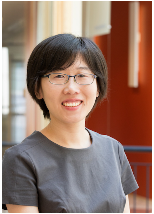
Information-theoretic, statistical and algorithmic foundations of reinforcement learning



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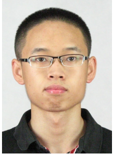
Tutorial, ISIT 2024
Part 1

Our wonderful collaborators



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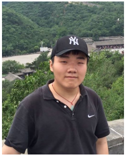

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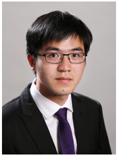

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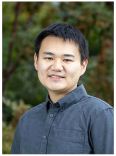

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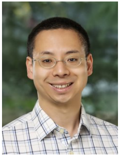

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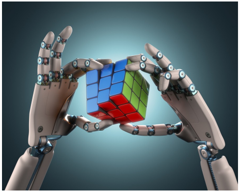
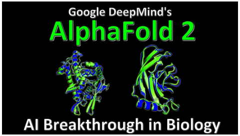
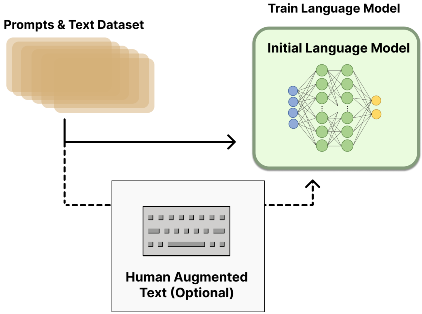
Recent successes in reinforcement learning (RL)





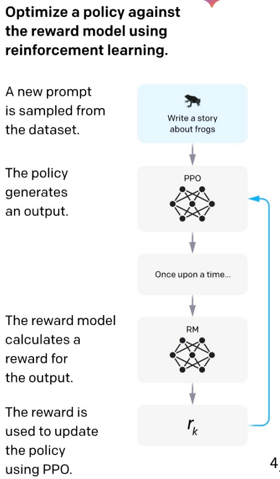
RL holds great promise in the era of AI

One more recent success: RLHF



ChatGPT

Bard

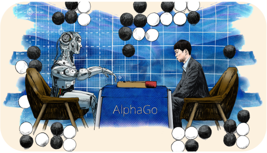


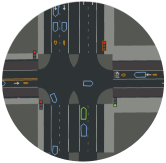
You

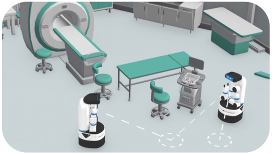
What is RLHF?

ChatGPT

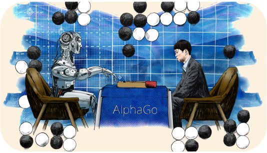
RLHF stands for Reinforcement Learning from Human Feedback. It's a technique used in machine learning and artificial intelligence where a model learns to perform tasks or make decisions based on feedback from human trainers, rather than solely relying on pre-existing data sets or explicit programming. This approach allows the

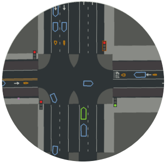


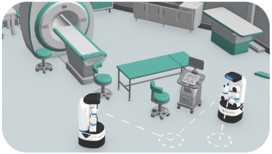




In RL, agent(s) often learn by probing the environment





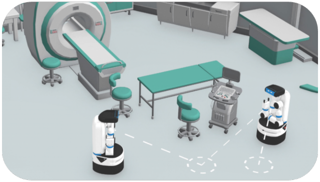


In RL, agent(s) often learn by probing the environment

- unknown environment
- explosion of dimensionality
- delayed feedback
- nonconvexity

Data efficiency

Data collection might be expensive, time-consuming, or high-stakes



clinical trials

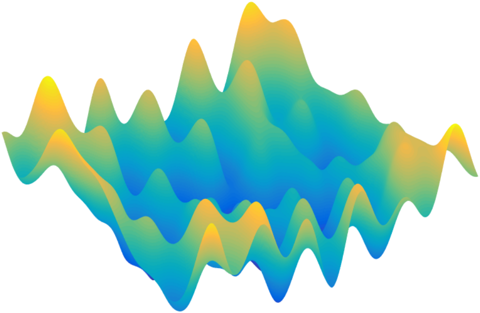
self-driving cars

Calls for design of sample-efficient RL algorithms!

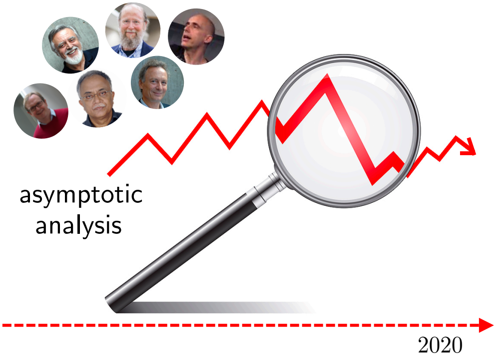
Computational efficiency

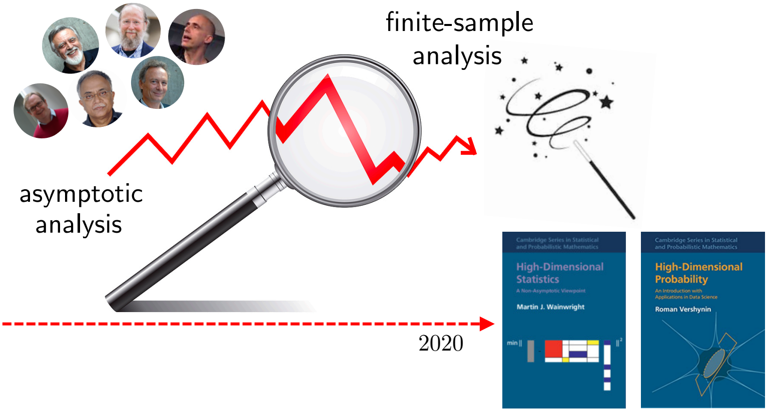
Running RL algorithms might take a long time ...

- enormous state-action space
- nonconvexity



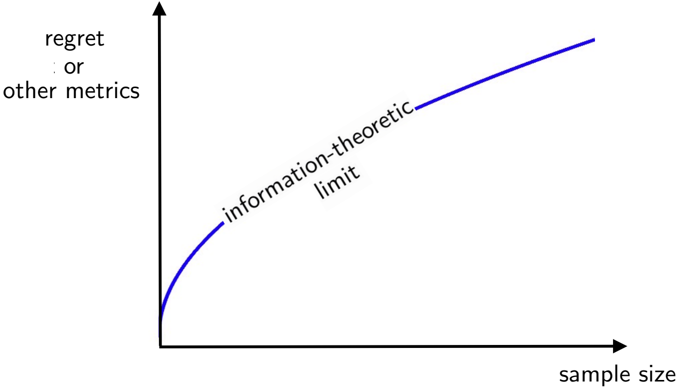
Calls for computationally efficient RL algorithms!


asymptotic
analysis
2020



Understanding efficiency of contemporary RL requires a modern suite of non-asymptotic analysis

Sample complexity issues that permeate state-of-the-art RL theory



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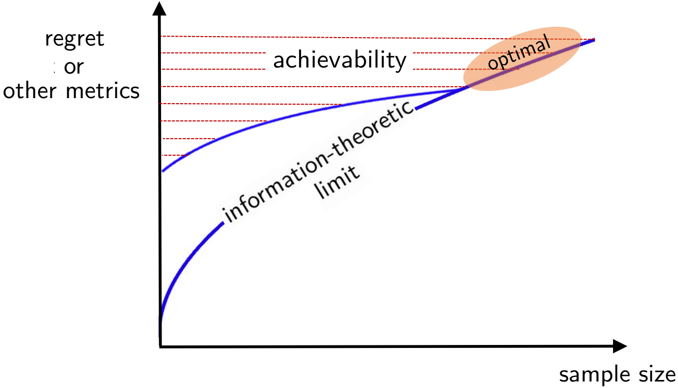
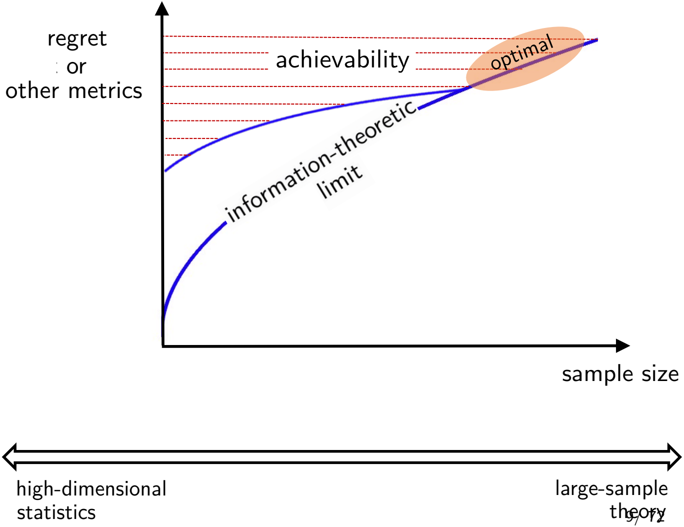


Sample complexity issues that permeate state-of-the-art RL theory



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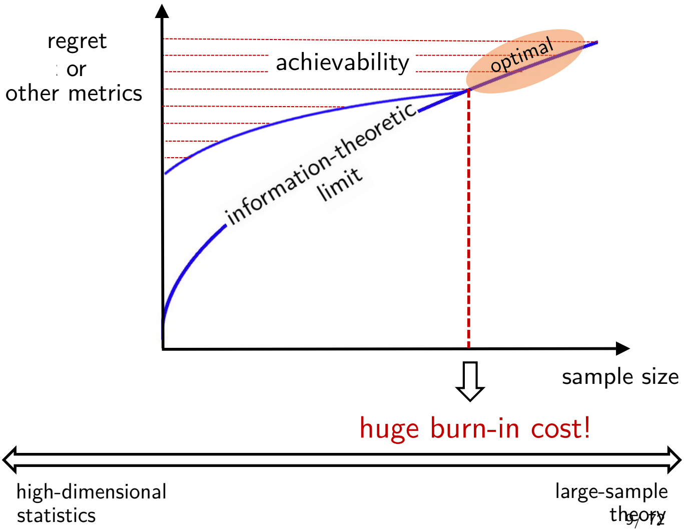

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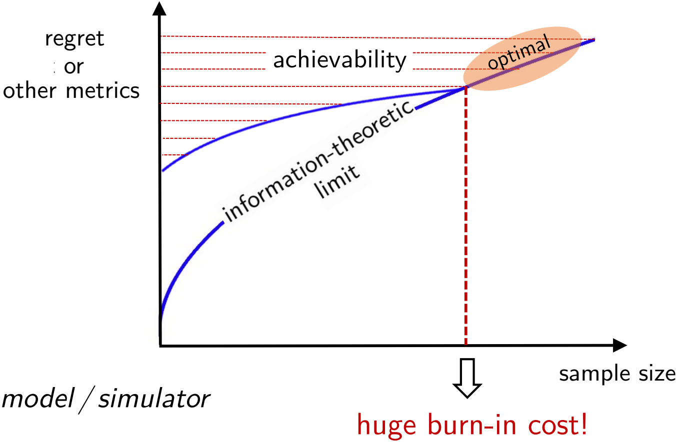
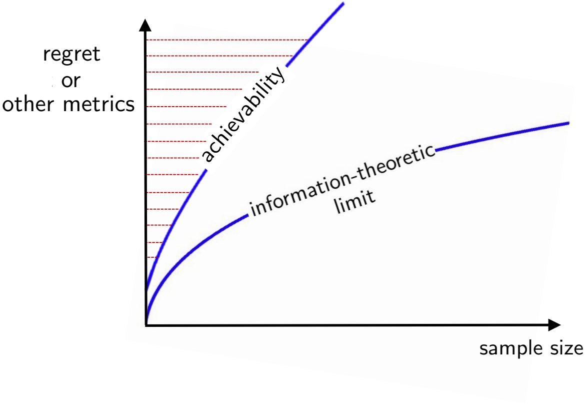


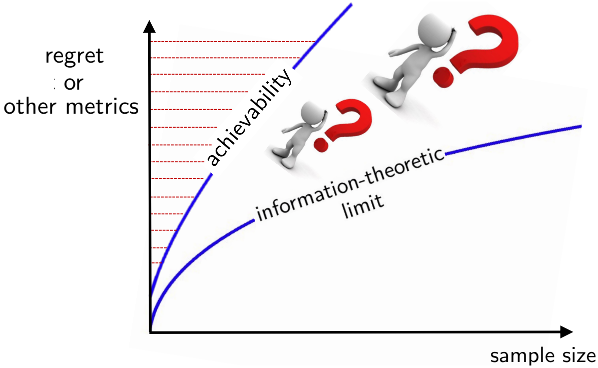
- *generative model / simulator*
- *online RL*
- *offline RL*
- ...

Sample complexity issues that permeate state-of-the-art RL theory



- *multi-agent RL*
- *partially observable MDPs*
- ...

Sample complexity issues that permeate state-of-the-art RL theory



- *multi-agent RL*
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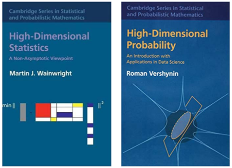
- ...

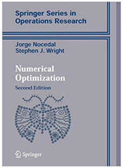
This tutorial

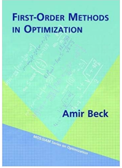


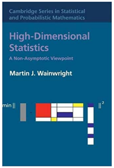
(large-scale) optimization (high-dimensional) statistics

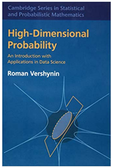
Design sample- and computationally-efficient RL algorithms

This tutorial









(large-scale) optimization (high-dimensional) statistics

Design sample- and computationally-efficient RL algorithms

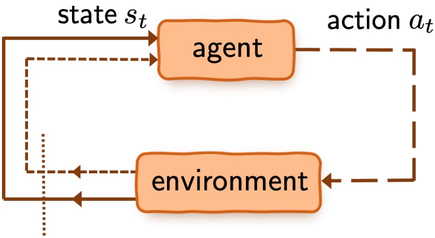
Part 1. basics, RL w/ a generative model

Part 2. online / offline RL, multi-agent / robust RL

Part 1

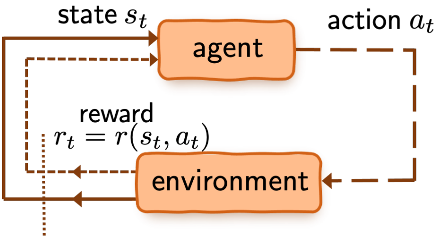
1. Basics: Markov decision processes
2. RL w/ a generative model (simulator)
   - model-based algorithms (a "plug-in" approach)
   - model-free algorithms

Markov decision process (MDP)



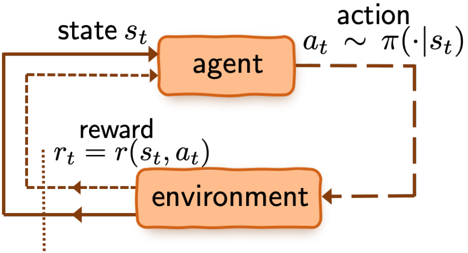
- $\mathcal{S} = \{1, \ldots, S\}$: state space (containing S states)
- $\mathcal{A} = \{1, \ldots, A\}$: action space (containing A actions)

Markov decision process (MDP)



- $\mathcal{S} = \{1, \ldots, S\}$: state space (containing S states)
- $\mathcal{A} = \{1, \ldots, A\}$: action space (containing A actions)
- $r(s, a) \in [0, 1]$: immediate reward

Discounted infinite-horizon MDPs



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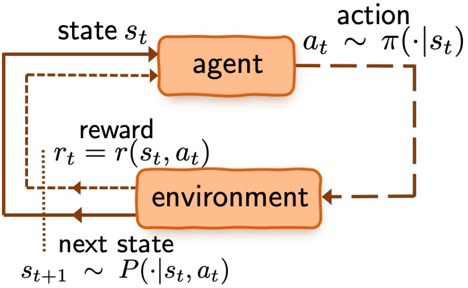
- $\pi(\cdot|s)$: policy (or action selection rule)

Discounted infinite-horizon MDPs



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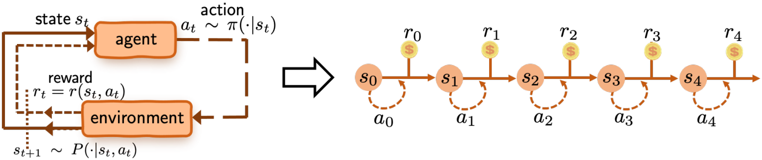
- $r(s, a) \in [0, 1]$: immediate reward
- $\pi(\cdot|s)$: policy (or action selection rule)
- $P(\cdot|s, a)$: unknown transition probabilities

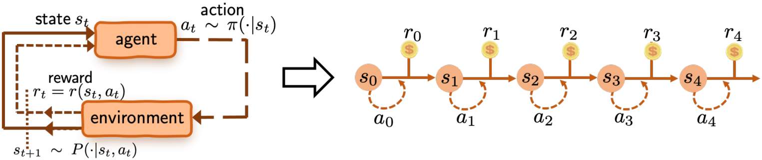
Value function



Value of policy π: cumulative discounted reward

$$\forall s \in \mathcal{S}: \quad V^{\pi}(s) := \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t r(s_t, a_t) \,\middle|\, s_0 = s\right]$$

Value function



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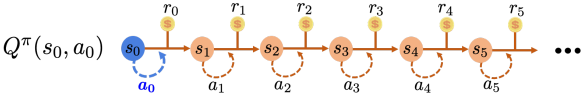
$$\forall s \in \mathcal{S}: \quad V^\pi(s) := \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t r(s_t, a_t) \,\middle|\, s_0 = s\right]$$

- $\gamma \in [0, 1)$: discount factor
    - take $\gamma \to 1$ to approximate long-horizon MDPs
    - **effective horizon**: $\frac{1}{1-\gamma}$

Q-function (action-value function)

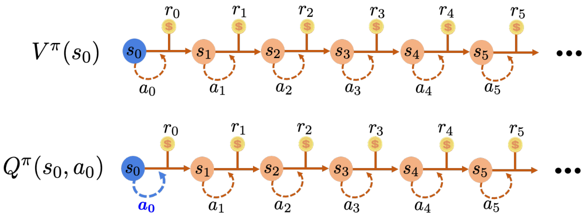


Q-function of policy π:

$$\forall (s,a) \in \mathcal{S} \times \mathcal{A}: \quad Q^\pi(s,a) := \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t r_t \,\middle|\, s_0 = s, a_0 = a\right]$$

- $(\cancel{a_0,}\, s_1, a_1, s_2, a_2, \cdots)$: induced by policy π

Q-function (action-value function)



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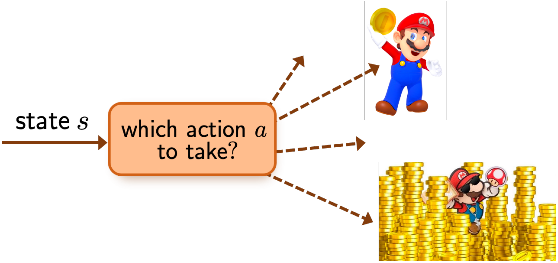
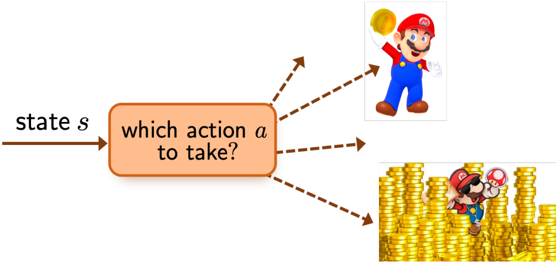
Optimal policy and optimal value



- **optimal policy** $\pi^\star$: maximizing value function $\max_\pi V^\pi$

Optimal policy and optimal value



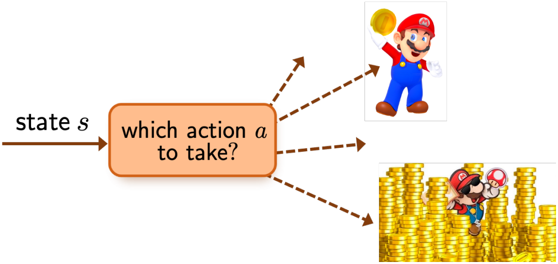
- **optimal policy** $\pi^\star$: maximizing value function $\max_\pi V^\pi$

Theorem (Puterman'94)

For infinite horizon discounted MDP, there always exists a deterministic policy $\pi^\star$, *such that*

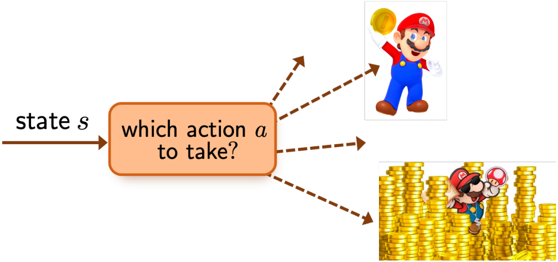
$$V^{\pi^\star}(s) \geq V^\pi(s), \quad \forall s, \text{ and } \pi.$$

Optimal policy and optimal value



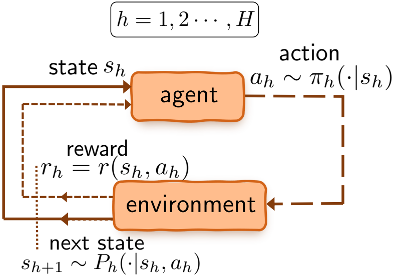
- **optimal policy** $\pi^\star$: maximizing value function $\max_{\pi} V^{\pi}$
- **optimal value / Q function**: $V^\star := V^{\pi^\star}$, $Q^\star := Q^{\pi^\star}$

Optimal policy and optimal value



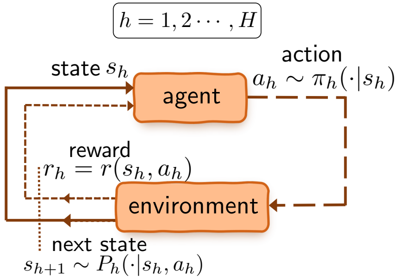
- **optimal policy** $\pi^\star$: maximizing value function $\max_\pi V^\pi$
- **optimal value / Q function**: $V^\star := V^{\pi^\star}$, $Q^\star := Q^{\pi^\star}$
- A question to keep in mind: *how to find optimal* $\pi^\star$*?*

Finite-horizon MDPs (nonstationary)



- H: horizon length
- $\mathcal{S}$: state space with size S
- $\mathcal{A}$: action space with size A
- $r_h(s_h, a_h) \in [0, 1]$: immediate reward in step h
- $\pi = \{\pi_h\}_{h=1}^{H}$: policy (or action selection rule)
- $P_h(\cdot \mid s, a)$: transition probabilities in step h

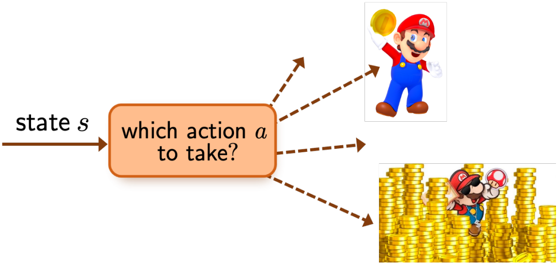
Finite-horizon MDPs (nonstationary)



value function: $V_h^\pi(s) := \mathbb{E}\left[\sum_{t=h}^{H} r_h(s_h, a_h) \,\middle|\, s_h = s\right]$

Q-function: $Q_h^\pi(s, a) := \mathbb{E}\left[\sum_{t=h}^{H} r_h(s_h, a_h) \,\middle|\, s_h = s, a_h = a\right]$

Optimal policy and optimal value



- **optimal policy** $\pi^\star$: maximizing value function at all steps
- **optimal value / Q function**: $V_h^\star := V_h^{\pi^\star}$, $Q_h^\star := Q_h^{\pi^\star}$, $\forall h$
- **Question:** *how to find optimal $\pi^\star$?*

Basic dynamic programming algorithms
when MDP specification is known

A simpler problem: **policy evaluation**

— given MDP $\mathcal{M}$ and policy π, how to compute V^π, Q^π?

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solution: Bellman's consistency equation

$$V^\pi(s) = \mathop{\mathbb{E}}_{a\sim\pi(\cdot|s)}\left[Q^\pi(s,a)\right]$$

$$Q^\pi(s,a) = \underbrace{r(s,a)}_{\text{immediate reward}} + \gamma \mathop{\mathbb{E}}_{s'\sim P(\cdot|s,a)}\Big[\underbrace{V^\pi(s')}_{\text{next state's value}}\Big]$$

- one-step look-ahead

Richard Bellman

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- one-step look-ahead
- P^π: state-action transition matrix induced by π:

$$Q^\pi = r + \gamma P^\pi Q^\pi \quad \Longrightarrow \quad Q^\pi = (I - \gamma P^\pi)^{-1} r$$

Richard Bellman

Back to main question: how to find optimal policy $\pi^\star$?

solution: Bellman's optimality principle

- Bellman operator:

$$\mathcal{T}(Q)(s,a) := \underbrace{r(s,a)}_{\text{immediate reward}} + \gamma \mathop{\mathbb{E}}_{s' \sim P(\cdot|s,a)} \underbrace{\left[\max_{a' \in \mathcal{A}} Q(s',a') \right]}_{\text{next state's value}}$$

  - one-step look-ahead
  - γ-contraction: $\|\mathcal{T}(Q_1) - \mathcal{T}(Q_2)\|_\infty \leq \gamma \|Q_1 - Q_2\|_\infty$

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  - one-step look-ahead
  - γ-contraction: $\|\mathcal{T}(Q_1) - \mathcal{T}(Q_2)\|_\infty \le \gamma \|Q_1 - Q_2\|_\infty$

- Bellman equation: $Q^\star$ is *unique* solution to

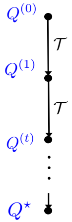
$$\mathcal{T}(Q^\star) = Q^\star$$

Two dynamic programming algorithms

Value iteration (VI)

For $t = 0, 1, \ldots$

$$Q^{(t+1)} = \mathcal{T}(Q^{(t)})$$

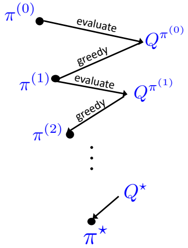


Policy iteration (PI)

For $t = 0, 1, \ldots$

policy evaluation: $Q^{(t)} = Q^{\pi^{(t)}}$

policy improvement: $\pi^{(t+1)}(s) = \arg\max_{a \in \mathcal{A}} Q^{(t)}(s, a)$



Iteration complexity

Theorem (Linear convergence of policy/value iteration)

$$\|Q^{(t)} - Q^\star\|_\infty \leq \gamma^t \|Q^{(0)} - Q^\star\|_\infty$$

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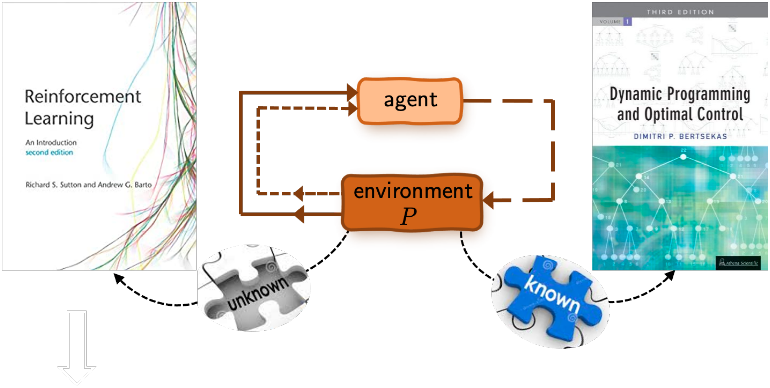
Linear convergence at a **dimension-free** rate!

When the model is unknown . . .



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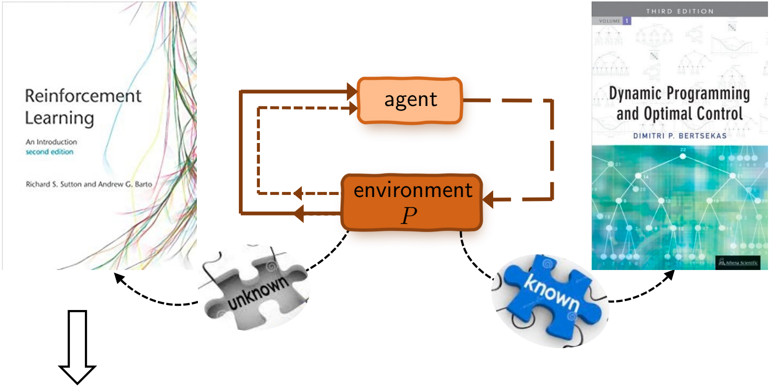
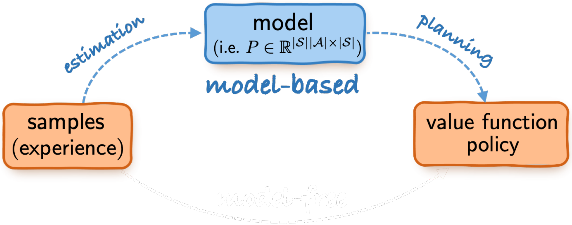


Need to learn optimal policy from samples w/o model specification

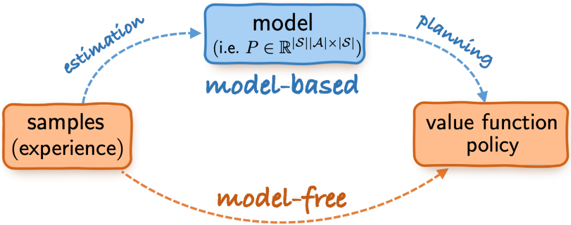
Two approaches



Model-based approach ("plug-in")

1. build an empirical estimate $\widehat{P}$ for P
2. planning based on the empirical $\widehat{P}$

Two approaches



Model-based approach ("plug-in")

1. build an empirical estimate $\widehat{P}$ for P
2. planning based on the empirical $\widehat{P}$

Model-free approach

— learning w/o estimating the model explicitly

Sampling mechanisms

1. RL w/ a generative model (a.k.a. simulator)
   ◦ can query arbitrary state-action pairs to draw samples

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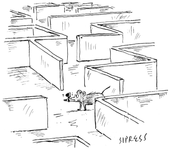
Question: *how many samples are sufficient to learn an* $\underbrace{\varepsilon\text{-optimal policy}}_{V^{\widehat{\pi}} \geq V^{\star} - \varepsilon}$*?*

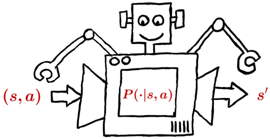
Exploration vs exploitation

Exploration

offline RL



online RL

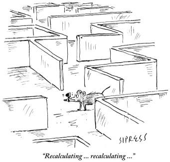


generative model

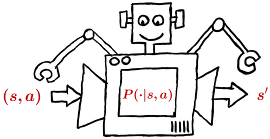
Exploration vs exploitation

Exploration

offline RL



online RL



generative model

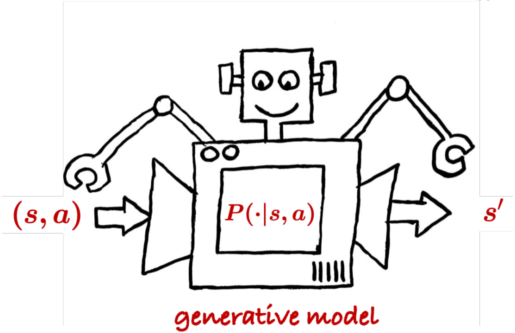
Varying levels of trade-offs between exploration and exploitation.

Part 1

1. Basics: Markov decision processes
2. RL w/ a generative model (simulator)
    - model-based algorithms (a "plug-in" approach)
    - model-free algorithms

A generative model / simulator

— *Kearns and Singh, 1999*



- **sampling:** for each (s, a), collect N samples $\{(s, a, s'_{(i)})\}_{1 \le i \le N}$

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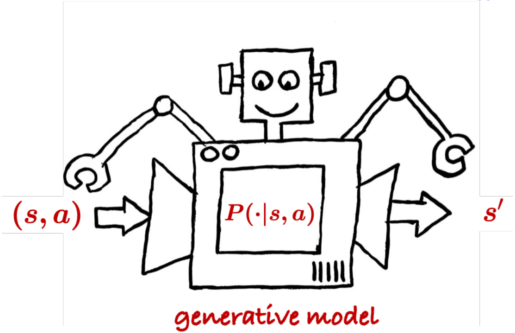

- **sampling:** for each (s, a), collect N samples $\{(s, a, s'_{(i)})\}_{1 \le i \le N}$
- construct $\widehat{\pi}$ based on samples (in total $SA \times N$)

ℓ_∞-**sample complexity:** how many samples are required to learn an $\underbrace{\varepsilon\text{-optimal policy}}_{\forall s:\ V^{\widehat{\pi}}(s) \geq V^{\star}(s) - \varepsilon}$?

Minimax lower bound

Theorem (minimax lower bound; Azar et al., 2013)

For all $\varepsilon \in [0, \frac{1}{1-\gamma})$, there exists some MDP such that the total number of samples need to be at least

$$\widetilde{\Omega}\left(\frac{|\mathcal{S}||\mathcal{A}|}{(1-\gamma)^3\varepsilon^2}\right)$$

to achieve $V^\star - V^{\widehat{\pi}} \leq \varepsilon$, where $\widehat{\pi}$ is the output of any RL algorithm.

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to achieve $V^{\star} - V^{\widehat{\pi}} \le \varepsilon$, where $\widehat{\pi}$ is the output of any RL algorithm.

- holds for both finding the optimal Q-function and the optimal policy over the entire range of ε
- much smaller than the model dimension $|\mathcal{S}|^2|\mathcal{A}|$

An incomplete list of works

- Kearns and Singh, 1999
- Kakade, 2003
- Kearns et al., 2002
- Azar et al., 2013
- Sidford et al., 2018a, 2018b
- Wang, 2019
- Agarwal et al., 2019
- Wainwright, 2019a, 2019b
- Pananjady and Wainwright, 2019
- Yang and Wang, 2019
- Khamaru et al., 2020
- Mou et al., 2020
- Cui and Yang, 2021
- ...

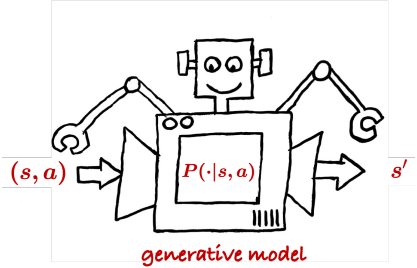
An even shorter list of prior art

algorithm	sample size range	sample complexity	ε-range
Empirical QVI Azar et al., 2013	$\left[\frac{S^2 A}{(1-\gamma)^2}, \infty\right)$	$\frac{SA}{(1-\gamma)^3 \varepsilon^2}$	$(0, \frac{1}{\sqrt{(1-\gamma)S}}]$
Sublinear randomized VI Sidford et al., 2018b	$\left[\frac{SA}{(1-\gamma)^2}, \infty\right)$	$\frac{SA}{(1-\gamma)^4 \varepsilon^2}$	$\left(0, \frac{1}{1-\gamma}\right]$
Variance-reduced QVI Sidford et al., 2018a	$\left[\frac{SA}{(1-\gamma)^3}, \infty\right)$	$\frac{SA}{(1-\gamma)^3 \varepsilon^2}$	$(0, 1]$
Randomized primal-dual Wang 2019	$\left[\frac{SA}{(1-\gamma)^2}, \infty\right)$	$\frac{SA}{(1-\gamma)^4 \varepsilon^2}$	$(0, \frac{1}{1-\gamma}]$
Empirical MDP + planning Agarwal et al., 2019	$\left[\frac{SA}{(1-\gamma)^2}, \infty\right)$	$\frac{SA}{(1-\gamma)^3 \varepsilon^2}$	$(0, \frac{1}{\sqrt{1-\gamma}}]$

important parameters $\Longrightarrow$

- # states S, # actions A
- the discounted complexity $\frac{1}{1-\gamma}$
- approximation error $\varepsilon \in (0, \frac{1}{1-\gamma}]$

Model estimation



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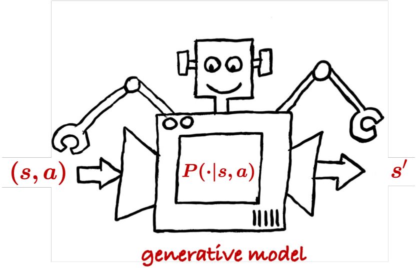


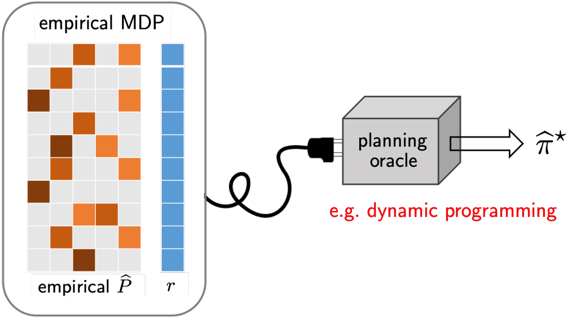
Sampling: for each (s,a), collect N ind. samples $\{(s,a,s'_{(i)})\}_{1\le i\le N}$

Empirical estimates:

$$\widehat{P}(s'|s,a) = \underbrace{\frac{1}{N}\sum_{i=1}^{N}\mathbb{1}\{s'_{(i)} = s'\}}_{\text{empirical frequency}}$$

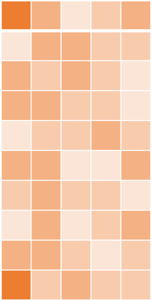
Empirical MDP + planning

— *Azar et al., 2013, Agarwal et al., 2019*

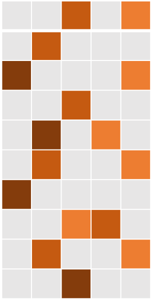


$\underbrace{\text{Find policy}}_{\text{using, e.g., policy iteration}}$ based on the $\underbrace{\text{empirical MDP}}_{(\widehat{P}, r)}$ (*empirical maximizer*)

Challenges in the sample-starved regime



truth: $P \in \mathbb{R}^{SA \times S}$



empirical estimate: $\widehat{P}$

- Can't recover P faithfully if sample size $\ll S^2 A$!

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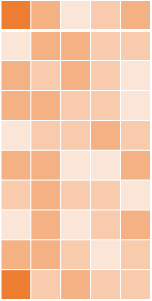

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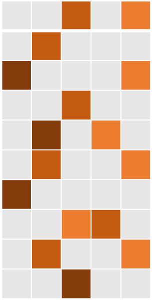

empirical estimate: $\widehat{P}$

- Can't recover P faithfully if sample size $\ll S^2 A$!
- Can we trust our policy estimate when reliable model estimation is infeasible?

ℓ_∞-based sample complexity

Theorem (Agarwal, Kakade, Yang '19)

For any $0 < \varepsilon \leq \frac{1}{\sqrt{1-\gamma}}$*, the optimal policy* $\widehat{\pi}^\star$ *of empirical MDP achieves*

$$\|V^{\widehat{\pi}^\star} - V^\star\|_\infty \leq \varepsilon$$

with high prob., with sample complexity at most

$$\widetilde{O}\left(\frac{SA}{(1-\gamma)^3\varepsilon^2}\right)$$

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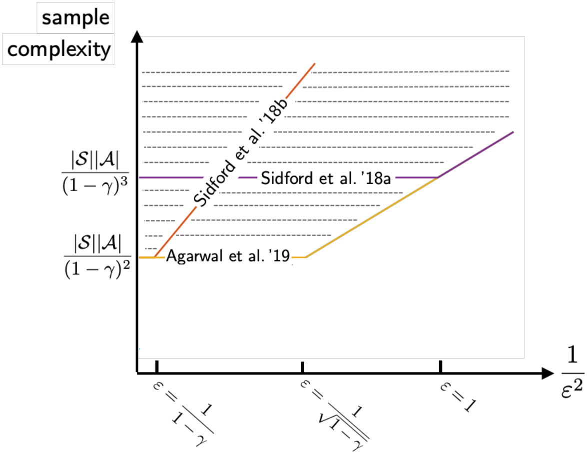
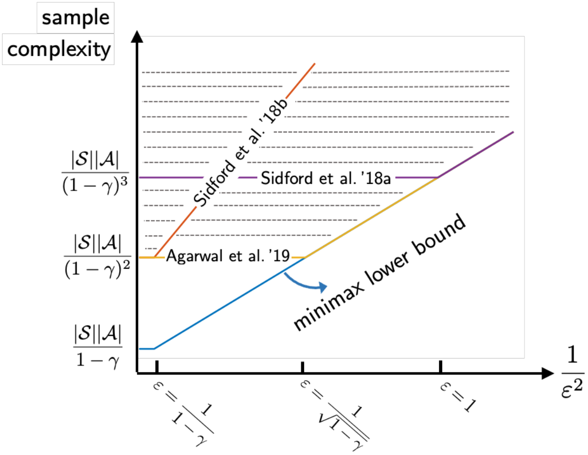
$$\widetilde{O}\left(\frac{SA}{(1-\gamma)^3\varepsilon^2}\right)$$

- matches minimax lower bound: $\widetilde{\Omega}(\frac{SA}{(1-\gamma)^3\varepsilon^2})$ when $\varepsilon \leq \frac{1}{\sqrt{1-\gamma}}$ (equivalently, when sample size exceeds $\frac{SA}{(1-\gamma)^2}$) Azar et al., 2013


sample
complexity
$\frac{|\mathcal{S}||\mathcal{A}|}{(1-\gamma)^3}$
$\frac{|\mathcal{S}||\mathcal{A}|}{(1-\gamma)^2}$
Sidford et al. '18b
Sidford et al. '18a
Agarwal et al. '19
$\varepsilon = \frac{1}{1-\gamma}$
$\varepsilon = \frac{1}{\sqrt{1-\gamma}}$
$\varepsilon = 1$
$\frac{1}{\varepsilon^2}$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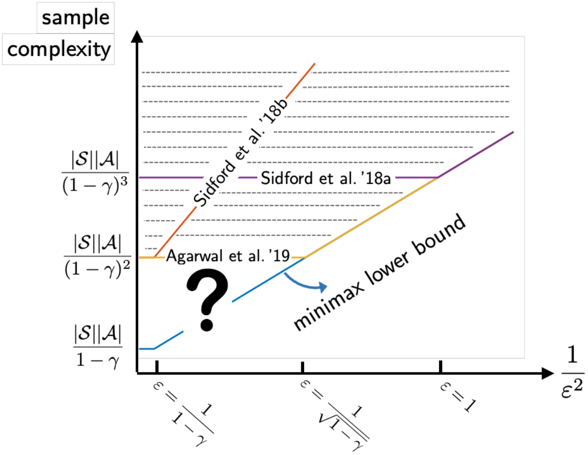
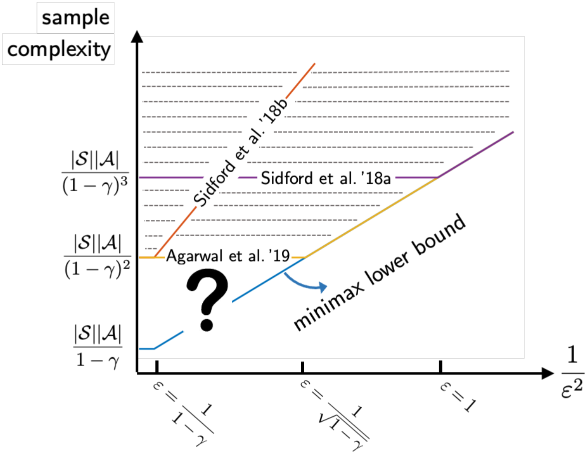


Agarwal et al., 2019 still requires a burn-in sample size $\gtrsim \frac{SA}{(1-\gamma)^2}$

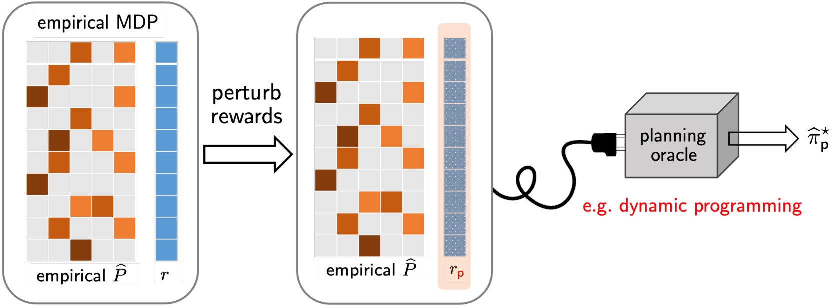


Agarwal et al., 2019 still requires a burn-in sample size $\gtrsim \frac{SA}{(1-\gamma)^2}$

Question: is it possible to break this sample size barrier?

Perturbed model-based approach (Li et al. '24)

— Li, Wei, Chi, Chen, 2024



Find policy based on empirical MDP w/ slightly perturbed rewards

Optimal ℓ_∞-based sample complexity

Theorem (Li, Wei, Chi, Chen '20; OR '24)

For any $0 < \varepsilon \leq \frac{1}{1-\gamma}$, *the optimal policy* $\widehat{\pi}_{\mathrm{p}}^{\star}$ *of perturbed empirical MDP achieves*

$$\|V^{\widehat{\pi}_{\mathrm{p}}^{\star}} - V^{\star}\|_{\infty} \leq \varepsilon$$

with high prob., with sample complexity at most

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Theorem (Li, Wei, Chi, Chen '20; OR '24)

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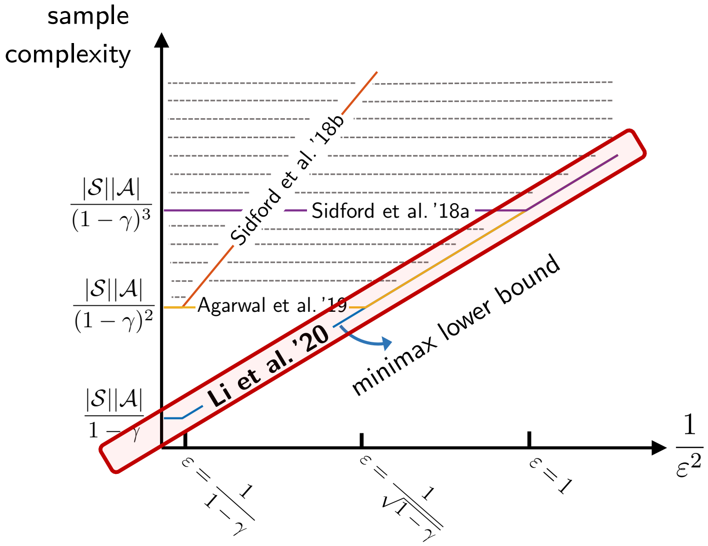
with high prob., with sample complexity at most

$$\widetilde{O}\left(\frac{SA}{(1-\gamma)^3\varepsilon^2}\right)$$

- matches minimax lower bound: $\widetilde{\Omega}(\frac{SA}{(1-\gamma)^3\varepsilon^2})$ Azar et al., 2013
- full ε-range: $\varepsilon \in (0, \frac{1}{1-\gamma}]$ $\longrightarrow$ no burn-in cost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Notation and Bellman equation

Bellman equation: $V^\pi = r_\pi + \gamma P_\pi V^\pi$

- V^π: value function under policy π
  - Bellman equation: $V^\pi = (I - \gamma P_\pi)^{-1} r_\pi$
- $\widehat{V}^\pi$: empirical version value function under policy π
  - Bellman equation: $\widehat{V}^\pi = (I - \gamma \widehat{P}_\pi)^{-1} r_\pi$

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- $\pi^\star$: optimal policy for V^π
- $\widehat{\pi}^\star$: optimal policy for $\widehat{V}^\pi$

Main steps

Elementary decomposition:

$$V^\star - V^{\widehat{\pi}^\star} = \left(V^\star - \widehat{V}^{\pi^\star}\right) + \left(\widehat{V}^{\pi^\star} - \widehat{V}^{\widehat{\pi}^\star}\right) + \left(\widehat{V}^{\widehat{\pi}^\star} - V^{\widehat{\pi}^\star}\right)$$
$$\leq \left(V^{\pi^\star} - \widehat{V}^{\pi^\star}\right) + 0 + \left(\widehat{V}^{\widehat{\pi}^\star} - V^{\widehat{\pi}^\star}\right)$$

Main steps

Elementary decomposition:

$$
\begin{aligned}
V^\star - V^{\widehat{\pi}^\star} &= \left(V^\star - \widehat{V}^{\pi^\star}\right) + \left(\widehat{V}^{\pi^\star} - \widehat{V}^{\widehat{\pi}^\star}\right) + \left(\widehat{V}^{\widehat{\pi}^\star} - V^{\widehat{\pi}^\star}\right) \\
&\le \left(V^{\pi^\star} - \widehat{V}^{\pi^\star}\right) + 0 + \left(\widehat{V}^{\widehat{\pi}^\star} - V^{\widehat{\pi}^\star}\right)
\end{aligned}
$$

- **Step 1:** control $V^\pi - \widehat{V}^\pi$ for a fixed π (called "policy evaluation")

  (Bernstein inequality + a peeling argument)

Main steps

Elementary decomposition:

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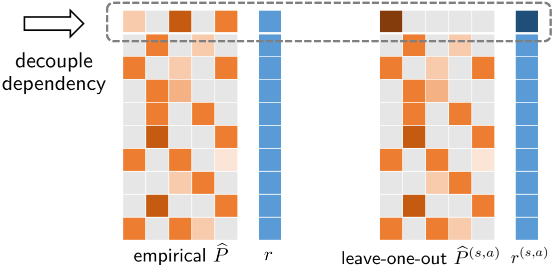
- **Step 1:** control $V^\pi - \widehat{V}^\pi$ for a fixed π (called "policy evaluation")
  (Bernstein inequality + a peeling argument)
- **Step 2:** extend it to control $\widehat{V}^{\widehat{\pi}^\star} - V^{\widehat{\pi}^\star}$ ($\widehat{\pi}^\star$ depends on samples)
  (decouple statistical dependency)

A glimpse of key analysis ideas

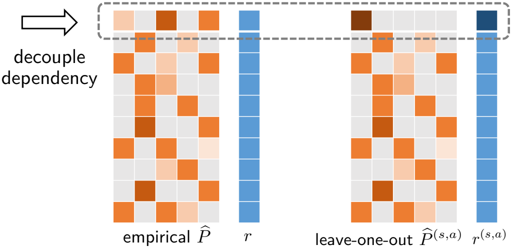
1. leave-one-out analysis: decouple statistical dependency



2. tie-breaking via random perturbation

Key idea 1: leave-one-out analysis

Decouple dependency by introducing auxiliary state-action absorbing MDPs by dropping randomness for each (s, a)



— *inspired by Agarwal et al. '19 but quite different . . .*

Key idea 1: leave-one-out analysis

- El Karoui, Bean, Bickel, Lim, Yu, 2013
- El Karoui, 2015
- Javanmard, Montanari, 2015
- Zhong, Boumal, 2017
- Lei, Bickel, El Karoui, 2017
- Sur, Chen, Candès, 2017
- Abbe, Fan, Wang, Zhong, 2017
- Chen, Fan, Ma, Wang, 2017
- Ma, Wang, Chi, Chen, 2017
- Chen, Chi, Fan, Ma, 2018
- Ding, Chen, 2018
- Dong, Shi, 2018
- Chen, Chi, Fan, Ma, Yan, 2019
- Chen, Fan, Ma, Yan, 2019
- Cai, Li, Poor, Chen, 2019
- **Agarwal, Kakade, Yang, 2019**
- Pananjady, Wainwright, 2019
- Ling, 2020
- Yan, Chen, Fan, 2024

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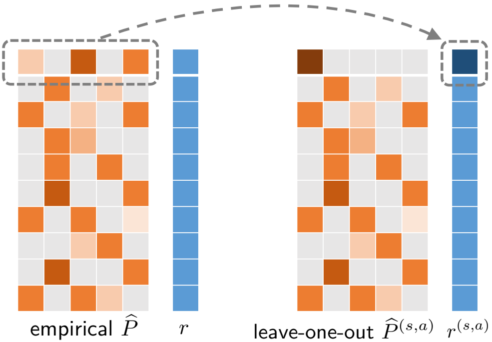
Spectral Methods for Data Science: A Statistical Perspective

Suggested Citation: Yuxin Chen, Yuejie Chi, Jianqing Fan and Cong Ma (2020), "Spectral Methods for Data Science: A Statistical Perspective", Foundations and Trends® in

Key idea 1: leave-one-out analysis



1. embed all randomness from $\widehat{P}_{s,a}$ into a single scalar (i.e. $r_{s,a}^{(s,a)}$)

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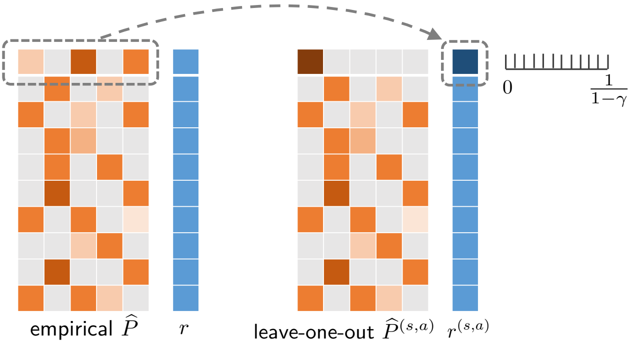

1. embed all randomness from $\widehat{P}_{s,a}$ into a single scalar (i.e. $r_{s,a}^{(s,a)}$)
2. build an ϵ-net for this scalar

works under a separation condition

$$\forall s, \quad \widehat{Q}^{\star}(s, \widehat{\pi}^{\star}(s)) - \max_{a:\, a \neq \widehat{\pi}^{\star}(s)} \widehat{Q}^{\star}(s,a) > 0$$

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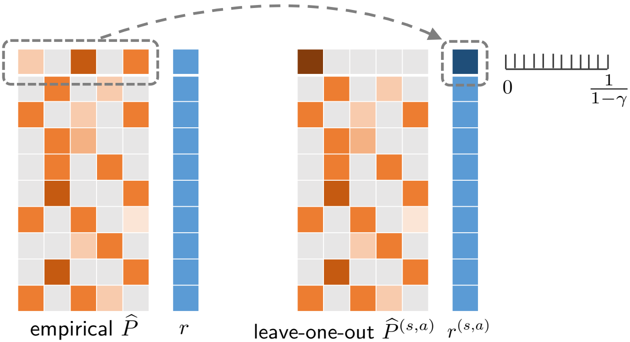

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Key idea 2: tie-breaking via perturbation

- How to ensure separation between the optimal policy and others?

$$\forall s, \quad \widehat{Q}^{\star}(s, \widehat{\pi}^{\star}(s)) - \max_{a:\, a \neq \widehat{\pi}^{\star}(s)} \widehat{Q}^{\star}(s, a) > 0$$

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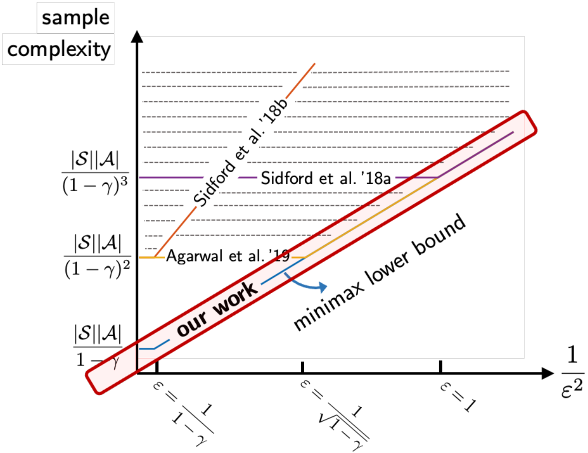
- **Solution:** *slightly perturb rewards* $r \implies \widehat{\pi}^{\star}_{\mathrm{p}}$
  - *ensures* $\widehat{\pi}^{\star}_{\mathrm{p}}$ *can be differentiated from others with high prob.*

Key idea 2: tie-breaking via perturbation

- How to ensure separation between the optimal policy and others?

$$\forall s, \quad \widehat{Q}^{\star}(s, \widehat{\pi}^{\star}(s)) - \max_{a:\, a \neq \widehat{\pi}^{\star}(s)} \widehat{Q}^{\star}(s, a) > \frac{(1-\gamma)\varepsilon}{S^5 A^5}$$

- **Solution:** *slightly perturb rewards* $r \implies \widehat{\pi}_{\mathrm{p}}^{\star}$
  - *ensures* $\widehat{\pi}_{\mathrm{p}}^{\star}$ *can be differentiated from others with high prob.*

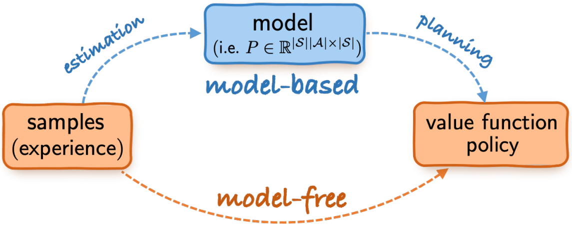


Model based RL is minimax optimal under generative models and does NOT suffer from a sample size barrier

Part 1

1. Basics: Markov decision processes
2. RL w/ a generative model (simulator)
   - model-based algorithms (a "plug-in" approach)
   - model-free algorithms

Model-based vs. model-free RL



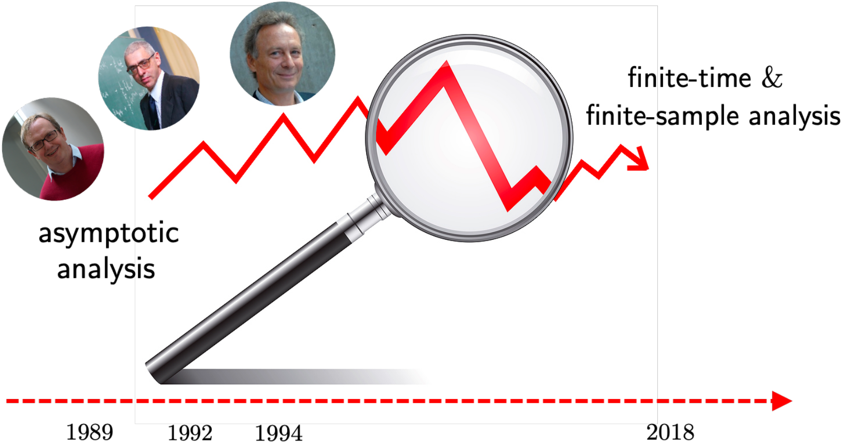
Model-based approach ("plug-in")

1. build empirical estimate $\widehat{P}$ for P
2. planning based on empirical $\widehat{P}$

Model-free / value-based approach

— learning w/o modeling & estimating environment explicitly

— memory-efficient, online, . . .



Focus of this part: classical **Q-learning** algorithm and its variants

A starting point: Bellman optimality principle

Bellman operator

$$\mathcal{T}(Q)(s,a) := \underbrace{r(s,a)}_{\text{immediate reward}} + \gamma \mathop{\mathbb{E}}_{s' \sim P(\cdot|s,a)} \underbrace{\left[\max_{a' \in \mathcal{A}} Q(s',a')\right]}_{\text{next state's value}}$$

- one-step look-ahead

A starting point: Bellman optimality principle

Bellman operator

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Bellman equation: $Q^\star$ is *unique* solution to

$$\mathcal{T}(Q^\star) = Q^\star$$

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- one-step look-ahead

Bellman equation: $Q^\star$ is *unique* solution to

$$\mathcal{T}(Q^\star) = Q^\star$$

- **takeaway message:** it suffices to solve the Bellman equation
- **challenge:** how to solve it using stochastic samples?

Richard Bellman

Q-learning: a stochastic approximation algorithm

Chris Watkins

Peter Dayan

Stochastic approximation for solving the **Bellman equation**

$\underbrace{\text{Stochastic approximation}}_{\text{Robbins \& Monro, 1951}}$

$$\mathcal{T}(Q) - Q = 0$$

where

$$\mathcal{T}(Q)(s,a) := \underbrace{r(s,a)}_{\text{immediate reward}} + \gamma \mathop{\mathbb{E}}_{s' \sim P(\cdot|s,a)} \underbrace{\left[\max_{a' \in \mathcal{A}} Q(s',a')\right]}_{\text{next state's value}}.$$

Q-learning: a stochastic approximation algorithm

Chris Watkins

Peter Dayan

Stochastic approximation for solving Bellman equation $\mathcal{T}(Q) - Q = 0$

$$\underbrace{Q_{t+1}(s,a) = Q_t(s,a) + \eta_t\big(\mathcal{T}_t(Q_t)(s,a) - Q_t(s,a)\big)}_{\text{sample transition } (s,a,s')}, \quad t \geq 0$$

Q-learning: a stochastic approximation algorithm

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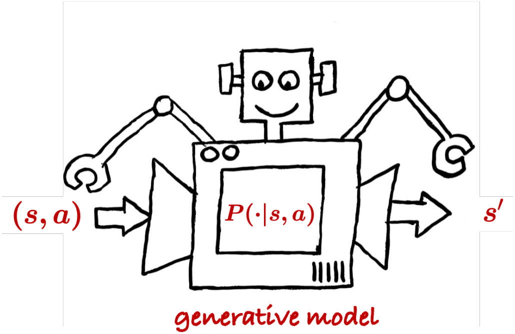
$$\mathcal{T}_t(Q)(s,a) = r(s,a) + \gamma \max_{a'} Q(s',a')$$

$$\mathcal{T}(Q)(s,a) = r(s,a) + \gamma \mathop{\mathbb{E}}_{s' \sim P(\cdot|s,a)} \Big[\max_{a'} Q(s',a')\Big]$$

A generative model / simulator

— *Kearns, Singh, 1999*



Each iteration, draw an independent sample (s, a, s') for given (s, a)

Synchronous Q-learning

Chris Watkins

Peter Dayan

for $t = 0, 1, \ldots, T$

for each $(s, a) \in \mathcal{S} \times \mathcal{A}$

draw a sample (s, a, s'), run

$$Q_{t+1}(s,a) = (1 - \eta_t) Q_t(s,a) + \eta_t \Big\{ r(s,a) + \gamma \max_{a'} Q_t(s', a') \Big\}$$

synchronous: all state-action pairs are updated simultaneously

- total sample size: TSA

Sample complexity of synchronous Q-learning

Theorem (Li, Cai, Chen, Wei, Chi '21, OR'24)

For any $0 < \varepsilon \le 1$, synchronous Q-learning yields $\|\widehat{Q} - Q^\star\|_\infty \le \varepsilon$ with high prob. and $\mathbb{E}[\|\widehat{Q} - Q^\star\|_\infty] \le \varepsilon$, with sample size at most

$$\begin{cases} \widetilde{O}\left(\frac{SA}{(1-\gamma)^4\varepsilon^2}\right) & \text{if } A \ge 2 \\ \widetilde{O}\left(\frac{S}{(1-\gamma)^3\varepsilon^2}\right) & \text{if } A = 1 \qquad (\textit{TD learning}) \end{cases}$$

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- Covers both *constant* and *rescaled linear* learning rates:

$$\eta_t \equiv \frac{1}{1 + \frac{c_1(1-\gamma)T}{\log^2 T}} \quad \text{or} \quad \eta_t = \frac{1}{1 + \frac{c_2(1-\gamma)t}{\log^2 T}}$$

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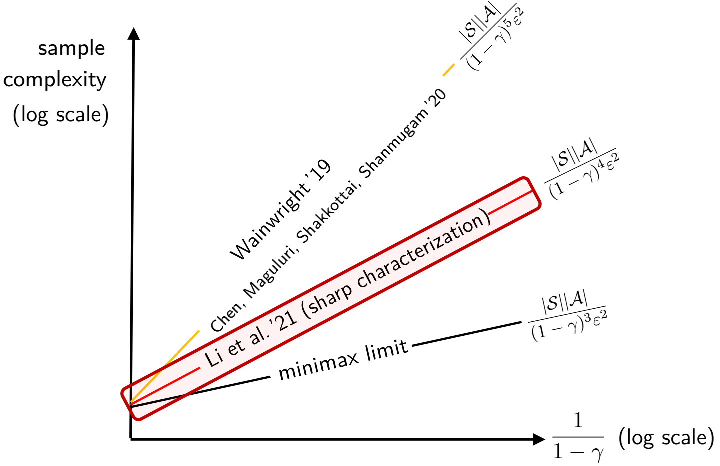
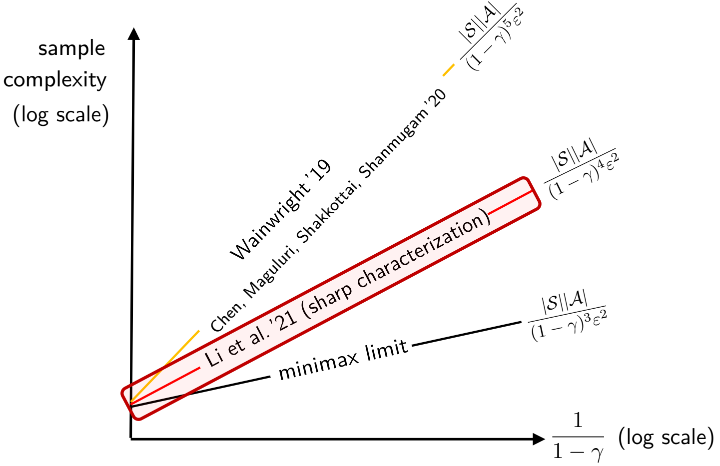
$$\begin{cases} \widetilde{O}\Big(\frac{SA}{(1-\gamma)^4\varepsilon^2}\Big) & \text{if } A \geq 2 \qquad \text{(?)} \\ \widetilde{O}\Big(\frac{S}{(1-\gamma)^3\varepsilon^2}\Big) & \text{if } A = 1 \qquad \text{(minimax optimal)} \end{cases}$$

other papers	sample complexity
Even-Dar & Mansour, 2003	$2^{\frac{1}{1-\gamma}} \frac{SA}{(1-\gamma)^4\varepsilon^2}$
Beck, Srikant, 2012	$\frac{S^2A^2}{(1-\gamma)^5\varepsilon^2}$
Wainwright, 2019	$\frac{SA}{(1-\gamma)^5\varepsilon^2}$
Chen, Maguluri, Shakkottai, Shanmugam, 2020	$\frac{SA}{(1-\gamma)^5\varepsilon^2}$

All this requires sample size at least $\frac{SA}{(1-\gamma)^4\varepsilon^2}$ $(A \geq 2)$ ...



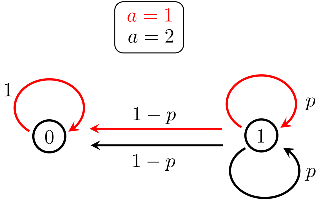
All this requires sample size at least $\frac{SA}{(1-\gamma)^4\varepsilon^2}$ $(A \geq 2)$ ...



Question: *Is Q-learning sub-optimal, or is it an analysis artifact?*

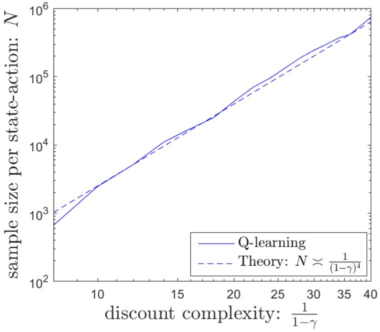
A numerical example: $\frac{SA}{(1-\gamma)^4\varepsilon^2}$ samples seem necessary ...

— *observed in Wainwright '19*



$$p = \frac{4\gamma - 1}{3\gamma}$$

$$r(0,1) = 0, \quad r(1,1) = r(1,2) = 1$$



Q-learning is NOT minimax optimal

Theorem (Li, Cai, Chen, Wei, Chi '21, OR'24)

For any $0 < \varepsilon \leq 1$, there exists an MDP with $A \geq 2$ such that to achieve $\|\widehat{Q} - Q^{\star}\|_{\infty} \leq \varepsilon$, synchronous Q-learning needs at least

$$\widetilde{\Omega}\left(\frac{SA}{(1-\gamma)^4\varepsilon^2}\right) \quad \text{samples}$$

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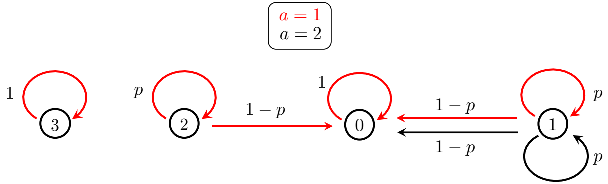
- Tight **algorithm-dependent** lower bound
- Holds for both constant and rescaled linear learning rates



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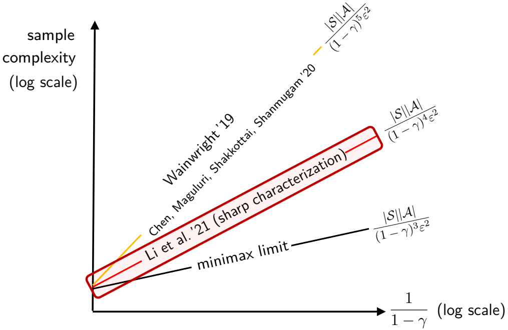

Why is Q-learning sub-optimal?

Over-estimation of Q-functions (Thrun & Schwartz '93; Hasselt '10)

- $\max_{a \in \mathcal{A}} \mathbb{E}[X(a)]$ tends to be over-estimated (high positive bias) when $\mathbb{E}[X(a)]$ is replaced by its empirical estimates using a small sample size
- often gets worse with a large number of actions (Hasselt, Guez, Silver '15)

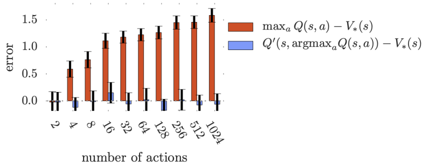

Figure 1: The orange bars show the bias in a single Q-learning update when the action values are $Q(s,a) = V_*(s) + \epsilon_a$ and the errors $\{\epsilon_a\}_{a=1}^m$ are independent standard normal random variables. The second set of action values Q', used for the blue bars, was generated identically and independently. All bars are the average of 100 repetitions.

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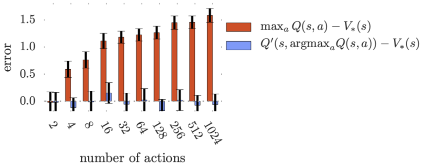

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A provable improvement: Q-learning with <u>variance reduction</u>

(Wainwright 2019)

Improving sample complexity via ***variance reduction***

— *a powerful idea from finite-sum stochastic optimization*

Variance-reduced Q-learning updates (Wainwright, 2019)

— *inspired by SVRG (Johnson & Zhang, 2013)*

$$Q_t(s,a) = (1-\eta)Q_{t-1}(s,a) + \eta\Big(\mathcal{T}_t(Q_{t-1}) \underbrace{-\mathcal{T}_t(\overline{Q}) + \widetilde{\mathcal{T}}(\overline{Q})}_{\text{use } \overline{Q} \text{ to help reduce variability}}\Big)(s,a)$$

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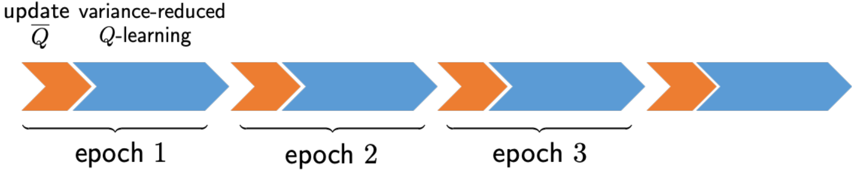
- $\overline{Q}$: some reference Q-estimate
- $\widetilde{\mathcal{T}}$: empirical Bellman operator (using a *batch* of samples)

$$\mathcal{T}_t(Q)(s,a) = r(s,a) + \gamma \max_{a'} Q(s',a')$$

$$\widetilde{\mathcal{T}}(Q)(s,a) = r(s,a) + \gamma \mathop{\mathbb{E}}_{s' \sim \widetilde{P}(\cdot|s,a)} \Big[\max_{a'} Q(s',a')\Big]$$

An epoch-based stochastic algorithm

— *inspired by Johnson & Zhang, 2013*



for each epoch

1. update $\overline{Q}$ and $\widetilde{\mathcal{T}}(\overline{Q})$ (which stay fixed in the rest of the epoch)
2. run variance-reduced Q-learning updates iteratively

Sample complexity of variance-reduced Q-learning

Theorem (Wainwright '19)

*For any $0 < \varepsilon \leq 1$, sample complexity for **variance-reduced synchronous Q-learning** to yield $\|\widehat{Q} - Q^{\star}\|_{\infty} \leq \varepsilon$ is at most*

$$\widetilde{O}\Big(\frac{SA}{(1-\gamma)^{3}\varepsilon^{2}}\Big)$$

- allows for more aggressive learning rates

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$$\widetilde{O}\Big(\frac{SA}{(1-\gamma)^3 \varepsilon^2}\Big)$$

- allows for more aggressive learning rates
- minimax-optimal for $0 < \varepsilon \leq 1$
  - remains suboptimal if $1 < \varepsilon < \frac{1}{1-\gamma}$

Reference: general RL textbooks I

- "*Reinforcement learning: An introduction*," R. S. Sutton, A. G. Barto, MIT Press, 2018
- "*Reinforcement learning: Theory and algorithms*," A. Agarwal, N. Jiang, S. Kakade, W. Sun, 2019
- "*Reinforcement learning and optimal control*," D. Bertsekas, Athena Scientific, 2019
- "*Algorithms for reinforcement learning*," C. Szepesvari, Springer, 2022
- "*Bandit algorithms*," T. Lattimore, C. Szepesvari, Cambridge University Press, 2020

Reference: model-based algorithms I

- "*Finite-sample convergence rates for Q-learning and indirect algorithms*," M. Kearns, S. Satinder, *NeurIPS*, 1998
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- "*A sparse sampling algorithm for near-optimal planning in large Markov decision processes*," M. Kearns, Y. Mansour, A. Y. Ng, *Machine learning*, 2002
- "*Minimax PAC bounds on the sample complexity of reinforcement learning with a generative model*," M. G. Azar, R. Munos, H. J. Kappen, *Machine learning*, 2013
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Reference: model-free algorithms I

- "*A stochastic approximation method,*" H. Robbins, S. Monro, *Annals of Mathematical Statistics*, 1951
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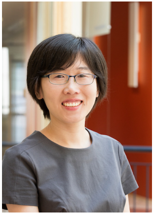
- "*Stochastic approximation with cone-contractive operators: Sharp ℓ_∞ bounds for Q-learning,*" M. Wainwright, 2019

Reference: model-free algorithms II

- "*Is Q-learning minimax optimal? a tight sample complexity analysis*," G. Li, C. Cai, Y. Chen, Y. Wei, Y. Chi, *Operations Research*, 2024
- "*Variance-reduced Q-learning is minimax optimal*," M. Wainwright, 2019
- "*Sample-optimal parametric Q-learning using linearly additive features,*" L. Yang, M. Wang, *ICML*, 2019
- "*Asynchronous stochastic approximation and Q-learning*," J. Tsitsiklis, *Machine learning*, 1994
- "*Finite-time analysis of asynchronous stochastic approximation and Q-learning*," G. Qu, A. Wierman, *COLT*, 2020
- "*Finite-sample analysis of contractive stochastic approximation using smooth convex envelopes*," Z. Chen, S. T. Maguluri, S. Shakkottai, K. Shanmugam, *NeurIPS*, 2020
- "*Sample complexity of asynchronous Q-learning: Sharper analysis and variance reduction*," G. Li, Y. Wei, Y. Chi, Y. Gu, Y. Chen, *IEEE Trans. on Information Theory*, 2022

Information-theoretic, statistical and algorithmic foundations of reinforcement learning



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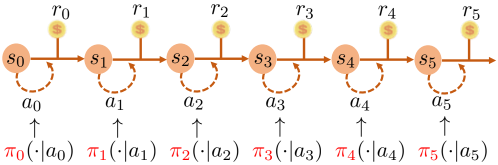
Tutorial, ISIT 2024
Part 2

Part 2

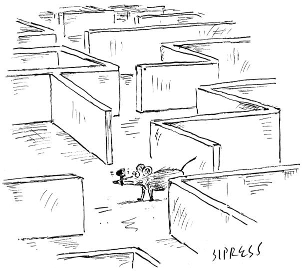
1. Online RL
2. Offline RL
3. Multi-agent RL
4. Robust RL

Online RL: interacting with real environment



exploration via adaptive policies

- trial-and-error
- sequential and online
- adaptive learning from data

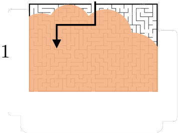


"Recalculating ... recalculating ..."

Online episodic RL

Sequentially execute MDP for K episodes, each consisting of H steps

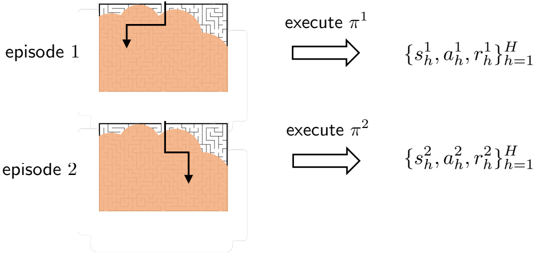
episode 1



execute π^1 $\Longrightarrow$ $\{s_h^1, a_h^1, r_h^1\}_{h=1}^H$

Online episodic RL

Sequentially execute MDP for K episodes, each consisting of H steps



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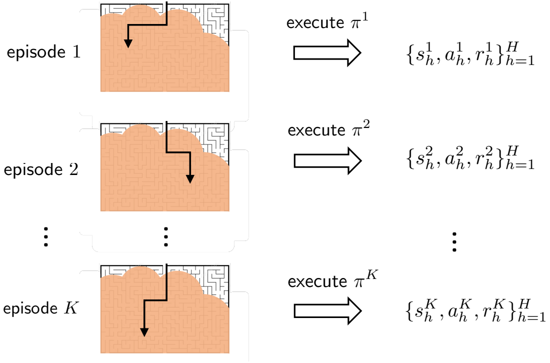
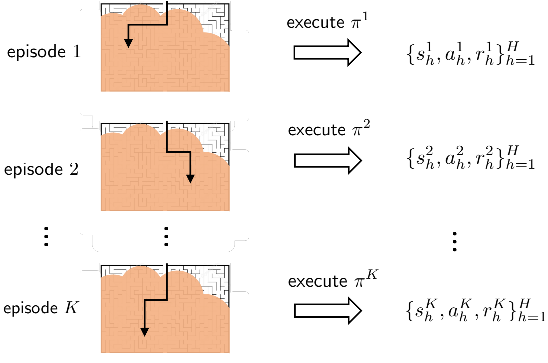


Online episodic RL

Sequentially execute MDP for K episodes, each consisting of H steps — *sample size: $T = KH$*



exploration (exploring unknowns) vs. **exploitation** (exploiting learned info)

Regret: gap between learned policy & optimal policy

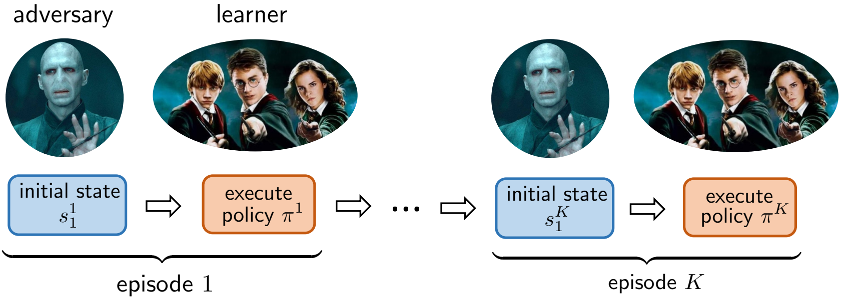
adversary

learner

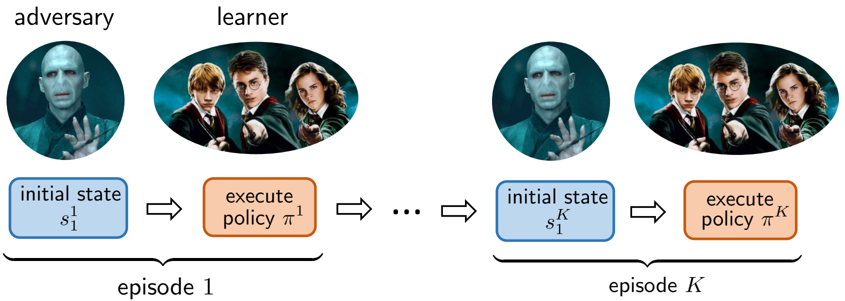
initial state s_1^1 $\Rightarrow$ execute policy π^1

episode 1

Regret: gap between learned policy & optimal policy



Regret: gap between learned policy & optimal policy



Performance metric: given initial states $\{s_1^k\}_{k=1}^K$, define

$$\text{Regret}(T) \quad := \quad \sum_{k=1}^{K} \left(V_1^{\star}(s_1^k) - V_1^{\pi^k}(s_1^k) \right)$$

Lower bound

(Domingues et al, 2021)

$$\text{Regret}(T) \gtrsim \sqrt{H^2SAT}$$

Existing algorithms

- UCB-VI: Azar et al, 2017
- UBEV: Dann et al, 2017
- UCB-Q-Hoeffding: Jin et al, 2018
- UCB-Q-Bernstein: Jin et al, 2018
- UCB2-Q-Bernstein: Bai et al, 2019
- EULER: Zanette et al, 2019
- UCB-Q-Advantage: Zhang et al, 2020
- MVP: Zhang et al, 2020
- UCB-M-Q: Menard et al, 2021
- Q-EarlySettled-Advantage: Li et al, 2021
- (modified) MVP: Zhang et al, 2024

Lower bound

(Domingues et al, 2021)

$$\text{Regret}(T) \gtrsim \sqrt{H^2SAT}$$

Existing algorithms

- UCB-VI: Azar et al, 2017
- UBEV: Dann et al, 2017
- UCB-Q-Hoeffding: Jin et al, 2018
- UCB-Q-Bernstein: Jin et al, 2018
- UCB2-Q-Bernstein: Bai et al, 2019
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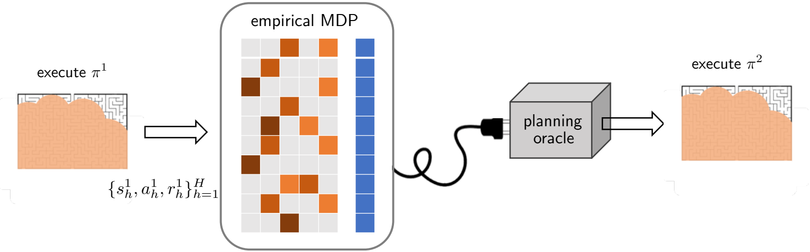
Which online RL algorithms achieve near-minimal regret?

Model-based online RL with UCB exploration

Model-based approach for online RL



repeat:

- use collected data to estimate transition probabilities
- apply planning to the estimated model to derive a new policy for sampling in the next episode

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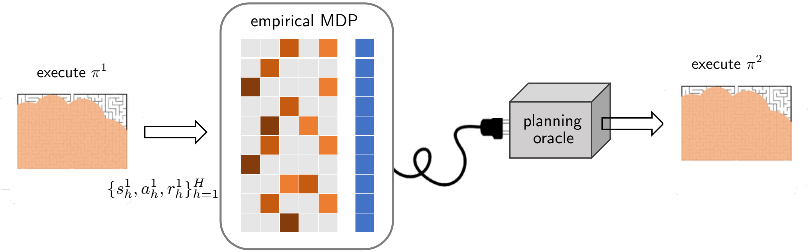

repeat:

- use collected data to estimate transition probabilities
- apply planning to the estimated model to derive a new policy for sampling in the next episode

How to balance exploration and exploitation in this framework?

T. L. Lai

H. Robbins

Optimism in the face of uncertainty:

- explores based on the best optimistic estimates associated with the actions!
- a common framework: utilize $\underbrace{\text{upper confidence bounds (UCB)}}_{\text{accounts for estimates + uncertainty level}}$

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Optimism in the face of uncertainty:

- explores based on the best optimistic estimates associated with the actions!
- a common framework: utilize upper confidence bounds (UCB) — accounts for estimates + uncertainty level

Optimistic model-based approach: incorporates UCB framework into model-based approach

UCB-VI (Azar et al. '17)

For each episode:

1. Backtrack $h = H, H-1, \ldots, 1$: run **value iteration**

$$Q_h(s_h, a_h) \leftarrow r_h(s_h, a_h) + \underbrace{\widehat{P}_{h,s_h,a_h}}_{\text{model estimate}} V_{h+1}$$

$$V_h(s_h) \leftarrow \max_{a \in \mathcal{A}} Q_h(s_h, a)$$

UCB-VI (Azar et al. '17)

For each episode:

1. Backtrack $h = H, H-1, \ldots, 1$: run **optimistic value iteration**

$$Q_h(s_h, a_h) \leftarrow r_h(s_h, a_h) + \underbrace{\widehat{P}_{h,s_h,a_h}}_{\text{model estimate}} V_{h+1} + \underbrace{b_h(s_h, a_h)}_{\text{bonus (upper confidence width)}}$$

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$$V_h(s_h) \leftarrow \max_{a \in \mathcal{A}} Q_h(s_h, a)$$

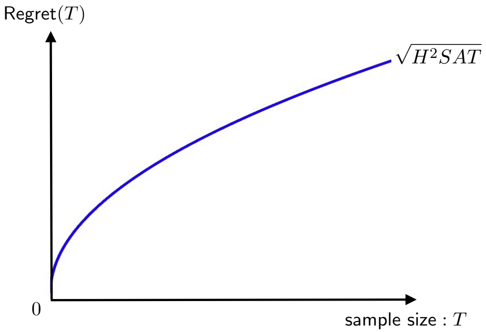
2. Forward $h = 1, \ldots, H$: take actions according to **greedy policy**

$$\pi_h(s) \leftarrow \text{argmax}_{a \in \mathcal{A}} Q_h(s, a)$$

to sample a new episode $\{s_h, a_h, r_h\}_{h=1}^{H}$

UCB-VI is asymptotically regret-optimal

— Azar, Osband, Munos, 2017



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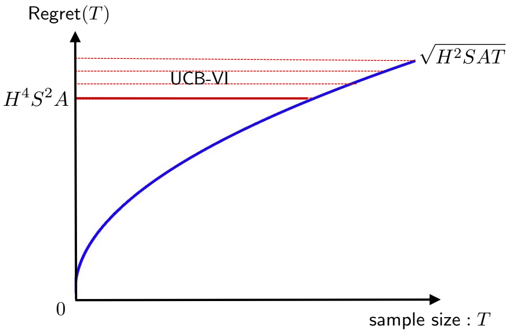

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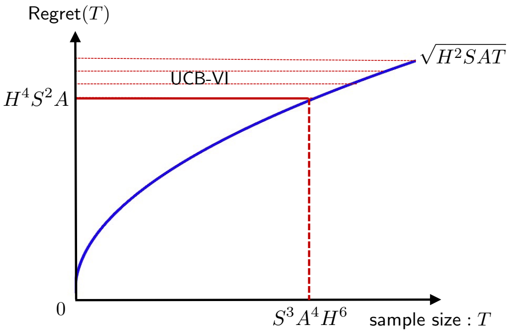

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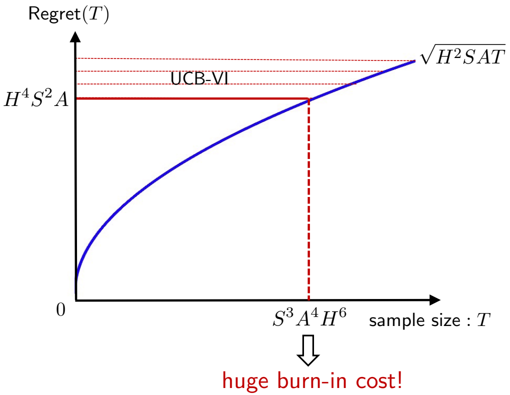

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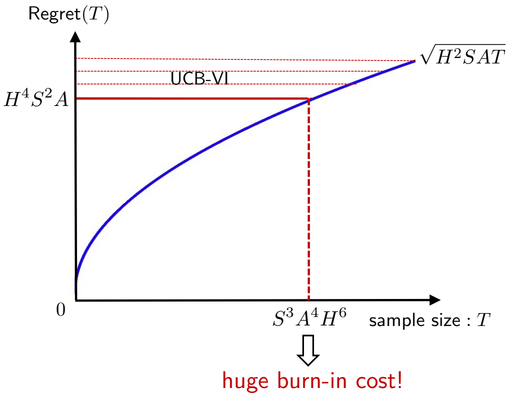

Issues: large burn-in cost

Other asymptotically regret-optimal algorithms

Algorithm	Regret upper bound	Range of K that attains optimal regret
UCBVI (Azar et al, 2017)	$\sqrt{SAH^2T} + S^2AH^3$	$[S^3AH^3, \infty)$
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Can we find a regre-optimal algorithm with no burn-in cost?

Monotonic Value Propagation

UCB-VI with doubling update rules and variance-aware bonus

- (s, a, h) is updated only when visited the $\{1, 3, 7, 15, \cdots\}$-th time

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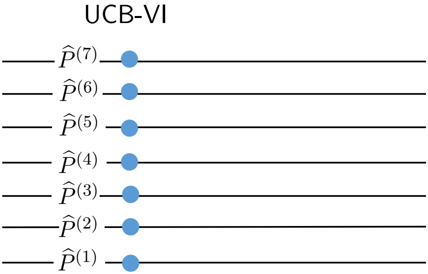

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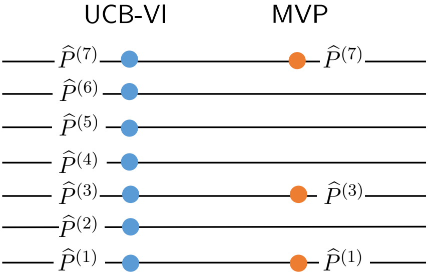

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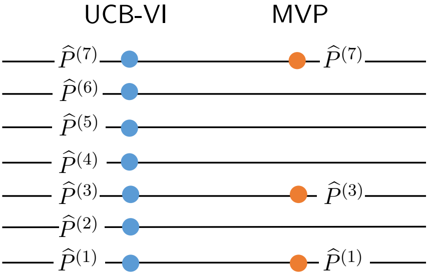

  - visitation counts change much less frequently
    $\longrightarrow$ reduces covering number dramatically

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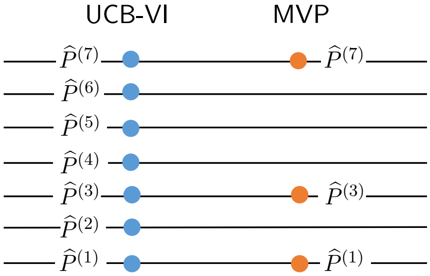
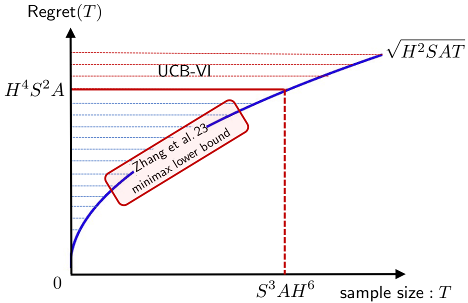


  - visitation counts change much less frequently
    $\longrightarrow$ reduces covering number dramatically

- data-driven bonus terms (chosen based on empirical variances)

Regret-optimal algorithm w/o burn-in cost

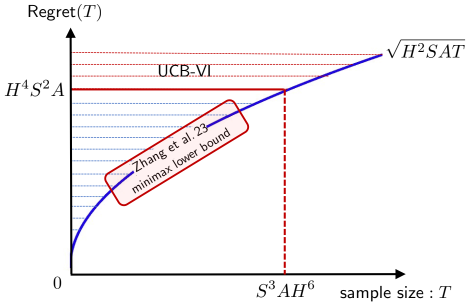


Theorem (Zhang, Chen, Lee, Du '24)

The model-based algorithm Monotonic Value Propagation achieves

$$\text{Regret}(T) \lesssim \widetilde{O}(\sqrt{H^2SAT})$$

Regret-optimal algorithm w/o burn-in cost



Theorem (Zhang, Chen, Lee, Du '24)

The model-based algorithm Monotonic Value Propagation achieves

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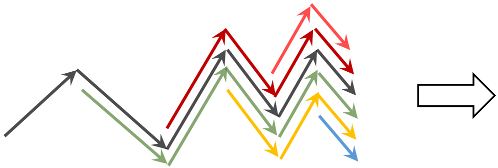
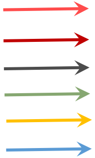
- the only algorithm so far that is regret-optimal w/o burn-ins

Key technical innovation



online data collection
w/ sample reuse



samples drawn
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Decoupling complicated statistical dependency during online learning

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Decoupling complicated statistical dependency during online learning

- couples online data collection with i.i.d. sampling

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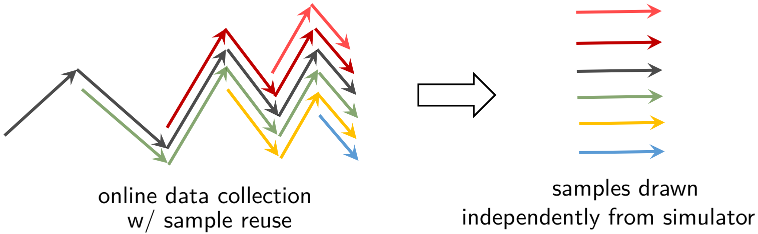

Decoupling complicated statistical dependency during online learning

- couples online data collection with i.i.d. sampling
- exploit *compressibility* of visitation counts
  - w/ the aid of doubling algorithmic trick

How about memory complexity?

Algorithm	Regret upper bound	Range of K that attains optimal regret	Memory complexity
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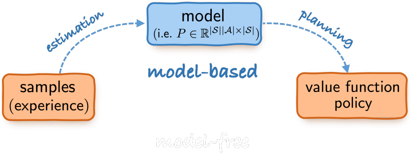
Can we find a regret-optimal algorithm with
(1) low burn-in cost and (2) low memory complexity?

Model-free RL is often more memory-efficient



store transition kernel estimates

$\rightarrow$ $O(S^2AH)$ *memory*

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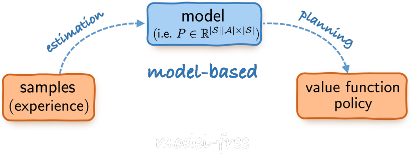

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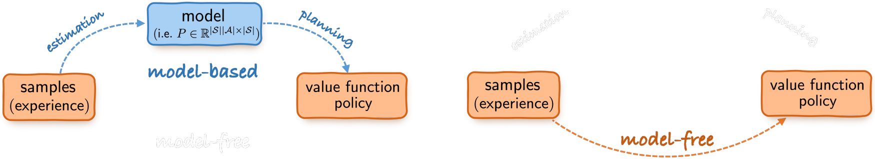

store transition kernel estimates
$\rightarrow$ $O(S^2AH)$ *memory*

maintain Q-estimates
$\rightarrow$ $O(SAH)$ *memory*

Definition (Jin et al. '18)

An RL algorithm is **model-free** if its space complexity is $o(S^2AH)$

Which model-free algorithms are sample-efficient for online RL?

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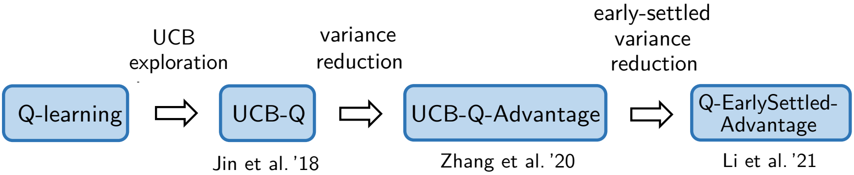

Q-learning: a classical model-free algorithm

Chris Watkins

Peter Dayan

Stochastic approximation for solving Bellman equation

$$Q_h(s_h, a_h) \longleftarrow (1-\eta_k)Q_h(s_h, a_h) + \eta_k \mathcal{T}_k(Q_{h+1})(s_h, a_h)$$

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$$\mathcal{T}_k(Q_h)(s_h, a_h) = r(s_h, a_h) + \max_{a'} Q(s_{h+1}, a')$$

using sample in k-th episode

Q-learning with UCB exploration (Jin et al., 2018)

$$Q_h(s_h, a_h) \leftarrow \underbrace{(1-\eta_k)Q_h(s_h, a_h) + \eta_k \mathcal{T}_k\left(Q_{h+1}\right)(s_h, a_h)}_{\text{classical Q-learning}} + \eta_k \underbrace{b_h(s_h, a_h)}_{\text{exploration bonus}}$$

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- $b_h(s,a)$: upper confidence bound
  — *optimism in the face of uncertainty*
- inspired by UCB bandit algorithm (Lai, Robbins '85)

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Issue: *large variability in stochastic update rules*

Q-learning with UCB and variance reduction

— *Zhang et al. '20*

Incorporates variance reduction into UCB-Q:

Q-learning with UCB and variance reduction

— *Zhang et al. '20*

Incorporates reference-advantage decomposition into UCB-Q:

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Incorporates reference-advantage decomposition into UCB-Q:

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$$+ \eta_k \Big(\underbrace{\mathcal{T}_k(Q_{h+1}) - \mathcal{T}_k(\overline{Q}_{h+1})}_{\text{advantage}} + \underbrace{\widehat{\mathcal{T}}(\overline{Q}_{h+1})}_{\text{reference}} \Big)(s_h, a_h)$$

- Reference $\overline{Q}_{h+1}$, batch estimate $\widehat{\mathcal{T}}$: help reduce variability

Q-learning with UCB and variance reduction

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Incorporates reference-advantage decomposition into UCB-Q:

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UCB-Q-Advantage is asymptotically regret-optimal

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UCB-Q-Advantage is asymptotically regret-optimal

Issue: *high burn-in cost* $O(S^6 A^4 H^{28})$

Diagnosis of UCB-Q-Advantage

Variance reduction requires sufficiently good references $\overline{Q}_h$

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$$\Downarrow$$

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Large burn-in cost

Diagnosis of UCB-Q-Advantage

Variance reduction requires sufficiently good references $\overline{Q}_h$

$\Downarrow$

Updating references $\overline{Q}_h$ and $\overline{V}_h$ many times

$\Downarrow$

Large burn-in cost

Key idea: early settlement of the reference as soon as it reaches a reasonable quality (e.g., $\overline{V}_h \leq V_h^\star + 1$)

Our algorithm: Q-EarlySettled-Advantage

Theorem (Li, Shi, Chen, Gu, Chi '21)

With high prob., Q-EarlySettled-Advantage *achieves (up to log factor)*

$$\text{Regret}(T) \lesssim \sqrt{H^2SAT} + H^6SA$$

with a memory complexity of $O(SAH)$

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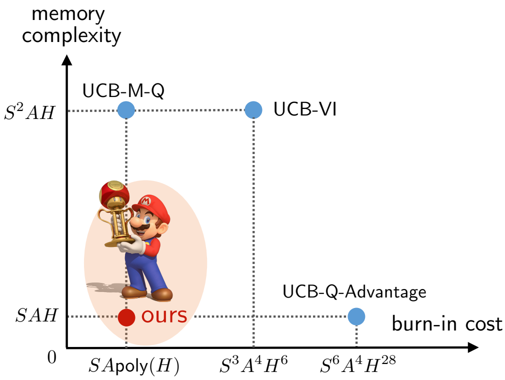
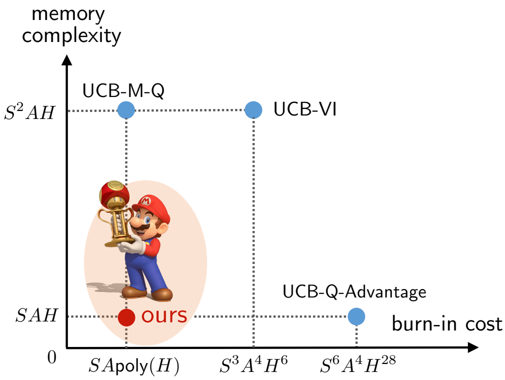
with a memory complexity of $O(SAH)$

- regret-optimal with burn-in cost $O(SA\text{poly}(H))$
  - optimal in SA, suboptimal in H
- memory-efficient $O(SAH)$
- computationally efficient: runtime $O(T)$



Model-free algorithms can simultaneously achieve

(1) regret optimality; (2) low burn-in cost; (3) memory efficiency



Model-free algorithms can simultaneously achieve

(1) regret optimality; (2) low burn-in cost; (3) memory efficiency

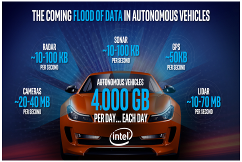
Part 2

1. Online RL
2. Offline RL
3. Multi-agent RL
4. Robust RL

Offline/batch RL

- Collecting new data might be costly, unsafe, unethical, or time-consuming

medical records



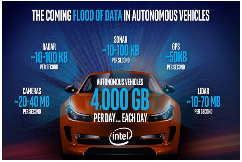
data of self-driving

clicking times of ads

Offline/batch RL

- Collecting new data might be costly, unsafe, unethical, or time-consuming
- But we have already stored tons of historical data

medical records



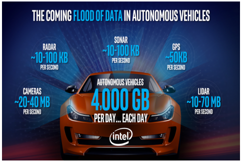
data of self-driving

clicking times of ads

Offline/batch RL

- Collecting new data might be costly, unsafe, unethical, or time-consuming
- But we have already stored tons of historical data

medical records

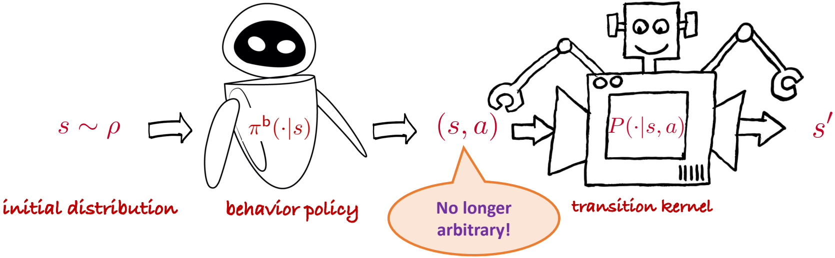


data of self-driving

clicking times of ads

Question: can we learn based solely on historical data w/o active exploration?

A mathematical model of offline data



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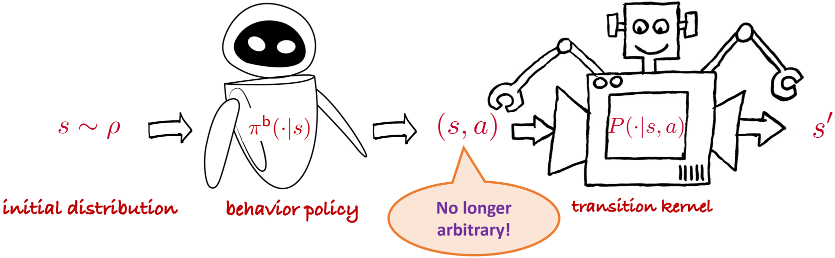
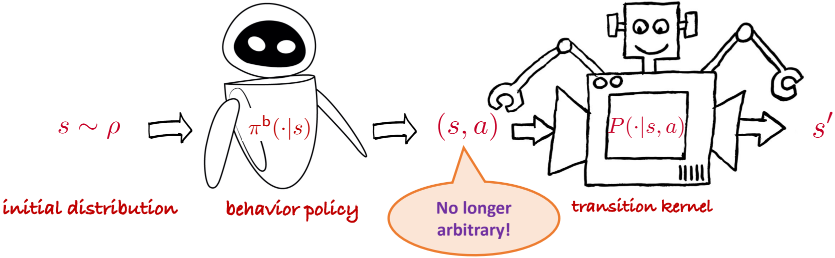


historical dataset $\mathcal{D} = \{(s^{(i)}, a^{(i)}, s'^{(i)})\}$**:** N independent copies of

$$s \sim \rho, \qquad a \sim \pi^{\mathsf{b}}(\cdot \,|\, s), \qquad s' \sim P(\cdot \,|\, s, a)$$

- ρ: initial state distribution; $\quad \pi^{\mathsf{b}}$: behavior policy

A mathematical model of offline data



Goal: given a target accuracy level $\varepsilon \in (0, H]$, find $\widehat{\pi}$ s.t.

$$V^{\star}(\rho) - V^{\widehat{\pi}}(\rho) := \mathop{\mathbb{E}}_{s\sim\rho}\left[V^{\star}(s)\right] - \mathop{\mathbb{E}}_{s\sim\rho}\left[V^{\widehat{\pi}}(s)\right] \leq \varepsilon$$

— *in a sample-efficient manner*

Challenges of offline RL

- **Distribution shift**:

$$\text{distribution}(\mathcal{D}) \neq \text{target distribution under optimal } \pi^\star$$

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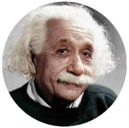
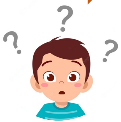
easier — harder → distance$(\pi^{\mathsf{b}}, \pi^\star)$



expert data

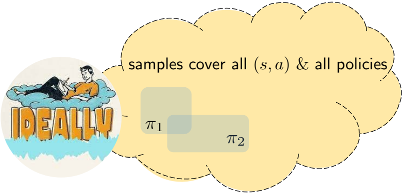


Challenges of offline RL

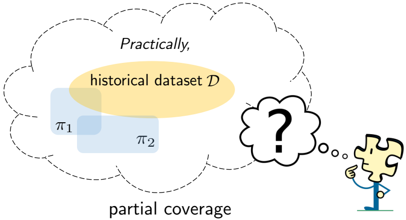
- **Distribution shift**:

$$\text{distribution}(\mathcal{D}) \neq \text{target distribution under optimal } \pi^\star$$

- **Partial coverage of state-action space**:



uniform coverage over entire space
(sufficiently explored)



partial coverage
(inadequately explored)

How to quantify quality of historical dataset $\mathcal{D}$ (induced by π^{b})?

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Single-policy concentrability coefficient (Rashidineiad et al. '21)

$$C^{\star} := \max_{s,a} \frac{d^{\pi^{\star}}(s,a)}{d^{\pi^{\mathsf{b}}}(s,a)} = \left\| \frac{\textit{occupancy distribution of } \pi^{\star}}{\textit{occupancy distribution of } \pi^{\mathsf{b}}} \right\|_{\infty} \geq 1$$

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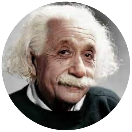
- captures distributional shift

$C^{\star} = O(1)$ —————————————————————→ large $C^{\star}$



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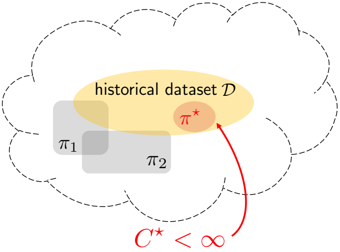
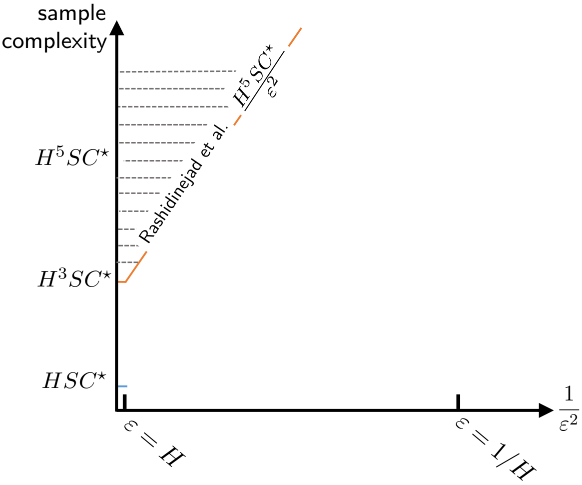
- captures distributional shift
- allows for partial coverage
  - as long as it covers the part reachable by $\pi^\star$



Prior art: sample complexity bounds



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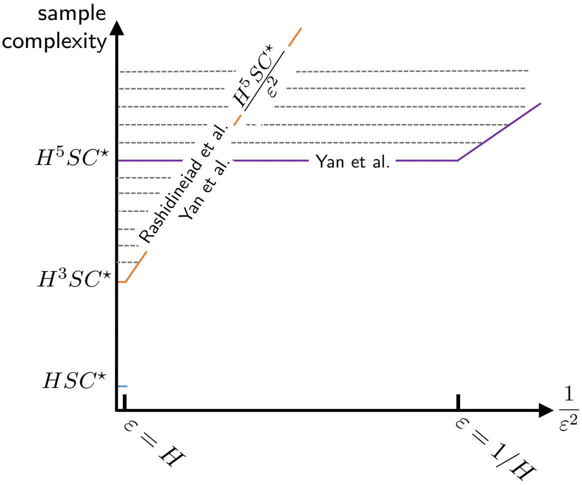

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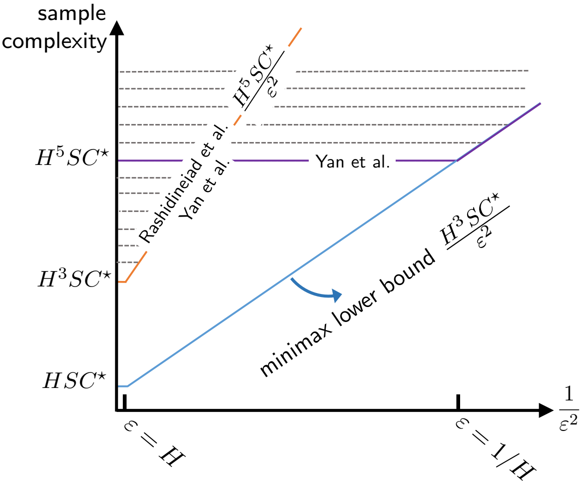

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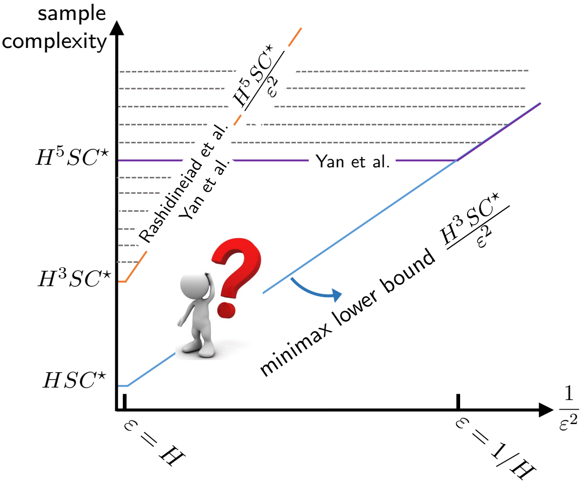
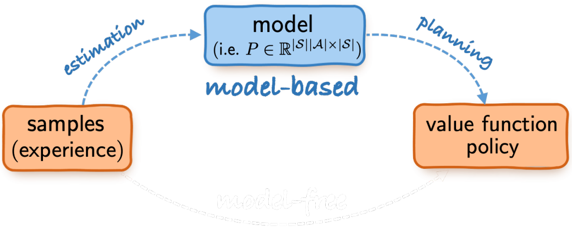


Can we close the gap between upper & lower bounds?

Model-based ("plug-in") approach?



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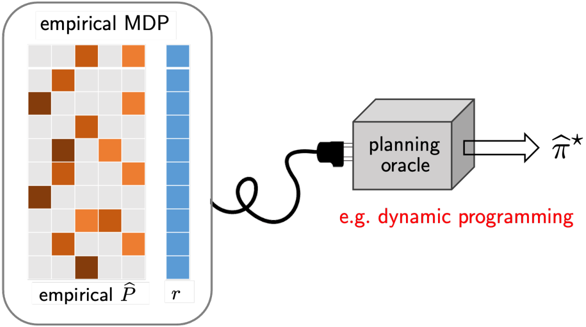
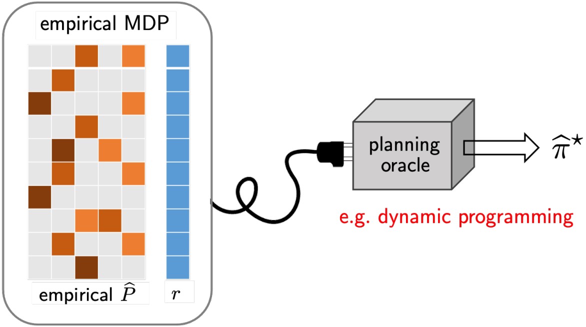


1. construct empirical model $\widehat{P}$:

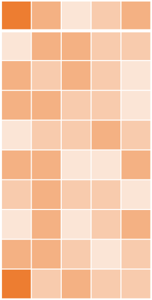
$$\widehat{P}(s' \mid s, a) = \underbrace{\frac{1}{N} \sum_{i=1}^{N} \mathbb{1}\{s'^{(i)} = s'\}}_{\text{empirical frequency}}$$

Model-based ("plug-in") approach?

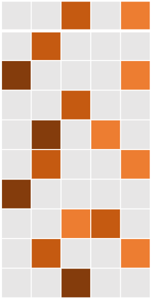


1. construct empirical model $\widehat{P}$
2. planning (e.g. value iteration) based on empirical MDP

Issues & challenges in the sample-starved regime



truth: $P \in \mathbb{R}^{SA \times S}$



empirical $\widehat{P}$ (simulator)

- can't recover P faithfully if sample size $\ll S^2 A$

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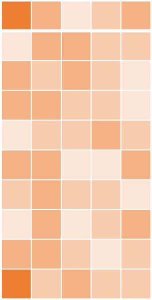

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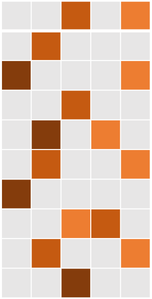

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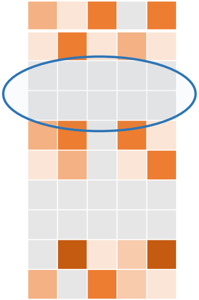

empirical $\widehat{P}$ (offline)

- can't recover P faithfully if sample size $\ll S^2 A$
- (possibly) insufficient coverage under offline data

Key idea: pessimism in the face of uncertainty

— Jin et al, 2020, Rashidinejad et al, 2021, Xie et al, 2021


online

upper confidence bounds

— promote exploration of under-explored (s, a)

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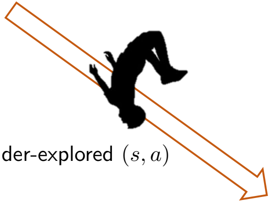

upper confidence bounds

— promote exploration of under-explored (s, a)

offline

lower confidence bounds

— stay cautious about under-explored (s, a)

Key idea: pessimism in the face of uncertainty

— *Jin et al, 2020, Rashidinejad et al, 2021, Xie et al, 2021*

1. build empirical model $\widehat{P}$
2. **(value iteration)** repeat: for all (s, a)

$$\widehat{Q}(s,a) \;\leftarrow\; \max\Big\{ r(s,a) + \gamma \langle \widehat{P}(\cdot \,|\, s,a), \widehat{V} \rangle,\; 0 \Big\}$$

where $\widehat{V}(s) = \max_a \widehat{Q}(s,a)$

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Penalize those poorly visited (s, a) ...

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compared w/ Rashidinejad et al, 2021

- sample-reuse across iterations
- Bernstein-style penalty

Sample complexity of model-based offline RL

Theorem (Li, Shi, Chen, Chi, Wei '24)

For any $0 < \varepsilon \leq \frac{1}{1-\gamma}$, *the policy* $\widehat{\pi}$ *returned by VI-LCB using a Bernstein-style penalty term achieves*

$$V^{\star}(\rho) - V^{\widehat{\pi}}(\rho) \leq \varepsilon$$

with high prob., with sample complexity at most

$$\widetilde{O}\left(\frac{SC^{\star}}{(1-\gamma)^{3}\varepsilon^{2}}\right)$$

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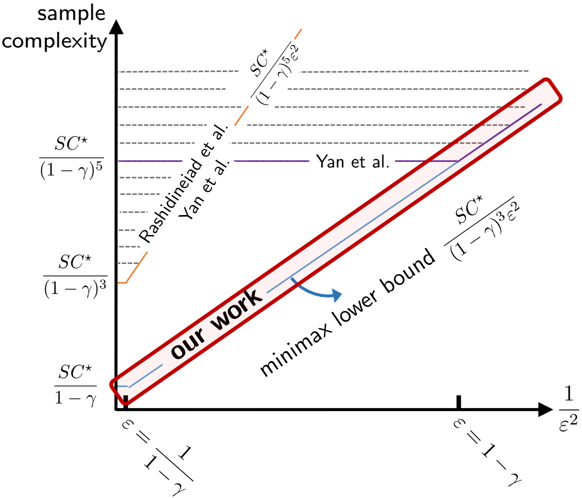
- depends on distribution shift (as reflected by $C^\star$)
- achieves minimax optimality
- full ε-range (no burn-in cost)



Model-based offline RL is minimax optimal with no burn-in cost!

Is it possible to design offline model-free algorithms with optimal sample efficiency?

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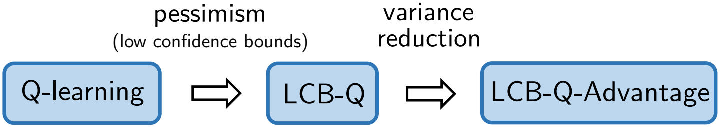

LCB-Q: Q-learning with LCB penalty

— *Shi et al, 2022, Yan et al, 2023*

$$Q_{t+1}(s_t, a_t) \leftarrow \underbrace{(1-\eta_t)Q_t(s_t, a_t) + \eta_t \mathcal{T}_t\left(Q_t\right)(s_t, a_t)}_{\text{classical Q-learning}} - \eta_t \underbrace{b_t(s_t, a_t)}_{\text{LCB penalty}}$$

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- $b_t(s, a)$: Hoeffding-style confidence bound
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- $b_t(s,a)$: Hoeffding-style confidence bound
- pessimism in the face of uncertainty

sample size: $\widetilde{O}\big(\frac{SC^\star}{(1-\gamma)^5\varepsilon^2}\big)$ $\Longrightarrow$ sub-optimal by a factor of $\frac{1}{(1-\gamma)^2}$

Issue: *large variability in stochastic update rules*

Q-learning with LCB and variance reduction

— *Shi et al, 2022, Yan et al, 2023*

$$Q_{t+1}(s_t, a_t) \leftarrow (1-\eta_t) Q_t(s_t, a_t) - \eta_t \underbrace{b_t(s_t, a_t)}_{\text{LCB penalty}}$$
$$+ \eta_t \Big(\underbrace{\mathcal{T}_t(Q_t) - \mathcal{T}_t(\overline{Q})}_{\text{advantage}} + \underbrace{\widehat{\mathcal{T}}(\overline{Q})}_{\text{reference}} \Big)(s_t, a_t)$$

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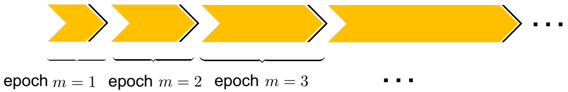
- incorporates variance reduction into LCB-Q



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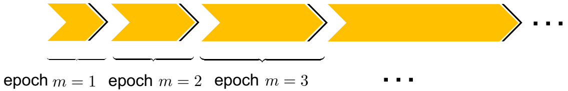
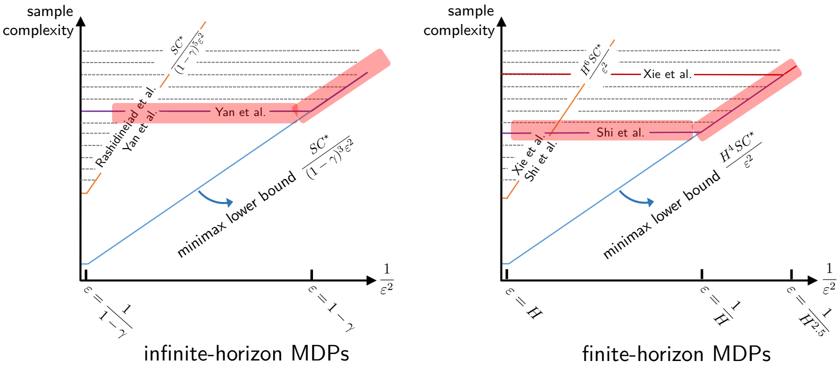


Theorem (Yan, Li, Chen, Fan '23, Shi, Li, Wei, Chen, Chi '22)

For $\varepsilon \in (0, 1-\gamma]$, LCB-Q-Advantage *achieves* $V^\star(\rho) - V^{\widehat{\pi}}(\rho) \le \varepsilon$ *with optimal sample complexity* $\widetilde{O}\big(\frac{SC^\star}{(1-\gamma)^3\varepsilon^2}\big)$



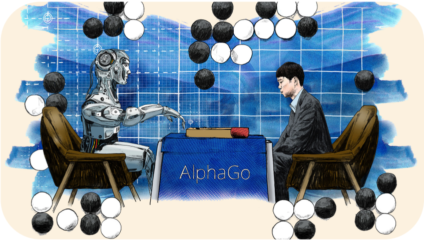
Model-free offline RL attains sample optimality too!

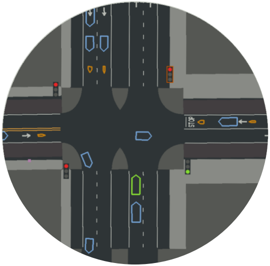
— *with some burn-in cost though . . .*

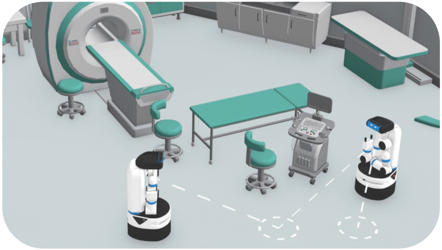
Part 2

1. Online RL
2. Offline RL
3. Multi-agent RL
4. Robust RL

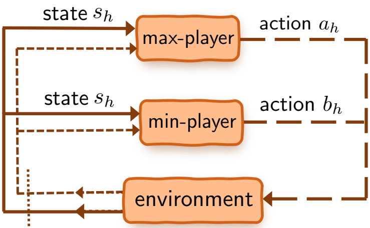
Multi-agent reinforcement learning (MARL)







Two-player zero-sum Markov games (finite-horizon)



- $\mathcal{S} = [S]$: state space
- H: horizon
- $\mathcal{A} = [A]$: action space of max-player
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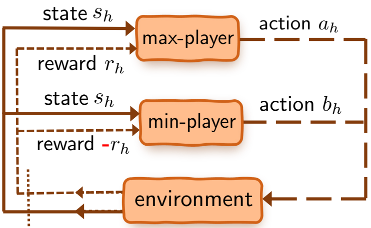

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- immediate reward: max-player $r(s, a, b) \in [0, 1]$
  min-player $-r(s, a, b)$

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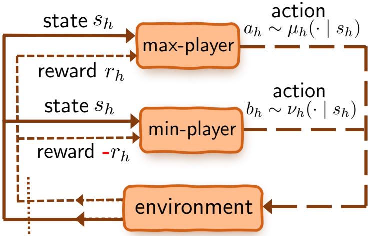

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- $\mu : \mathcal{S} \times [H] \to \Delta(\mathcal{A})$: policy of max-player
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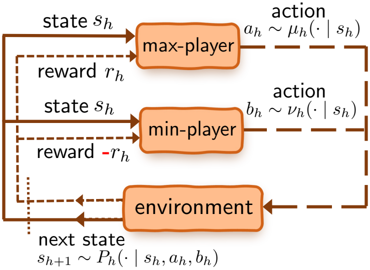

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- $\mu : \mathcal{S} \times [H] \to \Delta(\mathcal{A})$: policy of max-player
  $\nu : \mathcal{S} \times [H] \to \Delta(\mathcal{B})$: policy of min-player
- $P_h(\cdot \mid s,a,b)$: unknown transition probabilities

Value function under *independent* policies (μ, ν) (no coordination)

$$V^{\mu,\nu}(s) := \mathbb{E}\left[\sum_{h=1}^{H} r_h(s_h, a_h, b_h) \,\middle|\, s_1 = s\right]$$

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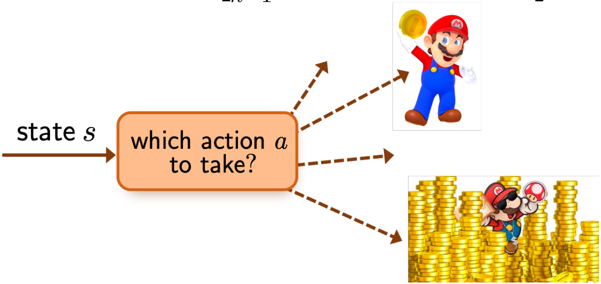

- Each agent seeks **optimal policy** maximizing her own value

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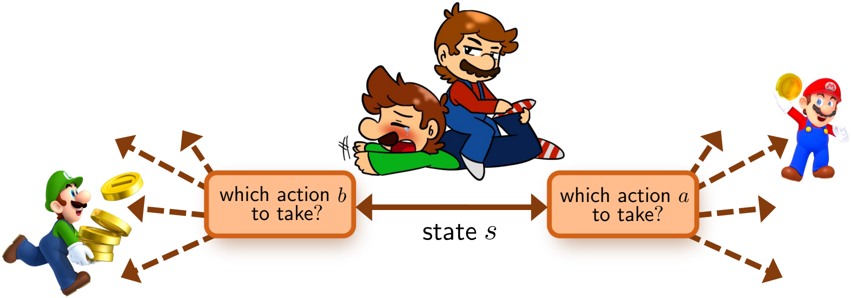

- Each agent seeks **optimal policy** maximizing her own value
- But two agents have conflicting goals ...

Compromise: Nash equilibrium (NE)

John von Neumann

John Nash

An NE policy pair $(\mu^\star, \nu^\star)$ obeys

$$\max_{\mu} V^{\mu,\nu^\star} = V^{\mu^\star,\nu^\star} = \min_{\nu} V^{\mu^\star,\nu}$$

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- no unilateral deviation is beneficial

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- no unilateral deviation is beneficial
- no coordination between two agents (they act *independently*)

Compromise: Nash equilibrium (NE)

John von Neumann

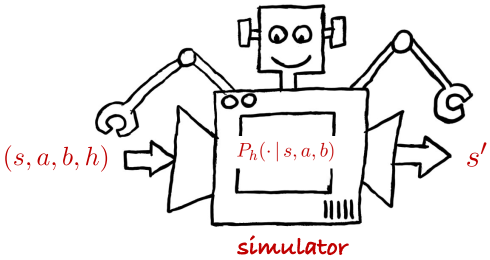
John Nash

An ε-NE policy pair $(\widehat{\mu}, \widehat{\nu})$ obeys

$$\max_{\mu} V^{\mu,\widehat{\nu}} - \varepsilon \le V^{\widehat{\mu},\widehat{\nu}} \le \min_{\nu} V^{\widehat{\mu},\nu} + \varepsilon$$

- no unilateral deviation is beneficial
- no coordination between two agents (they act *independently*)

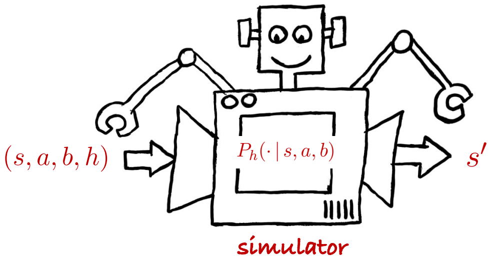
Learning NEs with a simulator



input: any (s, a, b, h)

output: an independent sample $s' \sim P_h(\cdot \mid s, a, b)$

Learning NEs with a simulator



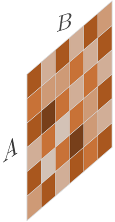
input: any (s,a,b,h)

output: an independent sample $s' \sim P_h(\cdot\,|\,s,a,b)$

Question: how many samples are sufficient to learn an ε-Nash policy pair?

Model-based approach (non-adaptive sampling)

— *Zhang, Kakade, Başar, Yang '20*

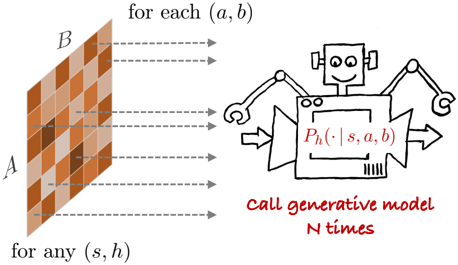


for any (s, h)

1. for each (s, a, b, h), call simulator N times

Model-based approach (non-adaptive sampling)

— *Zhang, Kakade, Başar, Yang '20*



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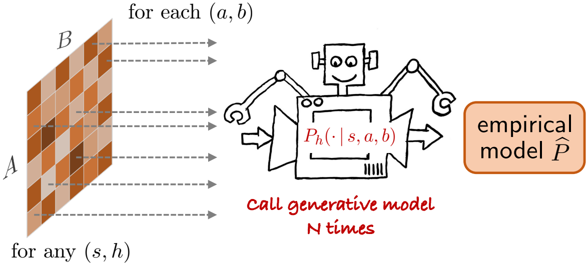

1. for each (s, a, b, h), call simulator N times
2. build empirical model $\widehat{P}$

Model-based approach (non-adaptive sampling)

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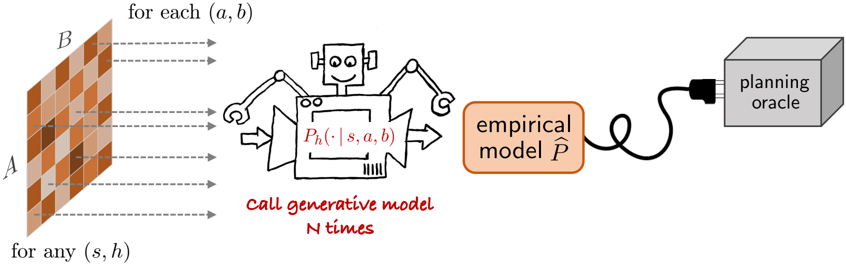
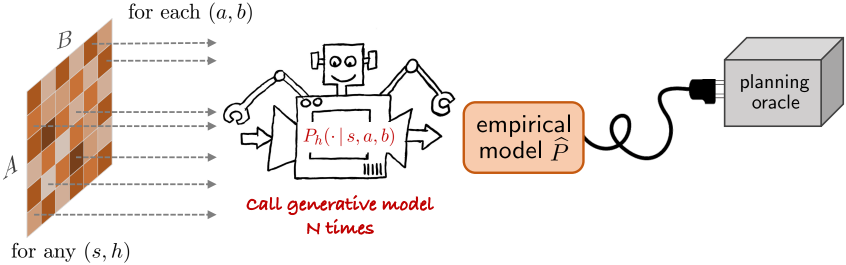


1. for each (s, a, b, h), call simulator N times
2. build empirical model $\widehat{P}$, and run "plug-in" methods

Model-based approach (non-adaptive sampling)

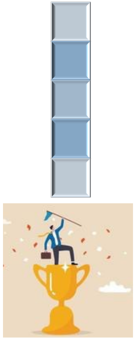
— *Zhang, Kakade, Başar, Yang '20*



1. for each (s, a, b, h), call simulator N times
2. build empirical model $\widehat{P}$, and run "plug-in" methods

sample complexity: $\frac{H^4 SAB}{\varepsilon^2}$

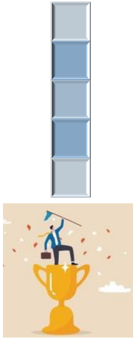
Curse of multiple agents



1 player: A

Let's look at the size of joint action space . . .

Curse of multiple agents



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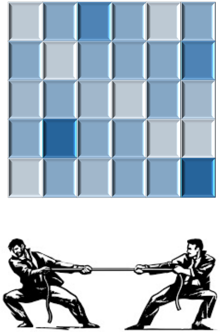
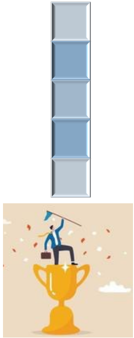


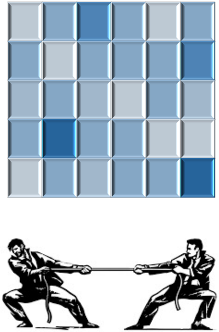
2 players: AB

Let's look at the size of joint action space . . .

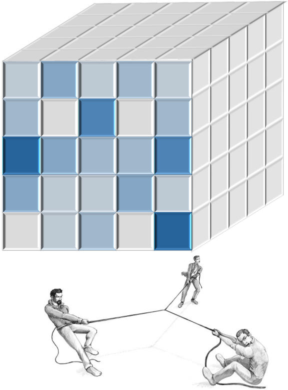
Curse of multiple agents



1 player: A



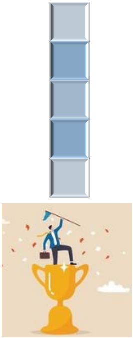
2 players: AB



m players: $A_1 A_2 \cdots A_m$

Let's look at the size of joint action space ...

Curse of multiple agents



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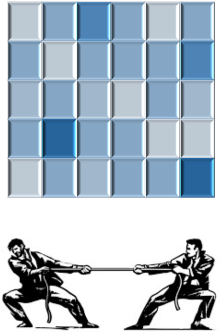
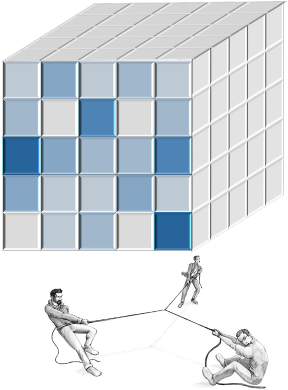
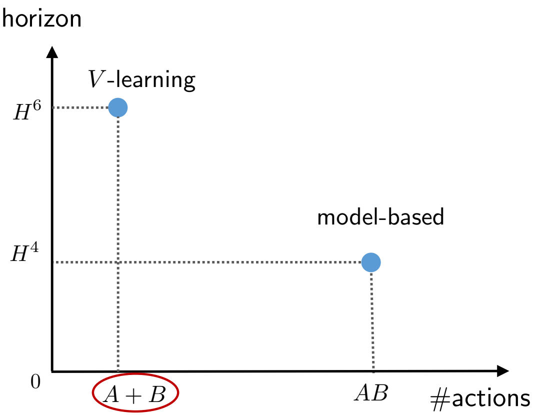


2 players: AB

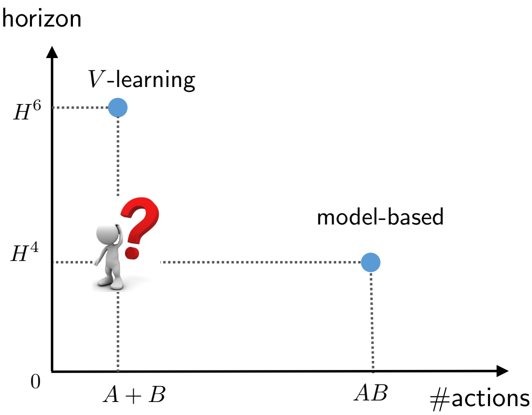


m players: $A_1 A_2 \cdots A_m$

joint actions blows up geometrically in # players!



horizon
V-learning
H^6
model-based
H^4
0
$A+B$
AB
#actions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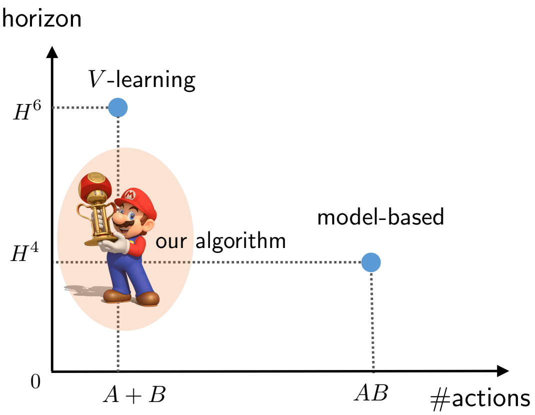


Theorem (Li, Chi, Wei, Chen '22)

For any $0 < \varepsilon \leq H$, one can design an algorithm that finds an ε-Nash policy pair $(\widehat{\mu}, \widehat{\nu})$ with high prob., with sample complexity at most

$$\widetilde{O}\Big(\frac{H^4 S(A+B)}{\varepsilon^2}\Big) \qquad \textit{(minimax-optimal } \forall \varepsilon)$$

Part 2

1. Online RL
2. Offline RL
3. Multi-agent RL
4. Robust RL

Safety and robustness in RL

(Zhou et al., 2021; Panaganti and Kalathil, 2022; Yang et al., 2022;)

Training environment $\neq$ Test environment

Safety and robustness in RL

(Zhou et al., 2021; Panaganti and Kalathil, 2022; Yang et al., 2022;)

Training environment $\neq$

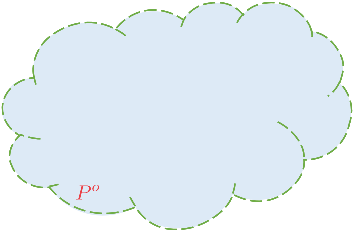
Test environment

Sim2Real Gap: Can we learn optimal policies that are robust to model perturbations?

Modeling environment uncertainty

Uncertainty set of the nominal transition kernel P^o:

$$\mathcal{U}^\sigma(P^o) = \{P : \rho(P, P^o) \le \sigma\}$$



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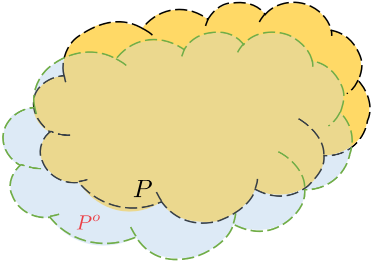

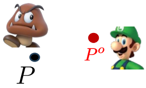

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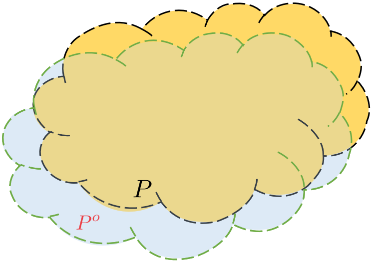

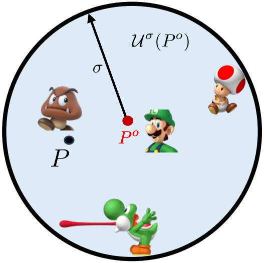

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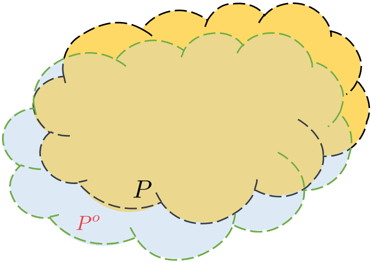
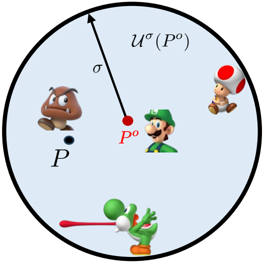
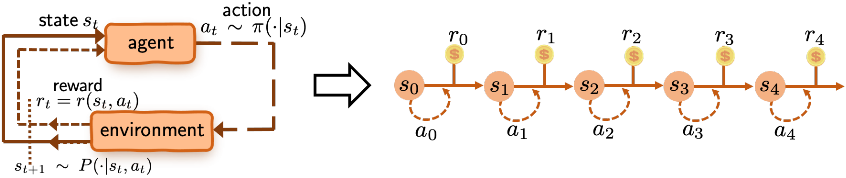




- Examples of ρ: f-divergence (TV, χ^2, KL...)

Robust value/Q function



Robust value/Q function of policy π:

$$\forall s \in \mathcal{S}: \qquad V^{\pi,\sigma}(s) := \inf_{P \in \mathcal{U}^{\sigma}(P^{o})} \mathbb{E}_{\pi,P}\left[\sum_{t=0}^{\infty} \gamma^t r_t \,\Big|\, s_0 = s\right]$$

$$\forall (s,a) \in \mathcal{S} \times \mathcal{A}: \quad Q^{\pi,\sigma}(s,a) := \inf_{P \in \mathcal{U}^{\sigma}(P^{o})} \mathbb{E}_{\pi,P}\left[\sum_{t=0}^{\infty} \gamma^t r_t \,\Big|\, s_0 = s, a_0 = a\right]$$

Measures the worst-case performance of the policy in the uncertainty set.

Distributionally robust MDP

Robust MDP

Find the policy $\pi^\star$ *that maximizes* $V^{\pi,\sigma}$

(Iyengar. '05, Nilim and El Ghaoui. '05)

Distributionally robust MDP

Robust MDP

Find the policy $\pi^\star$ that maximizes $V^{\pi,\sigma}$

(Iyengar. '05, Nilim and El Ghaoui. '05)

Robust Bellman's optimality equation: the optimal robust policy $\pi^\star$ and optimal robust value $V^{\star,\sigma} := V^{\pi^\star,\sigma}$ satisfy

$$Q^{\star,\sigma}(s,a) = r(s,a) + \gamma \inf_{P_{s,a}\in\mathcal{U}^\sigma\left(P^o_{s,a}\right)} \left\langle P_{s,a}, V^{\star,\sigma}\right\rangle,$$

$$V^{\star,\sigma}(s) = \max_a Q^{\star,\sigma}(s,a)$$

Distributionally robust MDP

Robust MDP

Find the policy $\pi^\star$ *that maximizes* $V^{\pi,\sigma}$

(Iyengar. '05, Nilim and El Ghaoui. '05)

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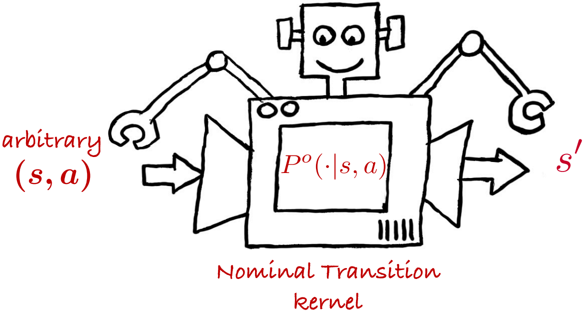
$$V^{\star,\sigma}(s) = \max_a Q^{\star,\sigma}(s,a)$$

Distributionally robust value iteration (DRVI):

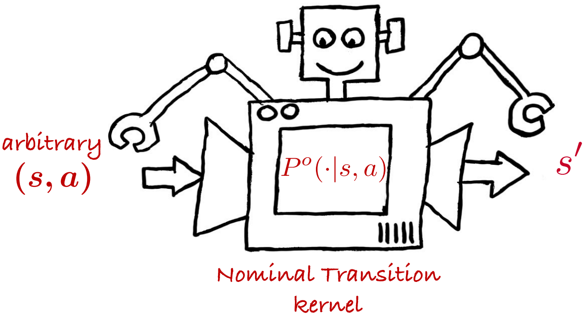
$$Q(s,a) \leftarrow r(s,a) + \gamma \inf_{P_{s,a} \in \mathcal{U}^\sigma(P^o_{s,a})} \langle P_{s,a}, V \rangle,$$

where $V(s) = \max_a Q(s,a)$.

Learning distributionally robust MDPs



Learning distributionally robust MDPs

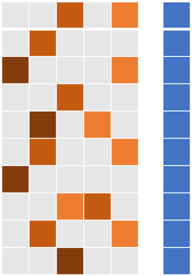


Goal of robust RL: given $\mathcal{D} := \{(s_i, a_i, s_i')\}_{i=1}^N$ from the *nominal* environment P^0, find an ε-optimal robust policy $\widehat{\pi}$ obeying

$$V^{\star,\sigma} - V^{\widehat{\pi},\sigma} \leq \varepsilon$$

— *in a sample-efficient manner*

A curious question

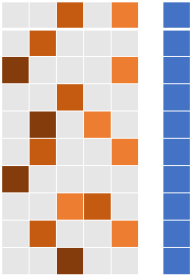


empirical MDP

Learn the optimal policy of the nominal MDP?

Learn the **robust** policy around the nominal MDP?

A curious question



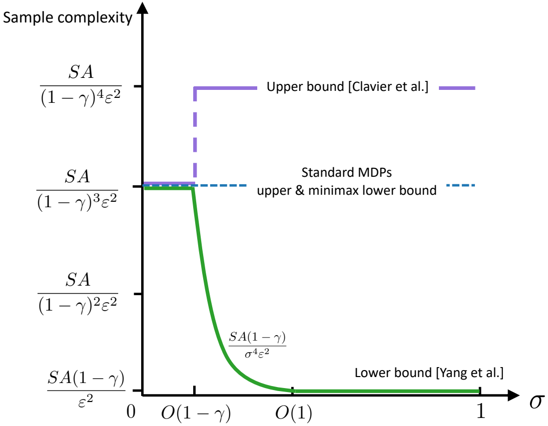
empirical MDP

Learn the optimal policy of the nominal MDP?

Learn the **robust** policy around the nominal MDP?

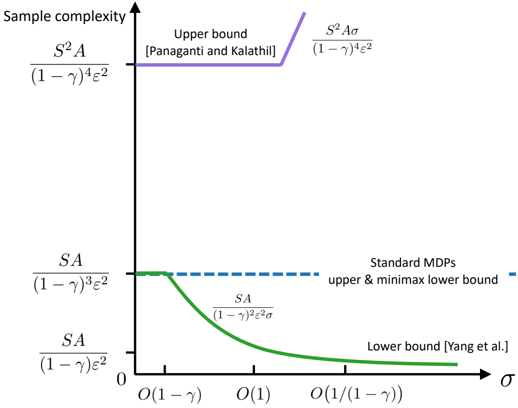
Robustness-statistical trade-off? Is there a statistical premium that one needs to pay in quest of additional robustness?

Prior art: TV uncertainty



- Large gaps between existing upper and lower bounds
- Unclear benchmarking with standard MDP

Prior art: χ^2 uncertainty



- Large gaps between existing upper and lower bounds
- Unclear benchmarking with standard MDP

Our theorem under TV uncertainty

Theorem (Shi et al., 2023)

Assume the uncertainty set is measured via the TV distance with radius $\sigma \in [0,1)$. For sufficiently small $\varepsilon > 0$, DRVI outputs a policy $\widehat{\pi}$ that satisfies $V^{\star,\sigma} - V^{\widehat{\pi},\sigma} \leq \varepsilon$ with sample complexity at most

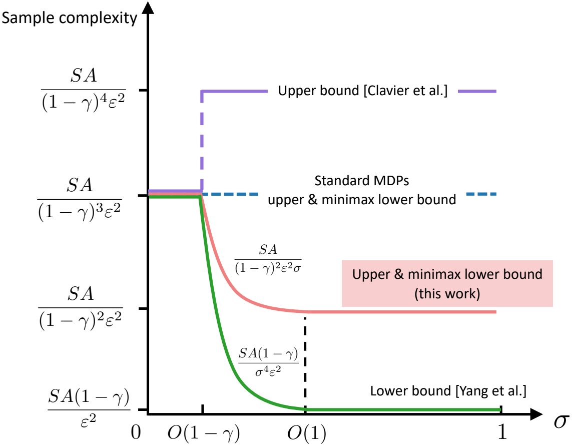
$$\widetilde{O}\left(\frac{SA}{(1-\gamma)^2 \max\{1-\gamma, \sigma\}\varepsilon^2}\right)$$

ignoring logarithmic factors. In addition, no algorithm can succeed if the sample size is below

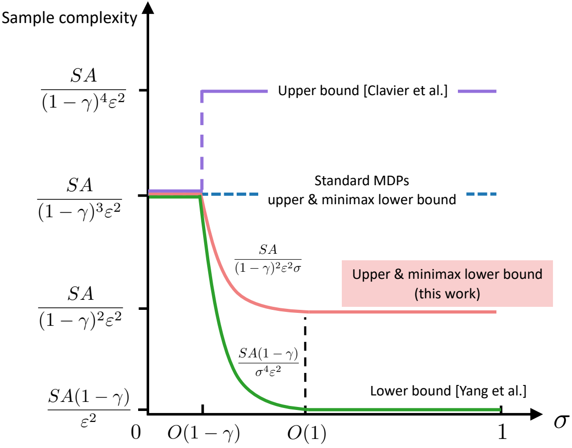
$$\widetilde{\Omega}\left(\frac{SA}{(1-\gamma)^2 \max\{1-\gamma, \sigma\}\varepsilon^2}\right).$$

- Establish the minimax optimality of DRVI for RMDP under the TV uncertainty set over the full range of σ.

When the uncertainty set is TV



When the uncertainty set is TV



RMDPs are **easier** to learn than standard MDPs.

Our theorem under χ^2 uncertainty

Theorem (Upper bound, Shi et al., 2023)

Assume the uncertainty set is measured via the χ^2 divergence with radius $\sigma \in [0, \infty)$. For sufficiently small $\varepsilon > 0$, DRVI outputs a policy $\widehat{\pi}$ that satisfies $V^{\star,\sigma} - V^{\widehat{\pi},\sigma} \leq \varepsilon$ with sample complexity at most

$$\widetilde{O}\left(\frac{SA(1+\sigma)}{(1-\gamma)^4\varepsilon^2}\right)$$

ignoring logarithmic factors.

Our theorem under χ^2 uncertainty

Theorem (Upper bound, Shi et al., 2023)

Assume the uncertainty set is measured via the χ^2 divergence with radius $\sigma \in [0, \infty)$. For sufficiently small $\varepsilon > 0$, DRVI outputs a policy $\widehat{\pi}$ that satisfies $V^{\star,\sigma} - V^{\widehat{\pi},\sigma} \leq \varepsilon$ with sample complexity at most

$$\widetilde{O}\left(\frac{SA(1+\sigma)}{(1-\gamma)^4\varepsilon^2}\right)$$

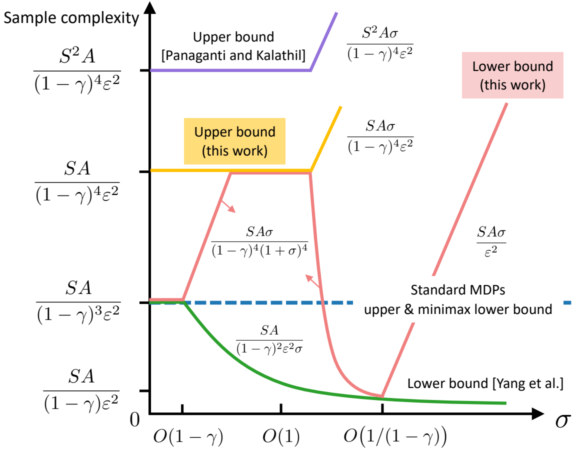
ignoring logarithmic factors.

Theorem (Lower bound, Shi et al., 2023)

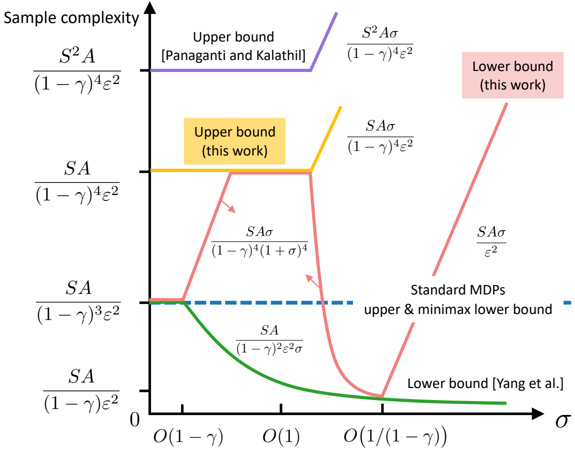
In addition, no algorithm succeeds when the sample size is below

$$\begin{cases} \widetilde{\Omega}\left(\frac{SA}{(1-\gamma)^3\varepsilon^2}\right) & \text{if } \sigma \lesssim 1-\gamma \\ \widetilde{\Omega}\left(\frac{\sigma SA}{\min\{1,(1-\gamma)^4(1+\sigma)^4\}\varepsilon^2}\right) & \text{otherwise} \end{cases}$$

When the uncertainty set is χ^2 divergence



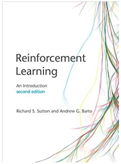
When the uncertainty set is χ^2 divergence

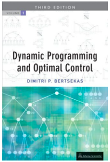


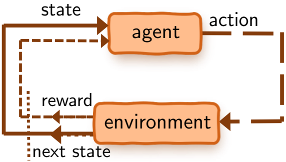
RMDPs can be **harder** to learn than standard MDPs.

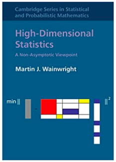
Concluding Remarks

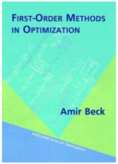
Concluding remarks











Understanding non-asymptotic performances of RL algorithms is a fruitful playground!

Promising directions:

- function approximation
- multi-agent/federated RL
- hybrid RL
- many more...

Beyond the tabular setting

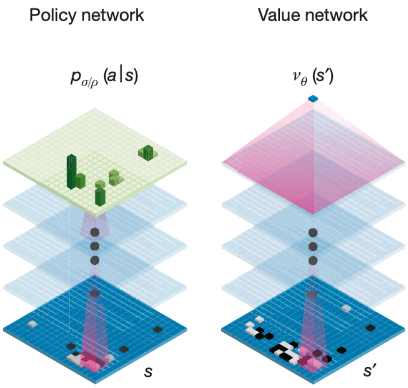
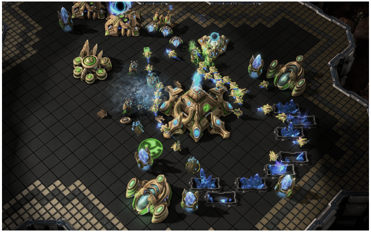


Figure credit: (Silver et al., 2016)

- function approximation for dimensionality reduction
- Provably efficient RL algorithms under minimal assumptions

(Osband and Van Roy, 2014; Dai et al., 2018; Du et al., 2019; Jin et al., 2020)

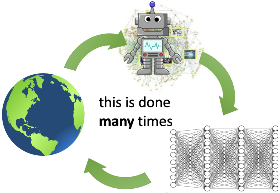
Multi-agent RL



- **Competitive setting:** finding Nash equilibria for Markov games
- **Collaborative setting:** multiple agents jointly optimize the policy to maximize the total reward

(Zhang, Yang, and Basar, 2021; Cen, Wei, and Chi, 2021)

Hybrid RL

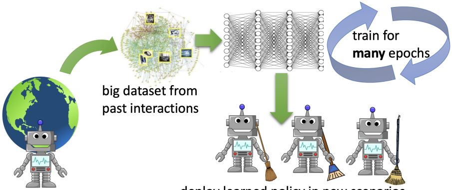


Online RL

- interact with environment
- actively collect new data

Offline/Batch RL

- no interaction
- data is given

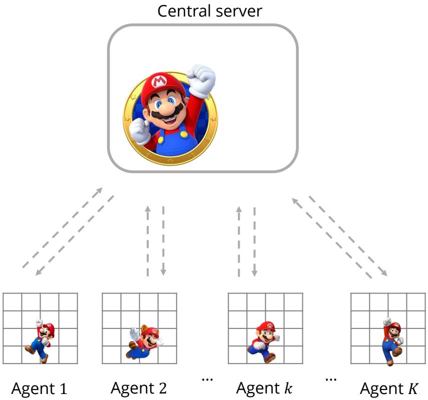


Can we achieve the best of both worlds?

(Wagenmaker and Pacchiano, 2022; Song et al., 2022; Li et al., 2023)

RL meets federated learning

Federated reinforcement learning enables multiple agents to collaboratively learn a global model without sharing datasets.



Can we achieve linear speedup via federated learning?

(Khodadadian et al., 2022; Woo et al., 2023)

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Thanks!

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