RLChina 2021

Sample Efficiency in Online RL

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Princeton $\longrightarrow$ Yale (2022)

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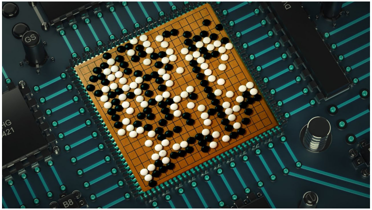
Motivation: sample complexity challenge in deep RL

Success and challenge of deep RL

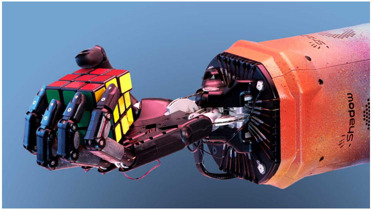
DRL = Representation (DL) + Decision Making (RL)

board games



computer games

robotic control



policy making

image source: Deepmind, OpenAI, Salesforce Research.

Success and challenge of deep RL

- AlphaGo: 3×10^7 games of self-play (data), 40 days of training (computation)
- AlphaStar: 2×10^2 years of self-play, 44 days of training
- Rubik's Cube: 10^4 years of simulation, 10 days of training

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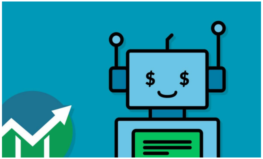
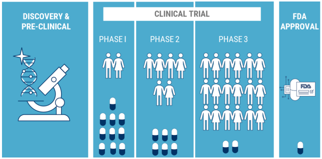
Massive Data Needed → Insufficient Data

↓

Massive Computation → Lack of Convergence

Insufficient Data, Lack of Convergence → **Unreliable AI**



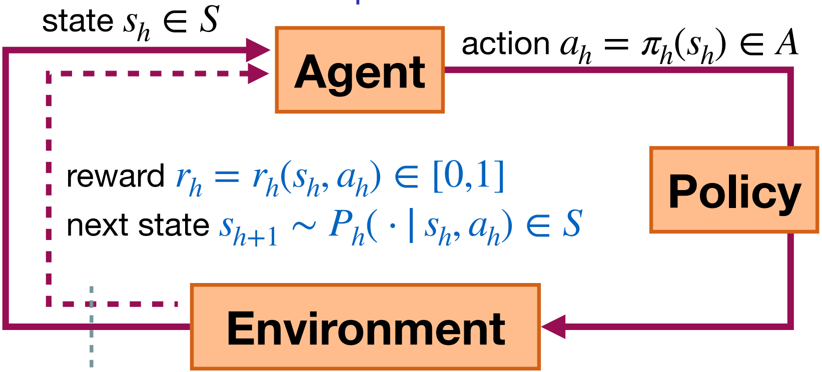


Our goal: provably efficient RL algorithms

- Sample efficiency: how many data points needed?
- Computational efficiency: how much computation needed?
- Function approximation: allow infinite number of observations?

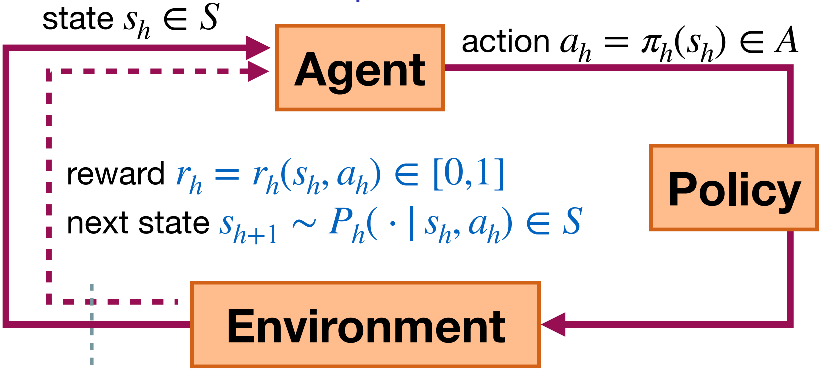
Background: Episodic Markov decision process

Episodic Markov decision process



- For $h \in [H]$, in the h-th step, observe state s_h, takes action a_h
- Receive immediate reward r_h, $\mathbb{E}[r_h | s_h = s, a_h = a] = r_h(s, a)$
- Environment evolves to a new state $s_{h+1} \sim P_h(\cdot | s_h, a_h)$

Episodic Markov decision process



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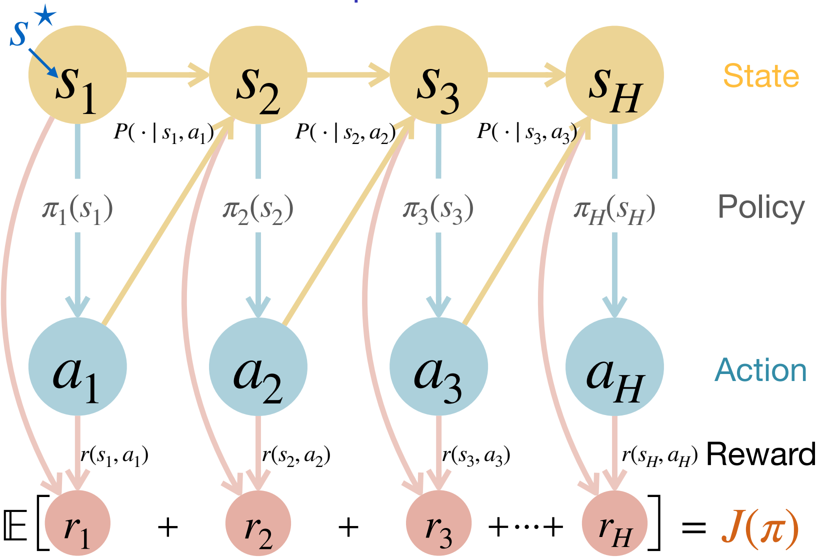
- Environment evolves to a new state $s_{h+1} \sim P_h(\cdot | s_h, a_h)$
- Policy $\pi_h \colon \mathcal{S} \to \mathcal{A}$: how agent takes action at h-th step
- Goal: find the policy $\pi^\star$ that maximizes $J(\pi) := \mathbb{E}_\pi[\sum_{h=1}^H r_h]$

Episodic Markov decision process



For simplicity, fix $s_1 = s^\star$, $r_h = r$, $P_h = P$ for all h.

Contextual bandit is a special case of MDP

- Contextual bandit (CB): observe context $s \in \mathcal{A}$, take action $a \in \mathcal{A}$, observe (random) reward r with mean $r^\star(s, a)$
- Optimal policy $\pi^\star(s) = \arg\max_{a \in \mathcal{A}} r^\star(s, a)$

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- Optimal policy $\pi^\star(s) = \arg\max_{a \in \mathcal{A}} r^\star(s, a)$
- CB is a MDP with $H = 1$
- Multi-armed bandit (MAB): $H = 1$, $|A|$ finite, and $|\mathcal{S}| = 1$

MDP is significantly **more challenging** than CB due to **temporal dependency** (i.e., state transitions)

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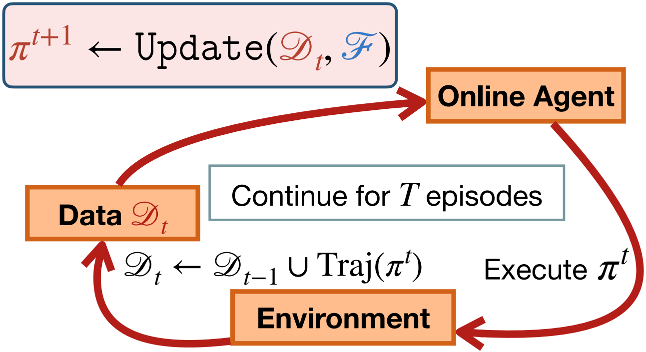
(i)	learning from model	query complexity
(ii)	learning from data	sample complexity
(iii)	learning by doing	sample complexity + exploration

Online RL: Pipeline



- Initialize $\pi^1 = \{\pi_h^1\}_{h \in [H]}$ arbitrarily
- For each $t \in [T]$, execute π^t, get a trajectory $\mathrm{Traj}(\pi^t)$
- Store $\mathrm{Traj}(\pi^t)$ into dataset $\mathcal{D}_t = \{\mathrm{Traj}(\pi^i), i \le t\}$
- Update the policy via RL algorithm (need our design)

Sample efficiency in online RL: regret

- Measure sample efficiency via regret:

$$\texttt{Regret}(T) = \sum_{t=1}^{T} \underbrace{[J(\pi^\star) - J(\pi^t)]}_{\text{suboptimality in } t\text{-th episode}}$$

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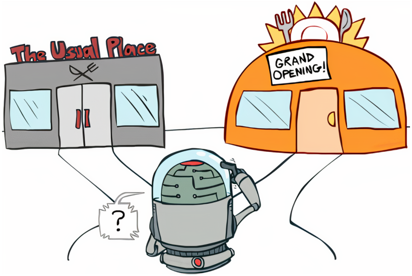
  - If $\texttt{Regret}(T) = o(T)$, when T sufficiency large, $\widetilde{\pi}^T$ is arbitrarily close to optimality
- Goal: $\texttt{Regret}(T) = \widetilde{\mathcal{O}}\big(\sqrt{T} \cdot \mathrm{poly}(H) \cdot \mathrm{poly}(\mathrm{dim})\big)$

Challenge of Online RL: exploration & uncertainty



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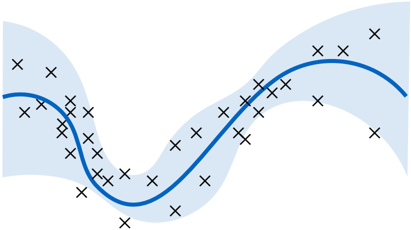

function estimation

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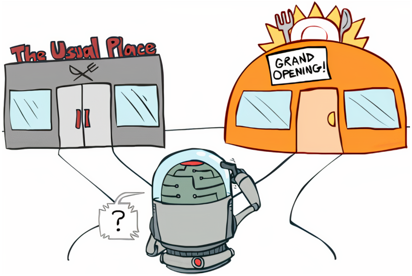

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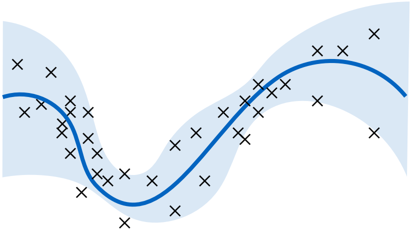

function estimation

How to assess estimation uncertainty based on adaptively acquired data?

Deep Exploration **Online RL** **Function Estimation**

How to construct exploration incentives tailored to function approximators?

Warmup example:
LinUCB for linear CB

Linear contextual bandit

- Setting of linear CB:
  - Observation structure: observe (perhaps adversarial) $s^t \in \mathcal{S}$, take action $a^t \in \mathcal{A}$, receive bounded reward $r^t \in [0, 1]$
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- Normalization condition: $\|\theta^\star\|_2 \leq \sqrt{d}$, $\sup_{s,a} \|\phi(s, a)\|_2 \leq 1$
  - Why? Include MAB as a special case: $|\mathcal{S}| = 1$, $d = |A|$, $\phi(s, a) = \mathbf{e}_a$, $\theta^\star = (\mu_1, \mu_2, \cdots, \mu_A)$ with $\mu_a \in [0, 1]$ for all $a \in \mathcal{A}$

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Intuition of OFU principle

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- $|r^{+,t}(s,a) - r^{-,t}(s,a)|$ reflects the uncertainty about a at context s
- By (2), $a^t = \arg\max_a r^{+,t}(s^t,a)$ — choose the action with either large uncertainty (explore) or large reward (exploit)

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- Define Θ^t as the *confidence ellipsoid*:

$$\Theta^t = \{\theta \in \mathbb{R}^d : \|\theta - \widehat{\theta}^t\|_{\Lambda^t} \le \beta\},$$

here define $\beta = C \cdot \sqrt{d \cdot \log(1 + T/\delta)}$, $\|x\|_M = \sqrt{x^\top M x}$

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  - For $t = 1, \dots, T$, in the beginning of t-th round
  - Observe context s_t
  - Compute $\widehat{\theta}^t$ via ridge regression and compute Hessian Λ^t
  - Choose $a^t = \arg\max_{a \in \mathcal{A}} r^{+,t}(s^t, a)$ and observe r^t

Regret Bound of LinUCB

Theorem. With probability $1 - \delta$, LinUCB satisfies

$$\texttt{Regret}(T) \leq \beta \cdot \sqrt{dT} \cdot \sqrt{\log T} = \widetilde{\mathcal{O}}(d\sqrt{T})$$

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- Independent of the size of context and action spaces, only depends on the dimension (linear in d)
- Depend on T through $\sqrt{T}$ (sample efficient)
- Computational cost $\mathrm{poly}(d, A, T)$ and memory requirement is $\mathrm{poly}(d, T)$ (Why?)

Regret Analysis of LinUCB (1/3)

Step 1. Conditioning on the event $\mathcal{E} = \{\forall t \in [T], \theta^\star \in \Theta^t\}$,
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Step 2. Regret decomposition:

$$
\begin{aligned}
&\max_a r^\star(s^t, a) - r^\star(s^t, a^t) \\
&\qquad = \left(\max_a r^\star(s^t, a) - r^{+,t}(s^t, a^t)\right) + \left(r^{+,t}(s^t, a^t) - r^\star(s^t, a^t)\right) \\
&\qquad \leq r^{+,t}(s^t, a^t) - r^{-,t}(s^t, a^t) \leq 2\beta \cdot \|\phi(s^t, a^t)\|_{(\Lambda^t)^{-1}}
\end{aligned}
$$

Regret Analysis of LinUCB (1/3)

Step 1. Conditioning on the event $\mathcal{E} = \{\forall t \in [T], \theta^\star \in \Theta^t\}$, $r^{-,t}(s,a) \leq r^\star(s,a) \leq r^{+,t}(s,a), \forall (x,a) \in \mathcal{S} \times \mathcal{A}$

Step 2. Regret decomposition:

$$\begin{aligned}
&\max_a r^\star(s^t,a) - r^\star(s^t,a^t) \\
&\qquad = \big(\max_a r^\star(s^t,a) - r^{+,t}(s^t,a^t)\big) + \big(r^{+,t}(s^t,a^t) - r^\star(s^t,a^t)\big) \\
&\qquad \leq r^{+,t}(s^t,a^t) - r^{-,t}(s^t,a^t) \leq 2\beta \cdot \|\phi(s^t,a^t)\|_{(\Lambda^t)^{-1}}
\end{aligned}$$

Thus we have shown

$$\max_a r^\star(s^t,a) - r^\star(s^t,a^t) \leq \beta \cdot \min\{1, \|\phi(s^t,a^t)\|_{(\Lambda^t)^{-1}}\}$$

Regret Analysis of LinUCB (2/3)

Step 3. Telescope the bonus: Cauchy-Schwarz + elliptical potential lemma

$$
\begin{aligned}
\texttt{Regret}(T) &\le 2\beta \cdot \sum_{t=1}^{T} \cdot \min\{1, \|\phi(s^t, a^t)\|_{(\Lambda^t)^{-1}}\} \\
&\le 2\beta\sqrt{T} \cdot \left[\sum_{t=1}^{T} \min\{1, \|\phi(s^t, a^t)\|^2_{(\Lambda^t)^{-1}}\} \right]^{1/2} \\
&\le 2\beta\sqrt{T} \cdot \sqrt{2 \mathrm{logdet}(\Lambda_T)} \lesssim \beta \cdot \sqrt{T} \cdot \sqrt{d \cdot \log T}
\end{aligned}
$$

Elliptical potential lemma

Lemma

$$\sum_{i=1}^{t-1} \min\{1, \|\phi(s^i, a^i)\|^2_{(\Lambda^t)^{-1}}\} \leq 2\mathrm{logdet}(\Lambda_T) \leq d \cdot \log T$$

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Bayesian perspective:

- Prior distribution $\theta^\star \sim N(0, I)$
- Likelihood $r_i = r^\star(s^i, a^i) + \varepsilon$, $\varepsilon \in N(0, 1)$
- Given dataset $\mathcal{D}_{t-1}$, the posterior distribution is $N(\widehat{\theta}^t, \Lambda^t)$

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- Given dataset $\mathcal{D}_{t-1}$, the posterior distribution is $N(\widehat{\theta}^t, \Lambda^t)$
- $\|\phi(s, a)\|^2_{(\Lambda^t)^{-1}} = I(\theta^\star, (s, a)|\mathcal{D}_{t-1}) = H(\theta^\star|\mathcal{D}_{t-1}) - H(\theta^\star|\mathcal{D}_{t-1} \cup \{(s, a)\})$ — conditional mutual information gain
- Elliptical potential lemma $\leftrightarrow$ chain rule of mutual information

Regret Analysis of LinUCB (3/3)

Step 4. Show optimism: $\theta^\star \in \Theta^t = \{\theta \in \mathbb{R}^d : \|\theta - \widehat{\theta}^t\|_{\Lambda^t} \leq \beta\}$

$$\theta^t - \theta^\star = (\Lambda^t)^{-1}\left[\sum_{i=1}^{t-1} \underbrace{(r^\star(s^i, a^i) + \varepsilon_i)}_{r_i} \cdot \phi(s^i, a^i) - (\Lambda^t) \cdot \theta^\star\right]$$

$$= (\Lambda^t)^{-1}\theta^\star + (\Lambda^t)^{-1} \sum_{i=1}^{t-1} \underbrace{\varepsilon_i}_{\text{martingale difference}} \cdot \phi(s^i, a^i)$$

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- $\|\theta^t - \theta^\star\|_{\Lambda^t} \approx \| \sum_{i=1}^{t-1} \varepsilon_i \cdot \phi(s^i, a^i)\|_{(\Lambda^t)^{-1}} \leq \beta$
- Concentration of self-normalized process (e.g., Abbasi-Yadkori et al, 2011)

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- Algorithm is based on the optimism principle
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  a. utilize optimism to bound instant regret by width of confidence region (bonus)
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  c. confidence region constructed via uncertainty quantification for ridge regression
- Extensions: generalized linear model, RKHS, overparameterized network, abstract function class with bounded eluder dimension, ...

From Linear CB to Linear RL

Value functions and Bellman equation

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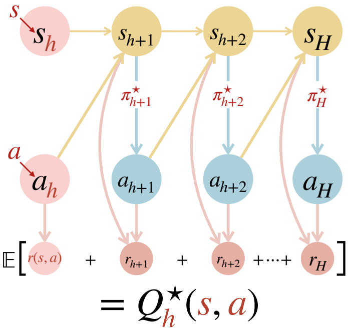
  - $Q_h^\star(s,a)$: optimal return starting from $s_h = s$ and $a_h = a$
  - $Q^\star$ is characterized by Bellman equation



- $\pi_h^\star(s) = \arg\max_a Q_h^\star(s,\cdot)$
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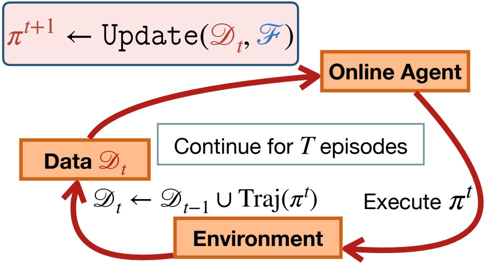
- RL with linear function approximation: use $\mathcal{F}_{\texttt{lin}} = \{\phi(s,a)^\top\theta \colon \mathcal{S}\times\mathcal{A}\to\mathbb{R}\}$ to approximate $\{Q^\star_h\}_{h\in[H]}$
  - $\phi\colon \mathcal{S}\times\mathcal{A}\to\mathbb{R}^d$: known feature mapping
  - Can allow known and step-varying features: $\{\phi_h\}_{h\in[H]}$

RL is more challenging than bandit



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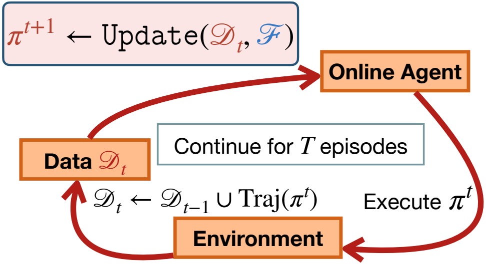

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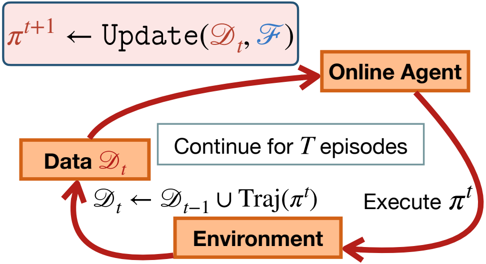

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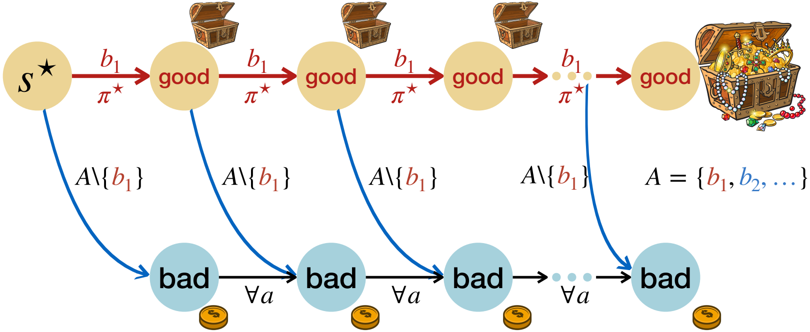
- Online RL $\neq$ a contextual bandit with TH rounds

> RL requires **deep exploration** for achieving $o(T)$ regret.

Deep Exploration



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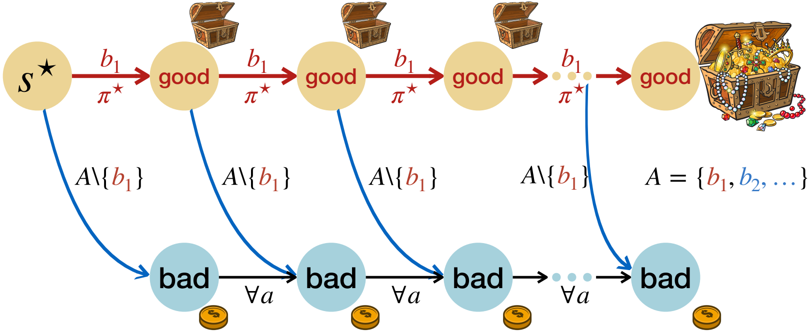

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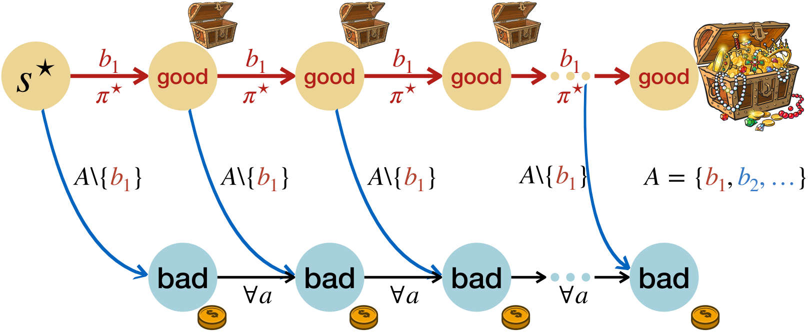

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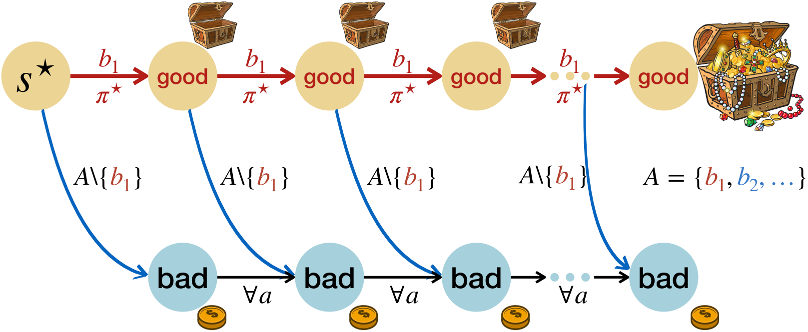

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- $\mathcal{O}(SAH)$ query complexity if have a generative model

What assumption should we impose?

- In CB, $\pi^\star$ is greedy with respect to $r^\star$, we assume $r^\star$ is linear
- In RL, $\pi^\star$ is greedy with respect to $Q^\star$
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> **Theorem** [Wang-Wang-Kakade-21] There exists a class of linearly realizable MDPs such that any online RL algorithm requires $\min\{\Omega(2^d), \Omega(2^H)\}$ samples to obtain a near optimal policy.

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  Theorem [Wang-Wang-Kakade-21] There exists a class of linearly realizable MDPs such that any online RL algorithm requires $\min\{\Omega(2^d), \Omega(2^H)\}$ samples to obtain a near optimal policy.

- Fundamentally different from supervised learning and bandits
- To achieve efficiency in online RL, we need stronger assumptions

Assumption: $\mathrm{Image}(\mathcal{B}) \subseteq \mathcal{F}_{\mathrm{lin}}$

- We assume the image set of the Bellman operator lies in $\mathcal{F}_{\mathrm{lin}}$:

For any $Q\colon \mathcal{S} \times \mathcal{A} \to [0, H]$, there exists $\theta^Q \in \mathbb{R}^d$ s.t.

$$(\mathcal{B}Q)(s,a) = r(s,a) + \mathbb{E}[\max_{a'} Q(s',a')] = \langle \phi(s,a), \theta^Q \rangle$$

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- Is there such an MDP? Yes, Linear MDP

> $r(s, a) \ = \ \langle \phi(s, a), \boldsymbol{\omega} \rangle \qquad P(s'|s, a) \ = \ \langle \phi(s, a), \boldsymbol{\mu}(s') \rangle$
> Normalization: $\|\boldsymbol{\omega}\|_2 \leq \sqrt{d}$, $\sum_{s'} \|\boldsymbol{\mu}(s')\|_2 \leq \sqrt{d}$

- Linear MDP contains tabular MDP as a special case: $\phi(s, a) = \mathbf{e}_{(s,a)}$, $d = |\mathcal{S}| \cdot |\mathcal{A}|$

Algorithm for linear RL: LSVI-UCB

Algorithm: LSVI + optimism

- In the beginning t-th episode, dataset $\mathcal{D}_{t-1} = \{(s_h^i, a_h^i, r_h^i), h \in [H]\}_{i<t}$

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$$y_h^i = r_h^i + \max_a Q_{h+1}^{+,t}(s_{h+1}, a)$$

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- UCB Q-function

$$Q_h^{+,t} = \mathrm{Trunc}_{[0,H]}\{\langle \phi(s, a), \widehat{\theta}_h^t \rangle + \Gamma_h^t(s, a)\}$$

- Execute $\pi_h^t(\cdot) = \arg\max_a Q_h^{+,t}(\cdot, a)$

A more abstract version of LSVI-UCB

- For $h = H, \ldots, 1$, backwardly solve least-squares regression:

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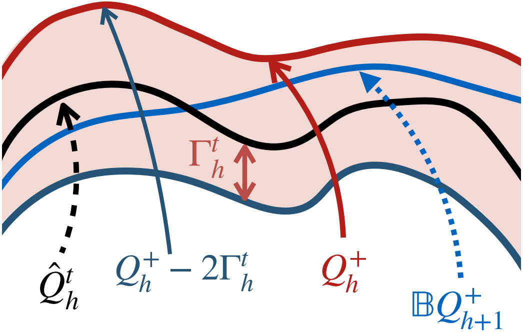
- Computation & memory cost independent of $|\mathcal{S}|$ (even for RKHS, overparameterized NN)

A more abstract version of LSVI-UCB



$$|\hat{Q}_h^t(s,a) - (\mathbb{B}Q_{h+1}^+)(s,a)| \le \Gamma_h^t(s,a), \ \forall t, h, s, a$$

$$Q_h^+(s,a) = \underbrace{\hat{Q}_h^t(s,a)}_{\text{LSVI}} + \underbrace{\Gamma_h^t(s,a)}_{\text{bonus}}$$

- Optimism gives: $\mathcal{B}Q_{h+1}^+ \in [Q_h^+ - 2\Gamma_h^t, Q_h^+]$
- Monotonicity of Bellman operator: $Q_h^+ \ge Q_h^\star$ (UCB)

Sample efficiency of LSVI-UCB

LSVI-UCB achieves $\sqrt{T}$-regret

Theorem [Jin-Yang-Wang-Jordan-20] Choosing $\beta = \widetilde{\mathcal{O}}(dH)$, with probability at least $1 - 1/T$,

$$\mathtt{Regret}(T) = \widetilde{\mathcal{O}}(\beta \cdot H \cdot \sqrt{dT}) = \widetilde{\mathcal{O}}(H^2 \cdot \sqrt{d^3 T})$$

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- Optimal regret $dH^2\sqrt{T}$ is achieved by [Zanette et al. 2020] with a relaxed model assumption. But the computation is intractable.

A general version of regret

Let $\mathcal{Q}_{ucb}$ be the function class containing the Q-functions constructed by LSVI-UCB

- $\mathcal{Q}_{ucb} = \left\{ \mathrm{Trunc}_{[0,H]}\{\phi(\cdot,\cdot)^\top \theta + \beta \cdot \|\phi(\cdot,\cdot)\|_{\Lambda^{-1}}\right\}$ for linear case

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> **Theorem** [Jin-Yang-Wang-Wang-Jordan-20] Choosing $\beta = \widetilde{\mathcal{O}}(H \cdot \sqrt{\log N_\infty(\mathcal{Q}_{ucb}, T^{-2})})$, with probability at least $1 - 1/T$,
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- d_{eff} is the effective dimension of RKHS or NTK
- For an abstract function class $\mathcal{F}$, d_{eff} can be set as the Bellman-Eluder dimension [Jin-Liu-Miryoosef-21]

Regret analysis

Regret analysis: sensitivity analysis + elliptical potential

A general sensitivity analysis

$$
\begin{aligned}
J(\pi^\star) - J(\pi^t) &= \underbrace{\textstyle\sum_{h\in[H]} \mathbb{E}_{\pi^\star}\left[Q_h^{+,t}(s_h,\pi_h^\star(s_h)) - Q_h^{+,t}(s_h,\pi_h^t(s_h))\right]}_{\text{(i) policy optimization error}} \\
&\quad + \underbrace{\textstyle\sum_{h\in[H]} \mathbb{E}_{\pi^t}\left[\left(Q_h^{+,t} - \mathcal{B}Q_{h+1}^{+,t}\right)\right]}_{\text{(ii) Bellman error on } \pi^t} \\
&\quad + \underbrace{\textstyle\sum_{h\in[H]} \mathbb{E}_{\pi^\star}\left[-\left(Q_h^{+,t} - \mathcal{B}Q_{h+1}^{+,t}\right)\right]}_{\text{(iii) Bellman error on } \pi^\star}
\end{aligned}
$$

- Term (i) ≤ 0 as π^t is greedy with respect to $Q_h^{+,t}$
- Optimism: $Q_{h+1}^{+,t} - 2\Gamma_h^t \le \mathcal{B}Q_{h+1}^{+,t} \le Q_h^{+,t}$, Term (iii) ≤ 0

Regret analysis: sensitivity analysis + elliptical potential

Therefore, we have

$$
\begin{aligned}
\texttt{Regret}(T) &= \sum_{t=1}^{T} J(\pi^\star) - J(\pi^t) \le 2\sum_{h\in[H]} \mathbb{E}_{\pi^t}\left[\Gamma_h^t(s_h, a_h)\right] \\
&= 2\sum_{h\in[H]} \left[\Gamma_h^t(s_h^t, a_h^t)\right] + \mathrm{martingale} - \mathrm{diff} \\
&= 2\beta\sum_{h\in[H]} \sum_{t\in[T]} \left[\|\phi(s_h^t, a_h^t)\|_{(\Lambda_h^t)^{-1}}\right] + H \cdot \sqrt{T} \\
&= \widetilde{\mathcal{O}}(\beta H\sqrt{dT})
\end{aligned}
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- Second line holds because $\{(s_h^t, a_h^t), h \in [H]\} \sim \pi^t$

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- It remains to conduct uncertainty quantification:

$$
\mathbb{P}\Big(\forall(t,h,s,a), |\widehat{Q}_h^t(s,a) - (\mathcal{B}Q_{h+1}^{+,t})(s,a)| \le \Gamma_h^t(s,a)\Big) \ge 1-\delta
$$

uniform concentration over $\mathcal{Q}_{ucb}$ (new for RL)+
self-normalized concentration (same as in CB)

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- LSVI-UCB explores by doing uncertainty quantification for LSVI estimator
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  - By construction, Q_1^+ contains the uncertainty about all $h \geq 1$
- LSVI-UCB achieves sample-efficiency and computational tractability in online RL with function approximation
- Similar principle can be extended to:
  - proximal policy optimization (use soft-greedy instead of greedy)
  - zero-sum Markov game (two-player extension)
  - constrained MDP (primal dual optimization)

References (a very incomplete list)

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References (a very incomplete list)

- RL with function approximation (incomplete list)
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  - [Jin et al, 2020] Provably Efficient Reinforcement Learning with Linear Function Approximation (this talk)
  - [Zanette et al, 2020] Learning near optimal policies with low inherent bellman error
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  - [Yang et al, 2020] On Function Approximation in Reinforcement Learning: Optimism in the Face of Large State Spaces (this talk)
  - [Jin et al, 2021] Bellman Eluder Dimension: New Rich Classes of RL Problems, and Sample-Efficient Algorithms