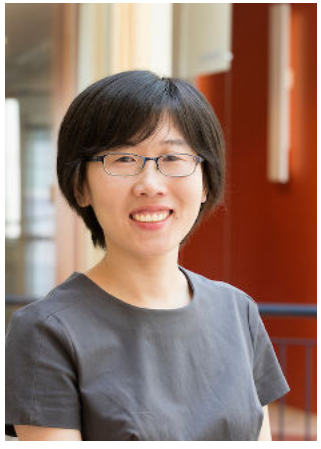
Recent Advances of Statistical Reinforcement Learning

Part 1



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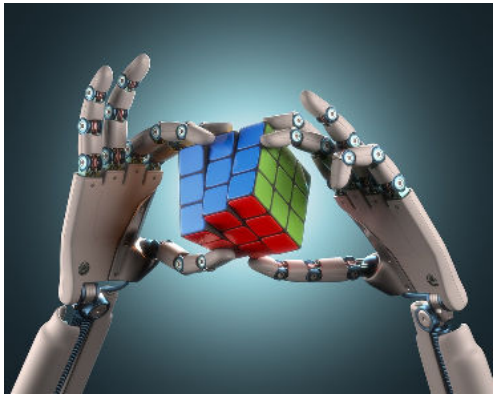
Tutorial, UAI 2024

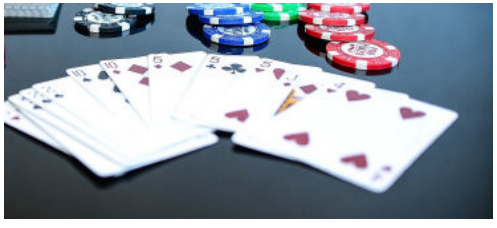
Acknowledgement

Yuxin Chen
UPenn

Yuting Wei
UPenn

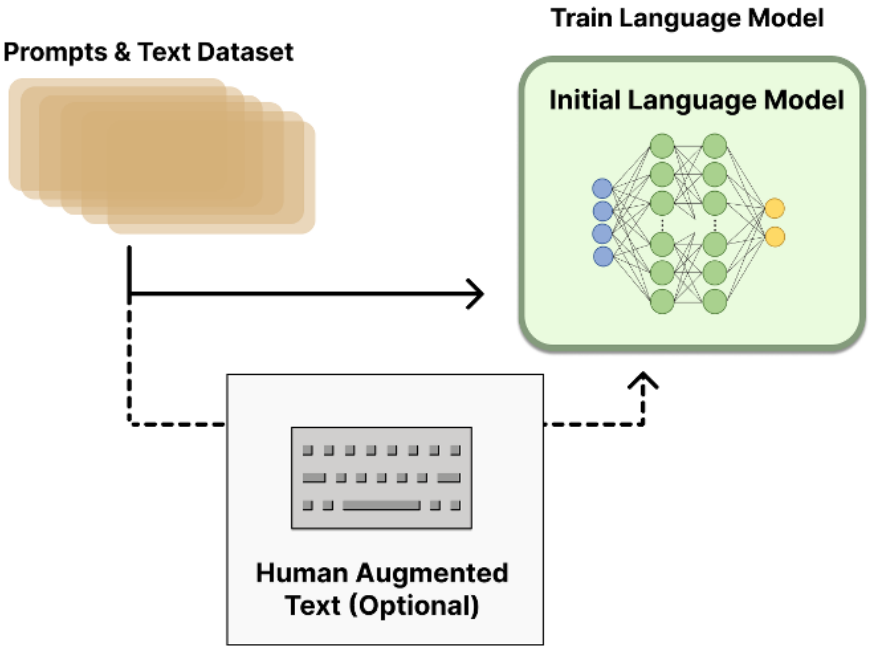
Recent successes in reinforcement learning (RL)





RL holds great promise in the era of AI

One more recent success: RLHF



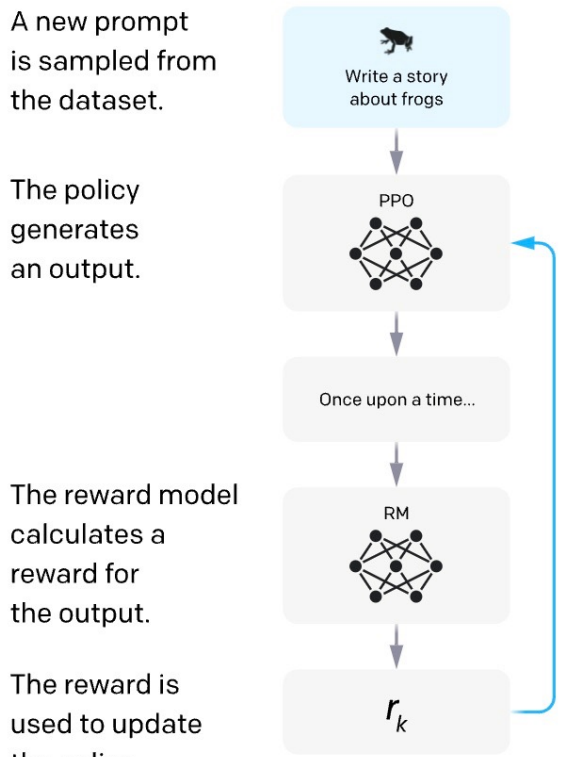
You
What is RLHF?

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

ChatGPT

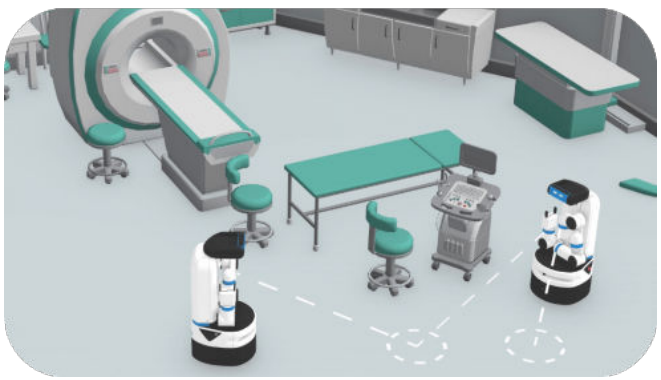
Bard

Optimize a policy against the reward model using reinforcement learning.



Data efficiency

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



clinical trials

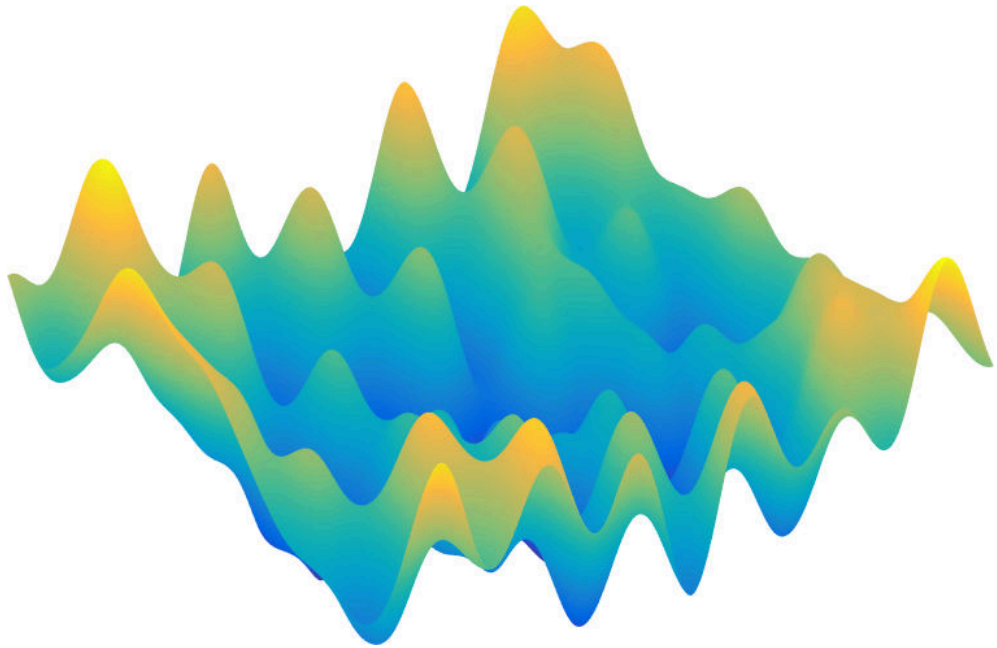
self-driving cars

Calls for design of sample-efficient RL algorithms!

Computational efficiency

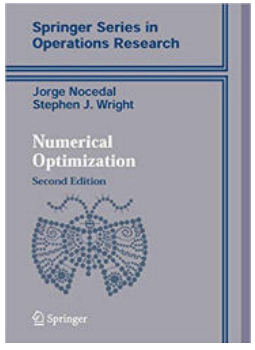
Running RL algorithms might take a long time . . .

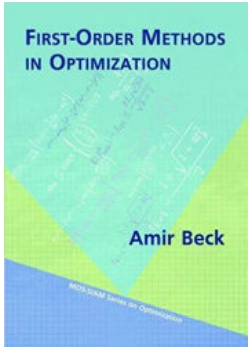
- enormous state-action space
- nonconvexity



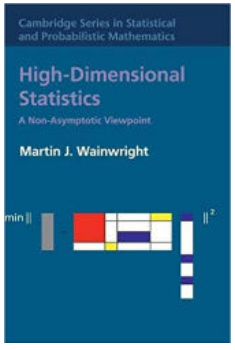
Calls for computationally efficient RL algorithms!

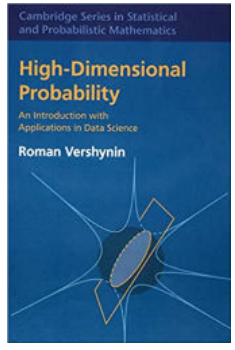
This tutorial





(large-scale) optimization





(high-dimensional) statistics

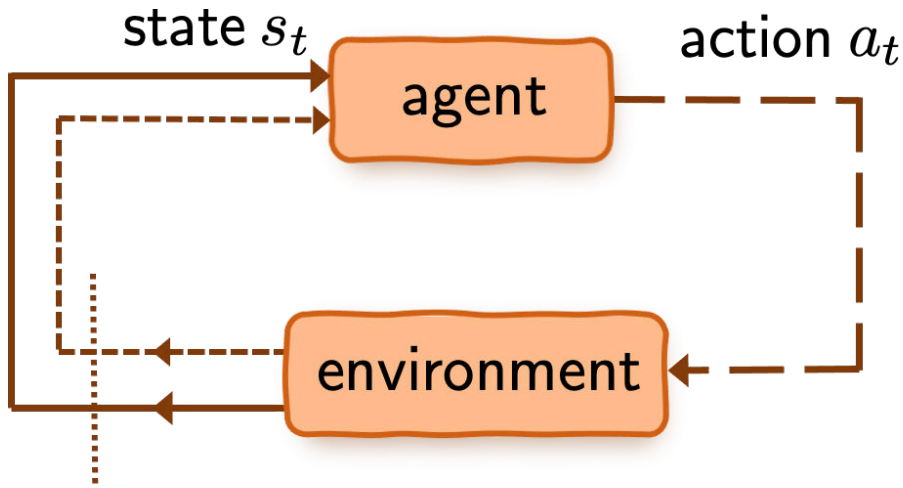
Part 1. Basics, statistical RL in the tabular setting

Part 2. Beyond the tabular setting

Part 1

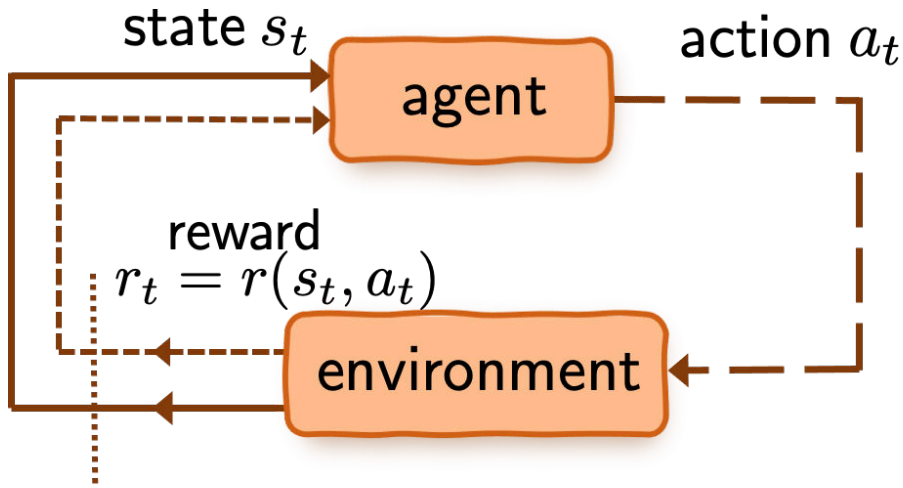
1. Basics: Markov decision processes
2. RL w/ a generative model (simulator)
3. Online RL
4. Offline RL

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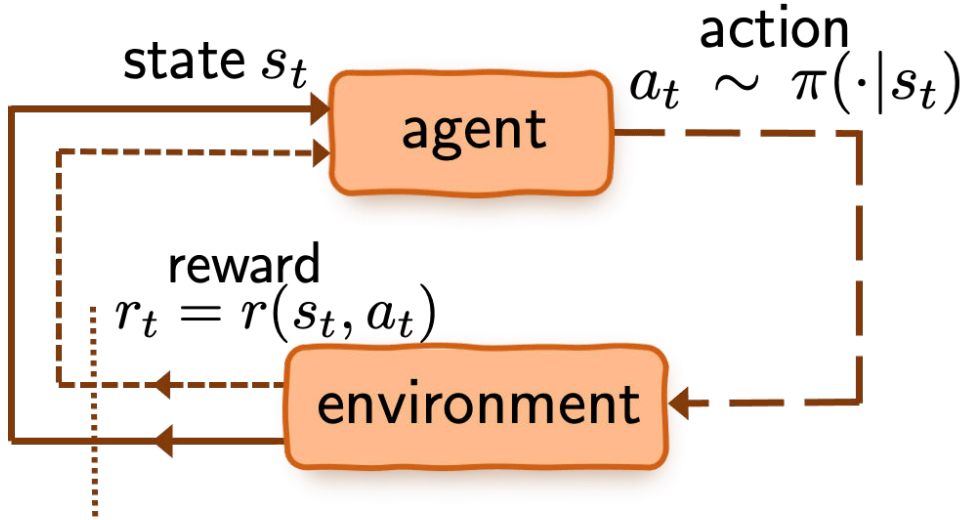
- $r(s, a) \in [0, 1]$: immediate reward

Discounted infinite-horizon MDPs



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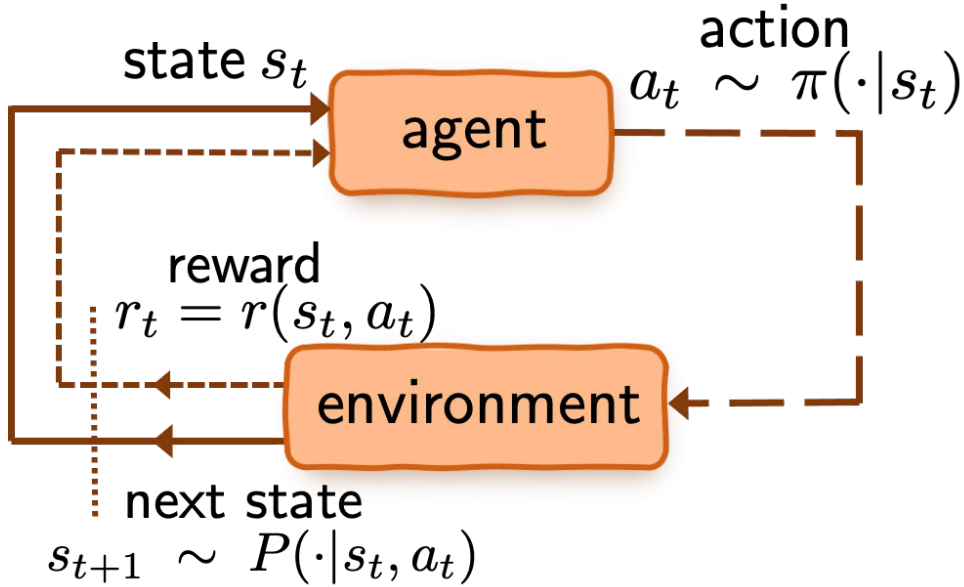

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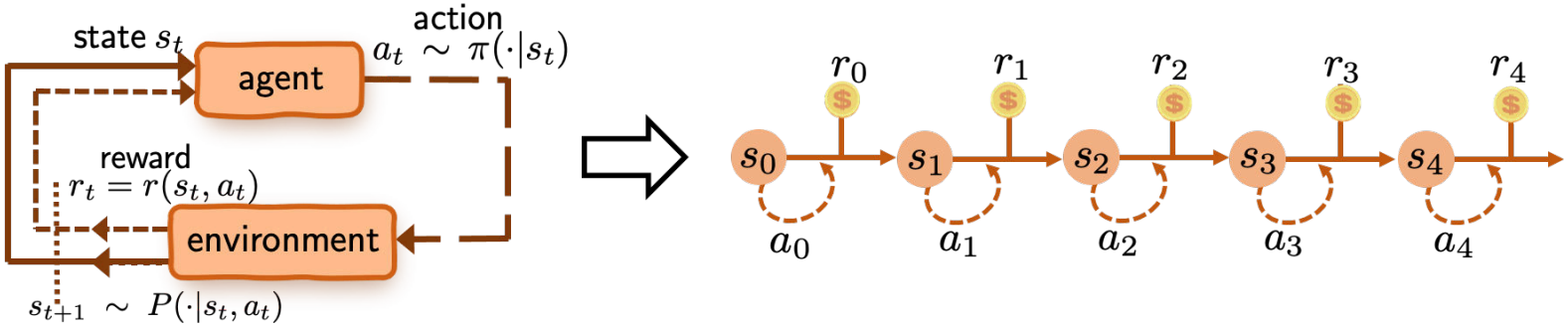
- $\pi(\cdot|s)$: policy (or action selection rule)
- $P(\cdot|s, a)$: unknown transition probabilities

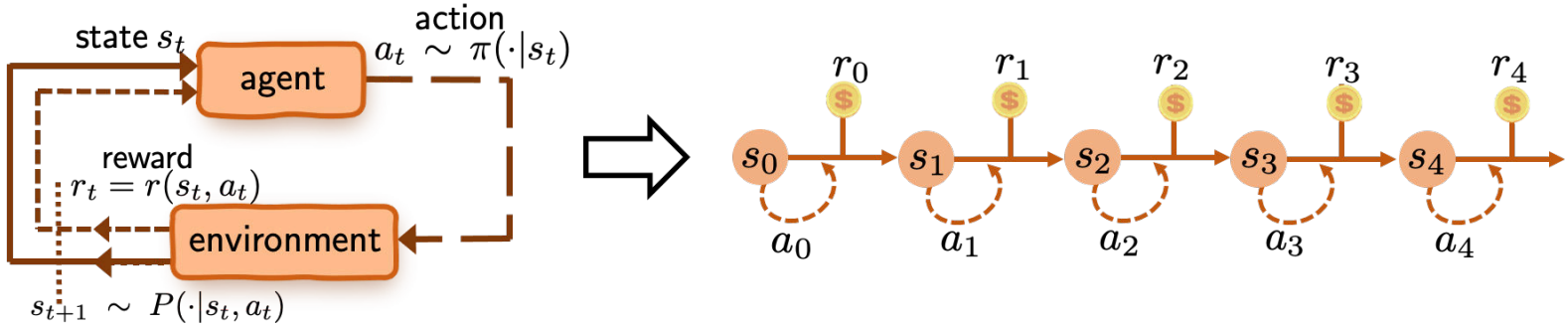
Value function



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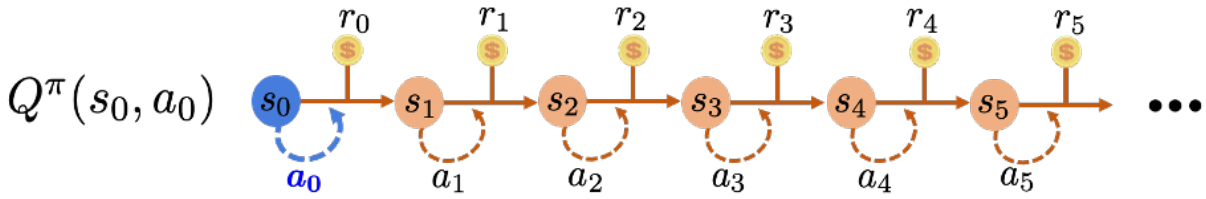
- $\gamma \in [0, 1)$: discount factor
  - take $\gamma \to 1$ to approximate long-horizon MDPs
  - **effective horizon**: $\frac{1}{1-\gamma}$

Q-function (action-value function)

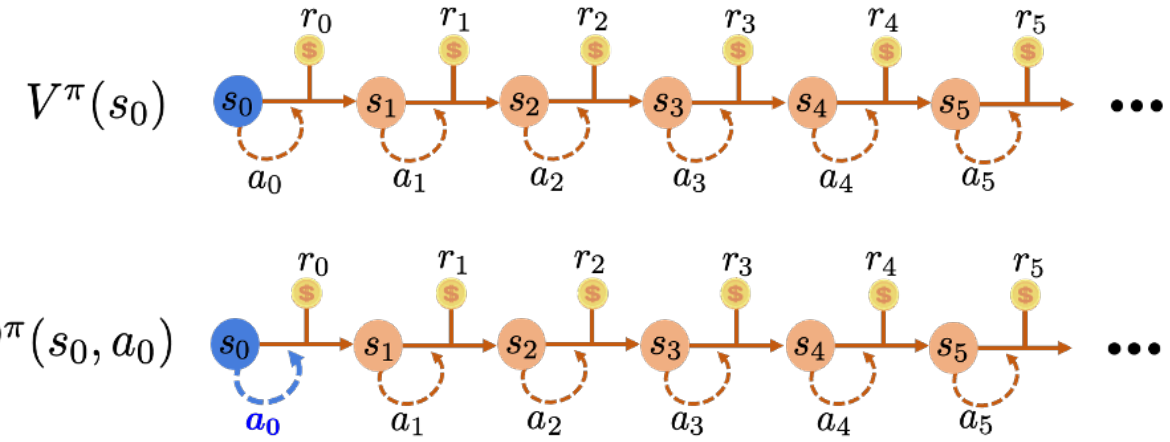


Q-function of policy π:

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

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

Q-function (action-value function)



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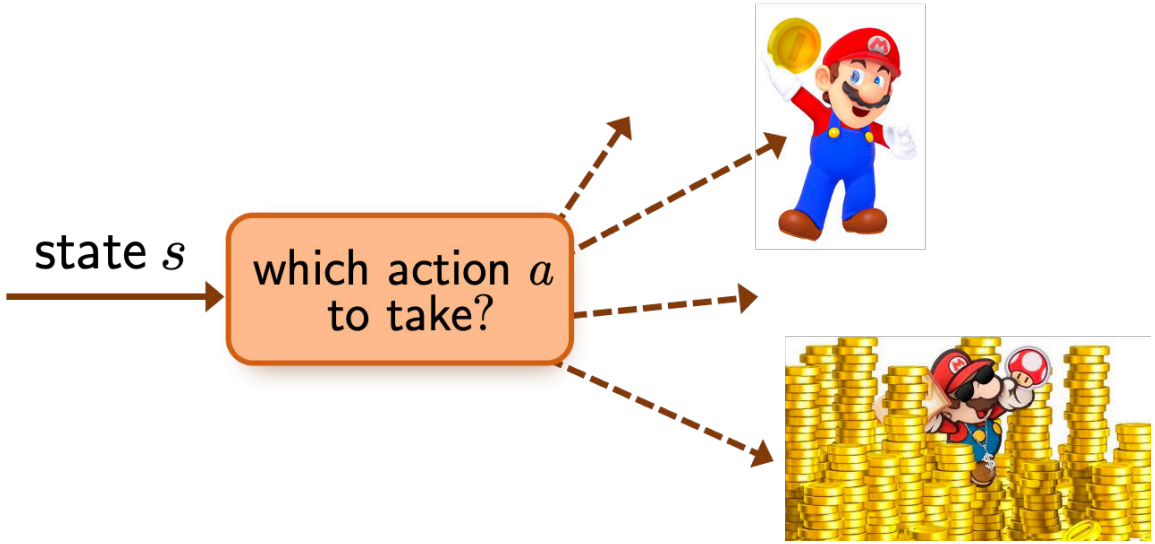
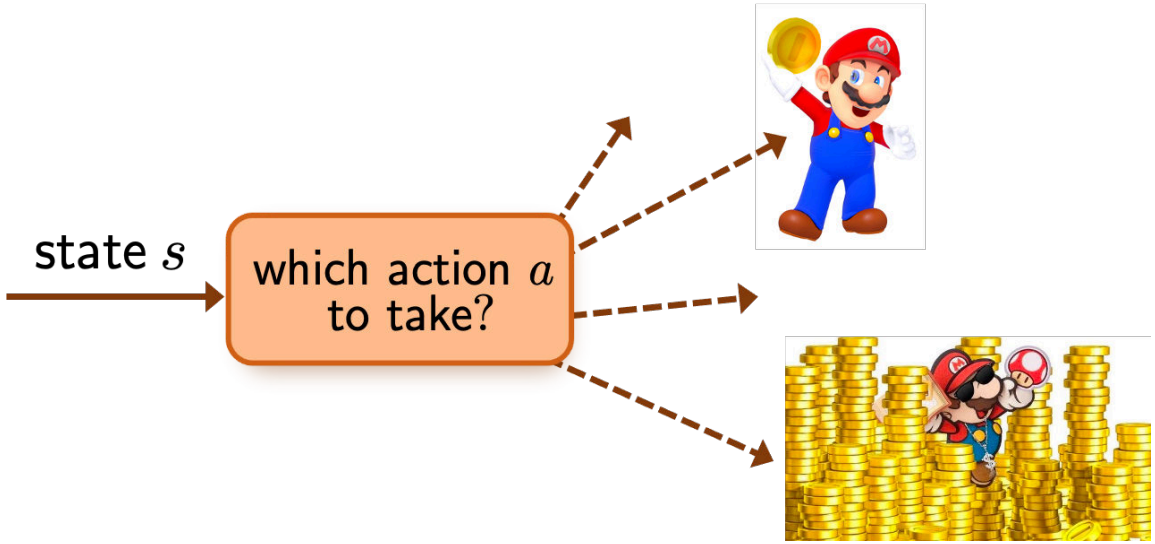
Optimal policy and optimal value



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

Optimal policy and optimal value



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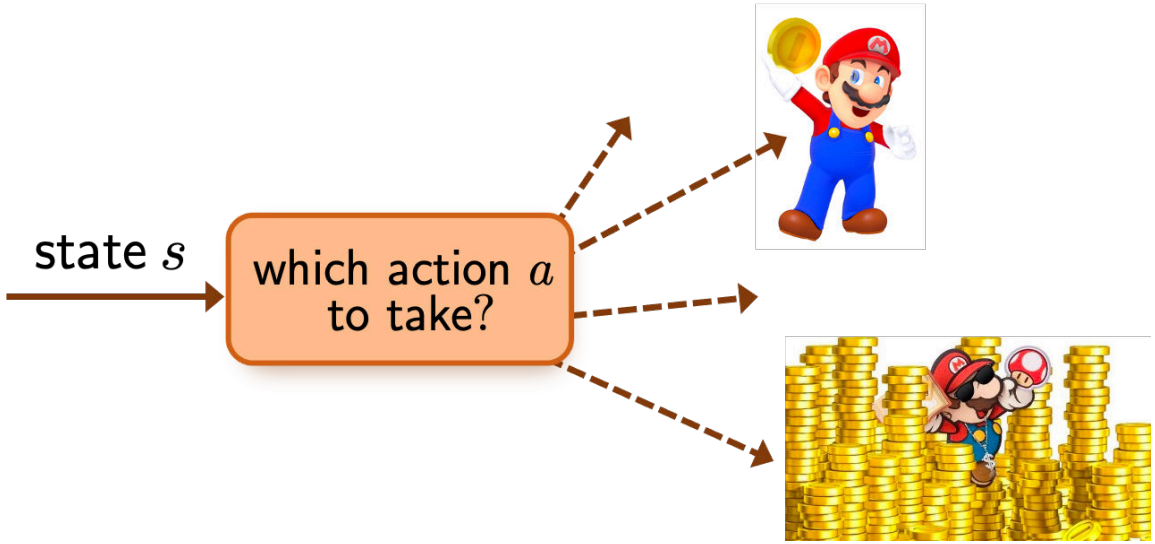
Theorem 1 (Puterman'94)

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



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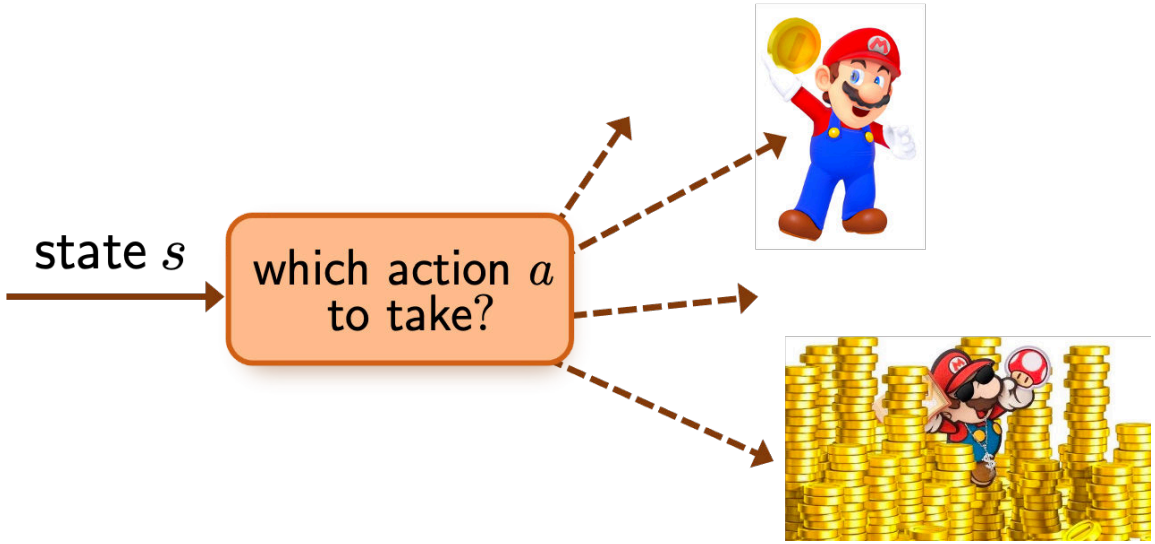
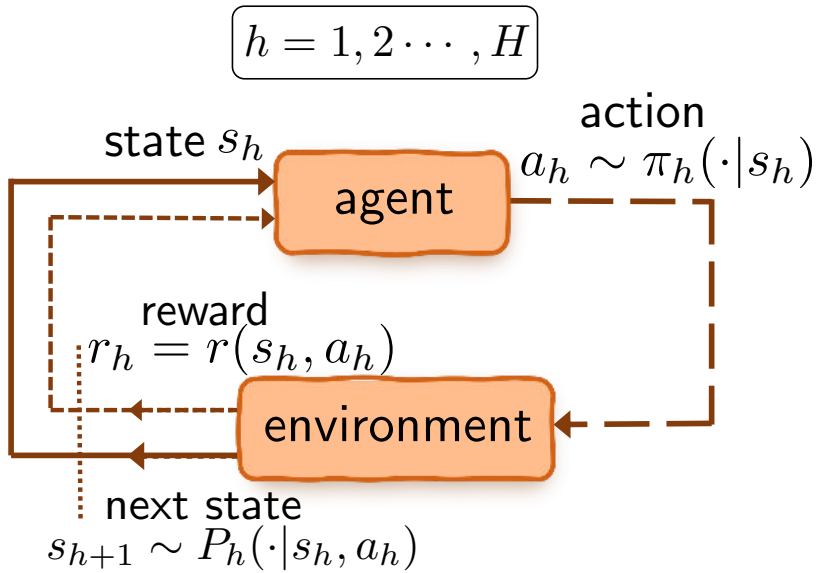
Optimal policy and optimal value



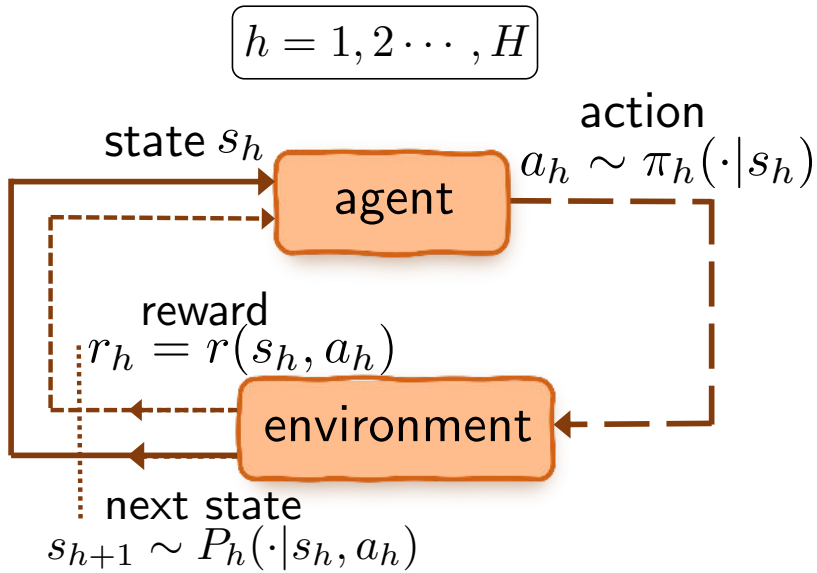
- **optimal policy** $\pi^\star$: maximizing value function $\max_\pi V^\pi$
- **optimal value / Q function**: $V^\star := V^{\pi^\star}$, $Q^\star := Q^{\pi^\star}$
- A question to keep in mind: *how to find optimal* $\pi^\star$*?*

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)
- $P_h(\cdot \,|\, s, a)$: transition probabilities in step h

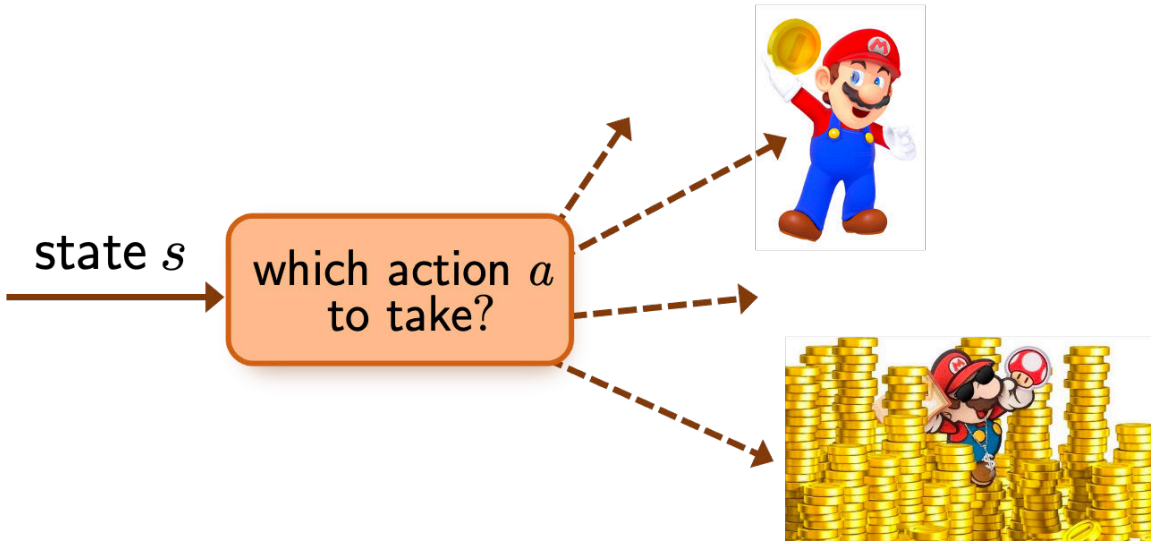
Finite-horizon MDPs (nonstationary)



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

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

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

- 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:

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

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

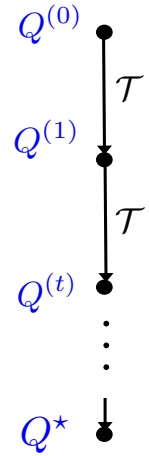
$$\mathcal{T}(Q^\star) = Q^\star$$

Two dynamic programming algorithms

Value iteration (VI)

For $t = 0, 1, \ldots$

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

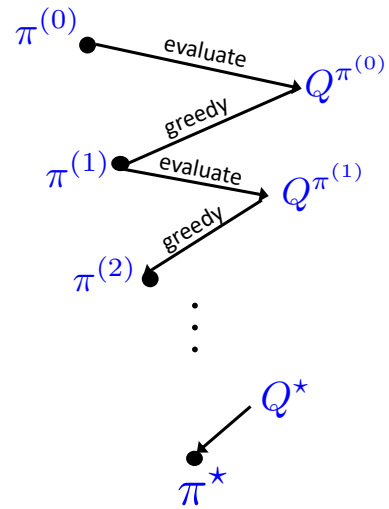


Policy iteration (PI)

For $t = 0, 1, \ldots$

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

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



Iteration complexity

Theorem 2 (Linear convergence of policy/value iteration)

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

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Implications: to achieve $\|Q^{(t)} - Q^\star\|_\infty \leq \varepsilon$, it takes no more than

$$\frac{1}{1-\gamma} \log\left(\frac{\|Q^{(0)} - Q^\star\|_\infty}{\varepsilon}\right) \quad \text{iterations}$$

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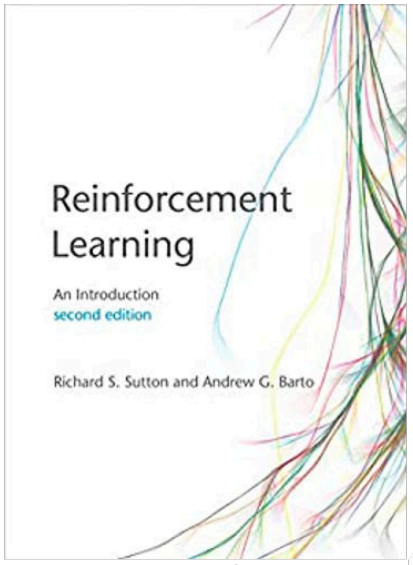
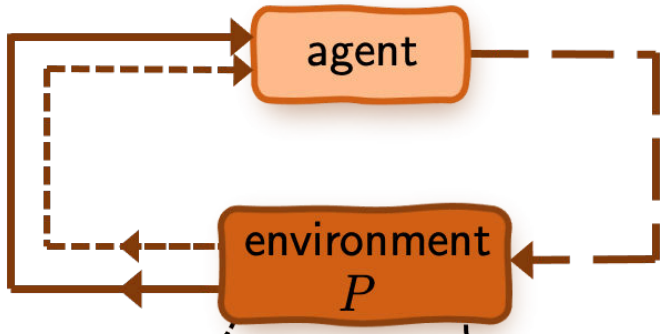
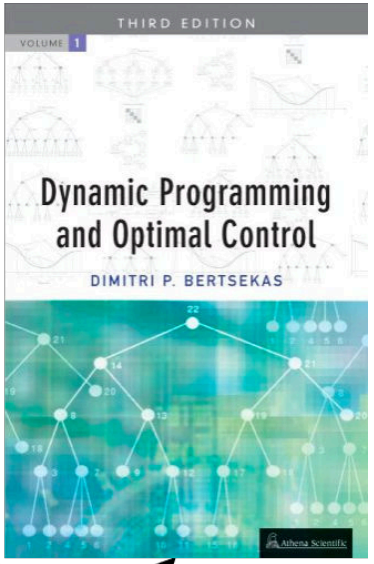
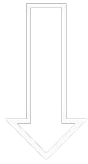
Linear convergence at a **dimension-free** rate!

When the model is unknown . . .









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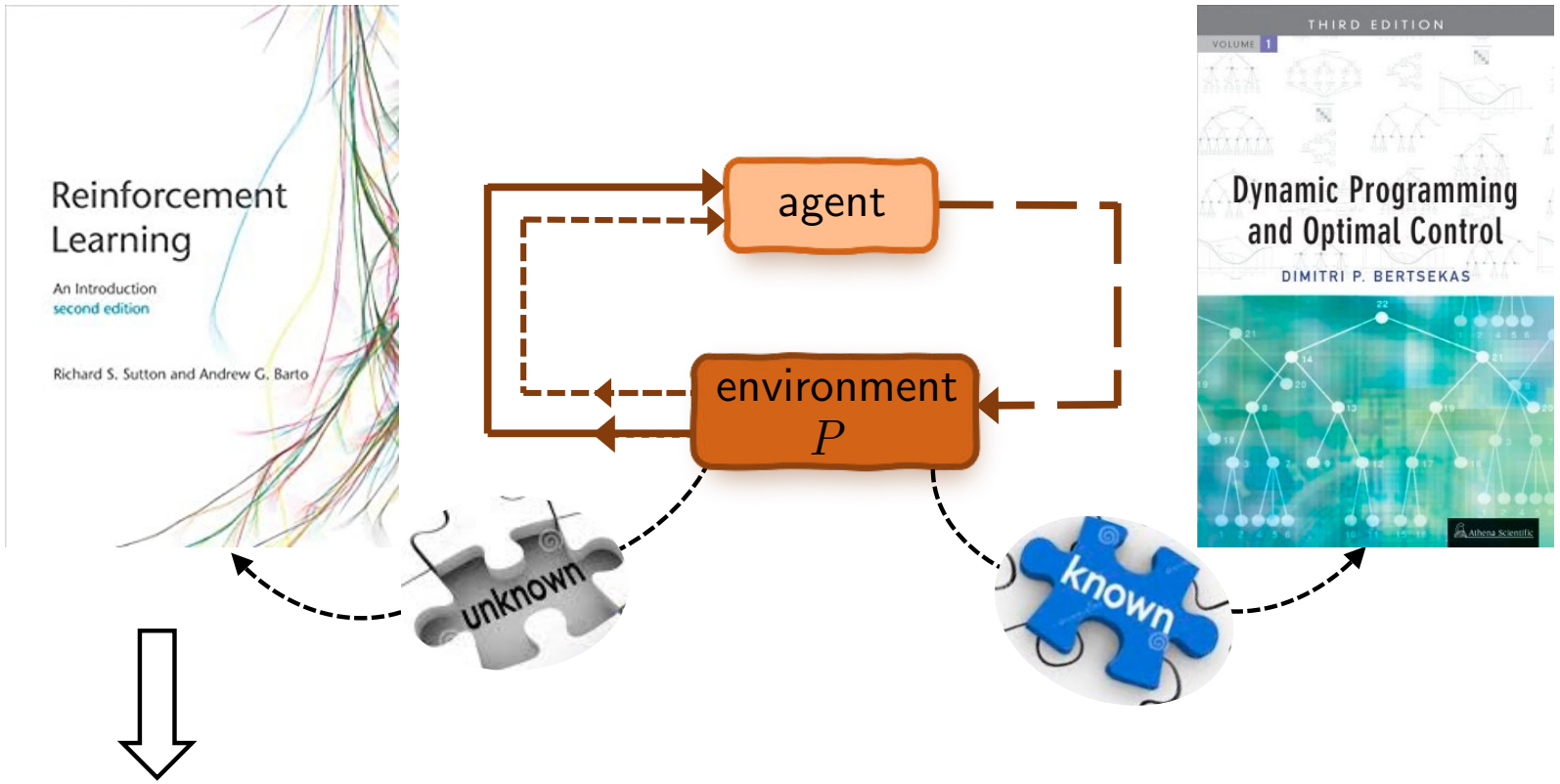
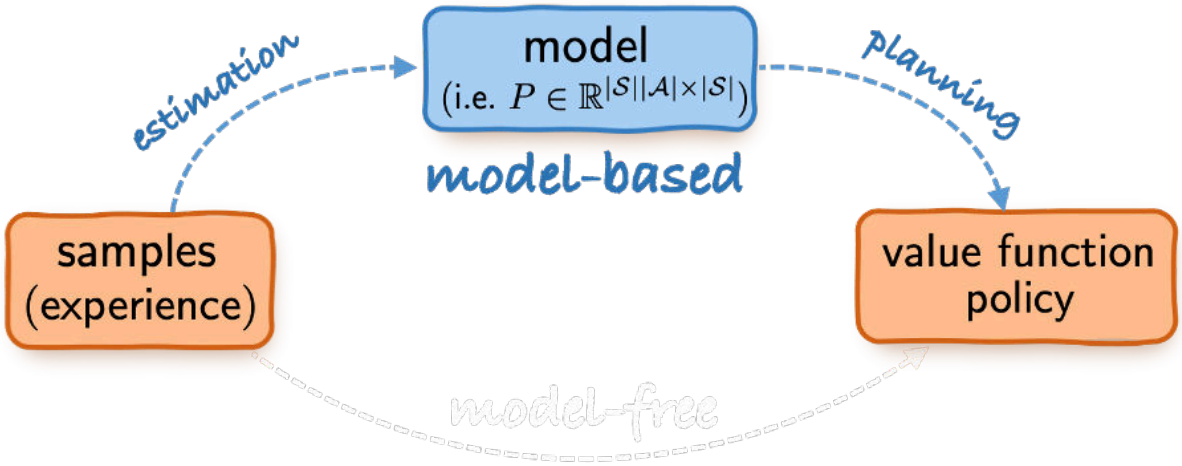


Need to learn optimal policy from samples w/o model specification

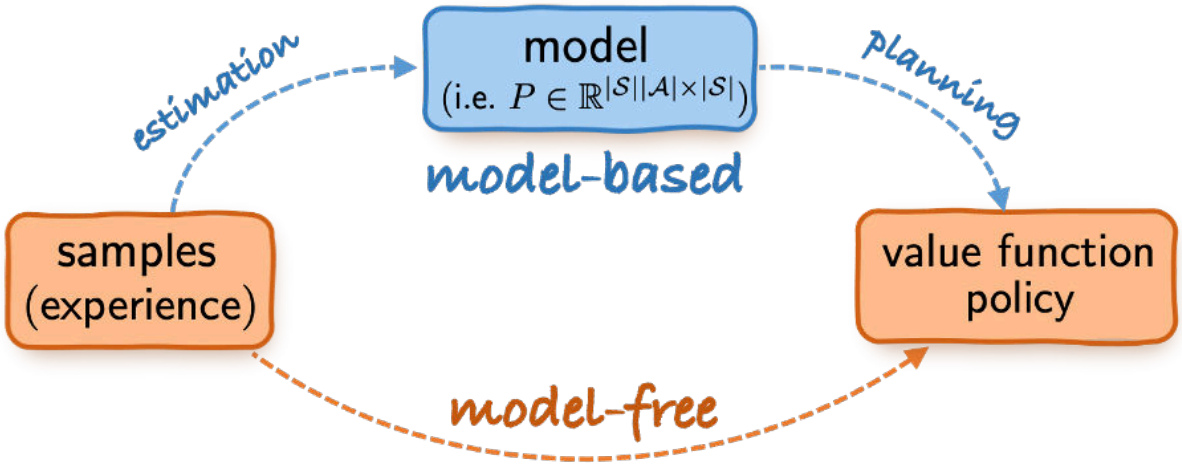
Two approaches



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 modeling & estimating environment explicitly

— memory-efficient, online, ...

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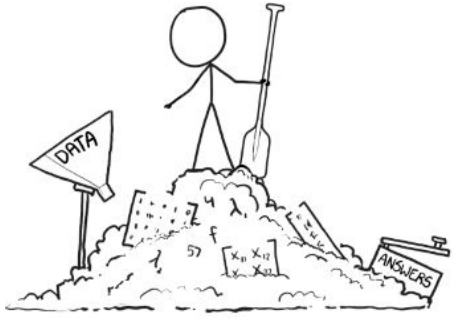
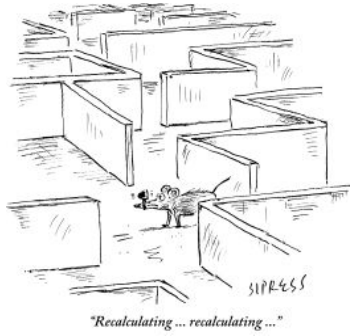
Question: *how many samples are sufficient to learn an* $\underbrace{\varepsilon\text{-optimal policy}}_{\widehat{V^{\pi}} \geq V^{\star} - \varepsilon}$*?*

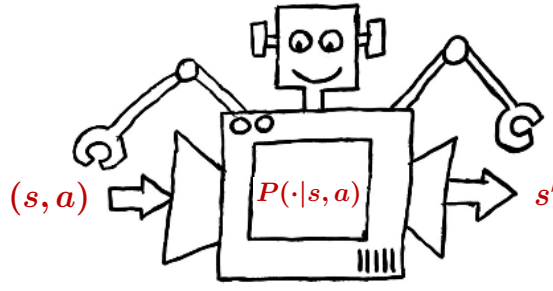
Exploration vs exploitation



offline RL

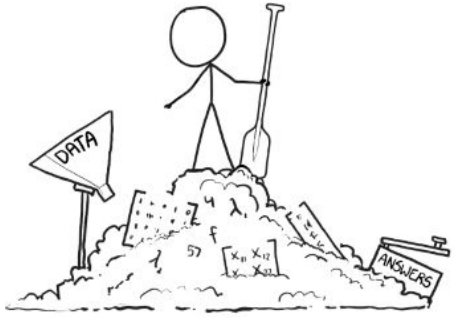


online RL



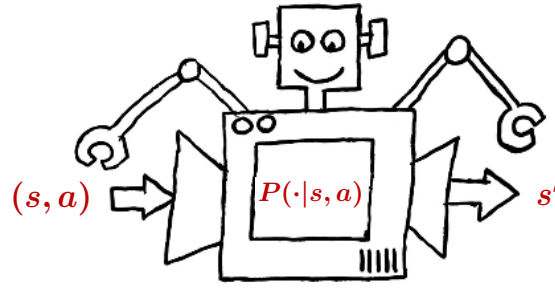
generative model

Exploration vs exploitation



offline RL

online RL



generative model

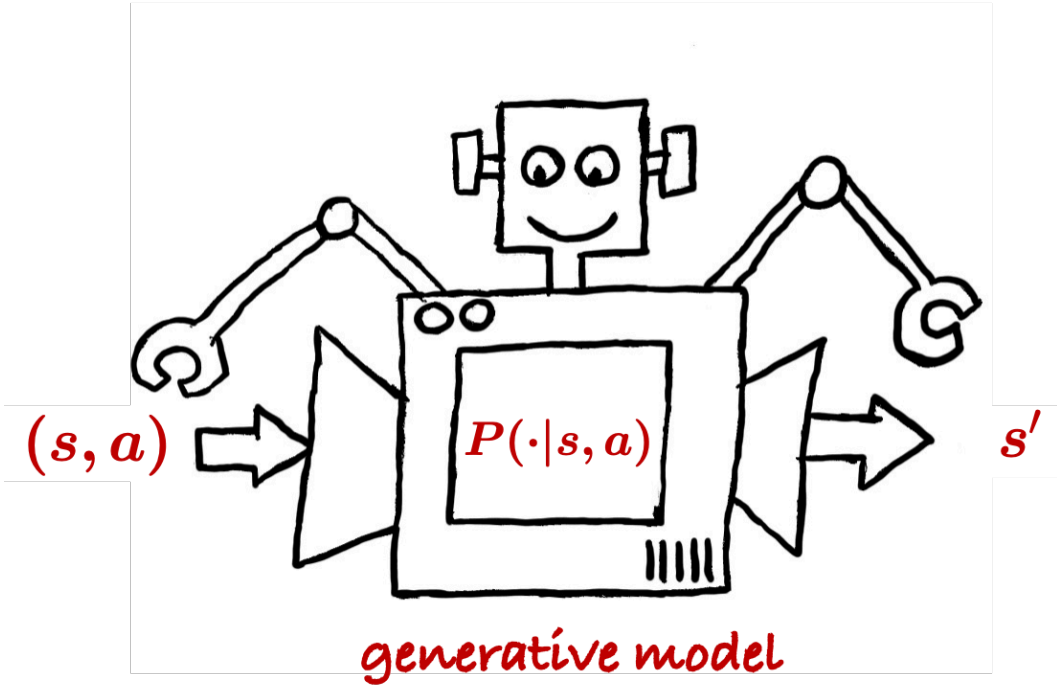
Varying levels of trade-offs between exploration and exploitation.

Part 1

1. Basics: Markov decision processes
2. RL w/ a generative model (simulator)
3. Online RL
4. Offline RL

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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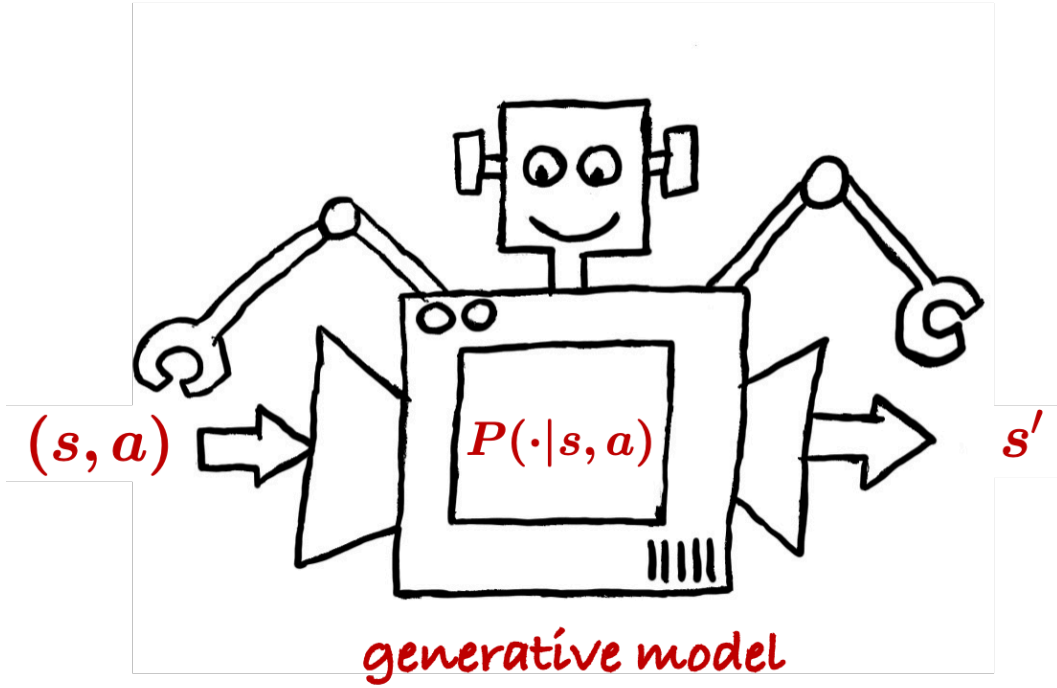


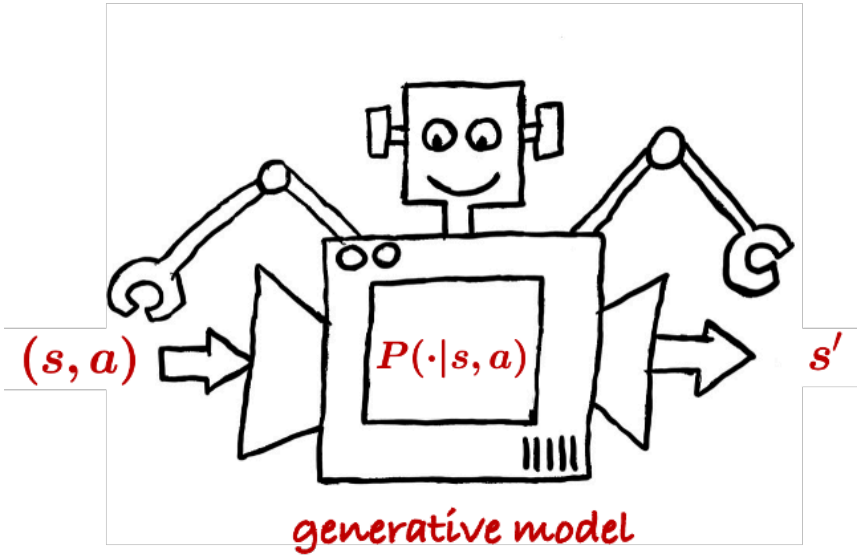
- **sampling:** for each (s, a), collect N samples $\{(s, a, s'_{(i)})\}_{1 \le i \le N}$
- construct $\widehat{\pi}$ based on samples (in total $SA \times N$)

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

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
- ...

Model estimation



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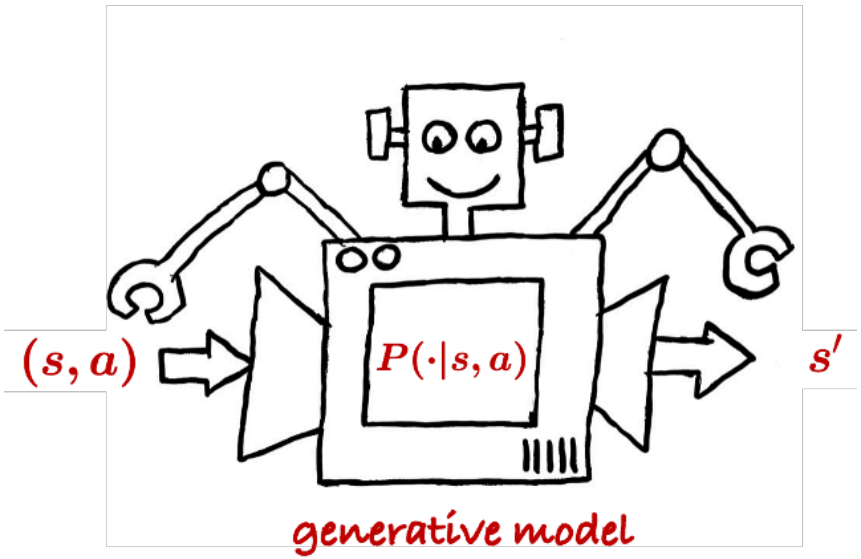


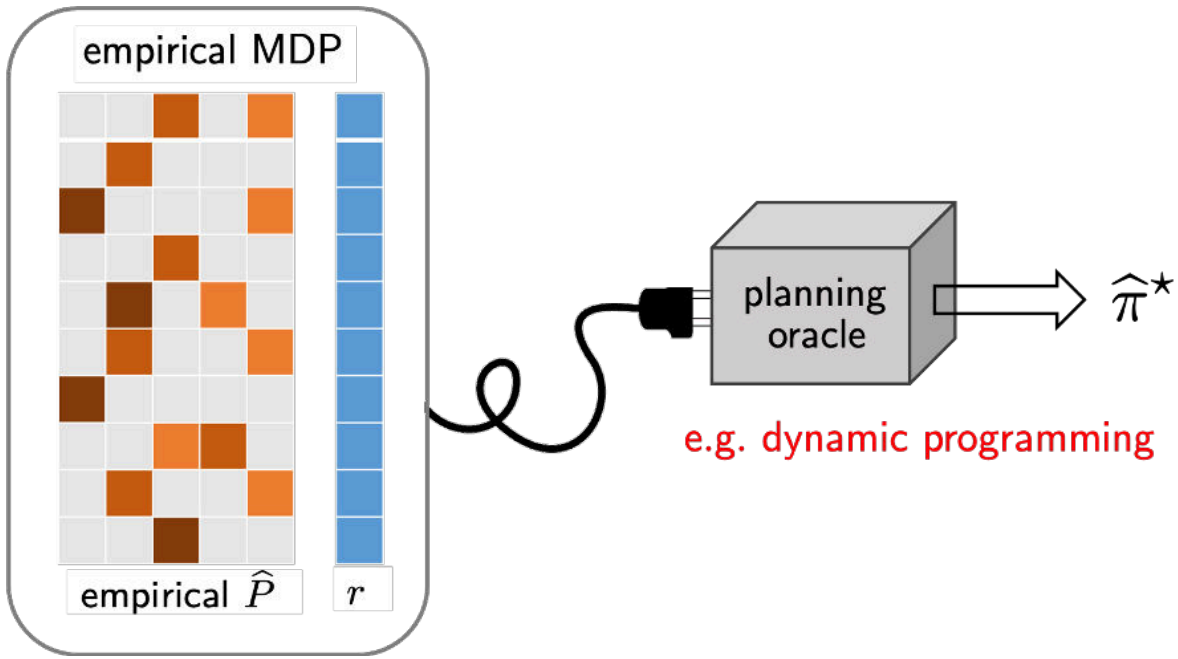
Sampling: for each (s, a), collect N ind. samples $\{(s, a, s'_{(i)})\}_{1 \le i \le N}$

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

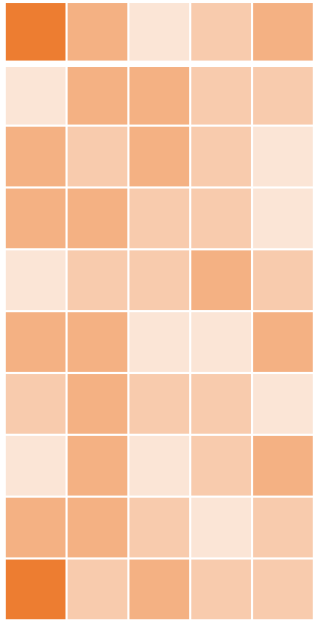


Find policy based on the empirical MDP (*empirical maximizer*)

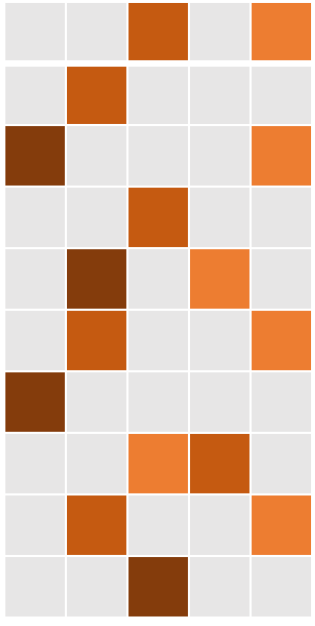
using, e.g., policy iteration

$(\widehat{P}, r)$

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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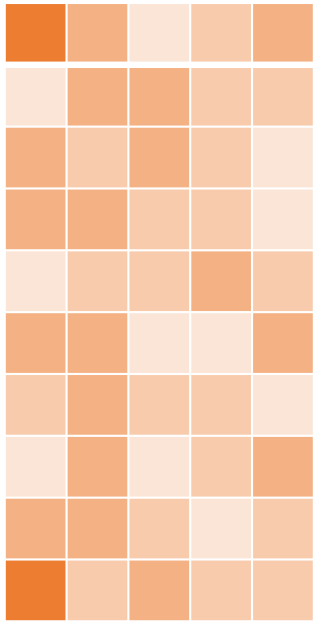

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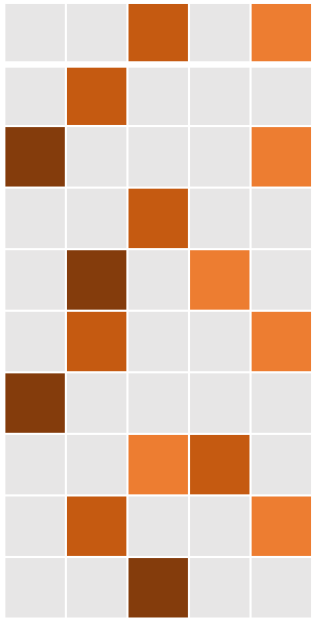

empirical estimate: $\widehat{P}$

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

ℓ_∞-based sample complexity

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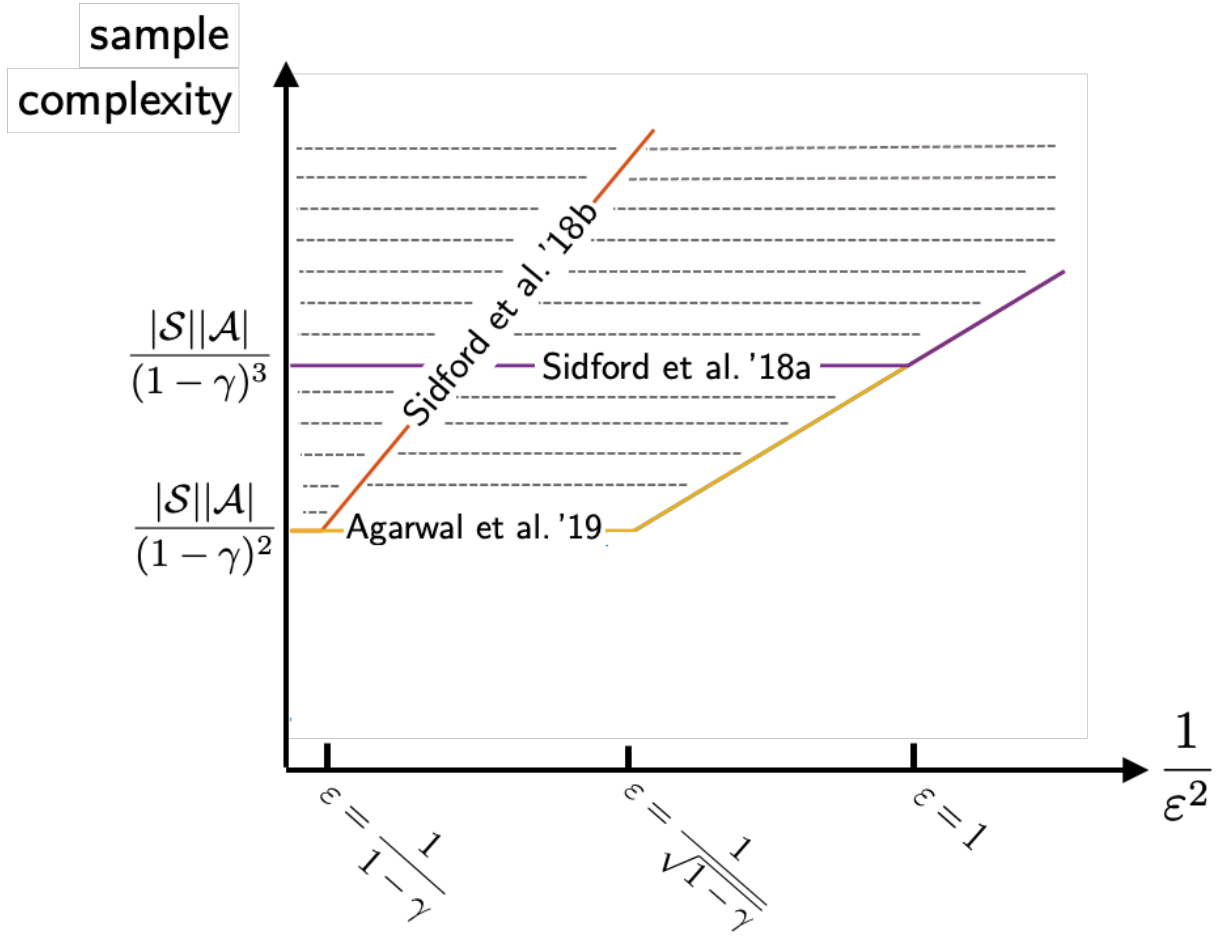
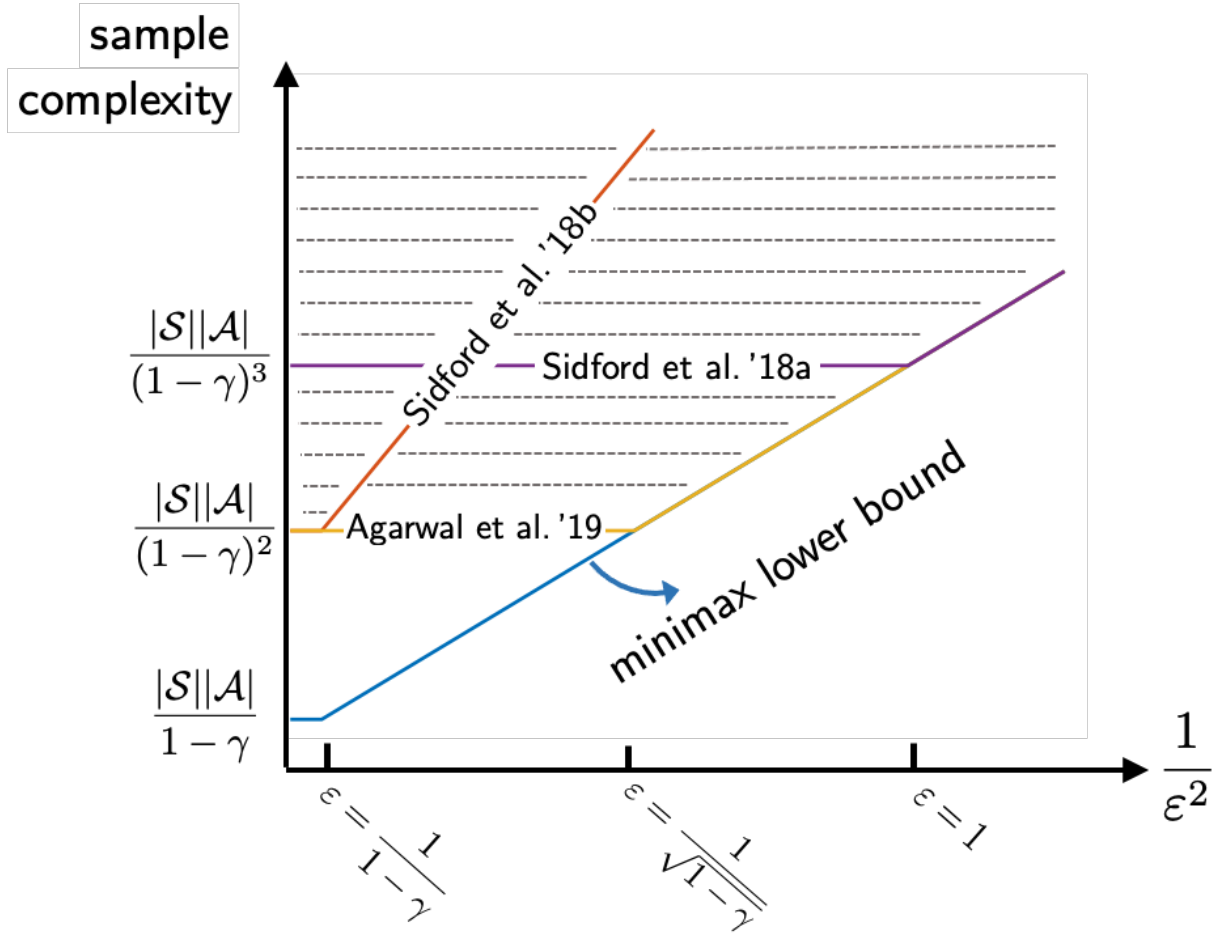
- matches minimax lower bound: $\widetilde{\Omega}(\frac{SA}{(1-\gamma)^3\varepsilon^2})$ when $\varepsilon \leq \frac{1}{\sqrt{1-\gamma}}$ (equivalently, when sample size exceeds $\frac{SA}{(1-\gamma)^2}$) Azar et al., 2013


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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minimax lower bound
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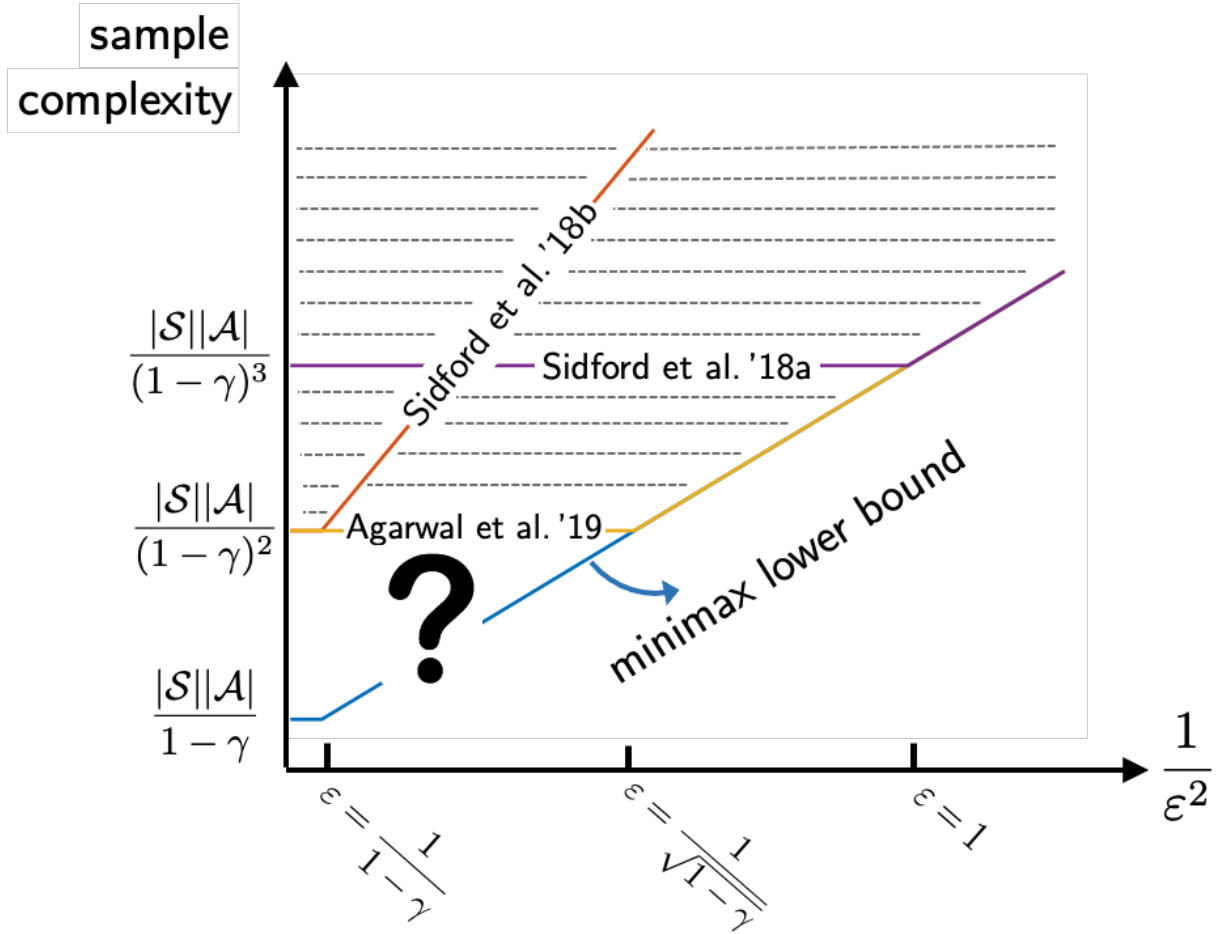
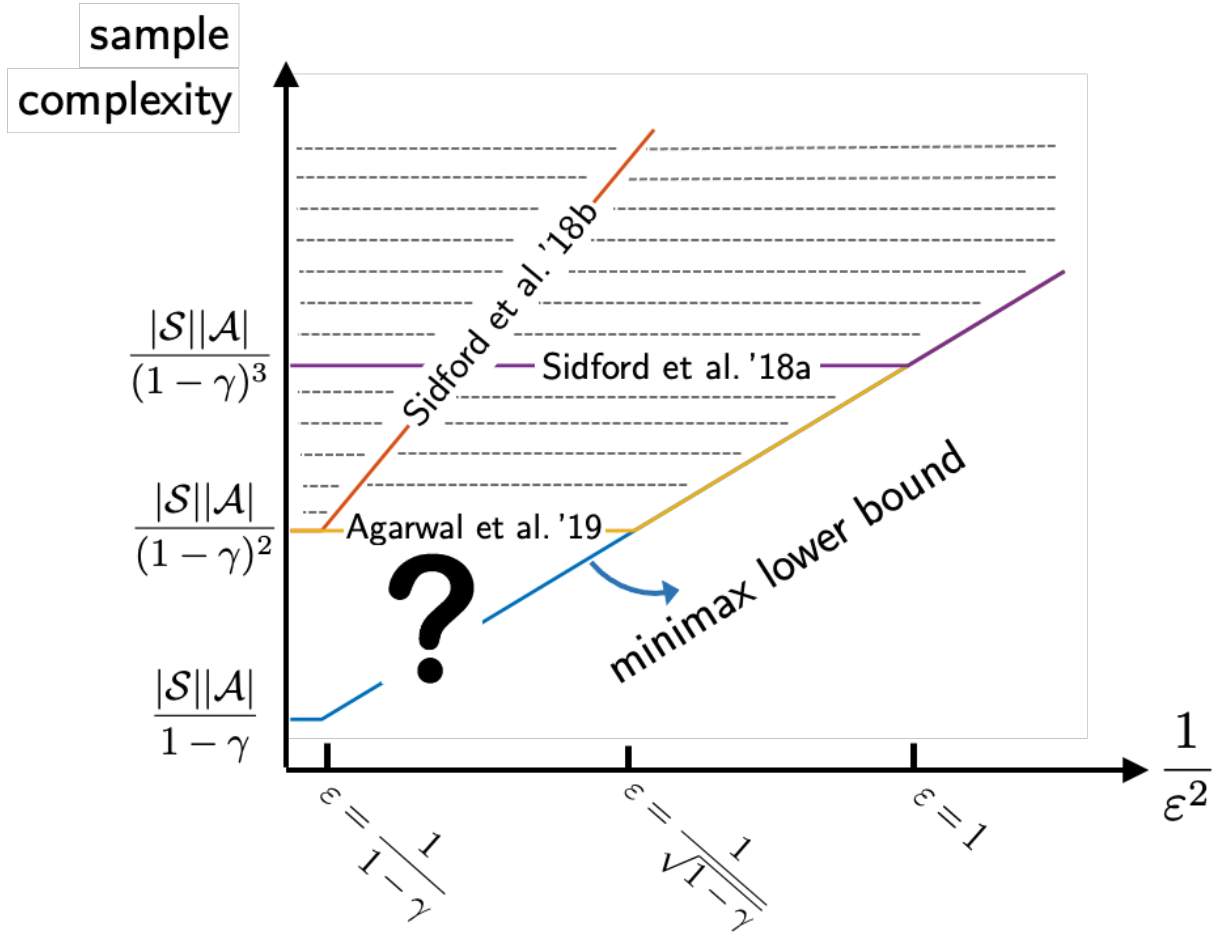


Agarwal et al., 2019 still requires a burn-in sample size $\gtrsim \frac{SA}{(1-\gamma)^2}$

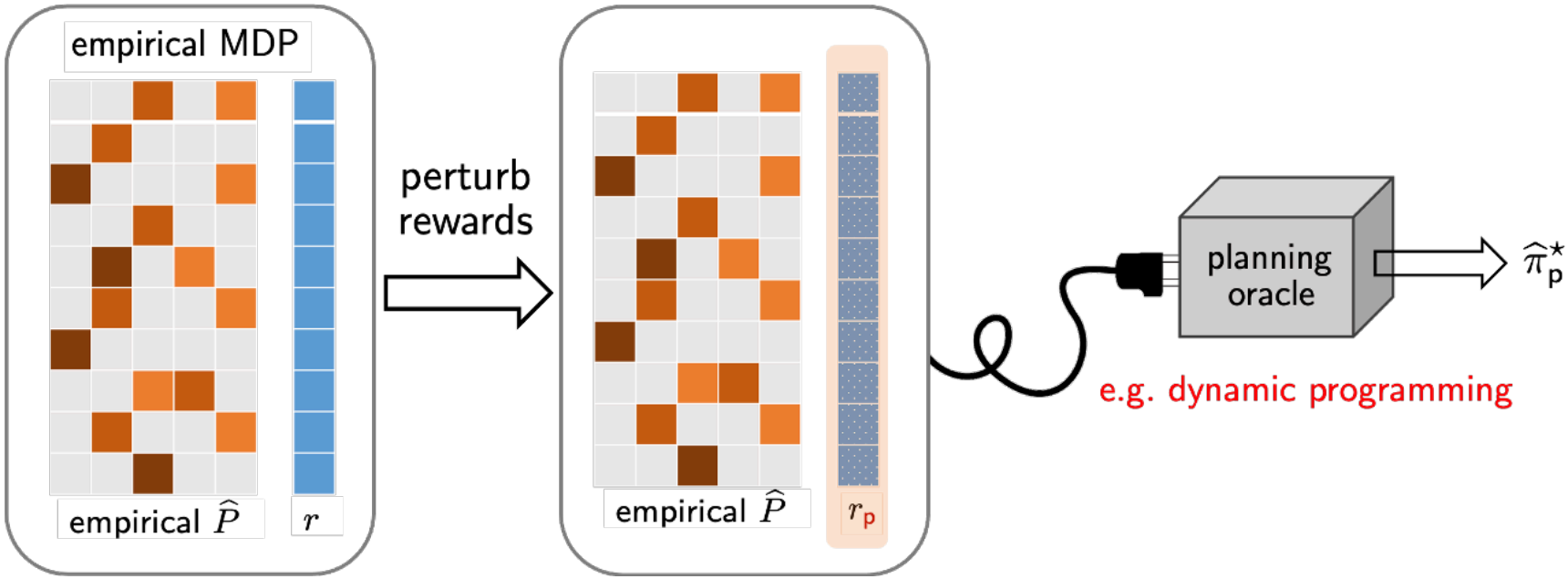


Agarwal et al., 2019 still requires a burn-in sample size $\gtrsim \frac{SA}{(1-\gamma)^2}$

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

Perturbed model-based approach (Li et al. '20)

— Li, Wei, Chi, Chen, '20, OR'24



Find policy based on empirical MDP w/ slightly perturbed rewards

Optimal ℓ_∞-based sample complexity

Theorem 4 (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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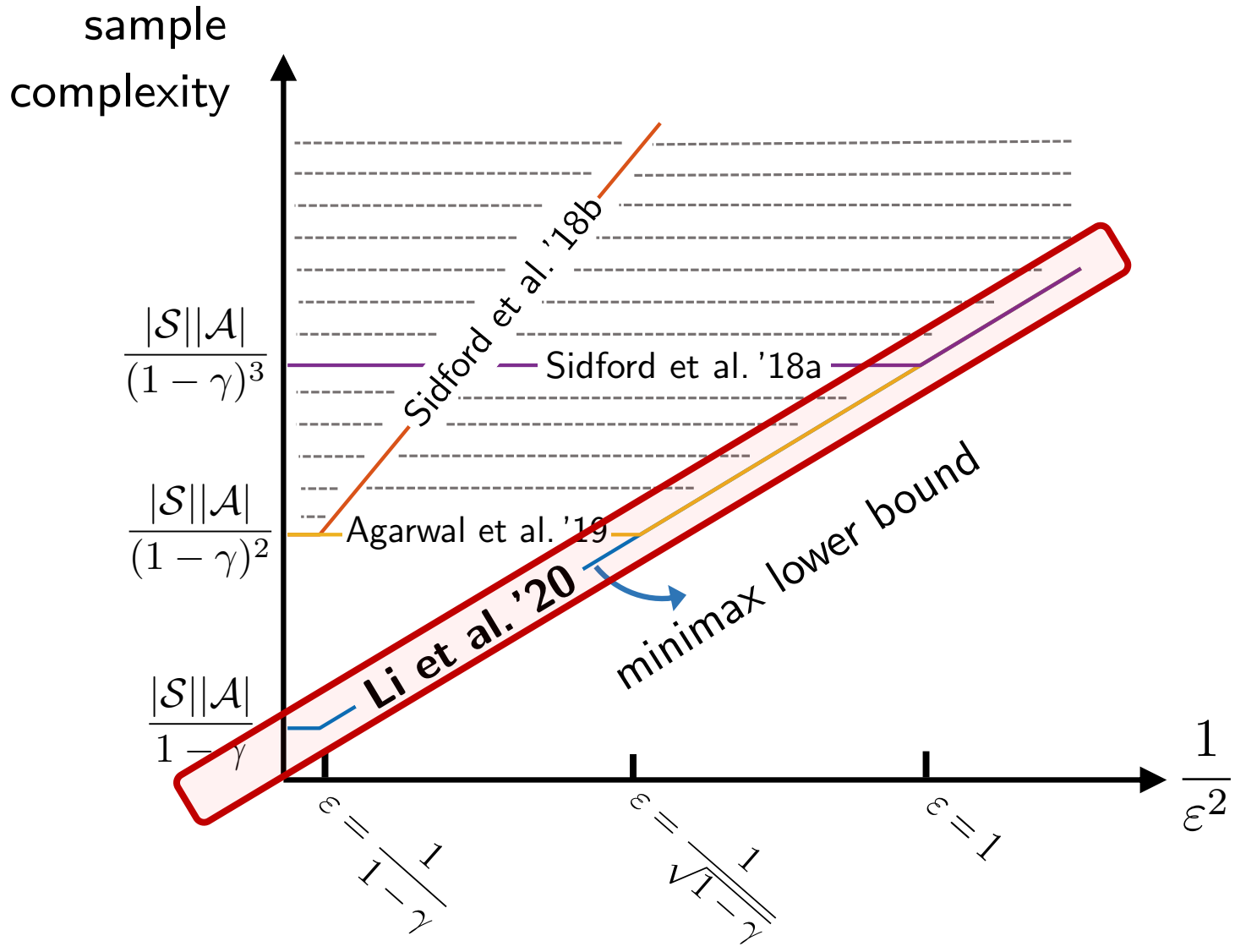
- matches minimax lower bound: $\widetilde{\Omega}(\frac{SA}{(1-\gamma)^3\varepsilon^2})$ Azar et al., 2013
- full ε-range: $\varepsilon \in (0, \frac{1}{1-\gamma}]$ $\longrightarrow$ no burn-in cost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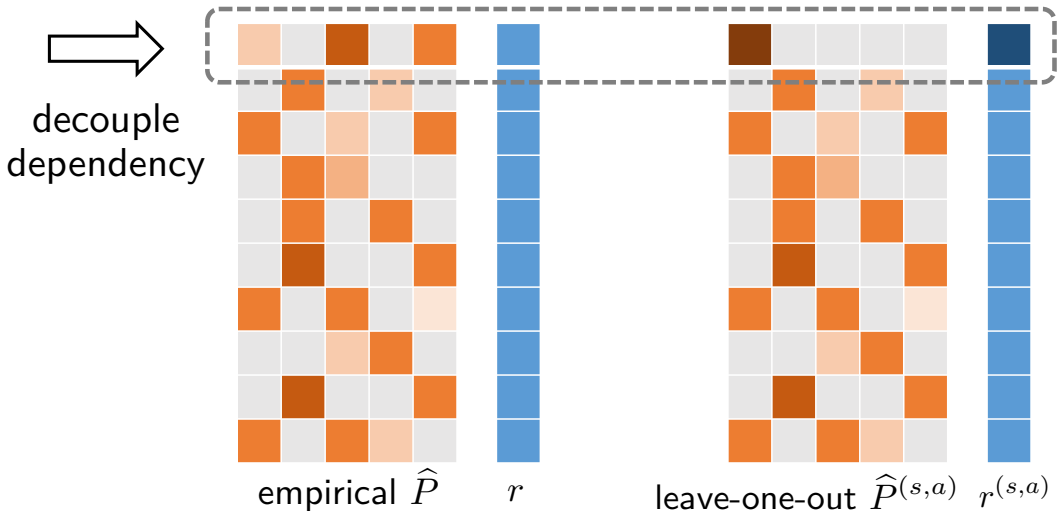
A glimpse of key analysis ideas

1. leave-one-out analysis: decouple statistical dependency by introducing auxiliary state-action absorbing MDPs by dropping randomness for each (s, a)



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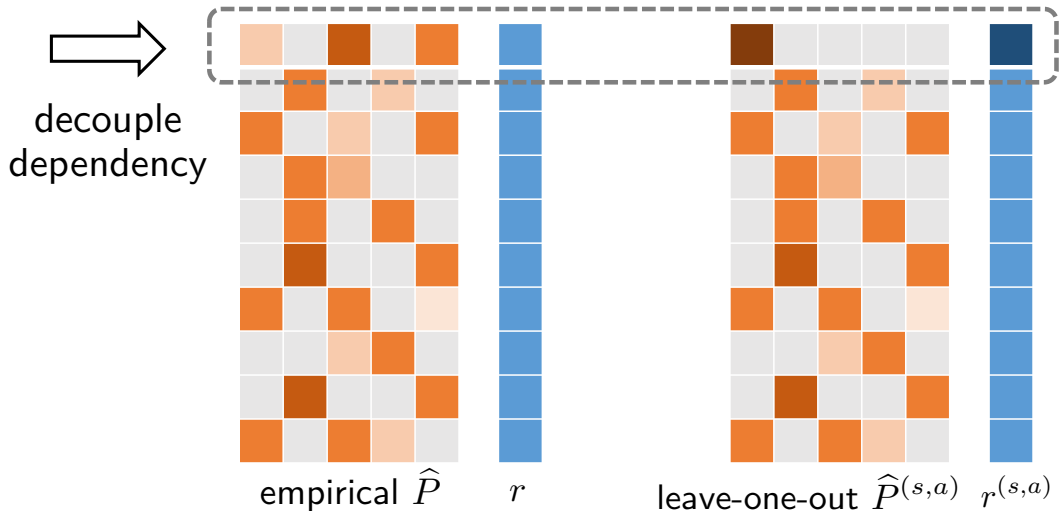

2. tie-breaking via random perturbation

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

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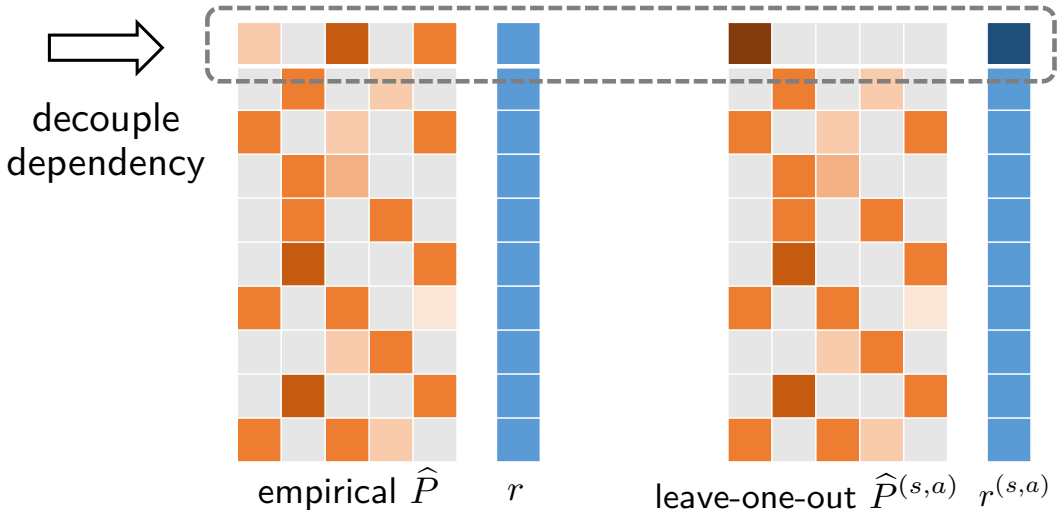

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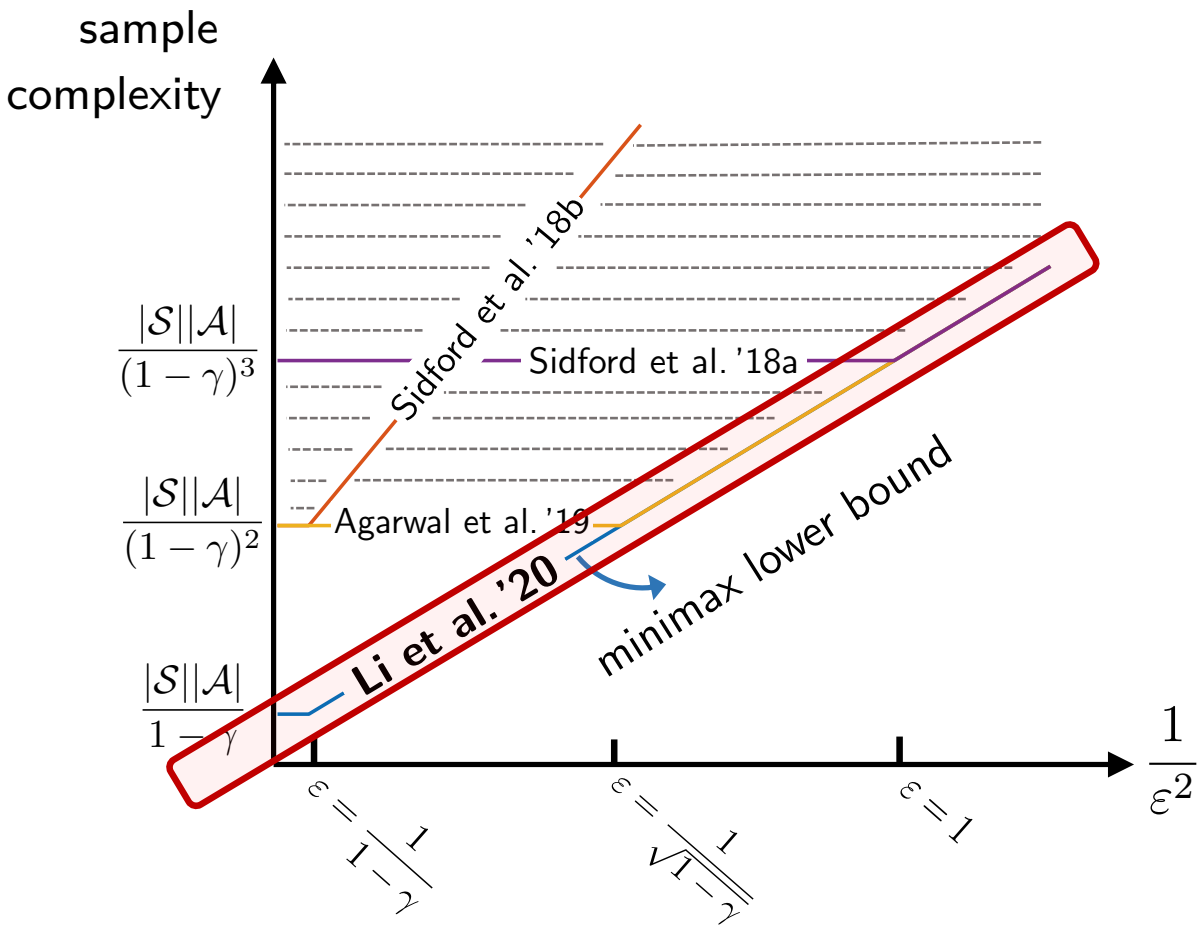
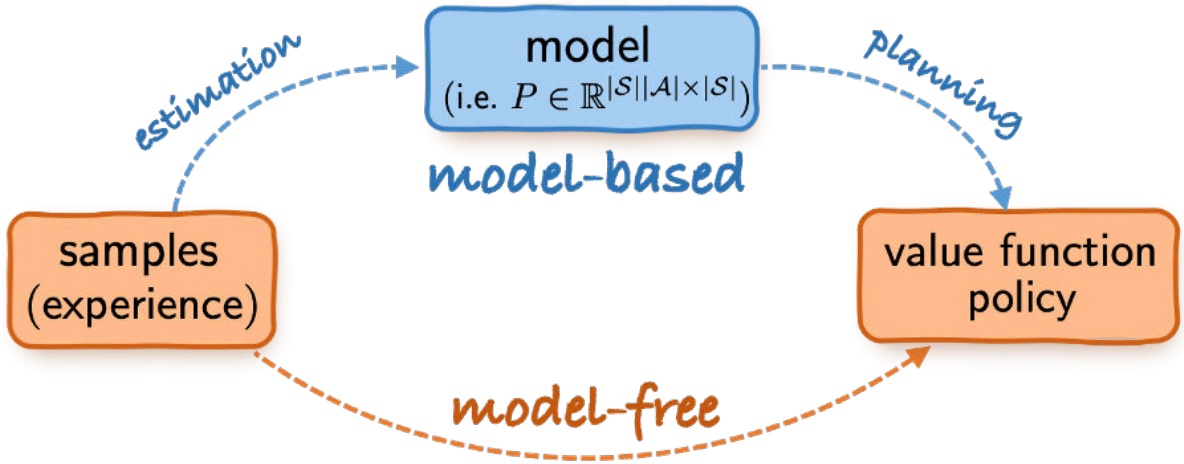
Solution: *slightly* perturb rewards $r \implies \widehat{\pi}^{\star}_{\mathrm{p}}$



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

Model-based vs. model-free RL



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Model-free / value-based approach

— learning w/o modeling & estimating environment explicitly

— memory-efficient, online, ...

Q-learning: a stochastic approximation algorithm

Chris Watkins

Peter Dayan

Stochastic approximation for solving the **Bellman equation**

Robbins & Monro, 1951

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

where

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

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

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

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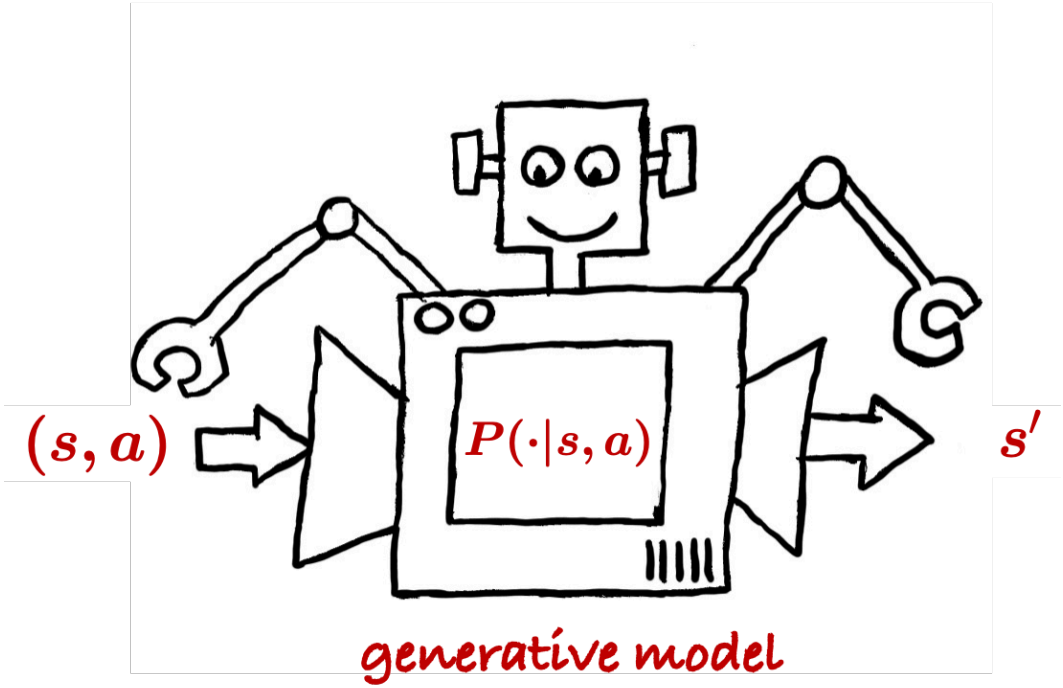
$$\mathcal{T}_t(Q)(s,a) = r(s,a) + \gamma \max_{a'} Q(s',a')$$

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

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

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

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

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

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

Sample complexity of synchronous Q-learning

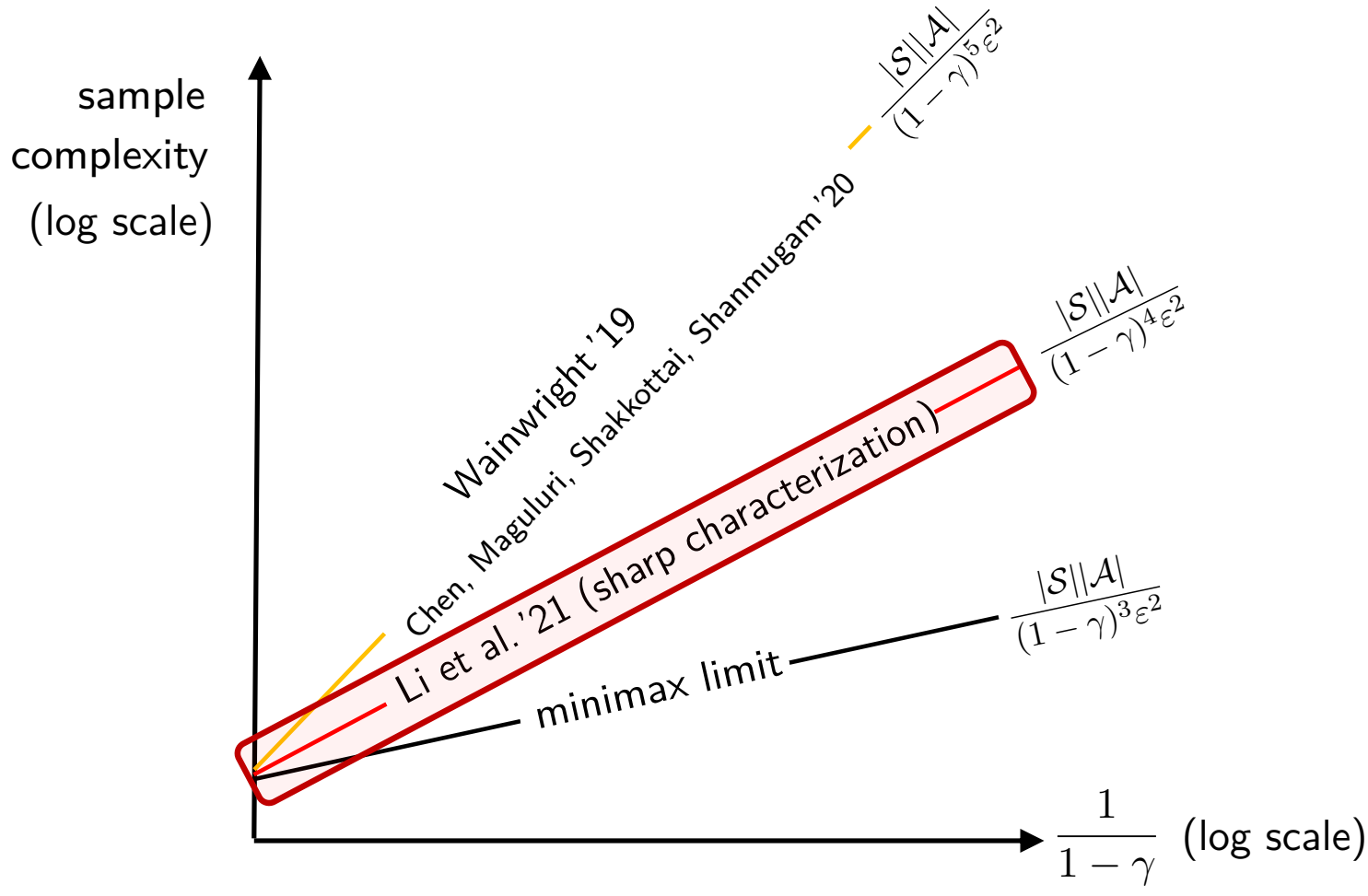
Theorem 5 (Li, Cai, Chen, Wei, Chi '21, OR'24)

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

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

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 $\frac{SA}{(1-\gamma)^4\varepsilon^2}$ $(A \geq 2)$ ...



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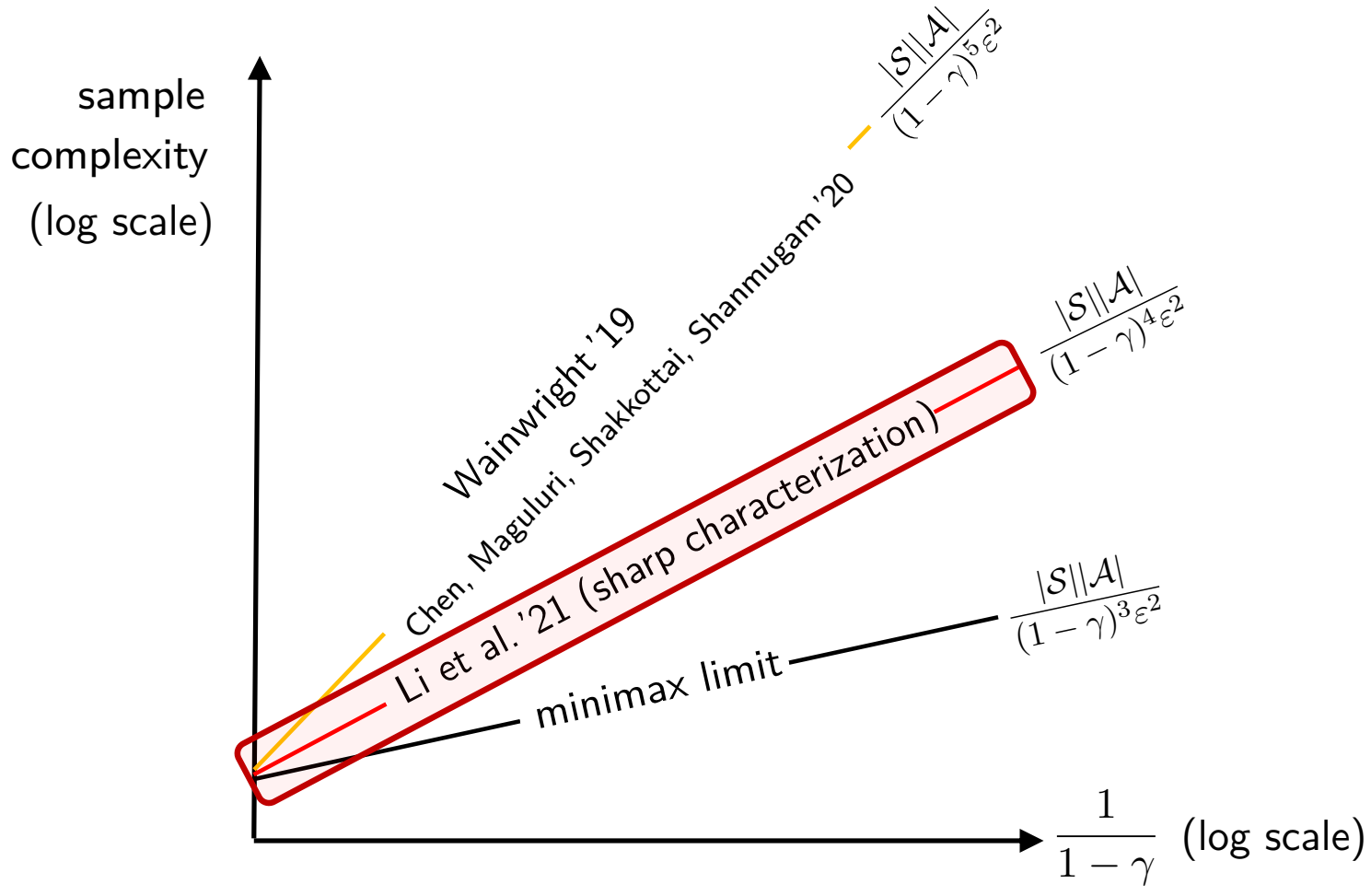

Question: *Is Q-learning sub-optimal, or is it an analysis artifact?*

Q-learning is NOT minimax optimal

Theorem 6 (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

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

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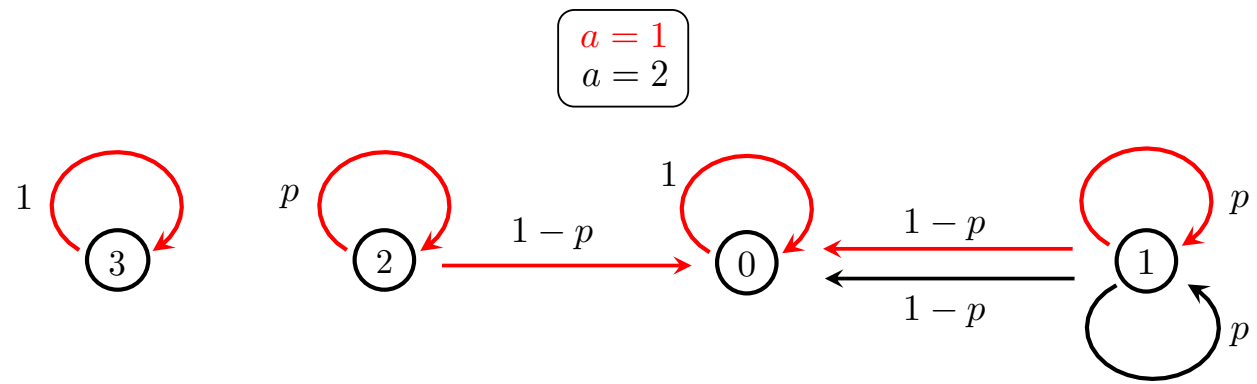
- Tight **algorithm-dependent** lower bound
- Holds for both constant and rescaled linear learning rates



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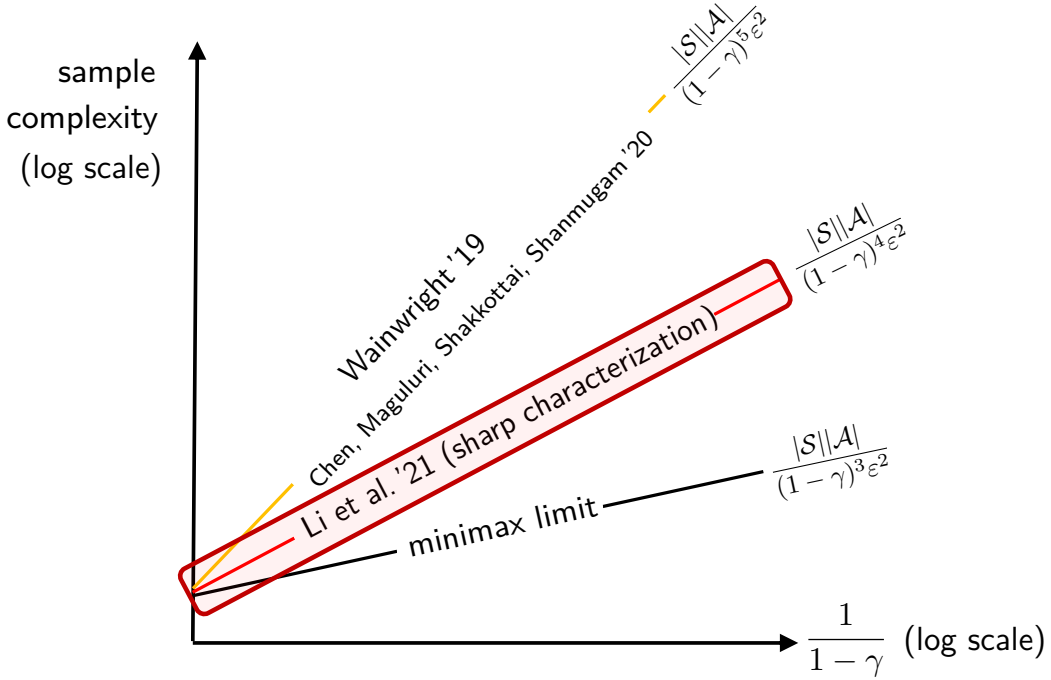

Why is Q-learning sub-optimal?

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)

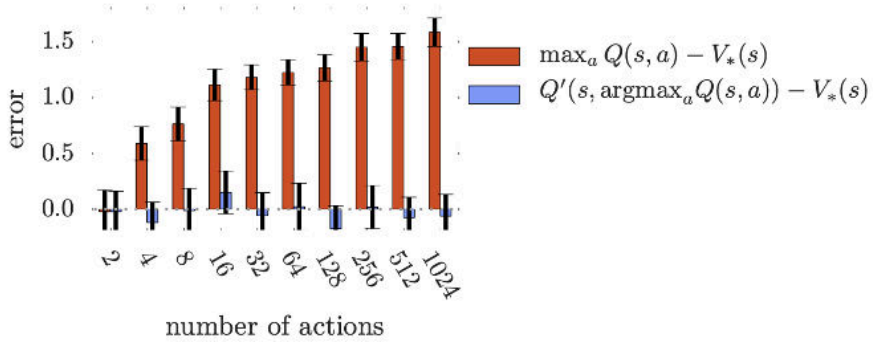

Figure 1: The orange bars show the bias in a single Q-learning update when the action values are $Q(s,a) = V_*(s) + \epsilon_a$ and the errors $\{\epsilon_a\}_{a=1}^m$ are independent standard normal random variables. The second set of action values Q', used for the blue bars, was generated identically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

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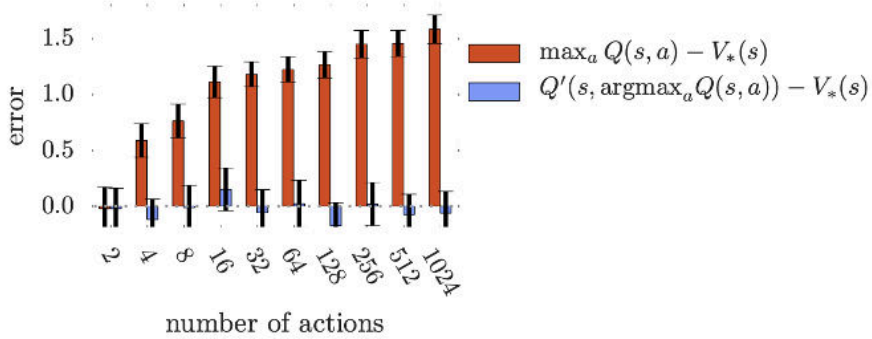

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A provable improvement: Q-learning with variance reduction

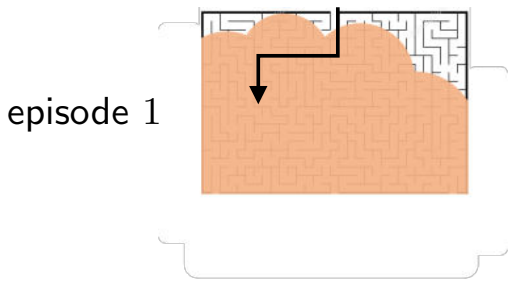
(Wainwright 2019)

Part 1

1. Basics: Markov decision processes
2. RL w/ a generative model (simulator)
3. Online RL
4. Offline RL

Online episodic RL

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

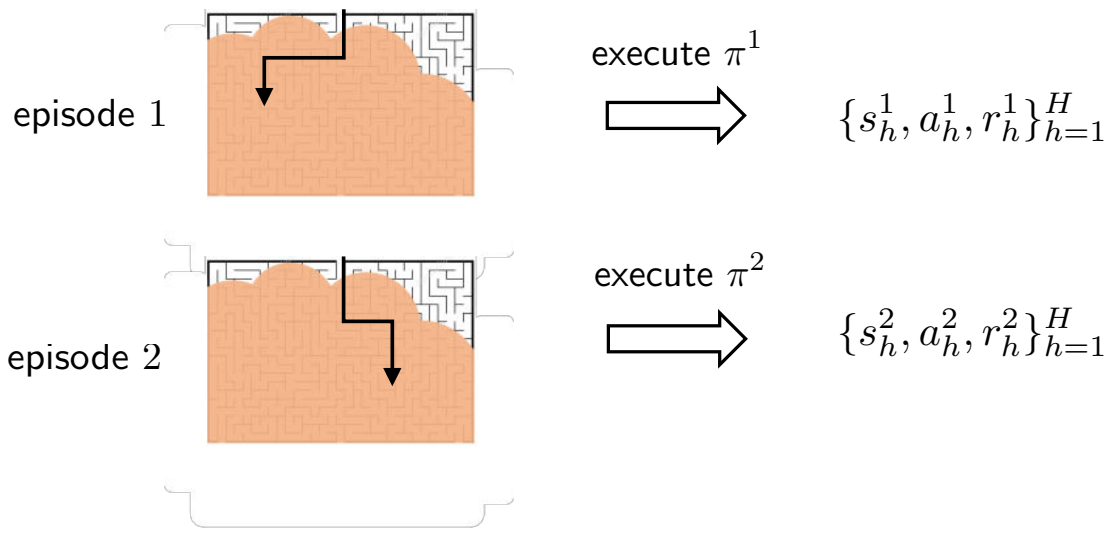


execute π^1

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

Online episodic RL

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



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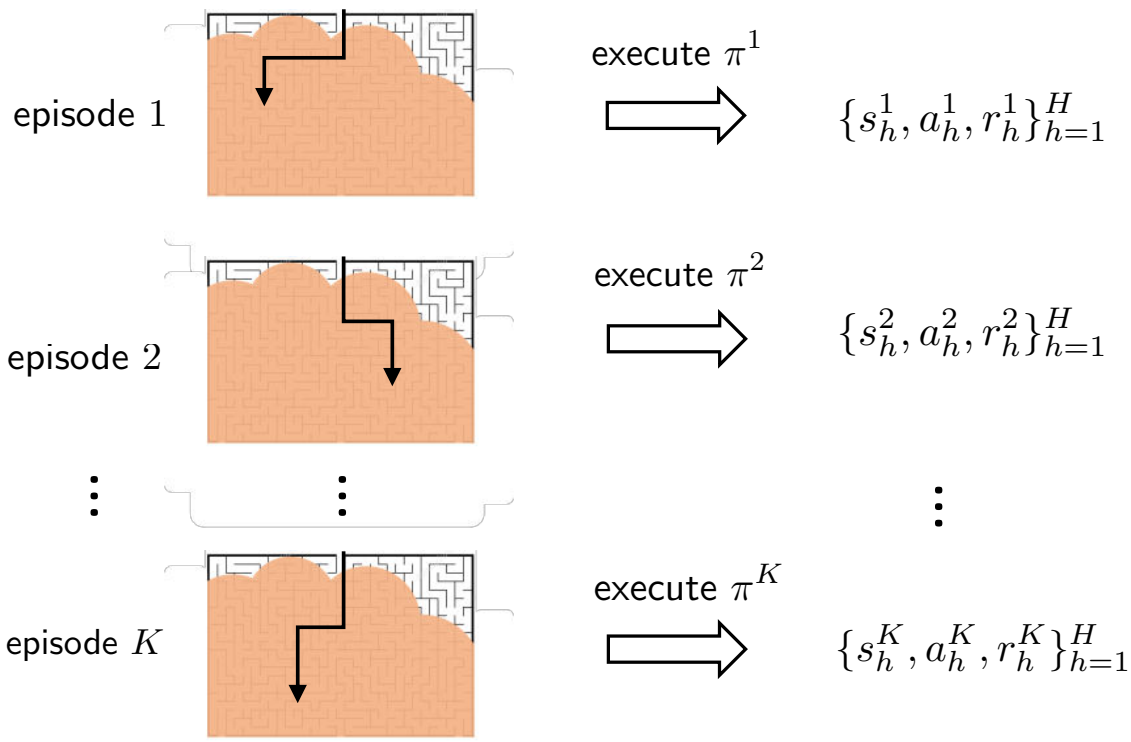
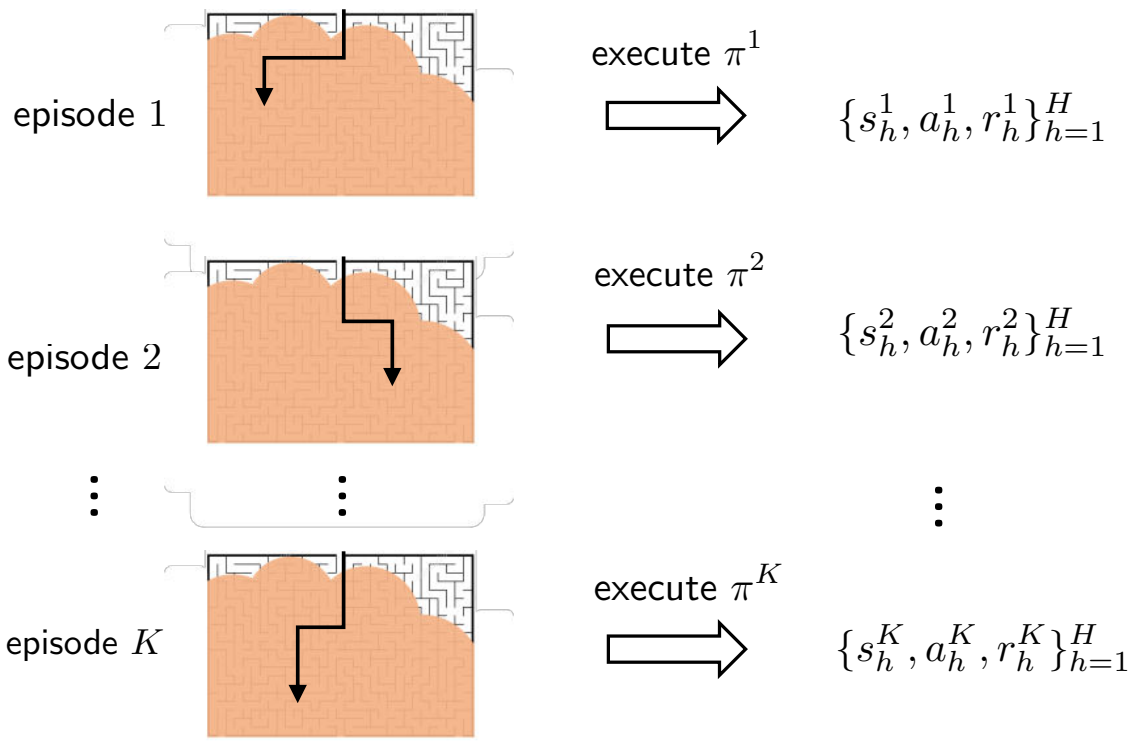


Online episodic RL

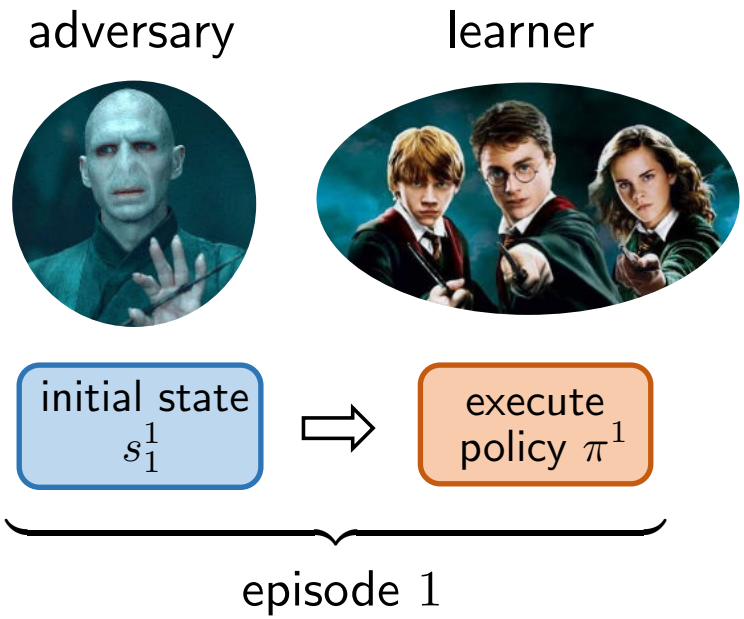
Sequentially execute MDP for K episodes, each consisting of H steps

— *sample size:* $T = KH$



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

Regret: gap between learned policy & optimal policy



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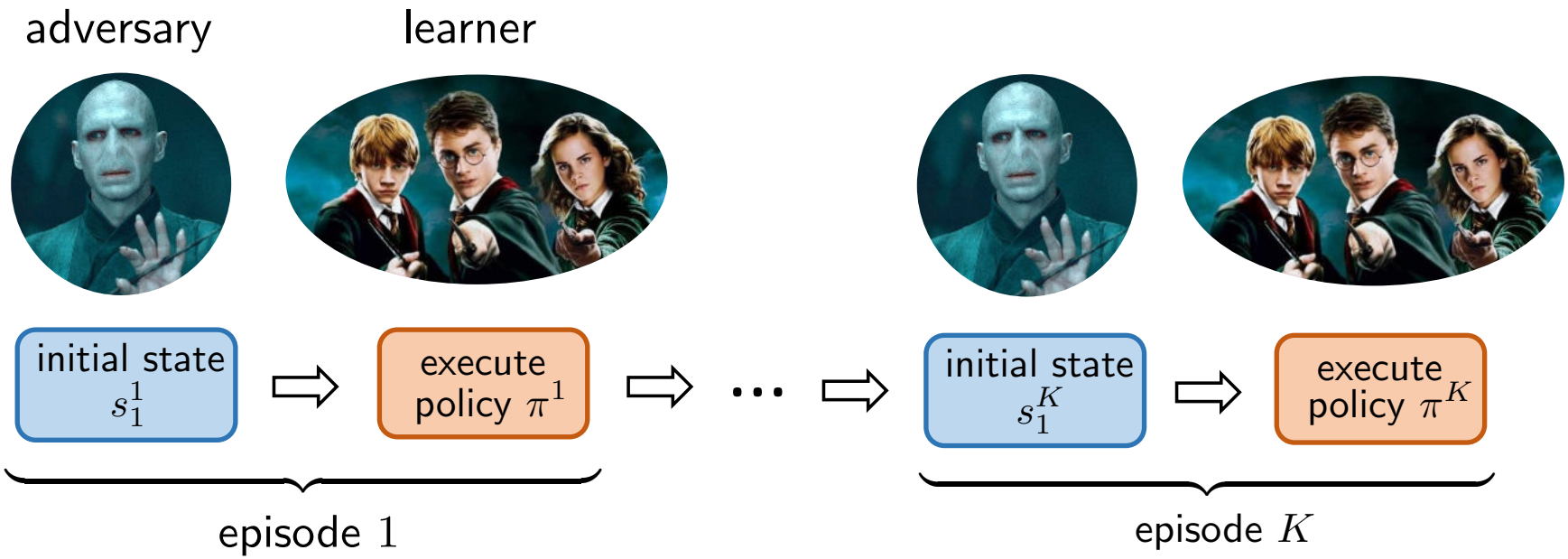

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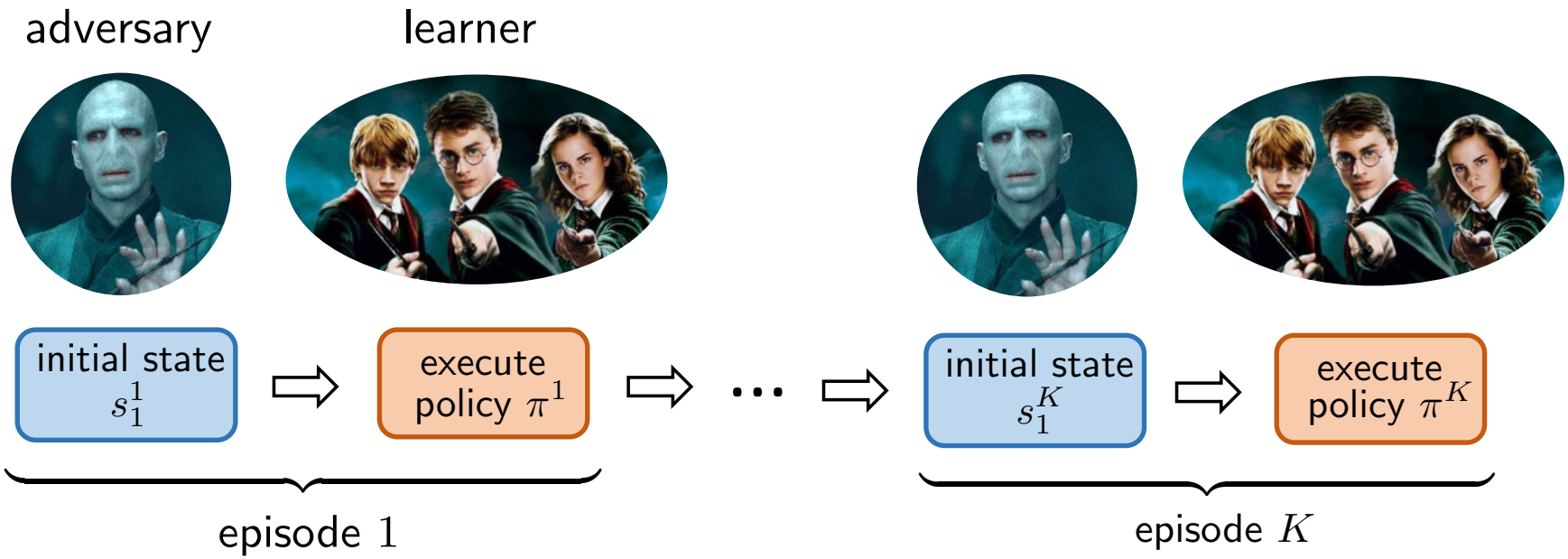

Performance metric: given initial states $\{s_1^k\}_{k=1}^K$, define

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

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
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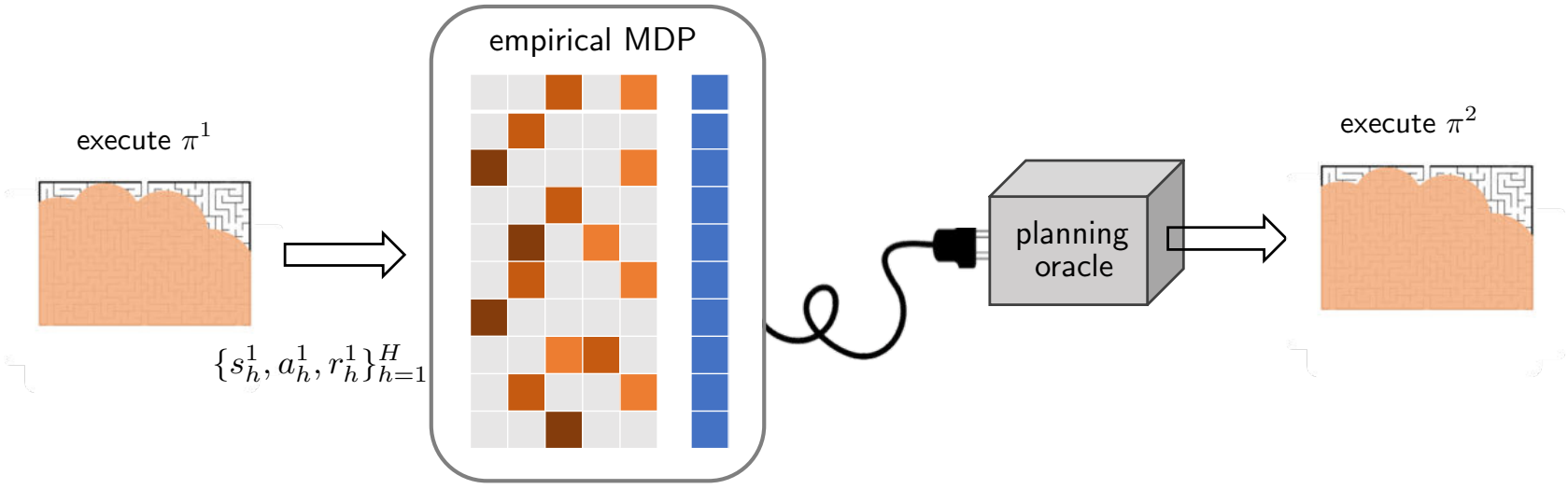
Which online RL algorithms achieve near-minimal regret?

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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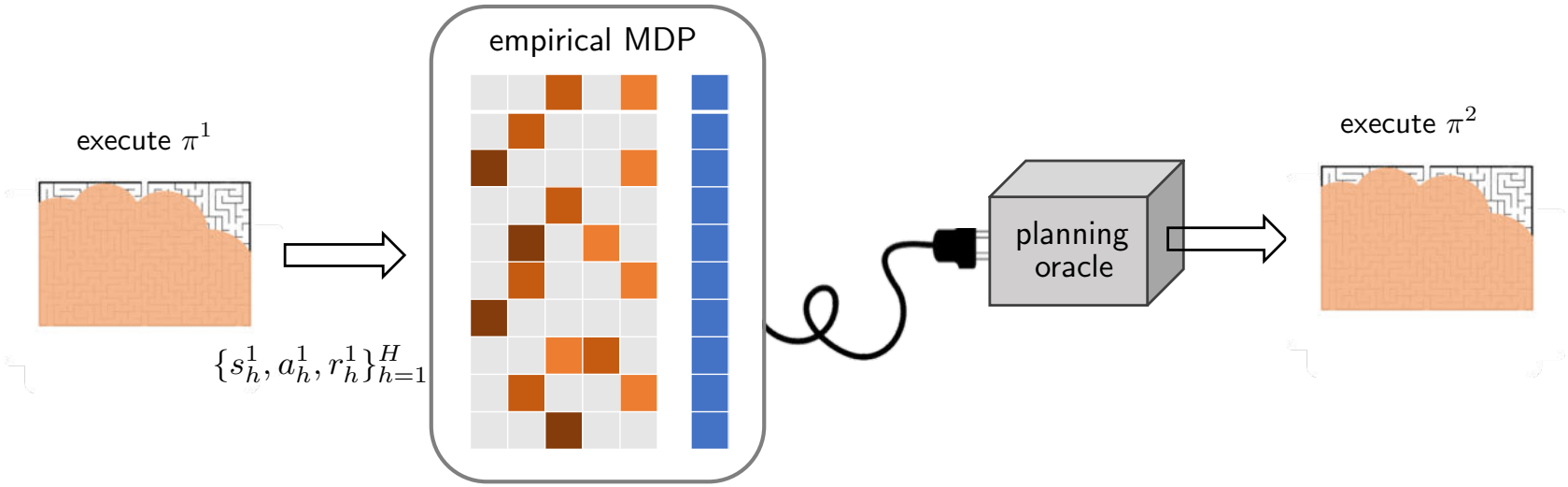

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How to balance exploration and exploitation in this framework?

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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- a common framework: utilize $\underbrace{\text{upper confidence bounds (UCB)}}_{\text{accounts for estimates + uncertainty level}}$

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**

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

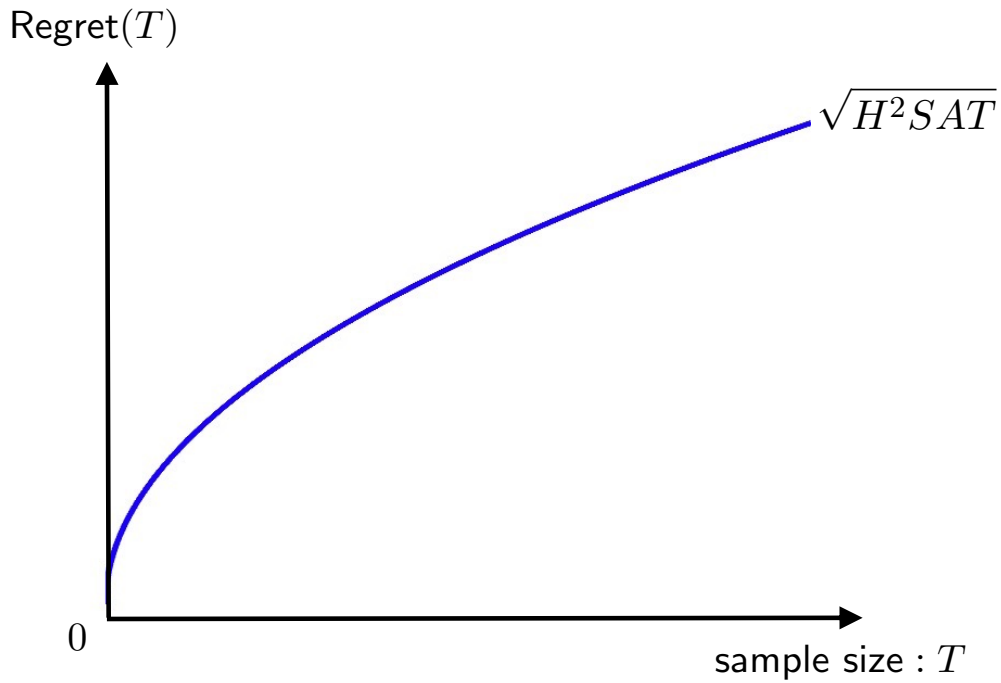
2. Forward $h = 1, \ldots, H$: take actions according to **greedy policy**

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

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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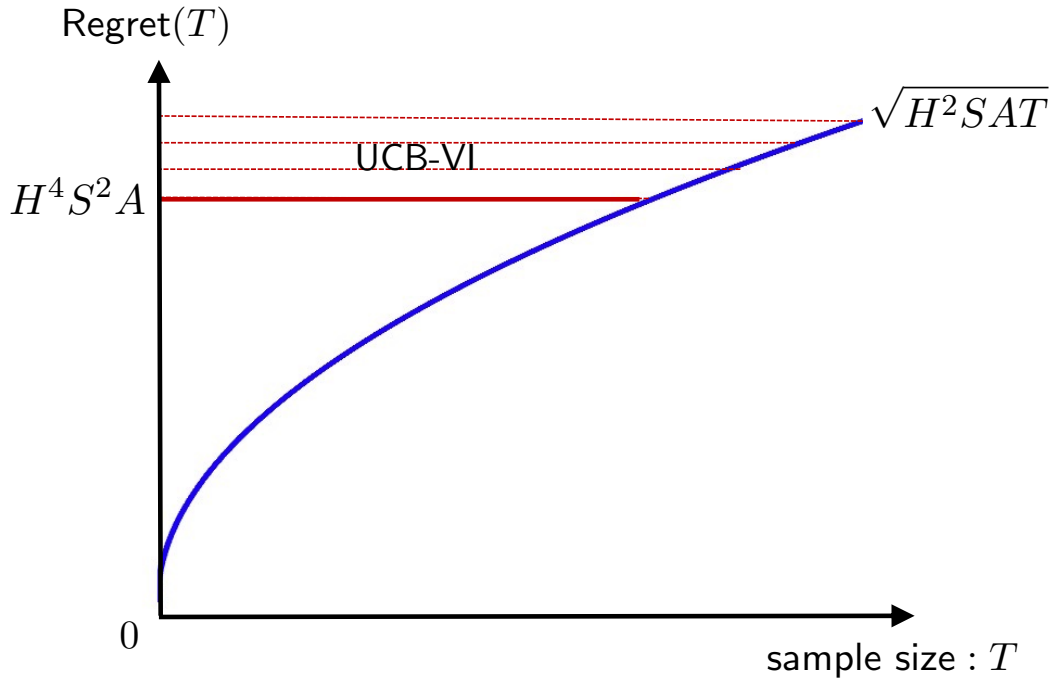

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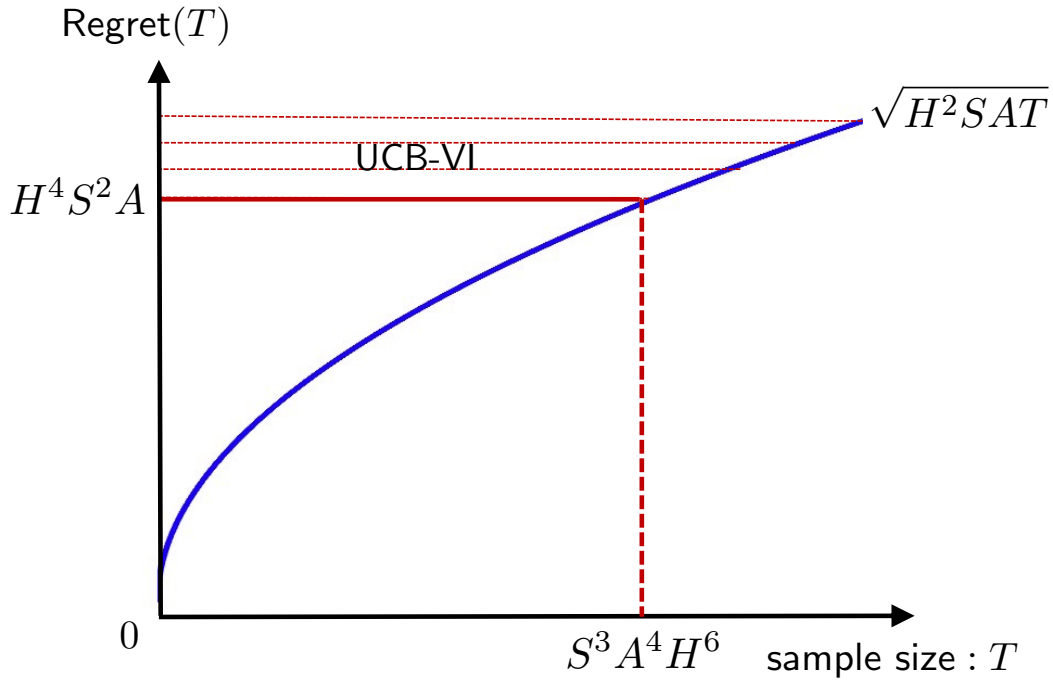

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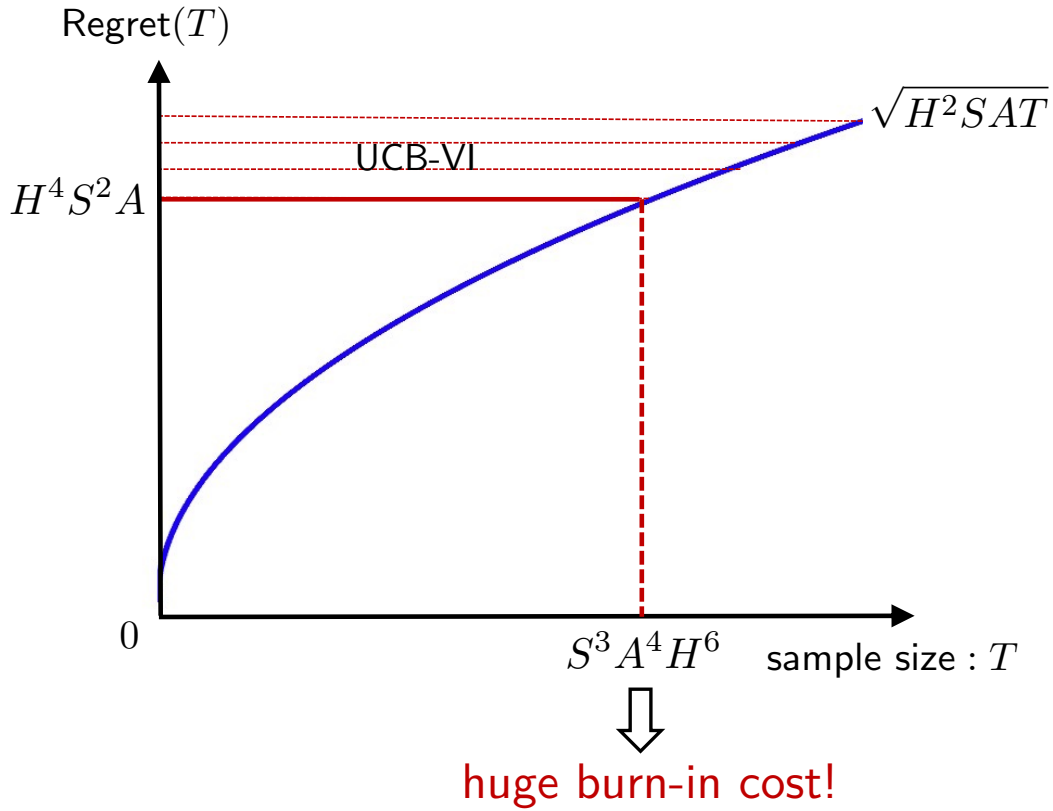

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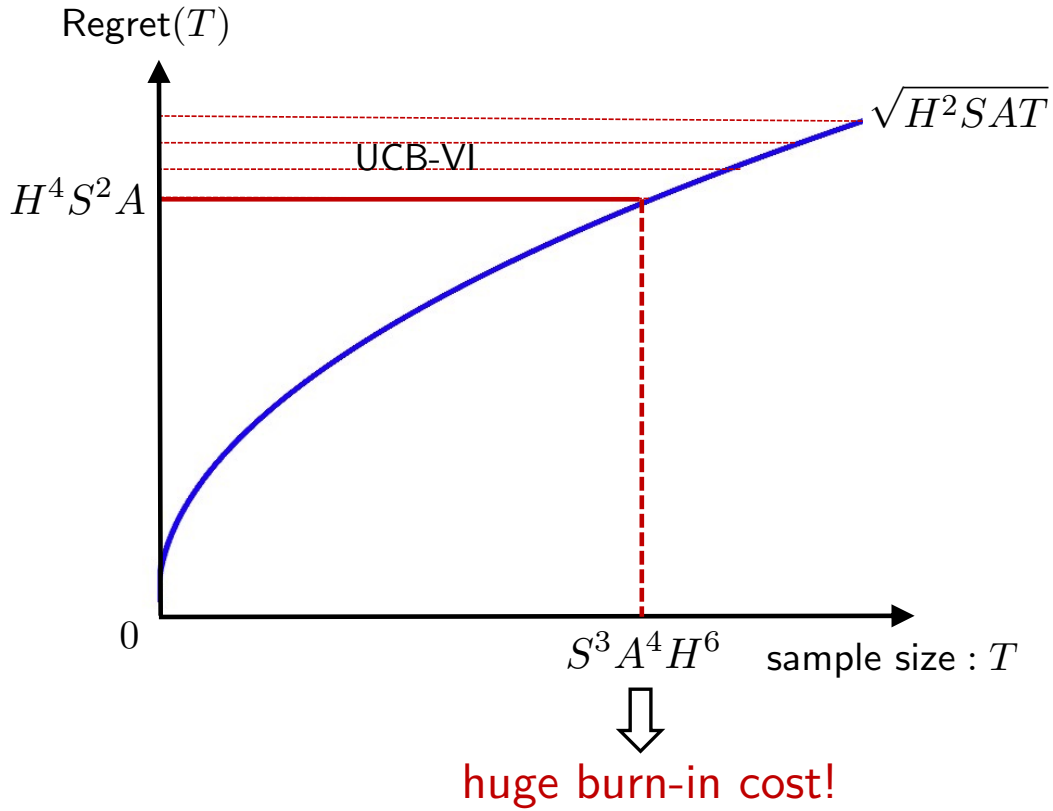

Issues: large burn-in cost

Other asymptotically regret-optimal algorithms

Algorithm	Regret upper bound	Range of K that attains optimal regret
UCBVI (Azar et al, 2017)	$\sqrt{SAH^2T} + S^2AH^3$	$[S^3AH^3, \infty)$
ORLC (Dann et al, 2019)	$\sqrt{SAH^2T} + S^2AH^4$	$[S^3AH^5, \infty)$
EULER (Zanette et al, 2019)	$\sqrt{SAH^2T} + S^{3/2}AH^3(\sqrt{S} + \sqrt{H})$	$[S^2AH^3(\sqrt{S} + \sqrt{H}), \infty)$
UCB-Adv (Zhang et al, 2020)	$\sqrt{SAH^2T} + S^2A^{3/2}H^{33/4}K^{1/4}$	$[S^6A^4H^{27}, \infty)$
MVP (Zhang et al, 2020)	$\sqrt{SAH^2T} + S^2AH^2$	$[S^3AH, \infty)$
UCB-M-Q (Menard et al, 2021)	$\sqrt{SAH^2T} + SAH^4$	$[SAH^5, \infty)$
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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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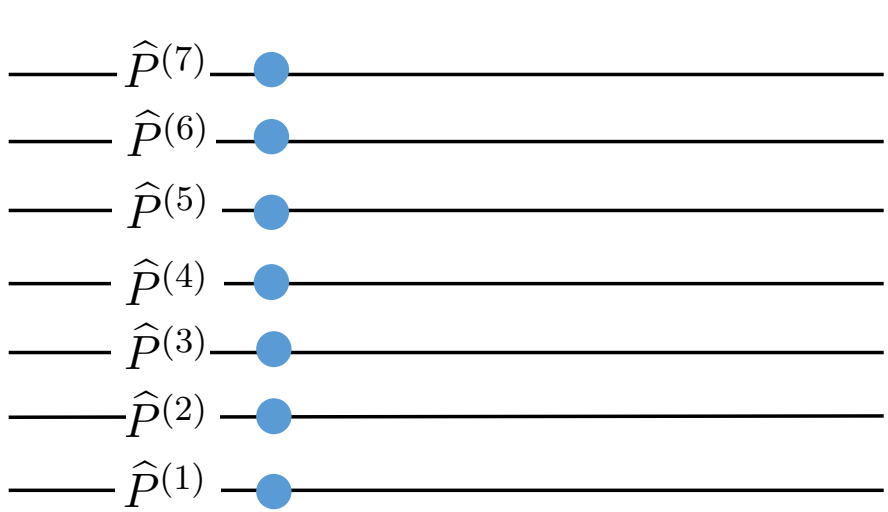

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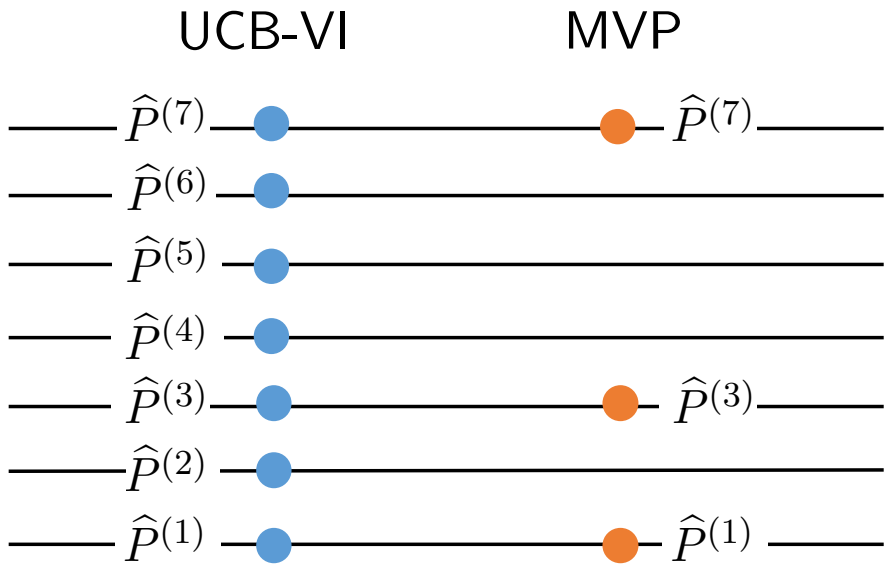

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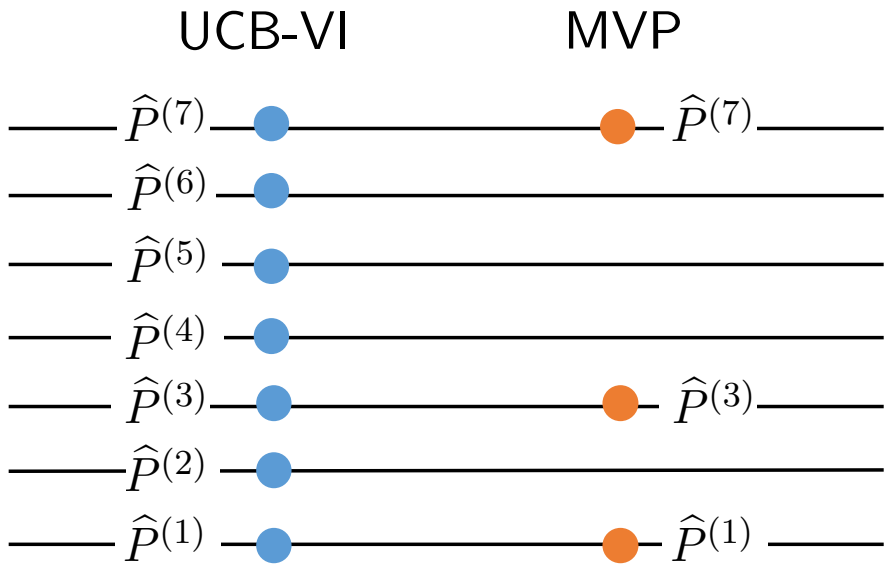

  - visitation counts change much less frequently
    $\longrightarrow$ reduces covering number dramatically

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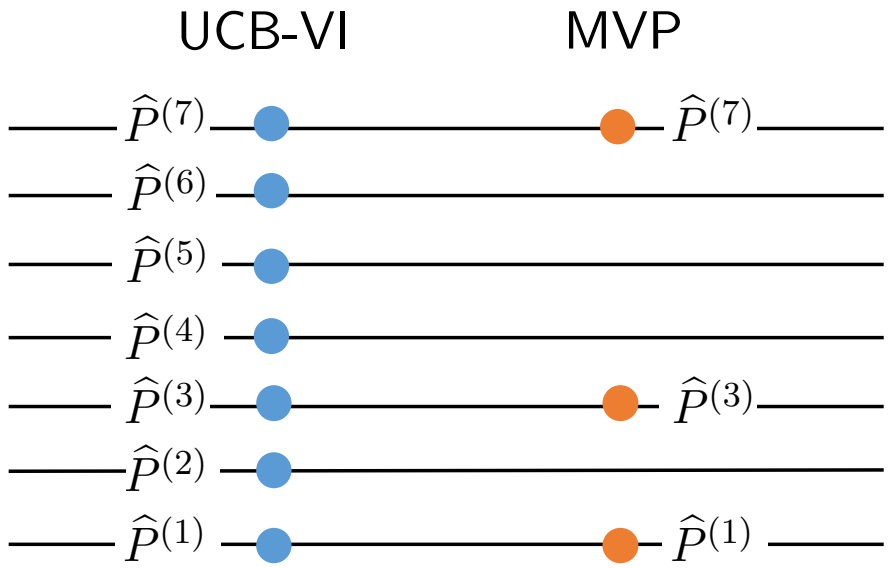

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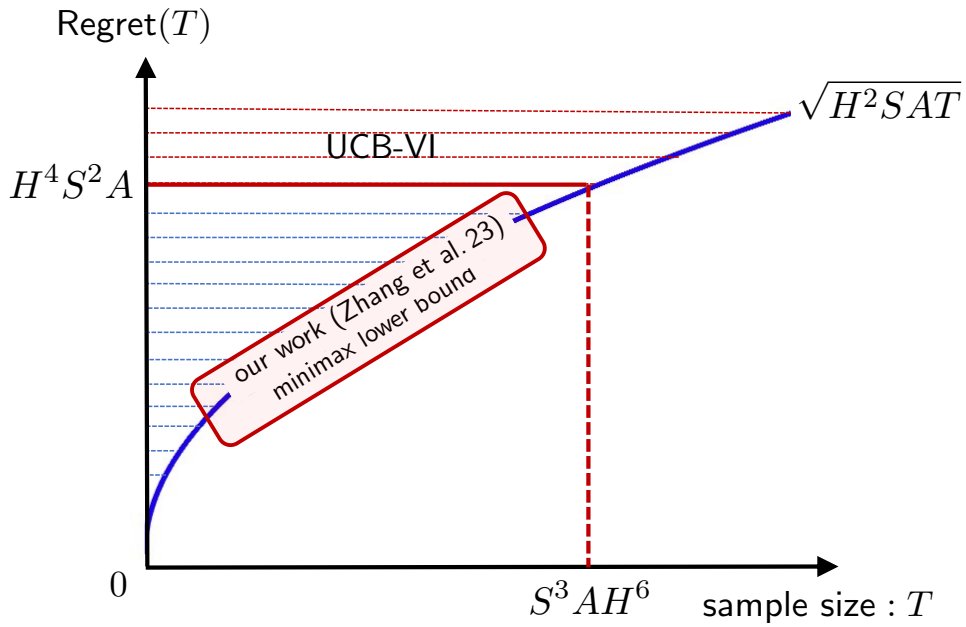
- data-driven bonus terms (chosen based on empirical variances)

Regret-optimal algorithm w/o burn-in cost

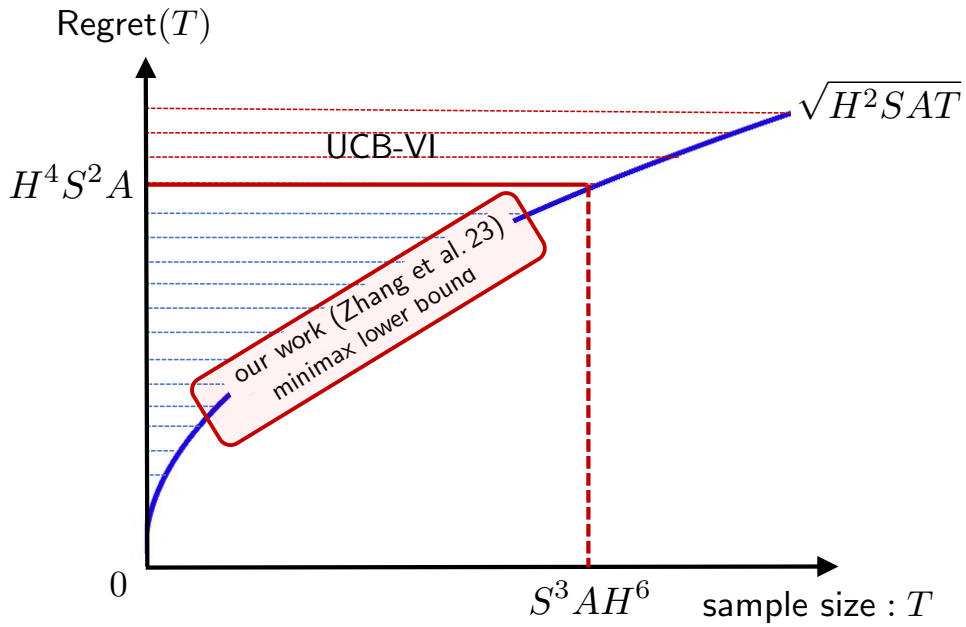


Theorem 7 (Zhang, Chen, Lee, Du '24)

The model-based algorithm Monotonic Value Propagation achieves

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

Regret-optimal algorithm w/o burn-in cost



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

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

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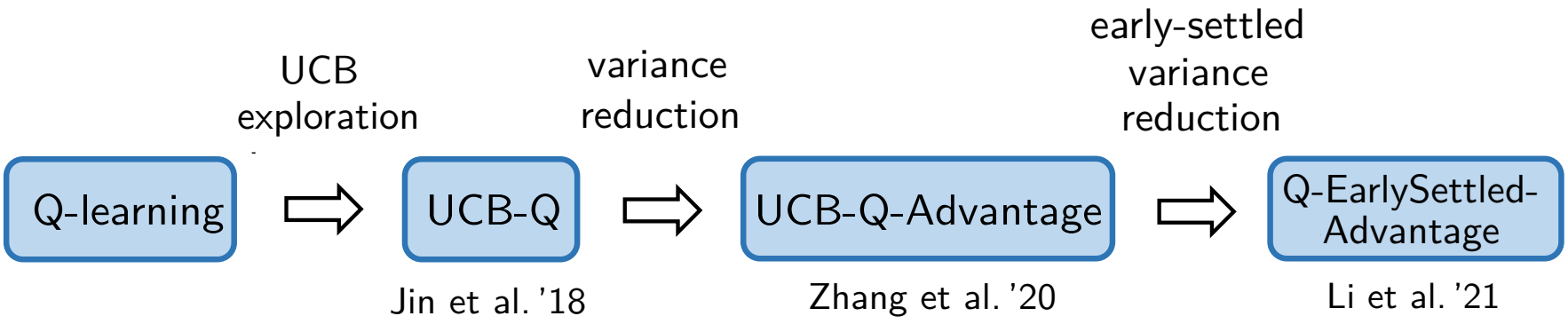

Q-learning with UCB exploration (Jin et al., 2018)

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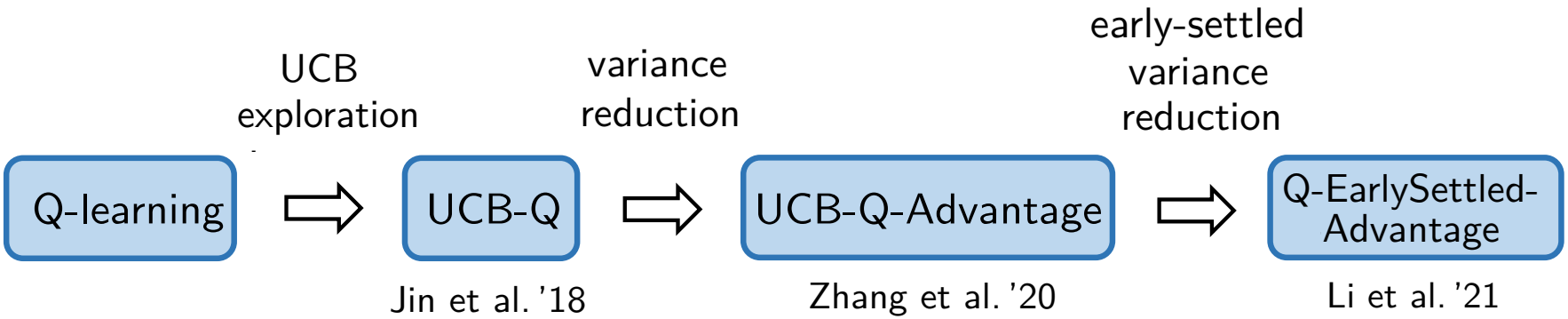
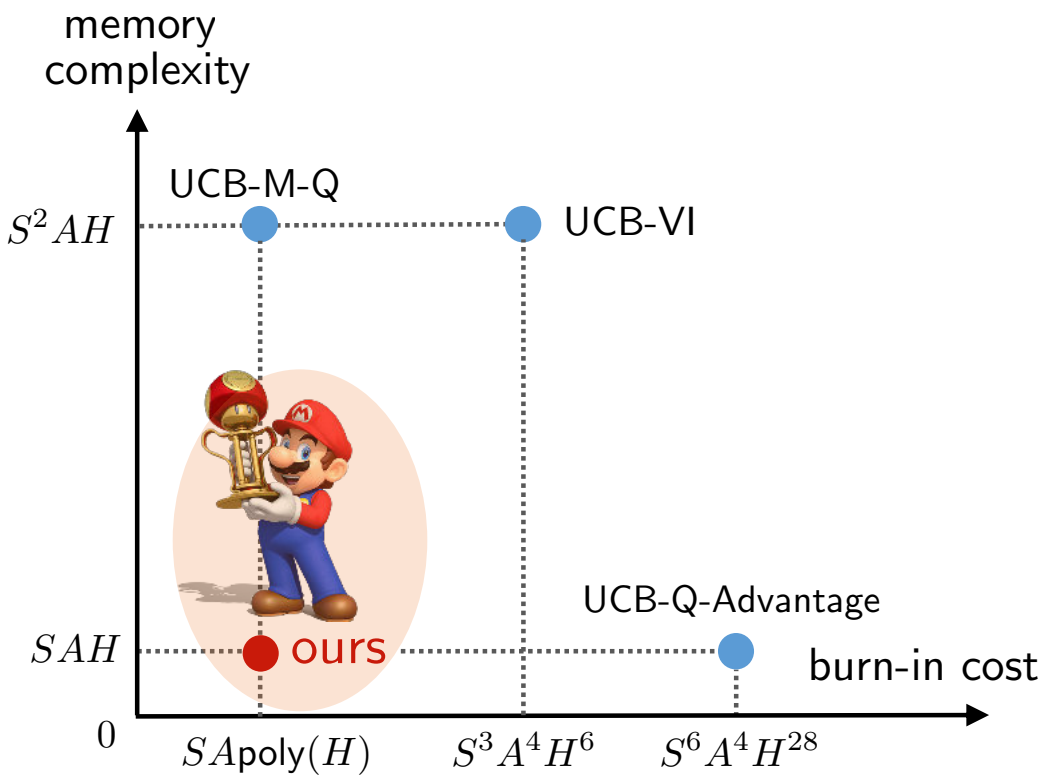
Issue: *large variability in stochastic update rules*

Further improvement

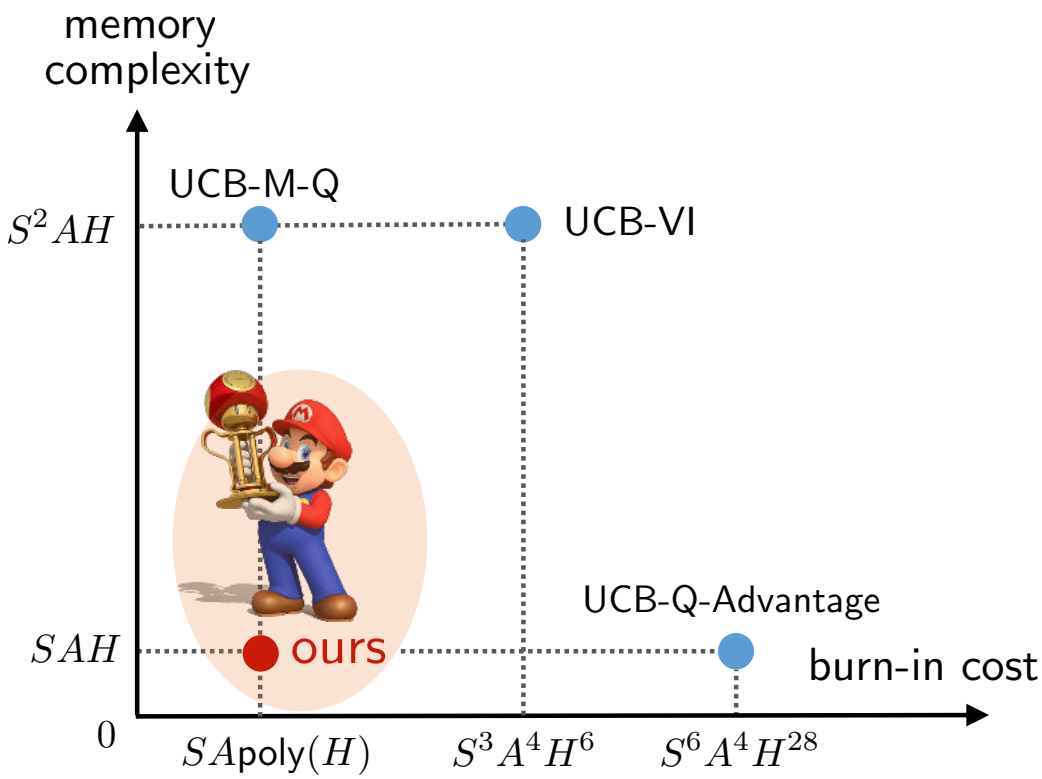


- UCB-Q-Advantage: use variance reduction to achieve near-optimal regret, but with large burn-in cost;
- Q-EarlySettled-Advantage: stop updating the reference as soon as possible to reduce burn-in cost.



Model-free algorithms can simultaneously achieve

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



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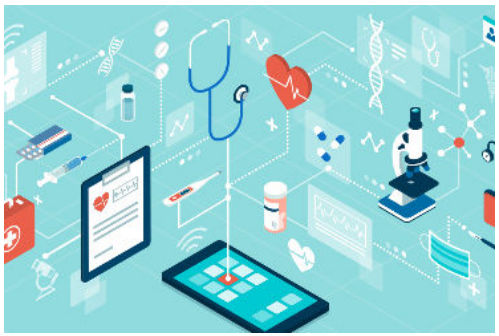
Part 1

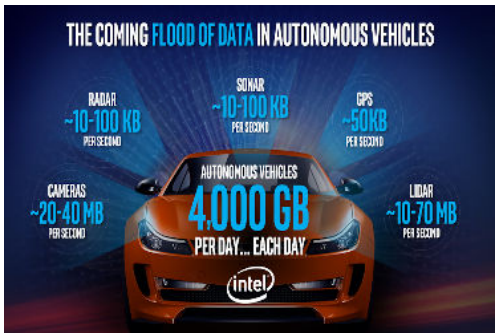
1. Basics: Markov decision processes
2. RL w/ a generative model (simulator)
3. Online RL
4. Offline RL

Offline/batch RL

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



medical records

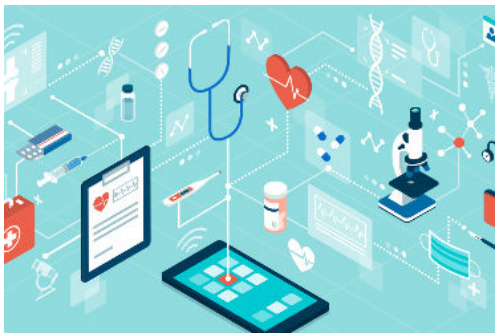


data of self-driving

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



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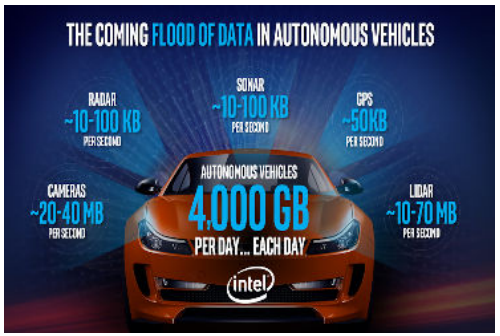

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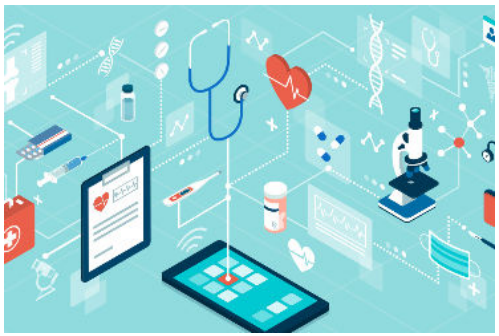

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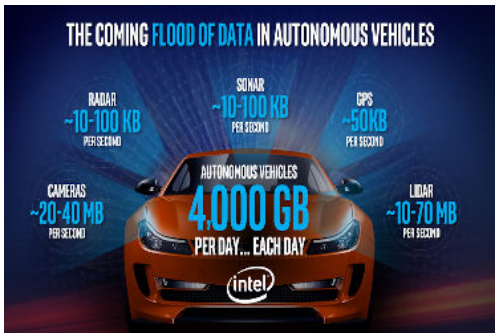
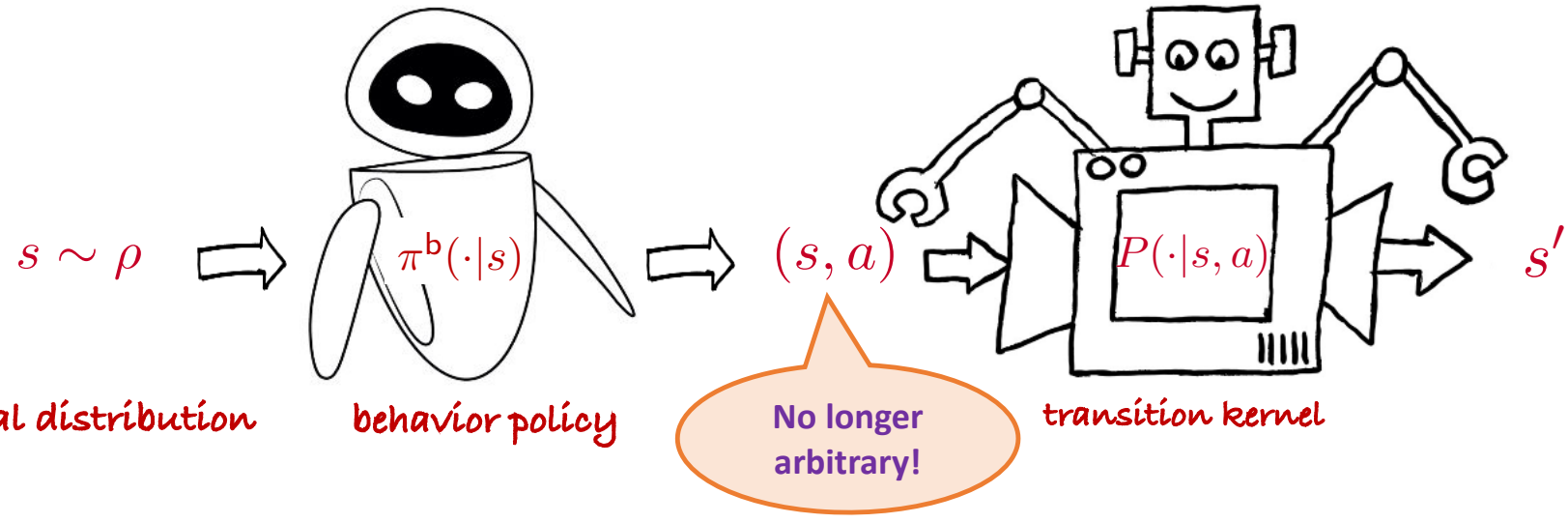


data of self-driving

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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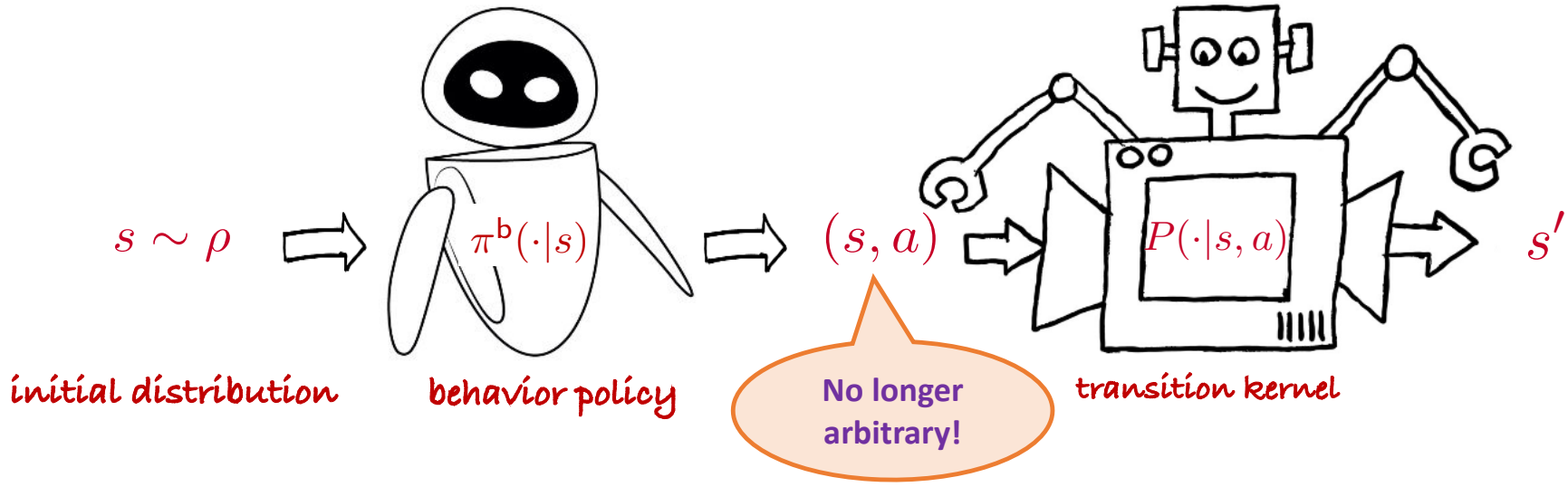
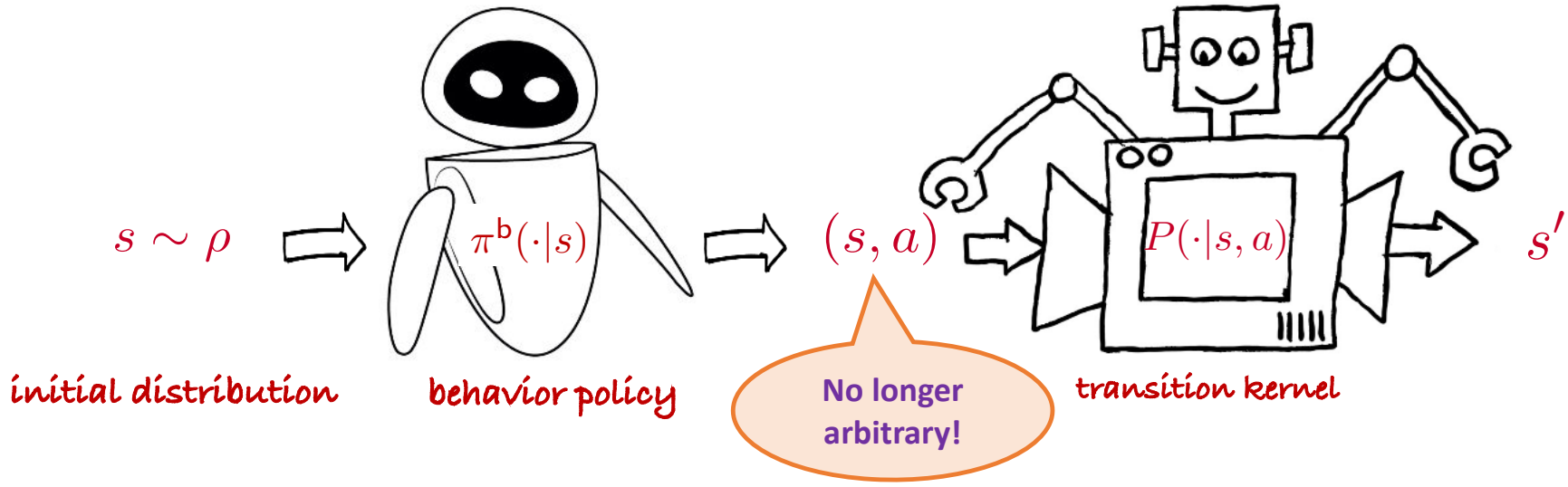


historical dataset $\mathcal{D} = \{(s^{(i)}, a^{(i)}, s'^{(i)})\}$**:** N independent copies of

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

- ρ: initial state distribution; π^{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*

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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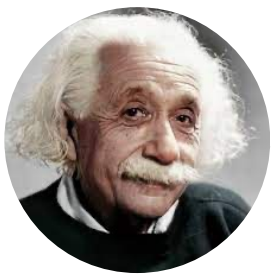
$C^\star = O(1)$ → large $C^\star$



expert data

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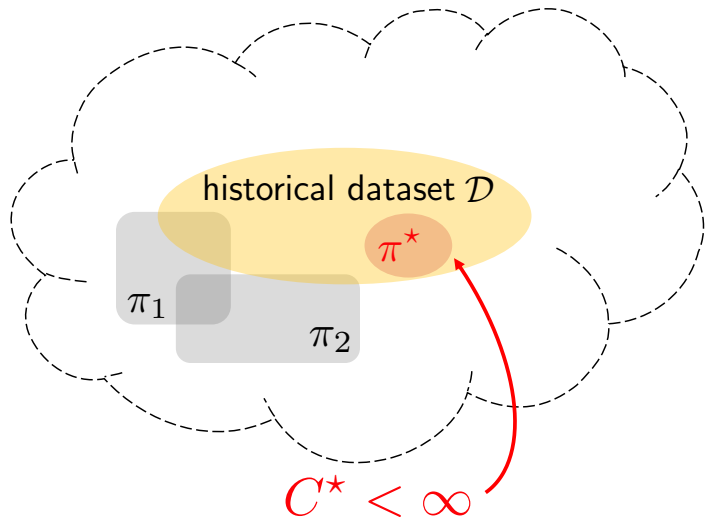
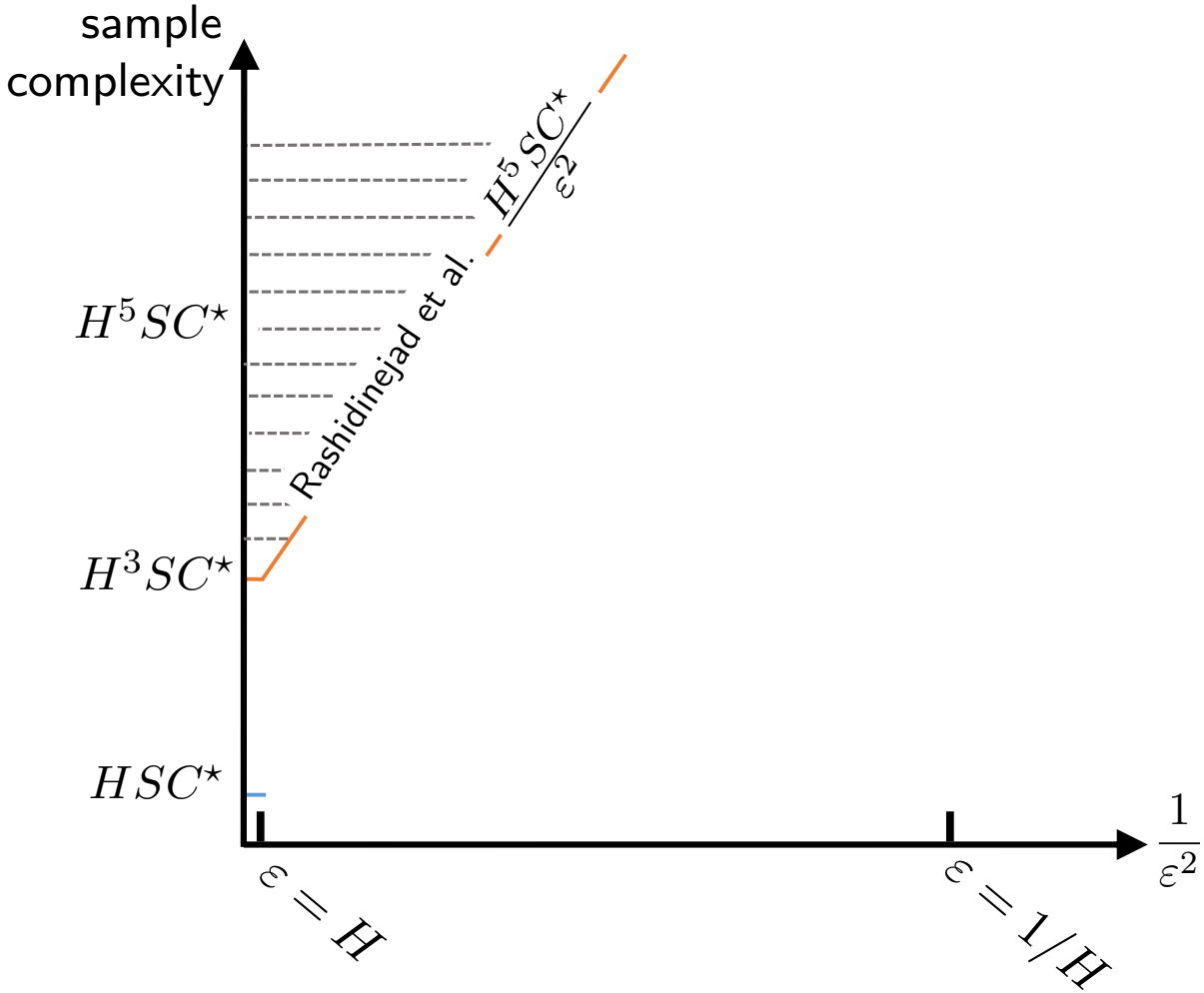
- captures distributional shift
- allows for partial coverage
  - as long as it covers the part reachable by $\pi^\star$



Prior art: sample complexity bounds



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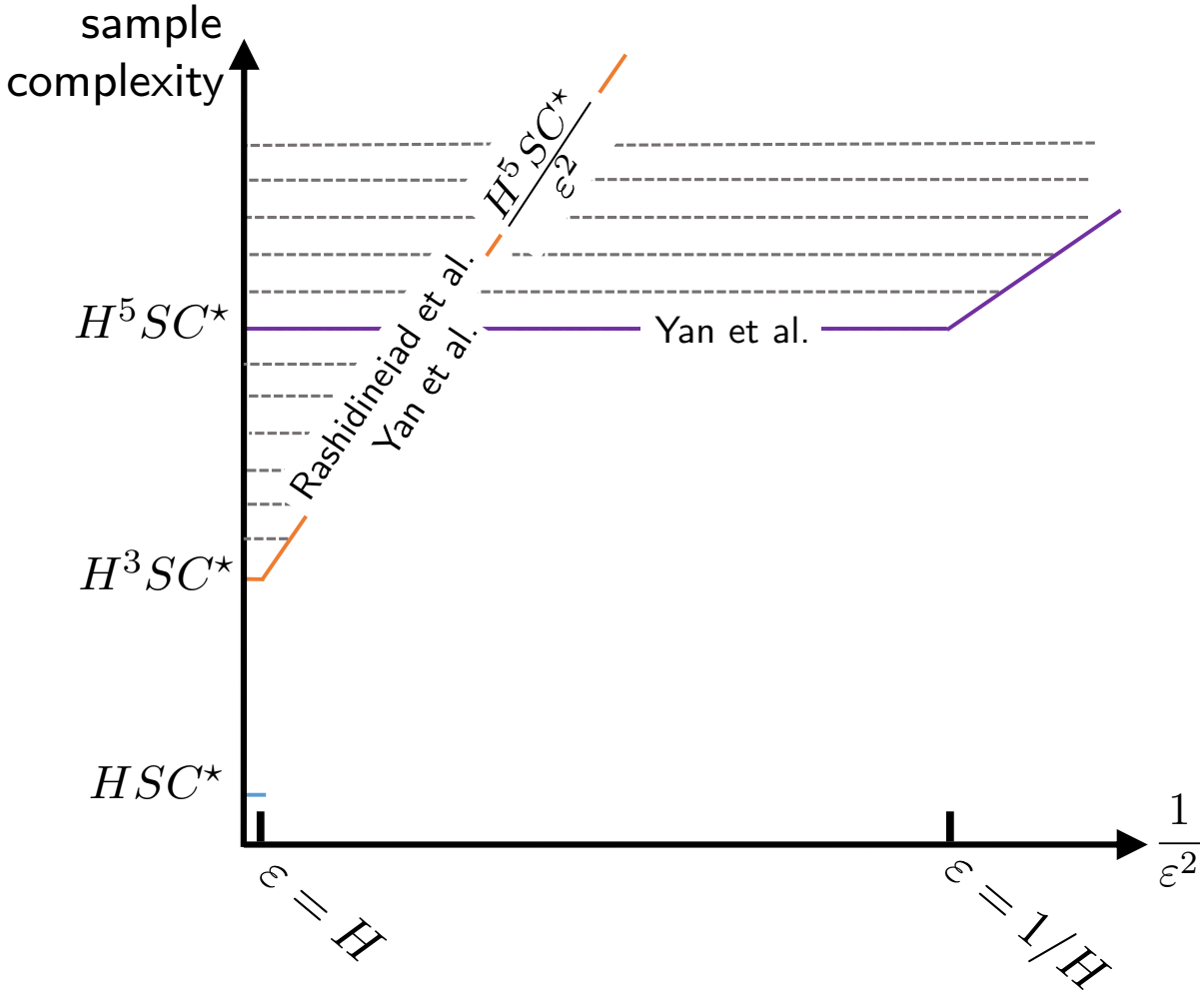

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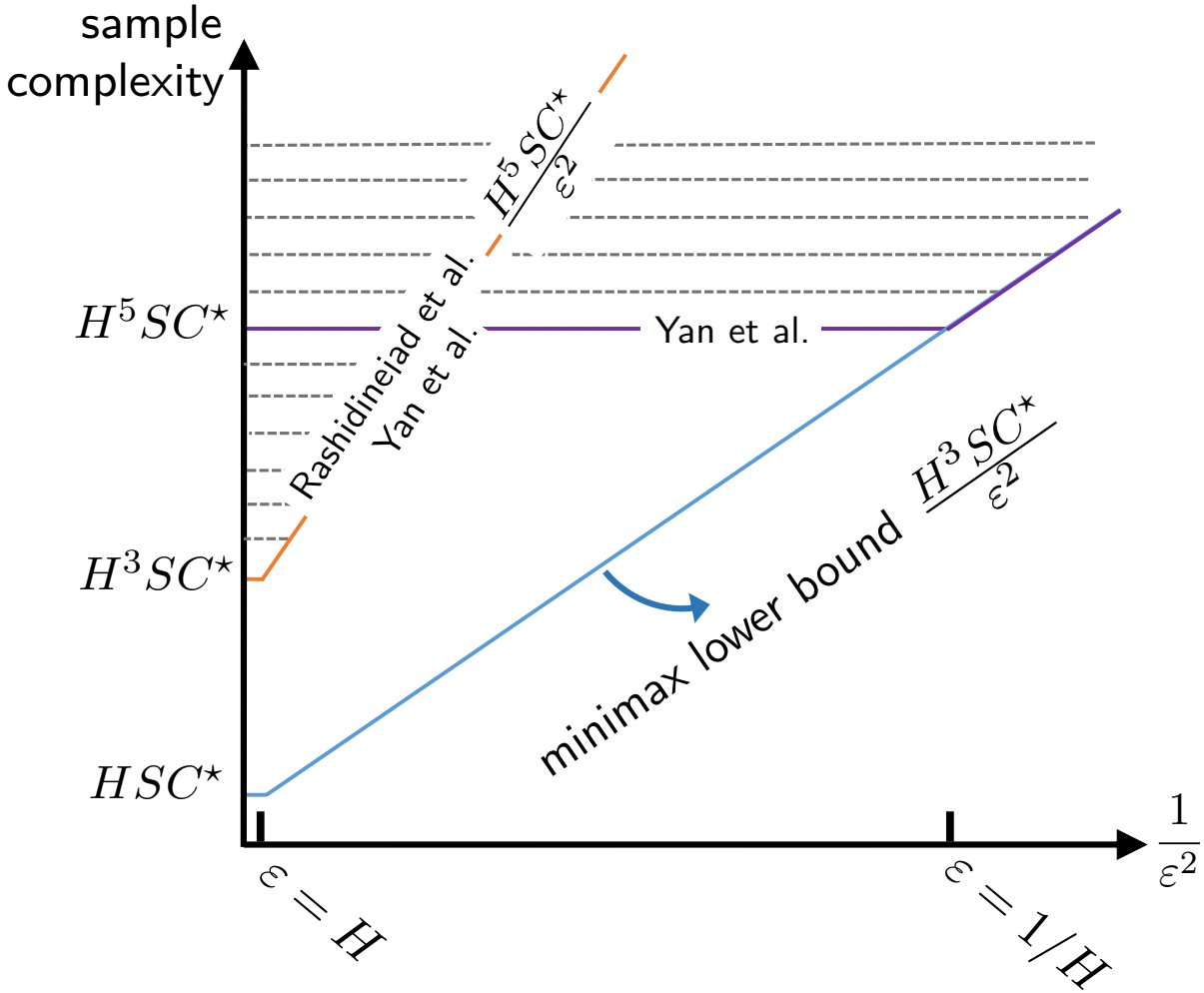

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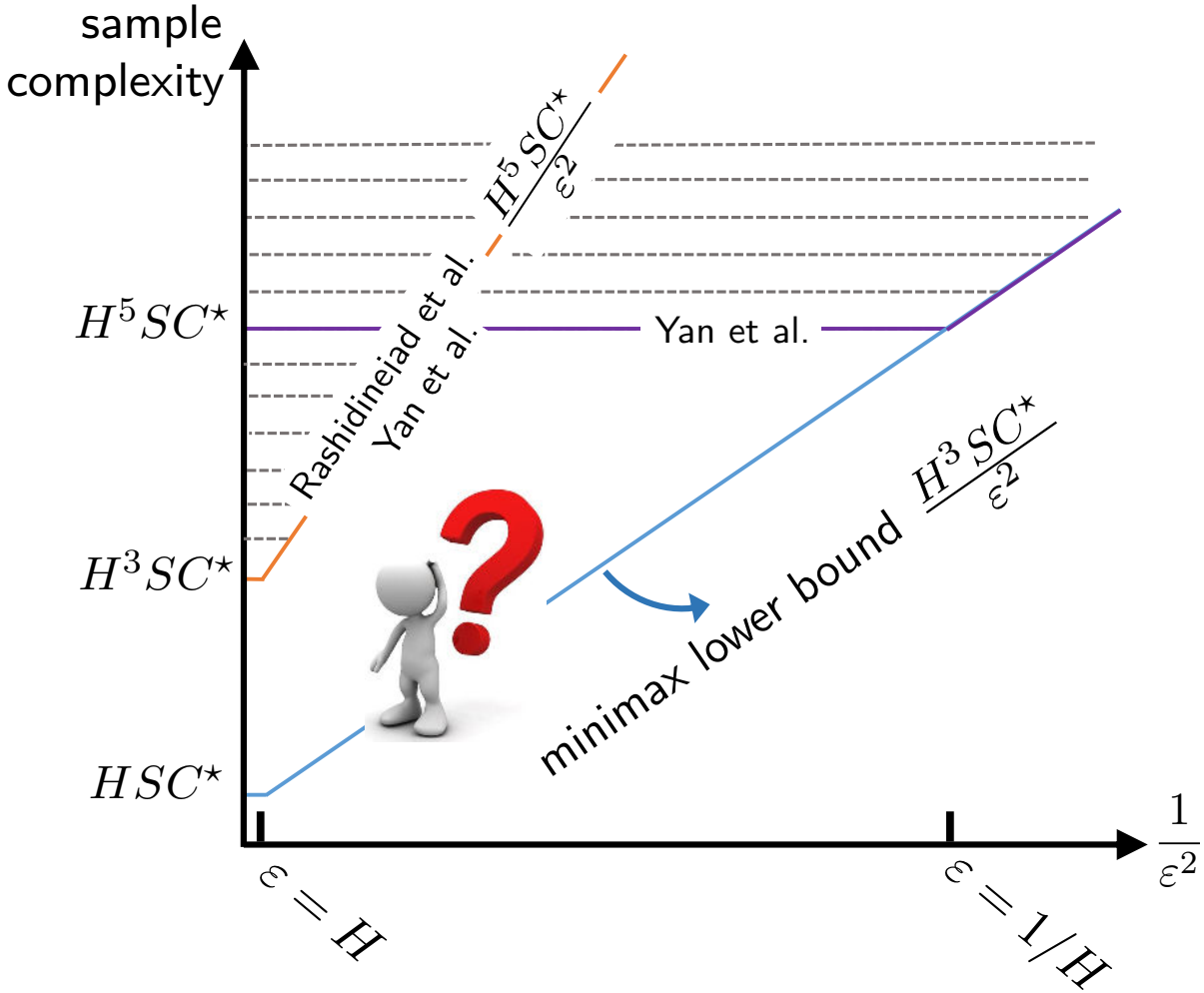
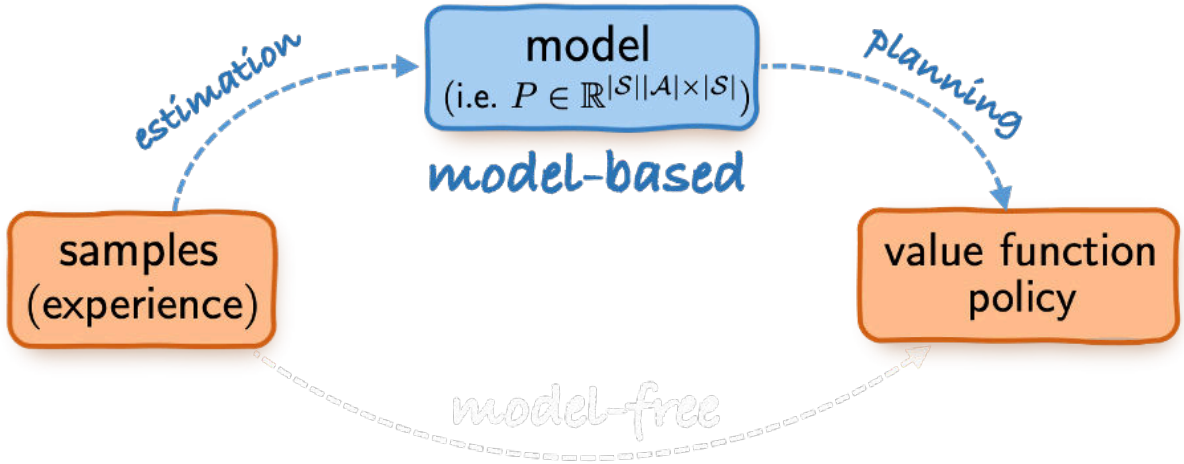


Can we close the gap between upper & lower bounds?

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



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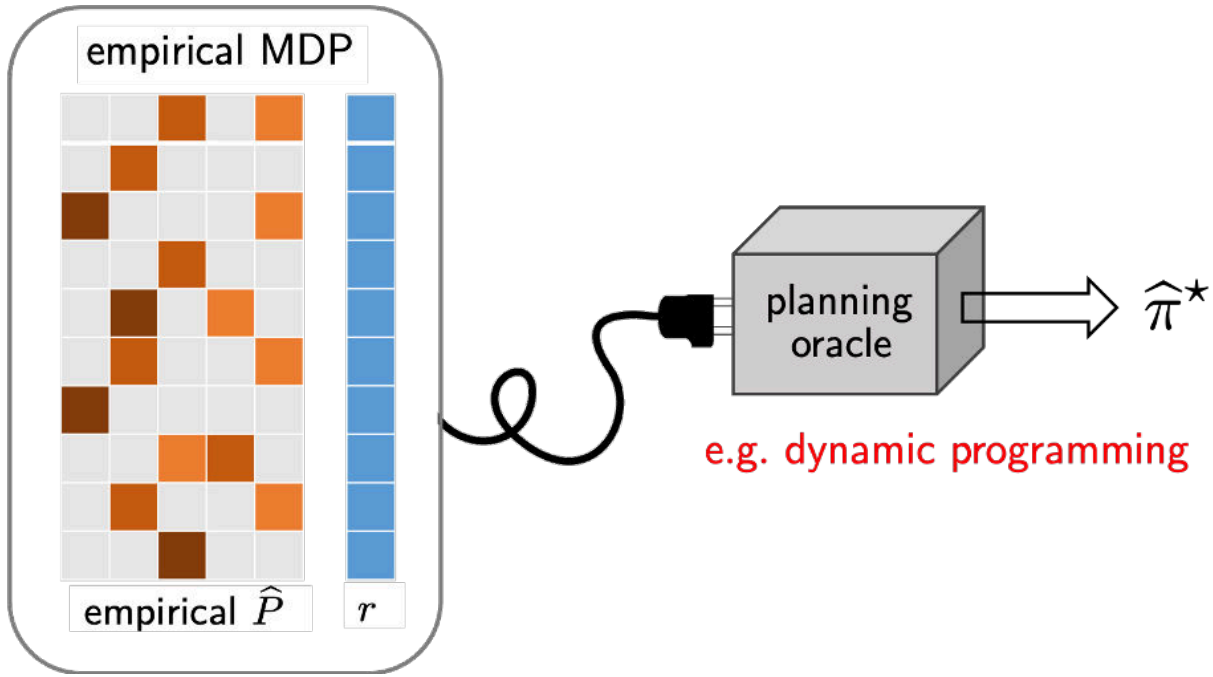
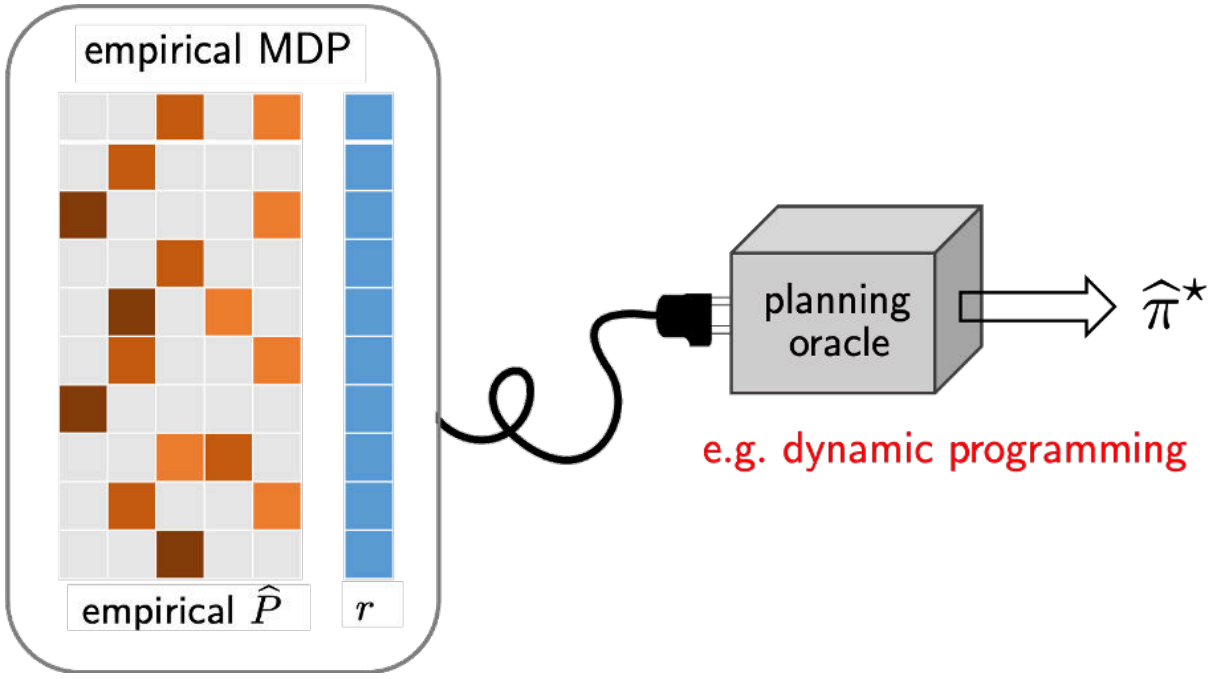


1. construct empirical model $\widehat{P}$:

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

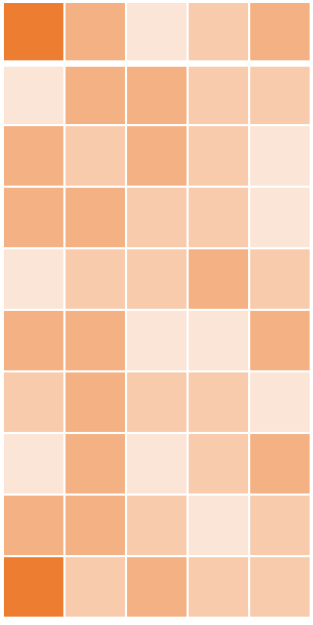
Model-based ("plug-in") approach?



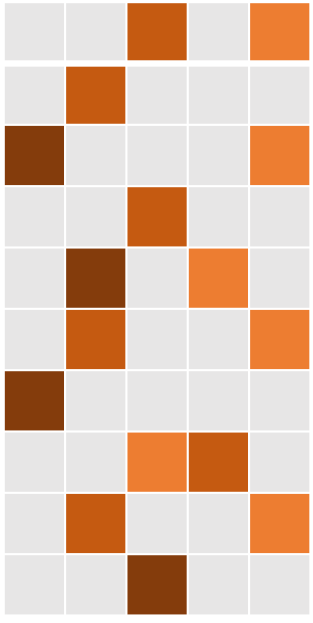
1. construct empirical model $\widehat{P}$

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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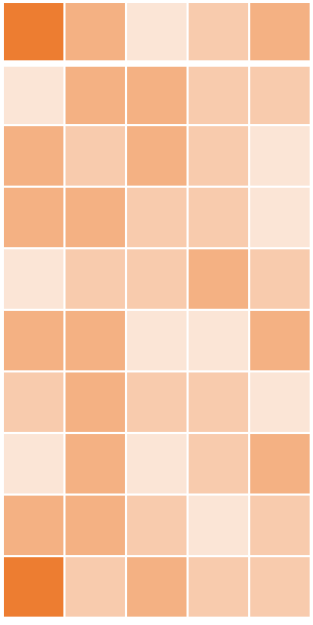

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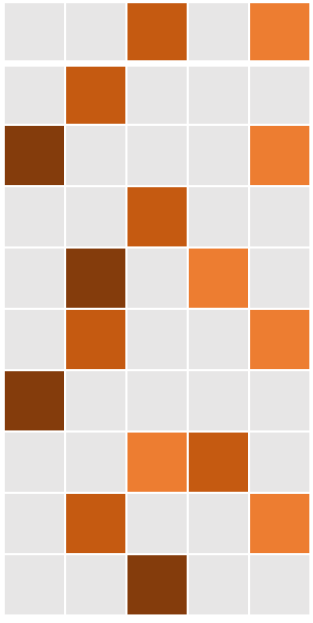

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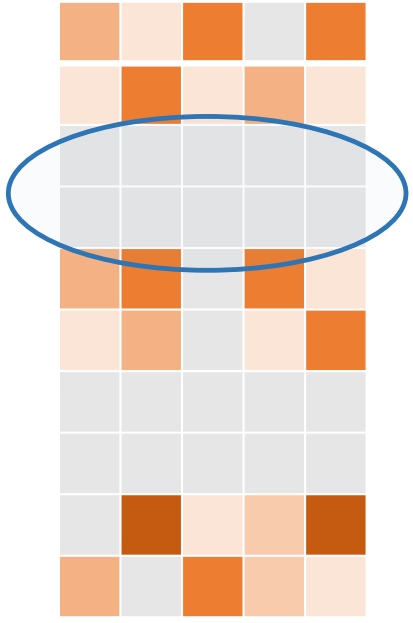

empirical $\widehat{P}$ (offline)

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

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)

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

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 8 (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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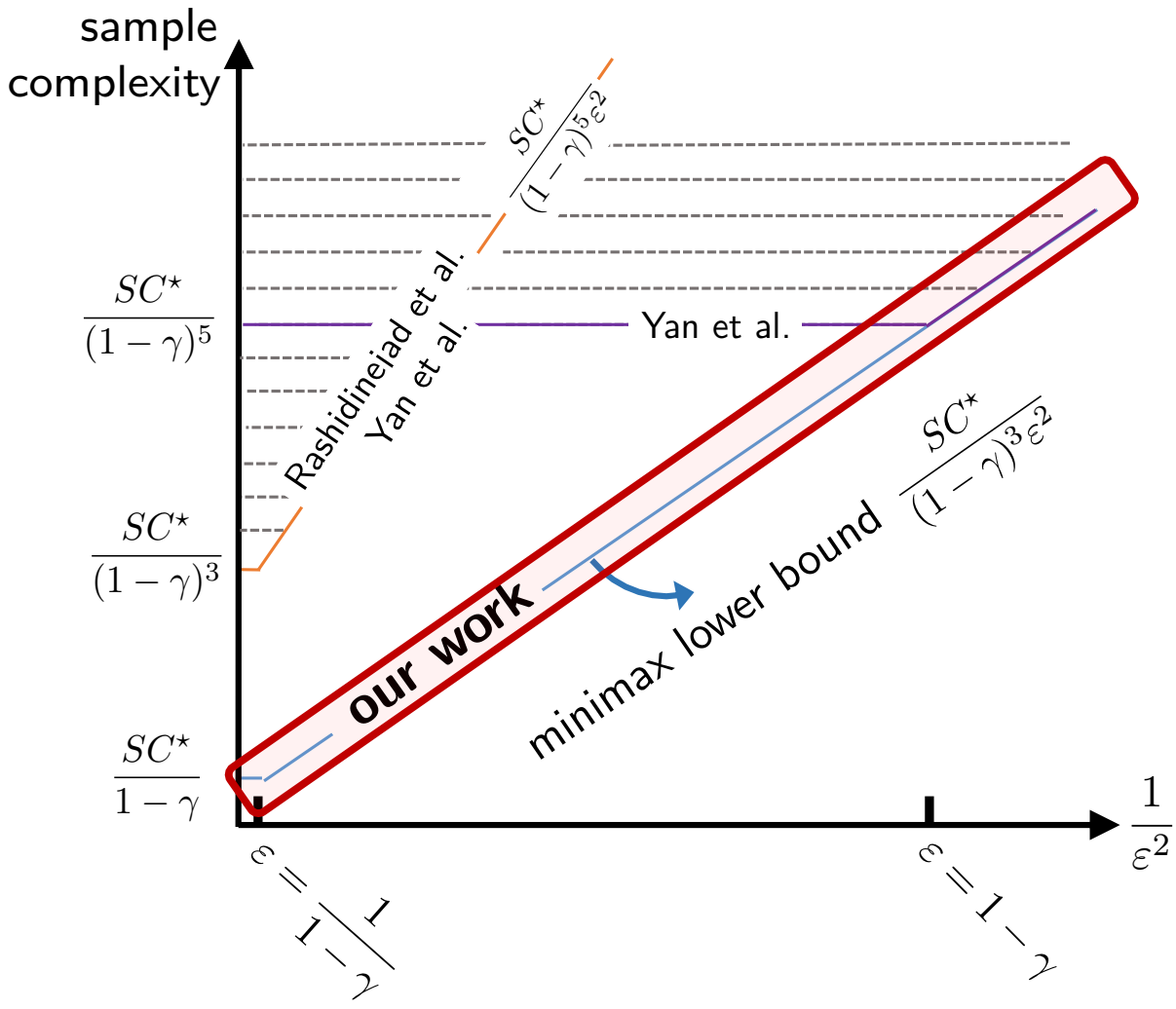
- depends on distribution shift (as reflected by $C^{\star}$)
- achieves minimax optimality
- full ε-range (no burn-in cost)



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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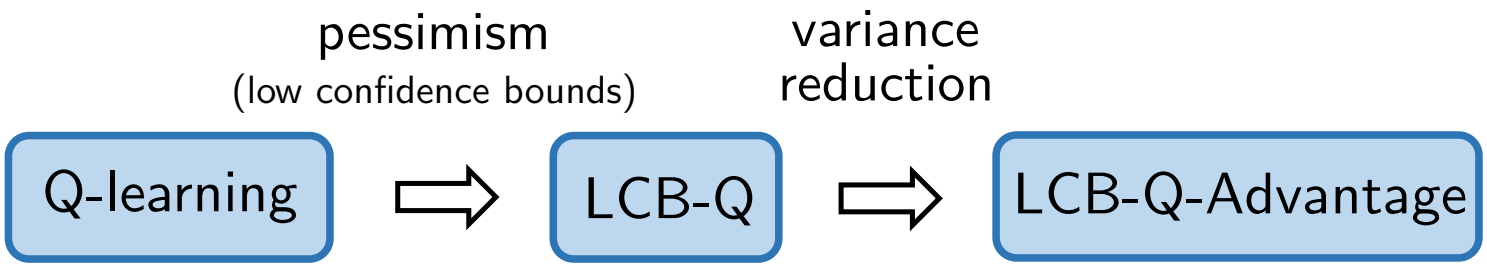

LCB-Q: Q-learning with LCB penalty

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

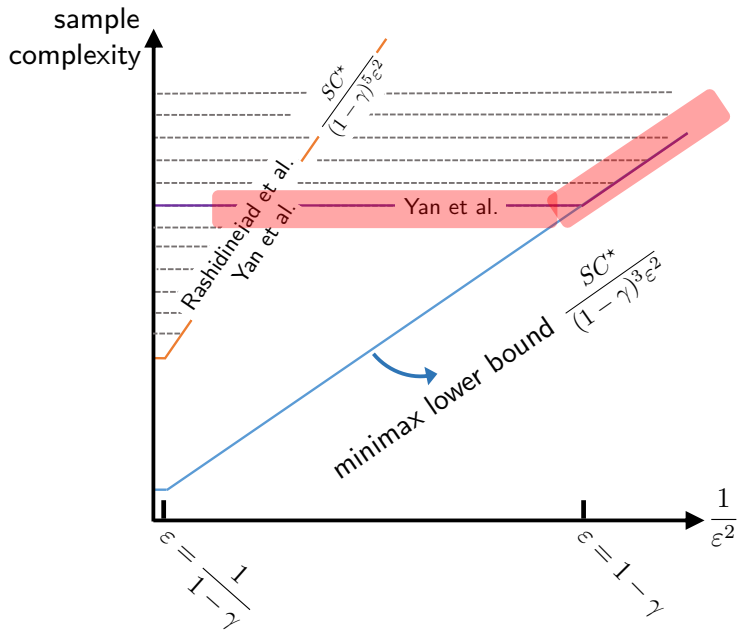
Issue: *large variability in stochastic update rules*

Further improvement

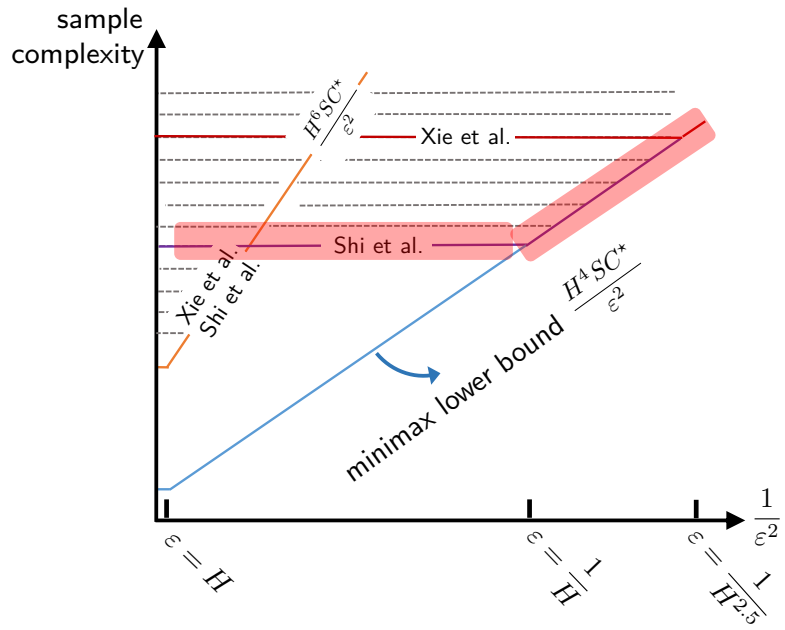
pessimism
(low confidence bounds)

variance
reduction

Q-learning ⇨ LCB-Q ⇨ LCB-Q-Advantage



infinite-horizon MDPs



finite-horizon MDPs

Model-free offline RL attains sample optimality too!

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

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
- "*On the sample complexity of reinforcement learning*," S. Kakade, 2003
- "*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
- "*Randomized linear programming solves the Markov decision problem in nearly linear (sometimes sublinear) time*," *Mathematics of Operations Research*, 2020
- "*Near-optimal time and sample complexities for solving Markov decision processes with a generative model*," A. Sidford, M. Wang, X. Wu, L. Yang, Y. Ye, *NeurIPS*, 2018

Reference: model-based algorithms II

- "*Variance reduced value iteration and faster algorithms for solving Markov decision processes*," A. Sidford, M. Wang, X. Wu, Y. Ye, *SODA*, 2018
- "*Model-based reinforcement learning with a generative model is minimax optimal*," A. Agarwal, S. Kakade, L. Yang, *COLT*, 2020
- "*Instance-dependent ℓ_∞-bounds for policy evaluation in tabular reinforcement learning*," A. Pananjady, M. J. Wainwright, *IEEE Trans. on Information Theory*, 2020
- "*Spectral methods for data science: A statistical perspective*," Y. Chen, Y. Chi, J. Fan, C. Ma, *Foundations and TrendsÂ® in Machine Learning*, 2021
- "*Breaking the sample size barrier in model-based reinforcement learning with a generative model,*" G. Li, Y. Wei, Y. Chi, Y. Chen, *Operations Research*, 2024

Reference: model-free algorithms I

- "*A stochastic approximation method,*" H. Robbins, S. Monro, *Annals of Mathematical Statistics*, 1951
- "*Robust stochastic approximation approach to stochastic programming,*" A. Nemirovski, A. Juditsky, G. Lan, A. Shapiro, *SIAM Journal on optimization*, 2009
- "*Q-learning,*" C. Watkins, P. Dayan, *Machine Learning*, 1992
- "*Learning rates for Q-learning,*" E. Even-Dar, Y. Mansour, *Journal of Machine Learning Research*, 2003
- "*Stochastic approximation with cone-contractive operators: Sharp ℓ_∞ bounds for Q-learning,*" M. Wainwright, 2019
- "*Is Q-learning minimax optimal? a tight sample complexity analysis*," G. Li, C. Cai, Y. Chen, Y. Wei, Y. Chi, *Operations Research*, 2024
- "*Accelerating stochastic gradient descent using predictive variance reduction*," R. Johnson, T. Zhang, *NeurIPS*, 2013
- "*Variance-reduced Q-learning is minimax optimal*," M. Wainwright, 2019

Reference: model-free algorithms II

- "*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

Reference: online RL I

- "*Asymptotically efficient adaptive allocation rules*," T. L. Lai, H. Robbins, *Advances in applied mathematics*, vol. 6, no. 1, 1985
- "*Finite-time analysis of the multiarmed bandit problem*," P. Auer, N. Cesa-Bianchi, P. Fischer, *Machine learning*, vol. 47, pp. 235-256, 2002
- "*Minimax regret bounds for reinforcement learning*," M. G. Azar, I. Osband, R. Munos, *ICML*, 2017
- "*Is Q-learning provably efficient?*" C. Jin, Z. Allen-Zhu, S. Bubeck, and M. Jordan, *NeurIPS*, 2018
- "*Provably efficient Q-learning with low switching cost*," Y. Bai, T. Xie, N. Jiang, Y. X. Wang, *NeurIPS*, 2019
- "*Episodic reinforcement learning in finite MDPs: Minimax lower bounds revisited*" O. D. Domingues, P. Menard, E. Kaufmann, M. Valko, *Algorithmic Learning Theory*, 2021
- "*Almost optimal model-free reinforcement learning via reference-advantage decomposition,*" Z. Zhang, Y. Zhou, X. Ji, *NeurIPS*, 2020

Reference: online RL II

- "*Is reinforcement learning more difficult than bandits? a near-optimal algorithm escaping the curse of horizon,*" Z. Zhang, X. Ji, and S. Du, *COLT*, 2021
- "*Breaking the sample complexity barrier to regret-optimal model-free reinforcement learning,*" G. Li, L. Shi, Y. Chen, Y. Gu, Y. Chi, *NeurIPS*, 2021
- "*Regret-optimal model-free reinforcement learning for discounted MDPs with short burn-in time,*" X. Ji, G. Li, *NeurIPS*, 2023
- "*Reward-free exploration for reinforcement learning*," C. Jin, A. Krishnamurthy, M. Simchowitz, T. Yu, *ICML*, 2020
- "*Minimax-optimal reward-agnostic exploration in reinforcement learning*," G. Li, Y. Yan, Y. Chen, J. Fan, *COLT*, 2024
- "*Settling the sample complexity of online reinforcement learning,*" Z. Zhang, Y. Chen, J. D. Lee, S. S. Du, *COLT*, 2024

Reference: offline RL I

- "*Bridging offline reinforcement learning and imitation learning: A tale of pessimism,*" P. Rashidinejad, B. Zhu, C. Ma, J. Jiao, S. Russell, *NeurIPS*, 2021
- "*Is pessimism provably efficient for offline RL?*" Y. Jin, Z. Yang, Z. Wang, *ICML*, 2021
- "*Settling the sample complexity of model-based offline reinforcement learning,*" G. Li, L. Shi, Y. Chen, Y. Chi, Y. Wei, *Annals of Statistics*, vol. 52, no. 1, pp. 233-260, 2024
- "*Pessimistic Q-learning for offline reinforcement learning: Towards optimal sample complexity*," L. Shi, G. Li, Y. Wei, Y. Chen, Y. Chi, *ICML*, 2022
- "*The efficacy of pessimism in asynchronous Q-learning*," Y. Yan, G. Li, Y. Chen, J. Fan, *IEEE Transactions on Information Theory*, 2023
- "*Policy finetuning: Bridging sample-efficient offline and online reinforcement learning*" T. Xie, N. Jiang, H. Wang, C. Xiong, Y. Bai, *NeurIPS*, 2021

Recent Advances of Statistical Reinforcement Learning

Part 2

Gergely Neu (Universitat Pompeu Fabra)
Sattar Vakili (MediaTek Research)

Tutorial, UAI 2024

Part 2

1. Introduction to structural complexity
2. Linear Function Approximation
3. Non-linear Function Approximation

Tabular Setting

Recall results for the tabular setting:

- Q-learning with UCB: [Jin et al., 2018]

$$\text{Regret}(T) = \mathcal{O}(\sqrt{H^3SAT})$$

- Sample complexity:

$$\tilde{\mathcal{O}}(\frac{\text{poly}(H)SA}{\epsilon^2})$$

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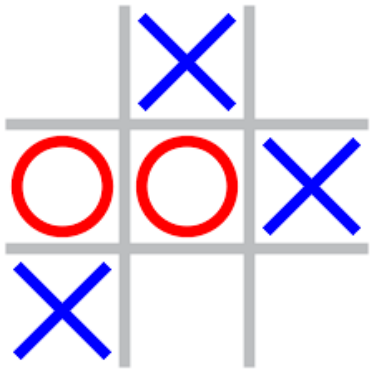
These are only meaningful if $T \ll S$ or $\epsilon \gg 1/\sqrt{S}$!

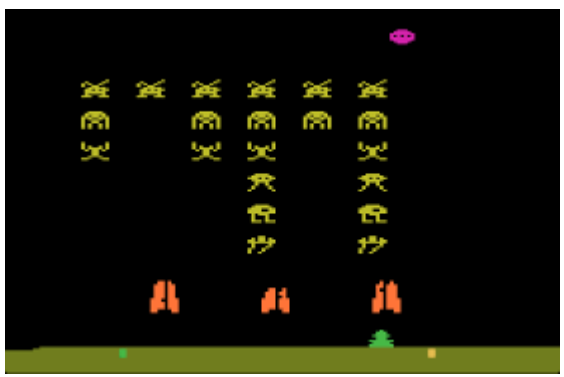
Why "Tabular"?



- Small size of state-action space
- $Q(s, a)$ can be represented as a table

Why Function Approximation?

Number of states S is enormous in real-world problems!



- Game of Go: 10^{170} states
- Atari: 10^{100} states
- Physical systems: continuum of states

Why Function Approximation?

Two types of challenges:

- Computational: Q and π cannot even be stored in memory, and Bellman equations are intractable to solve even if P and r were known
- Statistical: Most states are not visited even once! How could we expect to learn about P or r like that?

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- Statistical: Most states are not visited even once! How could we expect to learn about P or r like that?

We need to find a way to **generalize** knowledge from visited states to unvisited states by leveraging **structure**

RL with Function Approximation

- Approximate value function $Q(s, a)$ (or policy) in a class $\mathcal{F}$.
- Hope that $\mathcal{F}$ captures the MDP structure appropriately and leverage the information in structure of $\mathcal{F}$ to learn faster if possible.
- Typical function classes: Linear, Kernel-based, NN-based

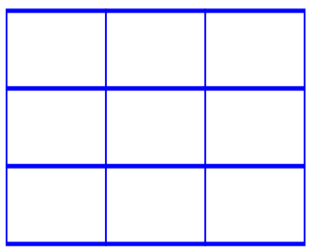
$$\text{Tabular} \rightarrow \text{Linear} \rightarrow \text{Nonlinear}$$

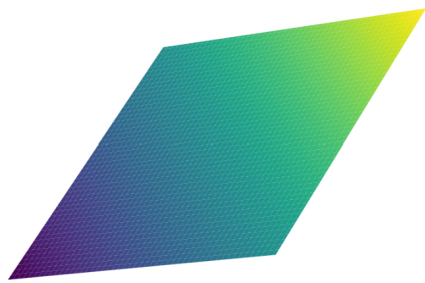
Setting

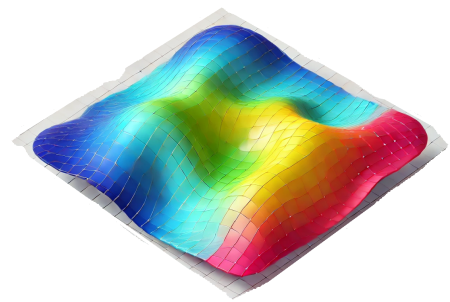
- Generative oracle, Offline, Online
- Episodic, Infinite horizon (discounted)
- Model-based, Model-free

In this part we focus on:

$$\text{Tabular} \rightarrow \text{Linear} \rightarrow \text{Nonlinear}$$







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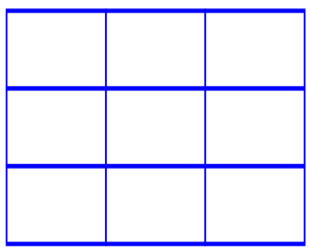
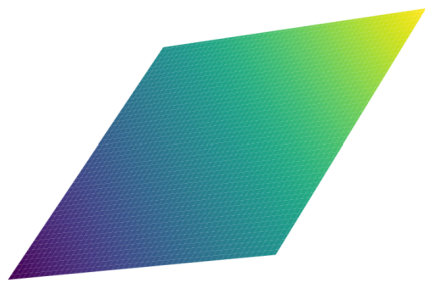
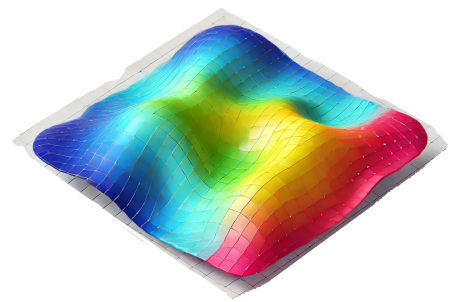
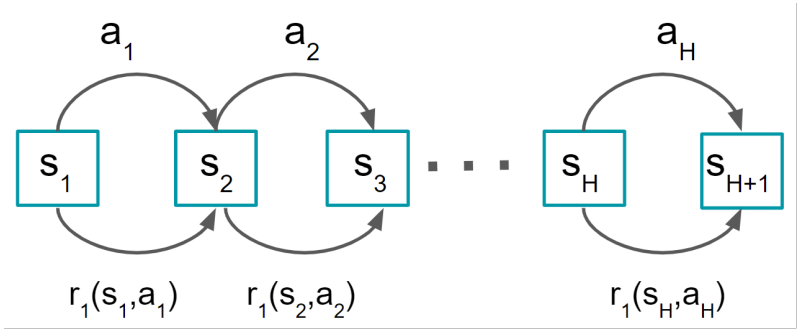






Setting

For a clear and sharp presentation we focus on episodic MDPs

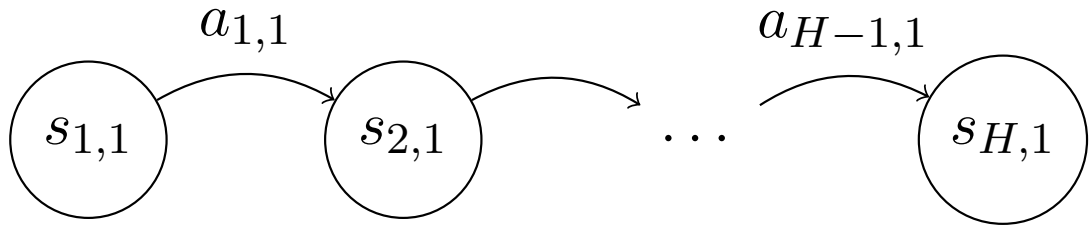


For simplicity, we assume r is known and deterministic

We focus on the structural complexity of $P(s'|s,a)$

Episodic MDP

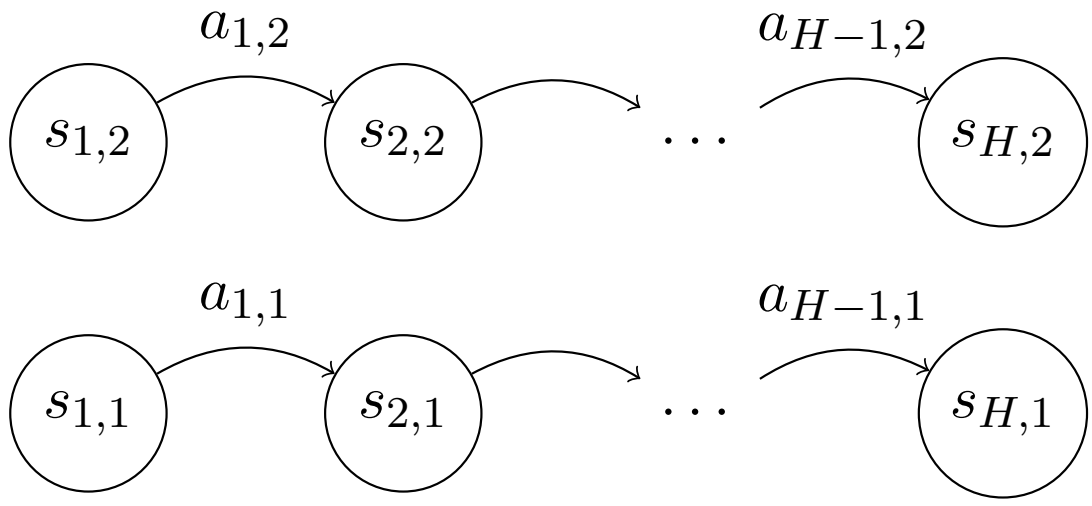
Episode 1:



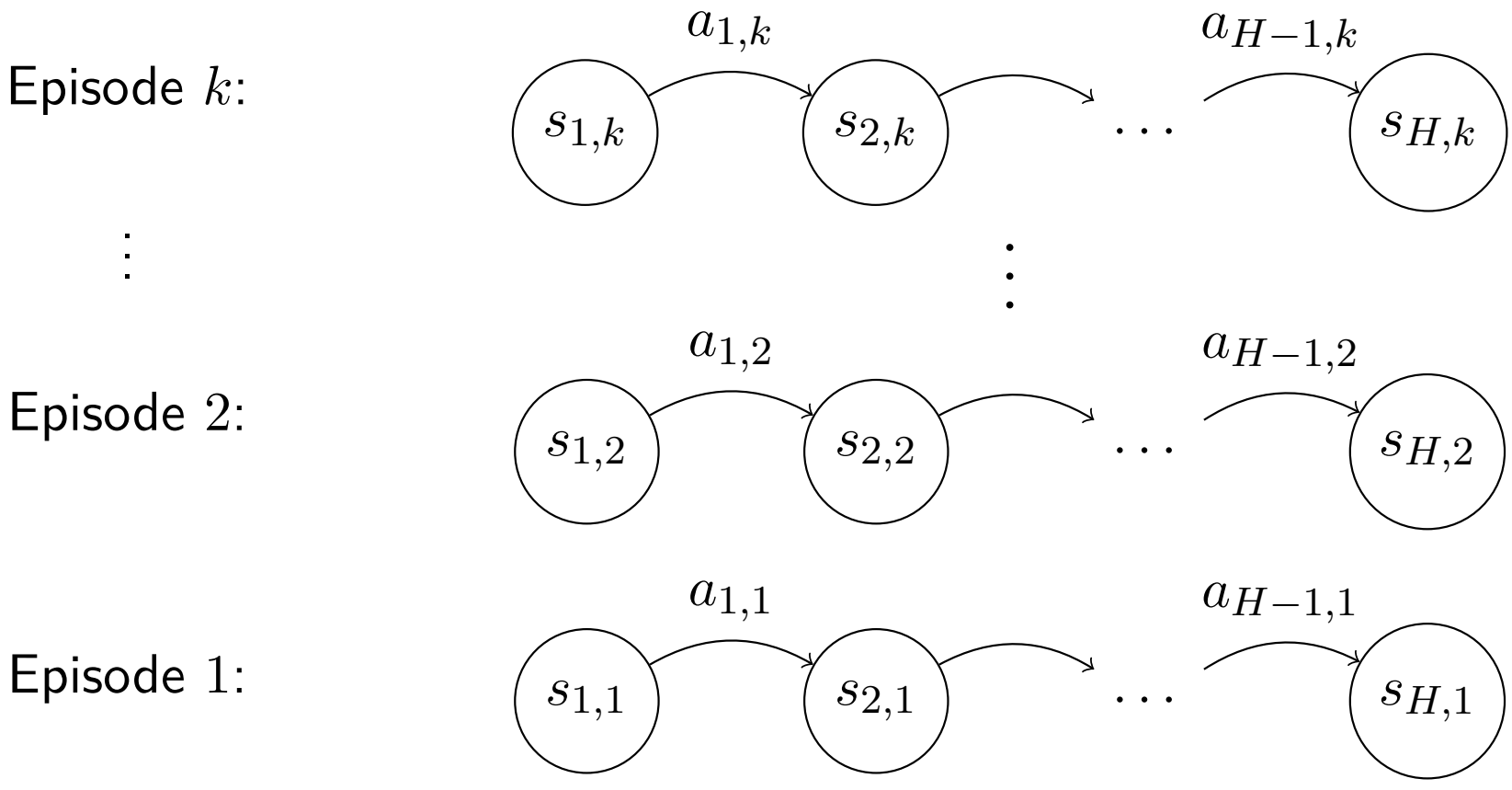
Episodic MDP

Episode 2:

Episode 1:



Episodic MDP



Part 2

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Linear Function Approximation

IDEA: approximate the Q-functions as linear functions of a given d-dimensional feature map $\boldsymbol{\phi} : \mathcal{S} \times \mathcal{A} \to \mathbb{R}^d$.

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Let $\Phi \in \mathbb{R}^{(\mathcal{S}\times\mathcal{A})\times d}$ be the "matrix" of stacked feature vectors $[\boldsymbol{\phi}(s_1, a_1) \dots \boldsymbol{\phi}(s_N, a_N)]^\top$ (where $N = |\mathcal{S} \times \mathcal{A}|$).

We need to find a parameter vector $\boldsymbol{\theta}^\star$ such that $Q^\star \approx \Phi\boldsymbol{\theta}^\star$.
(Meaning that $Q^\star(s, a) \approx \langle \boldsymbol{\theta}^\star, \boldsymbol{\phi}(s, a)\rangle$.)

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(Meaning that $Q^\star(s, a) \approx \langle \boldsymbol{\theta}^\star, \boldsymbol{\phi}(s, a)\rangle$.)

QUESTION: When can we learn $\boldsymbol{\theta}^\star$ efficiently?

Linear Function Approximation

Various conditions on the feature map Φ have been studied:

- Linear $Q^\star$: there exists a $\boldsymbol{\theta}^\star$ such that $Q^\star = \Phi\boldsymbol{\theta}^\star$.
- Linear Q^π: for every policy π, there exists a $\boldsymbol{\theta}^\pi$ such that $Q^\pi = \Phi\boldsymbol{\theta}^\pi$.
- Closure under Bellman operator: for any $Q_{\boldsymbol{\theta}} = \Phi\boldsymbol{\theta}$, $\mathcal{T}Q_{\boldsymbol{\theta}} \in \operatorname{span}(\Phi)$.
- Linear MDP: The transition and reward functions are linear in the features. This implies all of the above conditions.

A number of more refined conditions have been also studied, such as assuming linearity of $V^\star$ in some feature map, or other types of factorized transition models. We refer to Du et al. [2021], Jin et al. [2021] for more details on such extensions.

What can we hope for?

WANT: find an ϵ-optimal policy with a computational and sample complexity polynomial in d, $1/\epsilon$ and H, independently of S and A.

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- Situation is similar when only assuming closure under Bellman operator / Bellman completeness [Zanette et al., 2020b, Du et al., 2021].
- Linear MDP condition enables both statistical and computational efficiency!!! [Jin et al., 2023]

Linear MDPs

Linear transition function:

$$P_h(\cdot|s,a) = \langle \boldsymbol{\phi}(s,a), \boldsymbol{\mu}_h(\cdot) \rangle,$$

where $\boldsymbol{\mu}_h(\cdot) = [\mu_h^1(\cdot), \cdots, \mu_h^d(\cdot)]$ is a d-dimensional signed measure.

Linear rewards: $r_h(s,a) = \langle \boldsymbol{\phi}(s,a), \boldsymbol{\vartheta}_h \rangle$.

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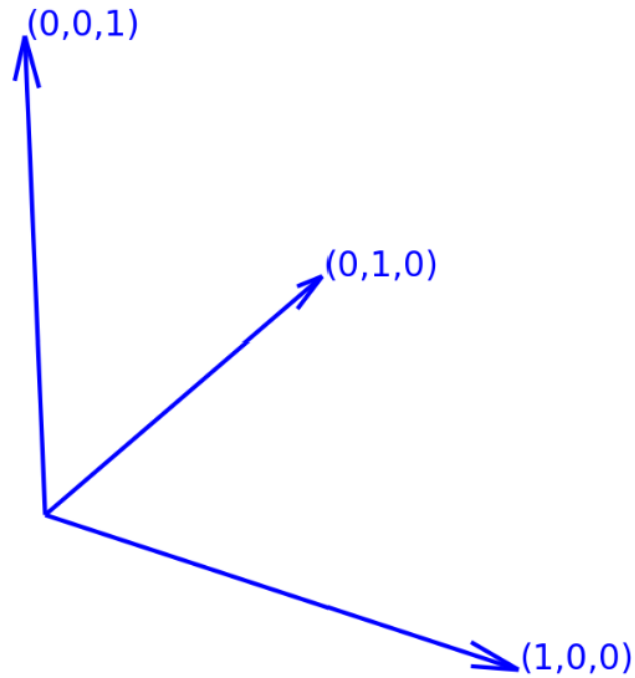
In matrix notation:

- Transition operator $P_h \in \mathbb{R}^{(\mathcal{S}\times\mathcal{A})\times\mathcal{S}}$ can be written as $P_h = \Phi M_h$ for some "matrix" $M_h \in \mathbb{R}^{\mathcal{S}\times d}$.
- Reward function can be written as $r_h = \Phi \boldsymbol{\vartheta}_h$ for some $\boldsymbol{\vartheta}_h \in \mathbb{R}^d$.

Tabular MDPs are linear

Tabular setting is a special case with dimension $d = SA$:

- Let $\boldsymbol{\phi}(s, a) = \boldsymbol{e}_{(s,a)}$ be the canonical basis in $\mathbb{R}^d$
- $P_h(\cdot|s, a) = \boldsymbol{e}_{s,a}^\top \boldsymbol{\mu}_h(\cdot)$



A magical property of linear MDPs

In a linear MDP, the Q-functions of all policies are linear in Φ:

$$\begin{aligned} Q_h^\pi &= r_h + P_h V_{h+1}^\pi = \Phi \vartheta_h + \Phi M_h V_{h+1}^\pi \\ &= \Phi \left(\vartheta_h + M_h V_{h+1}^\pi \right) = \Phi \boldsymbol{\theta}_h, \end{aligned}$$

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This implies linear $Q^\star$-realizability, linear Q^π-realizability, Bellman compleness, and many more useful properties for analysis! E.g., note that for any function $u \in \mathbb{R}^{\mathcal{S}}$, $P_h u = \Phi M_h u$ is linear in Φ.

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The structure of linear MDPs allows us to import tools from linear bandit literature [Abbasi-Yadkori et al., 2011, Lattimore and Szepesvári, 2020].

Optimistic approximate dynamic programming

IDEA: Combine the techniques for tabular MDPs with exploration bonuses borrowed from the linear bandit literature!

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UCB-VI [Azar et al., 2017]:

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

$$Q_h = r_h + \underbrace{\widehat{P}_h}_{\text{model estimate}} V_{h+1} + \underbrace{b_h}_{\text{exploration bonus}}$$

   and set $V_h(s) = \max_a Q_h(s,a)$ for all s, a.

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

$$\pi_h(s) = \arg\max_a Q_h(s,a).$$

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But how do we define $\widehat{P}_h$ and b_h?

Least Squares Value Iteration (LSVI)

Transition model $\widehat{P_h}$ can be defined implicitly via least-squares:

- Solve the regularized linear regression problem

$$\widehat{\boldsymbol{w}}_{h,k} = \arg\min_{\boldsymbol{w}} \sum_{t=1}^{k} (V_{h+1,k}(s_{h+1,t}) - \langle \boldsymbol{\phi}(s_{h,t}, a_{h,t}), \boldsymbol{w} \rangle)^2 + \lambda^2 \|\boldsymbol{w}\|^2$$

- That provides a prediction

$$\widehat{[P_h V_{h+1,k}]}(s,a) = \langle \boldsymbol{\phi}(s,a), \widehat{\boldsymbol{w}}_{h,k} \rangle$$

- Also, an uncertainty quantification (variance)

$$\sigma^2_{h,k}(s,a) = \|\boldsymbol{\phi}(s,a)\|^2_{(\lambda I + \Sigma_{h,k})^{-1}}$$

$$\Sigma_{h,k} = \sum_{t=1}^{k} \boldsymbol{\phi}^\top(s_{h,t}, a_{h,t}) \boldsymbol{\phi}(s_{h,t}, a_{h,t})$$

LSVI-UCB

The prediction and variance give us an upper confidence bound on $Q^\star$:

$$Q_{h,k}(s,a) = r_h(s,a) + \widehat{[P_h V_{h+1}]}(s,a) + \beta(\delta)\sigma_{h,k}(s,a)$$

This is then used to compute an UCB on $V^\star$ as

$$V_{h,k}(s) = \max_a Q_{h,k}(s,a)$$

Performance guarantees

Theorem [Jin et al., 2023] The regret of LSVI-UCB satisfies $\text{Regret}(K) = \tilde{\mathcal{O}}(H^2\sqrt{d^3K})$.

This implies a sample complexity guarantee of $\tilde{\mathcal{O}}(\frac{\text{poly}(H)d^3}{\epsilon^2})$.

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Proof ideas:

- Prove confidence bounds

$$|[\widehat{P_h V_{h+1,k}}](s,a) - [P_h V_{h+1,k}](s,a)| \leq \beta(\delta)\sigma_{h,k}(s,a).$$

- Using standard techniques (e.g., Azar et al., 2017), show

$$\text{Regret}(K) \lesssim \textstyle\sum_{h,k} \beta(\delta)\sigma_{h,k}(s_{h,k}, a_{h,k}).$$

- Use elliptical potential lemma (e.g., Abbasi-Yadkori et al., 2011) to show

$$\textstyle\sum_{h,k} \sigma_{h,k}(s_{h,k}, a_{h,k}) \lesssim H\sqrt{Kd\log(K)}.$$

Proving the confidence bounds

By standard results on least-squares estimators (e.g., Abbasi-Yadkori et al., 2011), one can prove the following confidence bound for any fixed $u \in \mathbb{R}^{\mathcal{S}}$ that holds with probability at least $1 - \delta$:

$$\left|\widehat{[P_h u]}(s,a) - [P_h u](s,a)\right| \leq \overline{\beta}(\delta)\sigma_{h,k}(s,a)$$

for some

$$\overline{\beta}(\delta) \approx \lambda^{\frac{1}{2}}\|M_h u\| + H\sqrt{d\log(\tfrac{K}{\delta})}$$

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Challenge: $u = V_{h+1,k}$ is not fixed, but depends on all past data!

Solution: Covering number argument

Covering Number Argument

- Notice that all value functions $V_{h,k}$ belong to the function class

$$\mathcal{V} = \left\{V(s) = \min\{H,\ \max_a \boldsymbol{\phi}^\top(s,a)\widehat{\boldsymbol{w}} + \beta\|\boldsymbol{\phi}(s,a)\|_{(\lambda I+\Sigma)^{-1}}\}\right\}.$$

- **Idea:** cover the space of functions $\mathcal{V}$ such that we can rewrite

$$\left|\widehat{[P_h V_{h+1,k}]}(s,a) - [P_h V_{h+1,k}](s,a)\right| \leq \epsilon + \sup_{u\in\mathcal{V}}\left|\widehat{[P_h u]}(s,a) - [P_h u](s,a)\right|.$$

- How many functions u are required to cover $\mathcal{V}$ up to ϵ error?

$$\mathcal{N}_\epsilon = \tilde{\mathcal{O}}(d^2)$$

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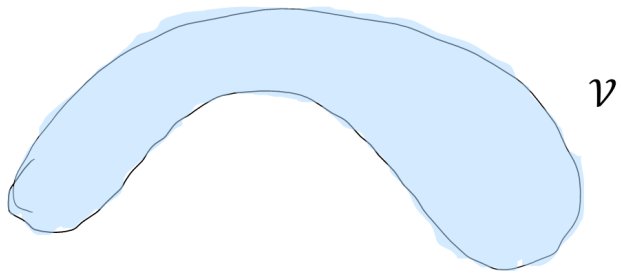

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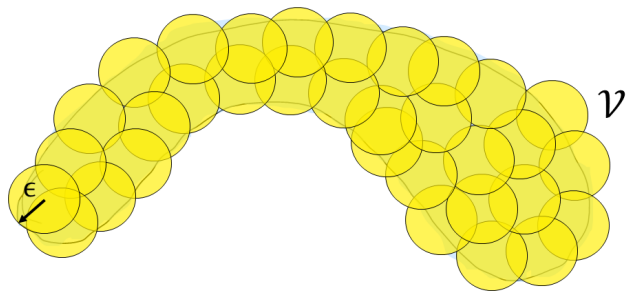


Covering Number Argument

- We can now use a union-bound argument to show that

$$\sup_{u \in \mathcal{V}} \left| \widehat{[P_h u]}(s,a) - [P_h u](s,a) \right| \leq \epsilon + \overline{\beta}(\delta/\mathcal{N}_\epsilon)\sigma_{h,k}(s,a)$$

holds with probability at least $1-\delta$.

- Choosing $\epsilon \approx 1/T$, we get

$$\beta(\delta) = \overline{\beta}(\delta/\mathcal{N}_\epsilon) \approx \lambda^{\frac{1}{2}}\|MV_{h,k}\| + H\sqrt{d\log(\tfrac{K\mathcal{N}_\epsilon}{\delta})} = \tilde{\mathcal{O}}(Hd)$$

Alternative linear models

Linear MDP model factorizes $P = \Phi M$ with some known $\Phi \in \mathbb{R}^{(\mathcal{S}\times\mathcal{A})\times d}$ and some unknown $M \in \mathbb{R}^{d\times\mathcal{S}}$.

Some alternative factorizations are:

- Linear mixture MDPs [Zhou et al., 2021]: $P = \Phi\boldsymbol{\theta}$ with some known $\Phi \in \mathbb{R}^{(\mathcal{S}\times\mathcal{A}\times\mathcal{S})\times d}$ and unknown $\boldsymbol{\theta} \in \mathbb{R}^d$. Analysis is simpler but the model doesn't allow simple and explicit Q-function approximation and leads to impractical algorithms.
- "MatrixRL" [Yang and Wang, 2020]: $P = \Phi M \Psi$ with some known $\Phi \in \mathbb{R}^{(\mathcal{S}\times\mathcal{A})\times m}$, another known $\Psi \in \mathbb{R}^{n\times\mathcal{S}}$, and an unknown $M \in \mathbb{R}^{m\times n}$. Can be shown to be a special case of linear mixture MDPs, and suffers from the same limitations.
- Low-rank MDPs [Modi et al., 2024]: Same as linear MDPs except both Φ and M are unknown and belong to finite model class. Requires much more sophisticated techniques, but algorithms are kind of tractable.

Some References

- Linear MDPs: Jin et al. [2020, 2023], Yang and Wang [2019, 2020], Neu and Pike-Burke [2020]
- Linear Bellman complete models: Zanette et al. [2020a]
- Linear mixture MDPs: Yang and Wang [2020], Ayoub et al. [2020], Zhou et al. [2021], Moulin and Neu [2023]
- Other model classes with hidden finite-dimensional linear structure: Du et al. [2021], Jin et al. [2021]

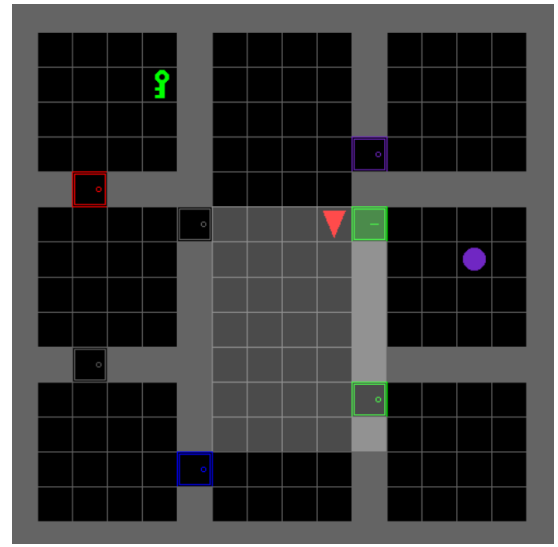
Part 2

1. Introduction to structural complexity
2. Linear Function Approximation
3. Non-linear Function Approximation

Limitations of the Linear Setting

Directly reachable states:

- $\mathcal{S}_{s,a} := \{s' \in \mathcal{S} : P(s'|s,a) > 0\}$
- $U := \max_{(s,a)\in\mathcal{S}\times\mathcal{A}} |\mathcal{S}_{s,a}|$



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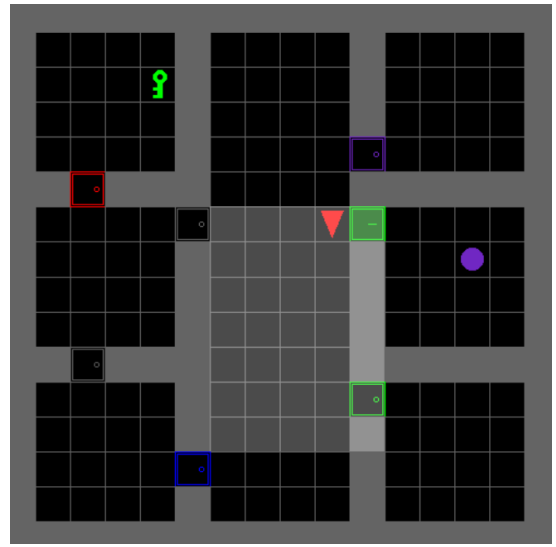
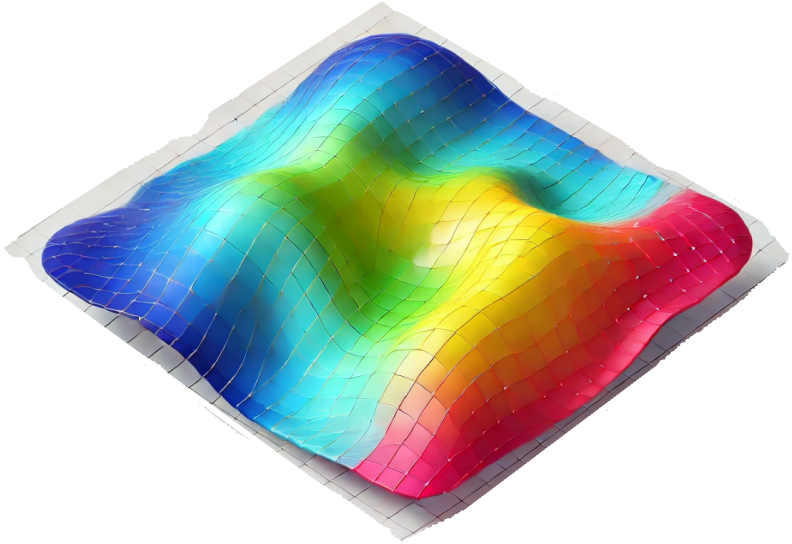


Theorem Lee and Oh [2024] For an MDP with a finite state space, the feature dimension d is lower bounded by

$$d \geq \lfloor \frac{|\mathcal{S}|}{U} \rfloor$$

Limitations of the Linear Setting

High dimensional problems



Nonlinear problems

Kernel-Based Setting

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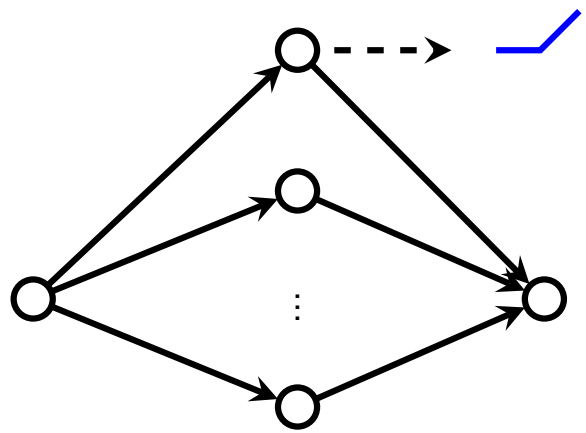
Tabular $\rightarrow$ Linear $\rightarrow$ Kernel-Based $\rightarrow$ NN-Based



Kernel-Based Setting

Function class:

$$\mathcal{F} = \left\{ f : \mathbb{R}^d \to \mathbb{R},\ f(\cdot) = \sum_{m=1}^{\infty} w_m \phi_m(\cdot) \right\}$$

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An extension of linear models to infinite dimensions in the feature space ϕ

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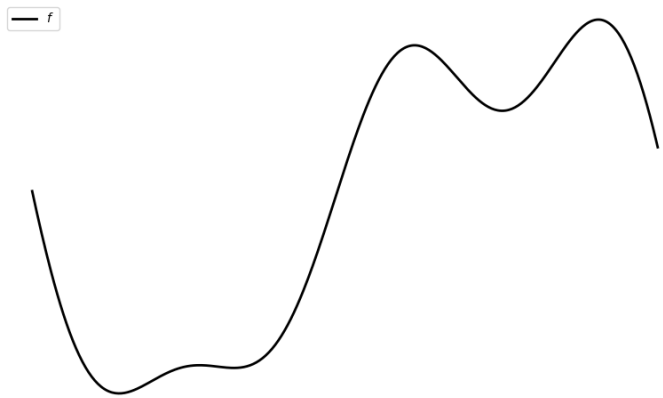
An extension of linear models to infinite dimensions in the feature space ϕ

Nonlinear functions in $\mathbb{R}^d$



Mercer Theorem

A positive definite kernel $\kappa : \mathcal{Z} \times \mathcal{Z} \to \mathbb{R}$

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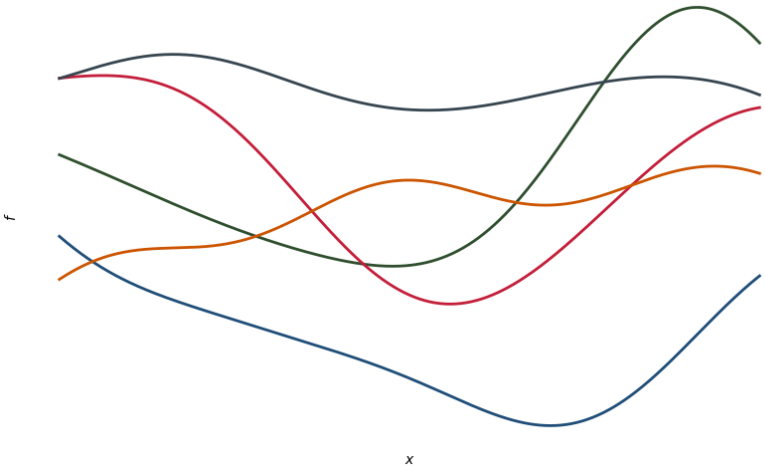
A positive definite kernel $\kappa : \mathcal{Z} \times \mathcal{Z} \to \mathbb{R}$

Theorem Any positive definite kernel can be written as

$$\kappa(z, z') = \sum_{m=1}^{\infty} \lambda_m \varphi_m(z) \varphi_m(z')$$

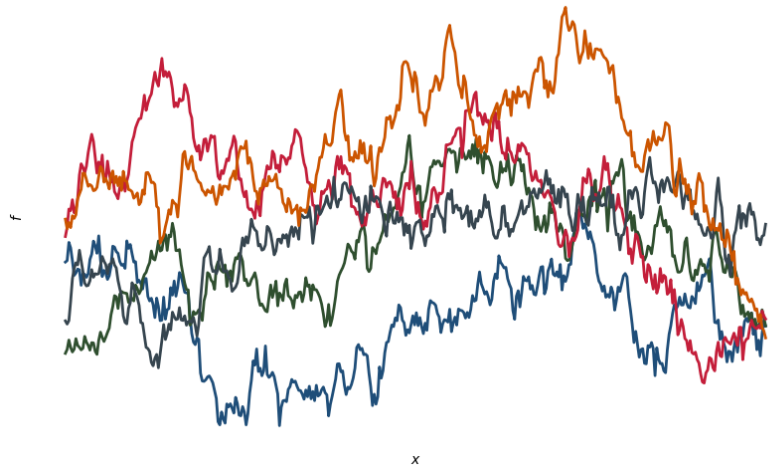
- The feature map $\phi_m(\cdot) = \lambda_m^{\frac{1}{2}} \varphi_m(\cdot)$ corresponding to κ
- λ_m are referred to as eigenvalues
- φ_m are referred to as eigenfunctions

Kernels



Squared Exponential kernel

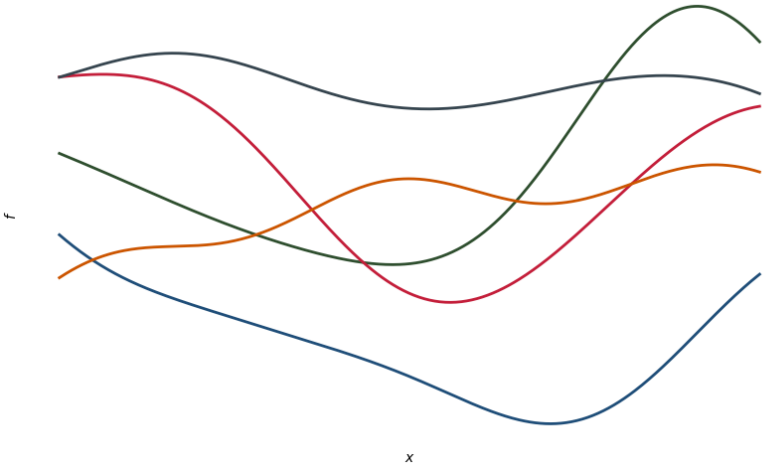
$$\kappa(z, z') = \exp\left(-\frac{\|z-z'\|^2}{2\ell^2}\right)$$

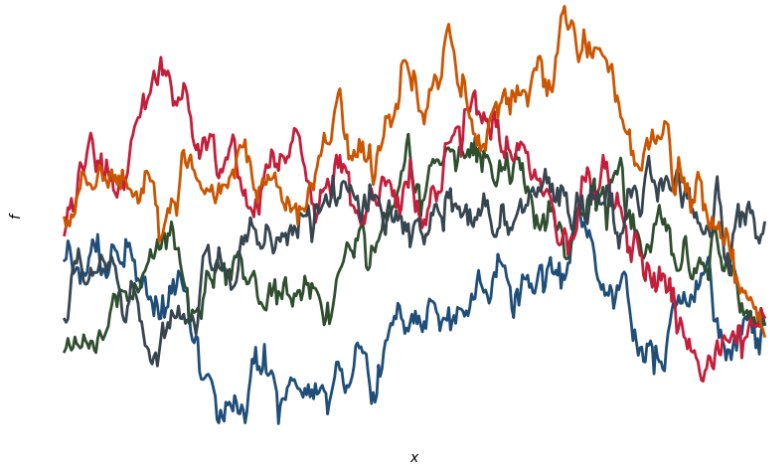


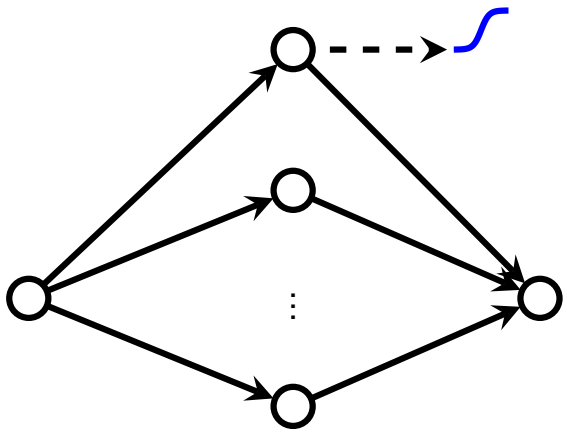
Matérn-ν kernel

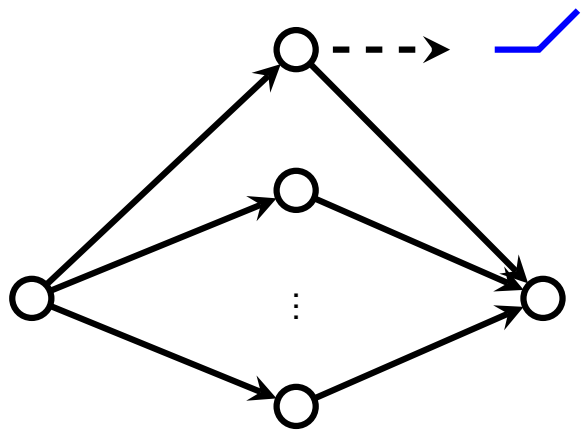
$$\kappa(z, z') = \frac{2^{1-\nu}}{\Gamma(\nu)}\left(\frac{\sqrt{2\nu}}{\ell}\|z - z'\|\right)^{\nu} K_\nu\left(\frac{\sqrt{2\nu}}{l}\|z - z'\|\right)$$

Kernels









Reproducing Kernel Hilbert Space

RKHS:

$$\mathcal{H}_\kappa = \{f(\cdot) = \sum_{m=1}^{\infty} w_m \phi_m(\cdot)\}$$

- Inner product $\langle f, g \rangle_k = \boldsymbol{w}_f^\top \boldsymbol{w}_g$
- $\|f\|_{\mathcal{H}_\kappa} = \|\mathbf{w}\|$
- $\phi_m = \sqrt{\lambda_m}\varphi_m$ form an orthonormal basis

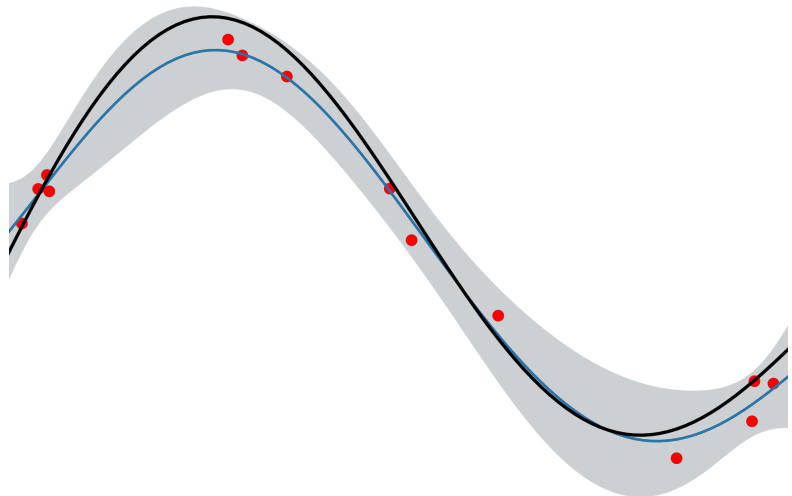
Kernel Based Regression

Provided a dataset of t observation:

$$\left\{(z_j, Y(z_j))\right\}_{j=1}^{t}, \; Y(z_j) = f(z_j) + \varepsilon_j$$

Regularized Least Squares Error:

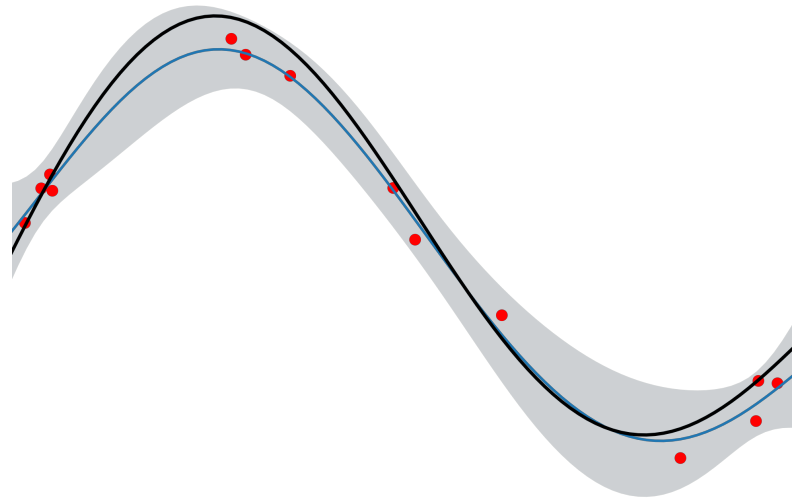
$$\hat{f} = \; \arg\min_{g \in \mathcal{H}_\kappa} \sum_{j=1}^{t} (Y(z_j) - g(z_j)) + \lambda \|g\|^2_{\mathcal{H}_\kappa}$$



Kernel-Based Regression

Predictor:

$$\hat{f}(z) = \boldsymbol{\kappa}_t^\top(z)(\mathbf{K}_t + \lambda I)^{-1}\mathbf{y}_t$$

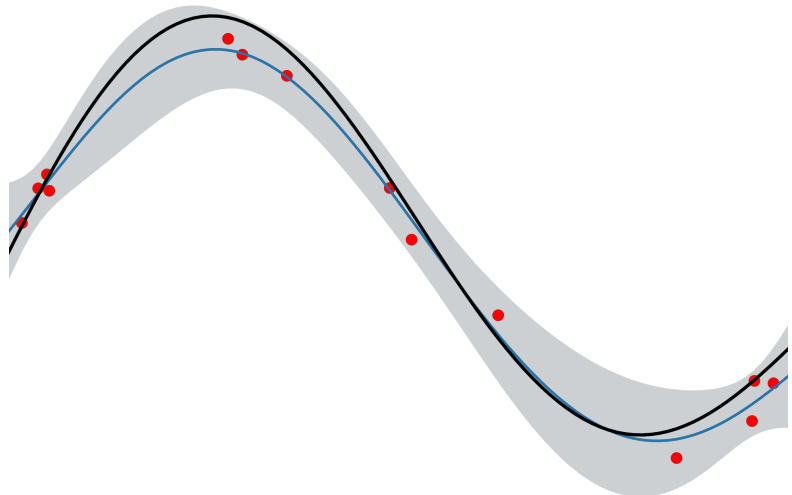


- $\boldsymbol{\kappa}_t(z) = [k(z_1, z), k(z_2, z), \cdots, k(z_t, z)]$
- $\mathbf{K}_t = [k(z_i, z_j)]_{i,j=1}^t$
- $\mathbf{y}_t = [Y(z_1), Y(z_2), \cdots, Y(z_t)]$

Kernel-Based Regression

Uncertainty estimator:

$$(\sigma_t(z))^2 = \kappa(z,z) - \boldsymbol{\kappa}_t^\top(z)(\mathbf{K}_t + \lambda I)^{-1}\boldsymbol{\kappa}_t(z)$$



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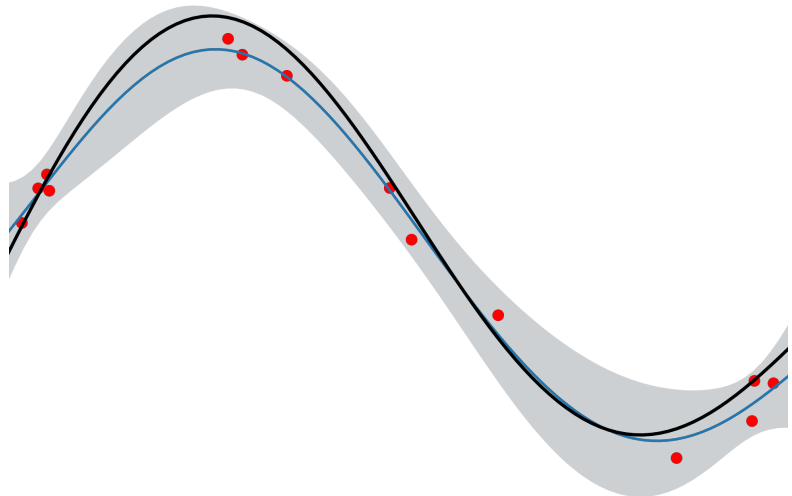

Closed from expressions for prediction and uncertainty quantification!

RL with kernel-based function approximation

IDEA: Approximate the Q-functions as a function in RKHS

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Want: Find an ϵ-optimal policy with a computational and sample complexity polynomial in $1/\epsilon$ and H

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$$\text{Sample complexity: } \tilde{\mathcal{O}}\left((\tfrac{1}{\epsilon})^2\right)$$

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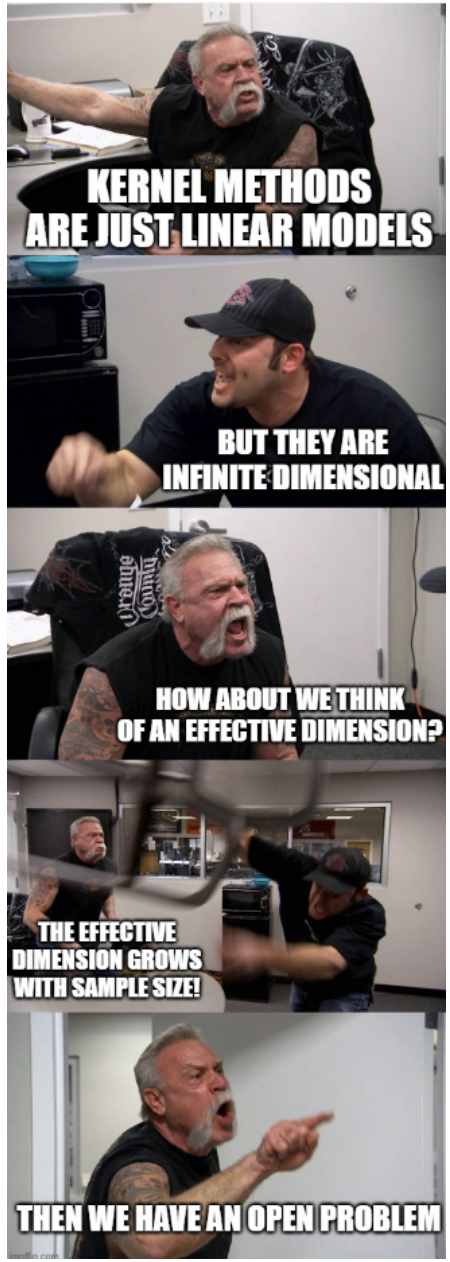

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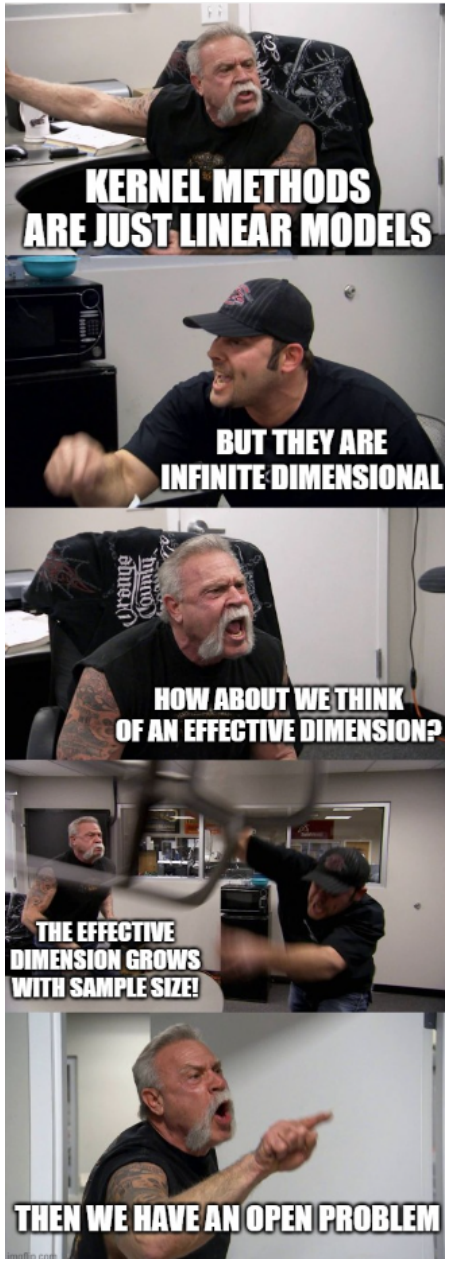

Effective Dimension:

$$\Big[\underbrace{\phi_1, \phi_2, \cdots, \phi_{\mathfrak{D}}}_{\mathfrak{D}\text{dimension}}, \ \phi_{\mathfrak{D}+1}, \cdots \Big]$$

$$\mathfrak{D} \approx \tfrac{1}{2} \log\det(I + \tfrac{1}{\lambda}\mathbf{K}_t)$$

- In the linear setting: $\mathfrak{D} \approx d$
- For Squared Exponential kernel: $\mathfrak{D} \approx \text{poly}\log(T)$
- For Matérn kernel: $\mathfrak{D} \approx T^{\frac{d}{d+\nu}}$ [Vakili et al., 2021]

RL with Kernel-based FA

Kernel-based transition assumption

For all s': $P(s'|s,a) \in \mathcal{H}_\kappa$

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$$\text{For all } s' \text{: } P(s'|s,a) \in \mathcal{H}_\kappa$$

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For integrable $V : \mathcal{S} \to \mathbb{R}$, $[PV] = \int_{s'} P(s'|s,a)V(s') \in \mathcal{H}_k$

Optimistic approximate DP goes kernelized

IDEA: Combine the techniques for tabular MDPs with exploration bonuses borrowed from the ~~linear~~ kernel bandit literature!

UCB-VI [Azar et al., 2017]:

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

$$Q_h = r_h + \underbrace{\widehat{P}_h}_{\text{model estimate}} V_{h+1} + \underbrace{b_h}_{\text{exploration bonus}}$$

   and set $V_h(s) = \max_a Q_h(s,a)$ for all s, a.

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

$$\pi_h(s) = \arg\max_a Q_h(s,a).$$

But how do we define $\widehat{P}_h$ and b_h?

Kernel-based optimistic value iteration (KOVI)

Transition model $\widehat{P_h}$ can be defined implicitly via least-squares:

- Solve the regularized linear regression problem

$$\hat{f}_h = \arg\min_{f \in \mathcal{H}_\kappa} \sum_{t=1}^{k} (V_{h+1}(s_{h+1,t}) - f(s_{h,t}, a_{h,t})^2 + \lambda \|f\|^2_{\mathcal{H}_\kappa}$$

- That provides a prediction

$$[\widehat{P_h V_{h+1,k}}](s,a) = \widehat{f}_h(s,a) = \boldsymbol{\kappa}_{h,k}^\top(s,a)(\mathbf{K}_{h,k} + \lambda I)^{-1}\mathbf{v}_{h,k}$$
$$\mathbf{v}_{h,k} = [V_{h+1}(s_{h+1,1}), V_{h+1}(s_{h+1,2}), \cdots, V_{h+1}(s_{h+1,k})]$$

- Also, an uncertainty quantification (variance)

$$\sigma^2_{h,k}(s,a) = \kappa\big((s,a),(s,a)\big) - \boldsymbol{\kappa}_{h,k}^\top(s,a)(\mathbf{K}_{h,k} + \lambda I)^{-1}\boldsymbol{\kappa}_{h,k}(s,a)$$

Kernel-based optimistic value iteration (KOVI)

The prediction and variance give us an upper confidence bound on $Q^\star$:

$$Q_{h,k}(s,a) = r_h(s,a) + \widehat{[P_h V_{h+1}]}(s,a) + \beta(\delta)\sigma_{h,k}(s,a)$$

This is then used to compute an UCB on $V^\star$ as

$$V_{h,k}(s) = \max_a Q_{h,k}(s,a)$$

Performance guarantees

Theorem [Yang et al., 2020] The regret of KOVI satisfies $\text{Regret}(K) = \tilde{\mathcal{O}}(H^2\sqrt{(\mathfrak{D}^2 + \mathfrak{D}\log\mathcal{N}_\epsilon)K})$.

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Proof ideas:

- Prove confidence bounds

$$|\widehat{[P_h V_{h+1,k}]}(s,a) - [P_h V_{h+1,k}](s,a)| \le \beta(\delta)\sigma_{h,k}(s,a).$$

- Using standard techniques, show

$$\text{Regret}(K) \lesssim \textstyle\sum_{h,k} \beta(\delta)\sigma_{h,k}(s_{h,k}, a_{h,k}).$$

- Kernelized elliptical potential lemma (e.g., Srinivas et al., 2010)

$$\textstyle\sum_{h,k} \sigma_{h,k}(s_{h,k}, a_{h,k}) \lesssim H\sqrt{K\mathfrak{D}\log(K)}.$$

Kernel-based Setting - Analysis

- We need a confidence bound of the form

$$\left|\hat{f}(s,a) - [P_h V_{h+1,k}](s,a)\right| \leq \beta(\delta)\sigma_h(s,a).$$

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Solution: Self-normalized concentration inequalities for vector-valued martingales extended to kernel setting [Abbasi-Yadkori, 2013, Whitehouse et al., 2023]:

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Solution: Covering number argument

Covering Number Argument

- Notice that all value functions $V_{h,k}$ belong to the function class

$$\mathcal{V} = \left\{ V(s) = \min\{H,\ \max_a \hat{f}(s,a) + \beta\sigma(s,a)\} \right\}$$

- How many functions V are required to cover $\mathcal{V}$ up to ϵ error?

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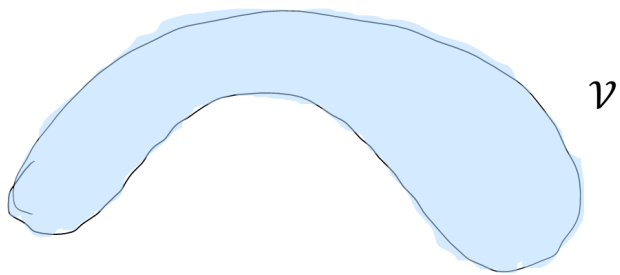

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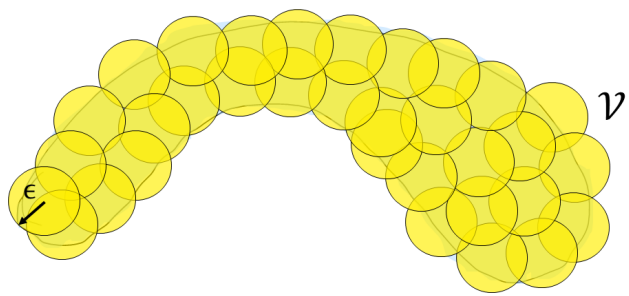

Covering Number Argument

- We can now use a union-bound argument

$$\beta(\delta) = \overline{\beta}(\delta/\mathcal{N}_\epsilon) \approx \|f\|_{\mathcal{H}_k} + \frac{H}{\sqrt{\lambda}}\sqrt{\mathfrak{D} + \log \mathcal{N}_\epsilon + \frac{1}{\delta}}$$

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- Regret ($\epsilon \approx \frac{1}{K}$) [Yang et al., 2020]

$$\text{Regret}(K) = \tilde{\mathcal{O}}(H^2\sqrt{\mathfrak{D}^2 K + \mathfrak{D}\log \mathcal{N}_\epsilon K})$$

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- Sample Complexity
  - Very smooth kernels $\mathfrak{D}$ and $\log(\mathcal{N}_\epsilon) \approx \text{poly}\log(K)$

$$\tilde{\mathcal{O}}\left(\frac{1}{\epsilon^2}\right)$$

  - In general could be vacuous!

Optimistic Closure

Chowdhury and Oliveira [2023] Optimistic Closure Assumption:

$$\mathcal{V} \in \mathcal{H}_{\kappa'}$$

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Idea: Leverage kernel mean embedding

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Doen not hold in the linear setting!

Open Problem Vakili [2024]

(a) Can a no-regret learning algorithm be designed?

(b) What is the minimum regret growth rate with K (and also H)? And, can a learning algorithm be designed to achieve order optimal (or near-optimal) regret performance, closely aligning with the established lower bound?

Some References

- Chowdhury and Gopalan [2019]
- Yang et al. [2020]
- Domingues et al. [2021]
- Vakili and Olkhovskaya [2023]
- ...

References I

Y. Abbasi-Yadkori. Online learning for linearly parametrized control problems. *PhD Thesis, University of Alberta*, 2013.

Y. Abbasi-Yadkori, D. Pál, and C. Szepesvári. Improved algorithms for linear stochastic bandits. *Advances in Neural Information Processing Systems*, 24, 2011.

A. Ayoub, Z. Jia, C. Szepesvari, M. Wang, and L. Yang. Model-based reinforcement learning with value-targeted regression. In *International Conference on Machine Learning*, pages 463–474. PMLR, 2020.

M. G. Azar, I. Osband, and R. Munos. Minimax regret bounds for reinforcement learning. In *International conference on machine learning*, pages 263–272. PMLR, 2017.

S. R. Chowdhury and A. Gopalan. Online learning in kernelized Markov decision processes. In *The 22nd International Conference on Artificial Intelligence and Statistics*, pages 3197–3205. PMLR, 2019.

S. R. Chowdhury and R. Oliveira. Value function approximations via kernel embeddings for no-regret reinforcement learning. In *Asian Conference on Machine Learning*, pages 249–264. PMLR, 2023.

O. D. Domingues, P. Ménard, M. Pirotta, E. Kaufmann, and M. Valko. Kernel-based reinforcement learning: A finite-time analysis. In *International Conference on Machine Learning*, pages 2783–2792. PMLR, 2021.

References II

S. Du, S. Kakade, J. Lee, S. Lovett, G. Mahajan, W. Sun, and R. Wang. Bilinear classes: A structural framework for provable generalization in RL. In *International Conference on Machine Learning*, pages 2826–2836. PMLR, 2021.

C. Jin, Z. Allen-Zhu, S. Bubeck, and M. I. Jordan. Is Q-learning provably efficient? *Advances in neural information processing systems*, 31, 2018.

C. Jin, Z. Yang, Z. Wang, and M. I. Jordan. Provably efficient reinforcement learning with linear function approximation. In *Conference on Learning Theory*, pages 2137–2143. PMLR, 2020.

C. Jin, Q. Liu, and S. Miryoosefi. Bellman eluder dimension: New rich classes of RL problems, and sample-efficient algorithms. *Advances in neural information processing systems*, 34:13406–13418, 2021.

C. Jin, Z. Yang, Z. Wang, and M. I. Jordan. Provably efficient reinforcement learning with linear function approximation. *Mathematics of Operations Research*, 48(3):1496–1521, 2023.

T. Lattimore and C. Szepesvári. *Bandit algorithms*. Cambridge University Press, 2020.

J. Lee and M.-h. Oh. Demystifying linear mdps and novel dynamics aggregation framework. In *The Twelfth International Conference on Learning Representations*, 2024.

References III

A. Modi, J. Chen, A. Krishnamurthy, N. Jiang, and A. Agarwal. Model-free representation learning and exploration in low-rank mdps. *Journal of Machine Learning Research*, 25 (6):1–76, 2024.

A. Moulin and G. Neu. Optimistic planning by regularized dynamic programming. In *International Conference on Machine Learning*, pages 25337–25357. PMLR, 2023.

G. Neu and C. Pike-Burke. A unifying view of optimism in episodic reinforcement learning. *Advances in Neural Information Processing Systems*, 33:1392–1403, 2020.

N. Srinivas, A. Krause, S. Kakade, and M. Seeger. Gaussian process optimization in the bandit setting: no regret and experimental design. In *Proceedings of the 27th International Conference on International Conference on Machine Learning*, pages 1015–1022, 2010.

S. Vakili. Open problem: Order optimal regret bounds for kernel-based reinforcement learning. In *The Thirty Seventh Annual Conference on Learning Theory*, pages 5340–5344. PMLR, 2024.

S. Vakili and J. Olkhovskaya. Kernelized reinforcement learning with order optimal regret bounds. *Advances in Neural Information Processing Systems*, 36, 2023.

S. Vakili, K. Khezeli, and V. Picheny. On information gain and regret bounds in Gaussian process bandits. In *International Conference on Artificial Intelligence and Statistics*, pages 82–90. PMLR, 2021.

References IV

G. Weisz, P. Amortila, and C. Szepesvári. Exponential lower bounds for planning in mdps with linearly-realizable optimal action-value functions. In *Algorithmic Learning Theory*, pages 1237–1264. PMLR, 2021.

G. Weisz, A. György, T. Kozuno, and C. Szepesvári. Confident approximate policy iteration for efficient local planning in q^π-realizable mdps. *Advances in Neural Information Processing Systems*, 35:25547–25559, 2022.

G. Weisz, A. György, and C. Szepesvári. Online RL in linearly q^π-realizable MDPs is as easy as in linear MDPs if you learn what to ignore. *Advances in Neural Information Processing Systems*, 36, 2023.

J. Whitehouse, A. Ramdas, and S. Z. Wu. On the sublinear regret of gp-ucb. *Advances in Neural Information Processing Systems*, 36, 2023.

L. Yang and M. Wang. Sample-optimal parametric q-learning using linearly additive features. In *International conference on machine learning*, pages 6995–7004. PMLR, 2019.

L. Yang and M. Wang. Reinforcement learning in feature space: Matrix bandit, kernels, and regret bound. In *International Conference on Machine Learning*, pages 10746–10756. PMLR, 2020.

References V

Z. Yang, C. Jin, Z. Wang, M. Wang, and M. Jordan. Provably efficient reinforcement learning with kernel and neural function approximations. *Advances in Neural Information Processing Systems*, 33:13903–13916, 2020.

A. Zanette, D. Brandfonbrener, E. Brunskill, M. Pirotta, and A. Lazaric. Frequentist regret bounds for randomized least-squares value iteration. In *International Conference on Artificial Intelligence and Statistics*, pages 1954–1964. PMLR, 2020a.

A. Zanette, A. Lazaric, M. Kochenderfer, and E. Brunskill. Learning near optimal policies with low inherent Bellman error. In H. D. III and A. Singh, editors, *Proceedings of the 37th International Conference on Machine Learning*, volume 119 of *Proceedings of Machine Learning Research*, pages 10978–10989. PMLR, 13–18 Jul 2020b.

D. Zhou, J. He, and Q. Gu. Provably efficient reinforcement learning for discounted mdps with feature mapping. In *International Conference on Machine Learning*, pages 12793–12802. PMLR, 2021.