline{m}, f\}
Construction Sketch: a Hard MDP Family
(A "leaking complete graph")

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- call the special state $\bar{f}$ a "terminal state".
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- call the special state $f$ a "terminal state".
- at state $\bar{i}$, the feasible actions set is $[m] \setminus \{i\}$
  at $f$, the feasible action set is $[m - 1]$.
  i.e. there are $m - 1$ feasible actions at each state.
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- each MDP in this family is specified by an index $a^* \in [m]$ and denoted by $M_{a^*}$.
  i.e. there are $m$ MDPs in this family.
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Lemma: For any $\gamma > 0$, there exist $m = \lceil \exp\left(\frac{1}{8}\gamma^2 d\right) \rceil$ unit vectors $\{v_1, \ldots, v_m\}$
in $\mathbb{R}^d$ s.t. $\forall i, j \in [m]$ and $i \neq j$, $|\langle v_i, v_j \rangle| \leq \gamma$.

We will set $\gamma = 1/4$.
(proof: Johnson-Lindenstrauss)
The construction, continued
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- **Transitions:** $s_0 \sim \text{Uniform}([m])$.
  
  $\Pr[f | \overline{a_1}, a^*] = 1,$

  $\Pr[ \cdot | \overline{a_1}, a_2] = \begin{cases} 
  \overline{a_2} : \left \langle v(a_1), v(a_2) \right \rangle + 2\gamma, & (a_2 \neq a^*, a_2 \neq a_1) \\
  f : 1 - \left \langle v(a_1), v(a_2) \right \rangle - 2\gamma 
  \end{cases}$

  $\Pr[f | f, \cdot ] = 1.$
The construction, continued

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  \[ \Pr[f | \overline{a_1}, a^*] = 1, \]

  \[ \Pr[\cdot | \overline{a_1}, a_2] = \begin{cases} 
  \overline{a_2} : \langle v(a_1), v(a_2) \rangle + 2\gamma 
  , (a_2 \neq a^*, a_2 \neq a_1) 
  
  f : 1 - \langle v(a_1), v(a_2) \rangle - 2\gamma 
  \end{cases} \]

  \[ \Pr[f | f, \cdot ] = 1. \]

- After taking action $a_2$, the next state is either $\overline{a_2}$ or $f$.
  This MDP looks like a "leaking complete graph".
The construction, continued

- **Transitions**: $s_0 \sim \text{Uniform}([m])$.
  \[
  \Pr[f|\overline{a_1}, a^*] = 1,
  \]

\[
\Pr[\cdot|\overline{a_1}, a_2] = \begin{cases} 
\overline{a_2} : \langle v(a_1), v(a_2) \rangle + 2\gamma, & (a_2 \neq a^*, a_2 \neq a_1) \\
 f : 1 - \langle v(a_1), v(a_2) \rangle - 2\gamma 
\end{cases}
\]

\[
\Pr[f|f, \cdot] = 1.
\]

- After taking action $a_2$, the next state is either $\overline{a_2}$ or $f$. This MDP looks like a "leaking complete graph".
- It is possible to visit any other state (except for $\overline{a^*}$); however, there is at least $1 - 3\gamma = 1/4$ probability of going to the terminal state $f$. 

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\end{cases}
\]
The construction, continued

- **Transitions:** \( s_0 \sim \text{Uniform}([m]) \).
  \[
  \Pr[f | \overline{a}_1, a^*] = 1, \quad \frac{1}{4} \leq \gamma \leq \frac{3}{4}
  \]
  \[
  \Pr[ \cdot | \overline{a}_1, a_2] = \begin{cases} 
  \overline{a}_2 : \langle v(a_1), v(a_2) \rangle + 2\gamma \\
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- After taking action \( a_2 \), the next state is either \( \overline{a}_2 \) or \( f \).
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- The transition probabilities are indeed valid, because
  \[
  0 < \gamma \leq \left\langle v(a_1), v(a_2) \right\rangle + 2\gamma \leq 3\gamma < 1.
  \]
The construction, continued
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- **Features:** of dimension $d$ defined as:

  $\phi(\overline{a_1}, a_2) := \left( \langle v(a_1), v(a_2) \rangle + 2\gamma \right) \cdot v(a_2), \quad \forall a_1 \neq a_2$

  $\phi(f, \cdot) := 0$

  note: the feature map does not depend of $a^*$. 

\[\begin{array}{cccc}
\overline{1} & \overline{2} & \overline{3} & \vdots \\
\overline{3} & \overline{3} & \overline{3} & \vdots \\
\overline{m} & \overline{m} & \overline{m} & \vdots \\
\overline{f} & \overline{f} & \overline{f} & \vdots \\
h = 1 & 2 & 3 & H \\
\end{array}\]
The construction, continued

- **Features:** of dimension $d$ defined as:
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  \]
  \[
  \phi(f, \cdot) := 0
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  note: the feature map does not depend of $a^*$.

- **Rewards:**
  for $1 \leq h < H$,
  \[
  R_h(\overline{a}_1, a^*) := \langle v(a_1), v(a^*) \rangle + 2\gamma,
  \]
  \[
  R_h(\overline{a}_1, a_2) := -2\gamma \left[ \langle v(a_1), v(a_2) \rangle + 2\gamma \right], \quad a_2 \neq a^*, a_2 \neq a_1
  \]
  \[
  R_h(f, \cdot) := 0.
  \]
  for $h = H$,
  \[
  r_H(s, a) := \langle \phi(s, a), v(a^*) \rangle
  \]
Verifying the Assumptions: Realizability and the Large Gap
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Lemma: For all $(s, a)$, we have $Q_h^*(s, a) = \langle \phi(s, a), v(a^*) \rangle$ and the “gap” is $\geq \gamma/4$. 
Verifying the Assumptions: Realizability and the Large Gap

**Lemma:** For all $(s, a)$, we have $Q^*_h(s, a) = \langle \phi(s, a), \nu(a^*) \rangle$ and the “gap” is $\geq \gamma/4$.

**Proof:** throughout $a_2 \neq a^*$
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Proof: throughout \(a_2 \neq a^*\)

- First, let’s verify \(Q^\pi(s, a) = \langle \phi(s, a), v(a^*) \rangle\) is the value of the policy \(\pi(a) = a^*\).

  By induction, we can show:

  \[
  Q_h^\pi(a_1, a_2) = \left( \langle v(a_1), v(a_2) \rangle + 2\gamma \right) \cdot \langle v(a_2), v(a^*) \rangle, \\
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- Proving optimality: for \(a_2 \neq a^*, a_1\)
  \[
  Q^\pi_h(\overline{a}_1, a_2) \leq 3\gamma^2, \quad Q^\pi_h(\overline{a}_1, a^*) = \langle v(a_1), v(a^*) \rangle + 2\gamma \geq \gamma > 3\gamma^2
  \]

\(\Rightarrow\) \(\pi\) is optimal
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  \[
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  \]

- Proving the large gap: for \(a_2 \neq a^*\)
  \[
  V^*_h(a_1) - Q^*_h(a_1, a_2) = Q^\pi_h(a_1, a^*) - Q^\pi_h(a_1, a_2) > \gamma - 3\gamma^2 \geq \frac{1}{4\gamma}.
  \]
The information theoretic proof:
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Proof: When is info revealed about $M_{a^*}$, indexed by $a^*$?
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- But there is always at least $1/4$ chance of moving to $f$
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Open Problem: Can we prove a lower bound with $A = 2$ actions?
Interlude:
Are these issues relevant in practice?
These Representational Issues are Relevant for Practice!

(related concepts: distribution shift, “the deadly triad”, offline RL)
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Theorem [Wang, Foster, K., ’20]:
Analogue for “offline” RL: linear realizability is also not sufficient.
These Representational Issues are Relevant for Practice!
(related concepts: distribution shift, “the deadly triad”, offline RL)

Theorem [Wang, Foster, K., ’20]:
Analogue for “offline” RL: linearity is also not sufficient.
Practice: [Wang, Wu, Salakhutdinov, K., 2021]:
Does it matter in practice? Say given good ““deep-pre-trained- features”? YES!

Offline dataset is a mix of two sources:
running & random

Use SL to evaluate the running policy with “deep-pre-trained- features”
Massive error amplification even with 50/50% mixed offline data
Part-3:
What are sufficient conditions?
Is there a common theme to positive results?
Provable Generalization in RL

Can we find an $\epsilon$-opt policy with no $S,A$ dependence and $\text{poly}(H,1/\epsilon, "\text{complexity measure"})$ samples?
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Agnostically/best-in-class? NO.
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- With various stronger assumptions, YES! Many special cases:
  - Linear Bellman Completion: [Munos, ’05, Zanette+ ‘19]
    - Linear MDPs: [Wang & Yang’18]; [Jin+ ’19] (the transition matrix is low rank)
    - Linear Quadratic Regulators (LQR): standard control theory model
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  - almost: **Bellman rank** [Jiang+ ‘17]; **Witness rank** [Wen+ ’19]
Intuition: properties of linear bandits
(back to $H = 1$ RL problem)
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An important structural property:

• **Data reuse:** difference between $f$ and $r$ is estimable when playing $\pi_g$  
  
  \[
  E_{a \sim \pi_g} [f(s, a) - r] = \langle w(f) - w^*, E_{\pi_g} [\phi(s, a)] \rangle
  \]
Special case: linear Bellman complete classes
(stronger conditions over linear realizability)
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  \[
  E_{\pi_g}[Q_f(s_h, a_h) - r(s_h, a_h) - V_f(s_{h+1})] \leq \langle w_h(f) - \mathcal{T}(w_h(f)), E_{\pi_g}[\phi(s_h, a_h)] \rangle
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  (where expectation is with respect to trajectories under \( \pi_g \))
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- (recall) Bellman optimality: suppose \( Q^* - \mathcal{T}(Q^*) = 0 \)
BiLinear Regret Classes: structural properties to enable generalization in RL
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• Hypothesis class: \( \{ f \in \mathcal{F} \} \),
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  \]

• Data reuse: there is function \( \ell_f(s, a, s', g) \) s.t.
  \[
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Theorem: Structural Commonalities and Bilinear Classes
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- Theorem: [Du, K., Lee, Lovett, Mahajan, Sun, Wang ’19]
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- Bilinear classes generalize the: **Bellman rank** [Jiang+ ‘17]; **Witness rank** [Wen+ ’19]
- The framework easily leads to new models (see paper).
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- **return**: the best policy $\pi_f$ found
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Theorem: [Du, K., Lee, Lovett, Mahajan, Sun, Wang ’19]
Assume $\mathcal{F}$ is a bilinear class and the class is realizable, i.e. $Q^* \in \mathcal{F}$. Using $\gamma_T^3 \cdot poly(H) \cdot \log(1/\delta)/\epsilon^2$ trajectories, the BiLin-UCB algorithm returns an $\epsilon$-opt policy (with prob. $\geq 1 - \delta$).
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- again, $\gamma_T$ is the max. info. gain $\gamma_T := \max_{f_0 \ldots f_{T-1} \in \mathcal{F}} \ln \det \left( I + \frac{1}{\lambda} \sum_{t=0}^{T-1} \Phi(f_t)\Phi(f_t)^T \right)$
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- The proof is “elementary” using the elliptical potential function. [Dani, Hayes, K. ’08]
Thanks!

- A generalization theory in RL is possible and different from SL!
  - necessary: linear realizability insufficient. need much stronger assumptions.
  - sufficient: lin. bandit theory → RL theory (bilinear classes) is rich.
    - covers known cases and new cases
  - practice: these issues are relevant ("deadly triad"/RL can be unstable)

See https://rltheorybook.github.io/ for forthcoming book!