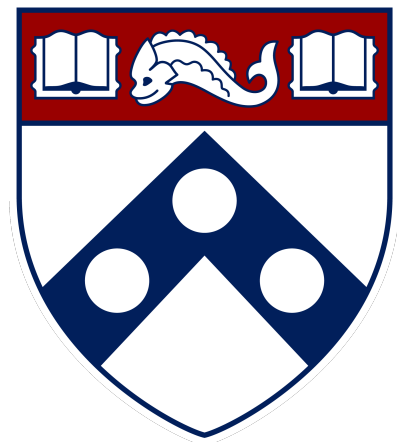
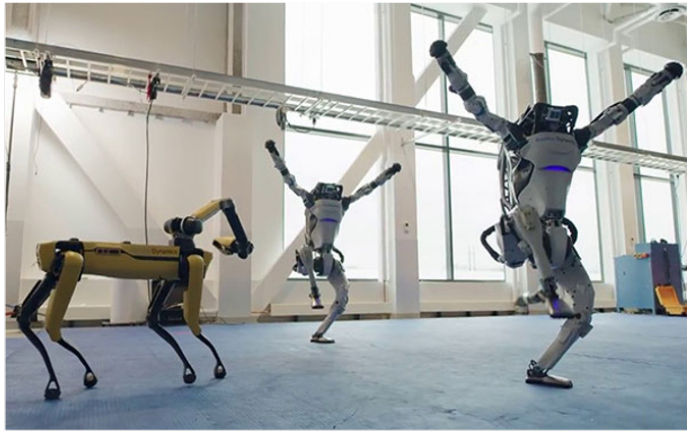
Reinforcement learning (Part 1): Basics and Model-based RL



Yuxin Chen

Wharton Statistics & Data Science, Spring 2022

Successes of reinforcement learning (RL)



Supervised learning

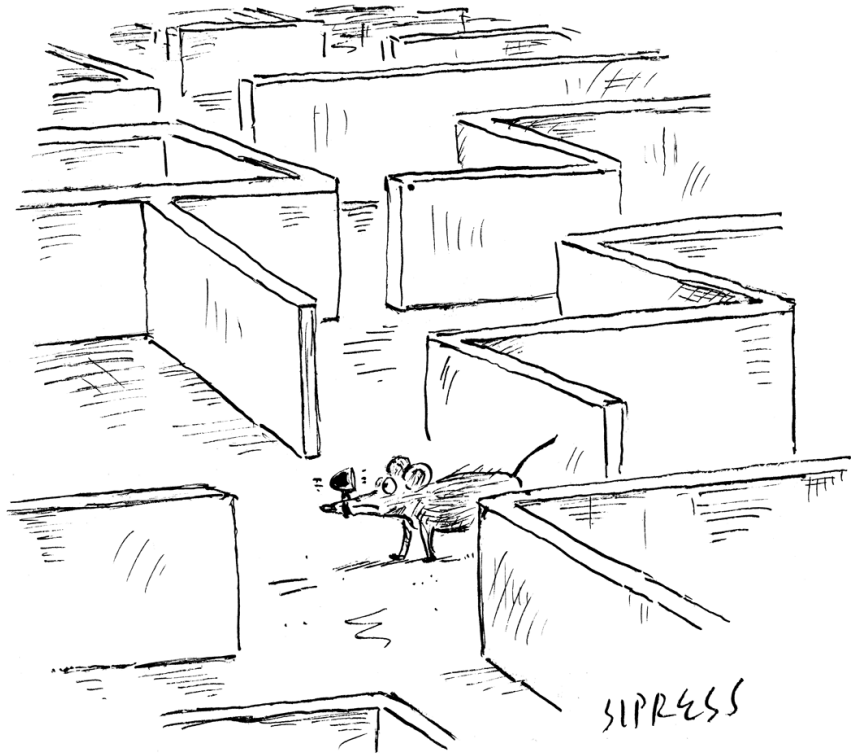
Given i.i.d. training data, the goal is to make prediction on unseen data:

— *pic from internet*

Reinforcement learning (RL)

In RL, an agent learns by interacting with an environment

- no training data
- maximize total rewards
- trial-and-error
- sequential and online

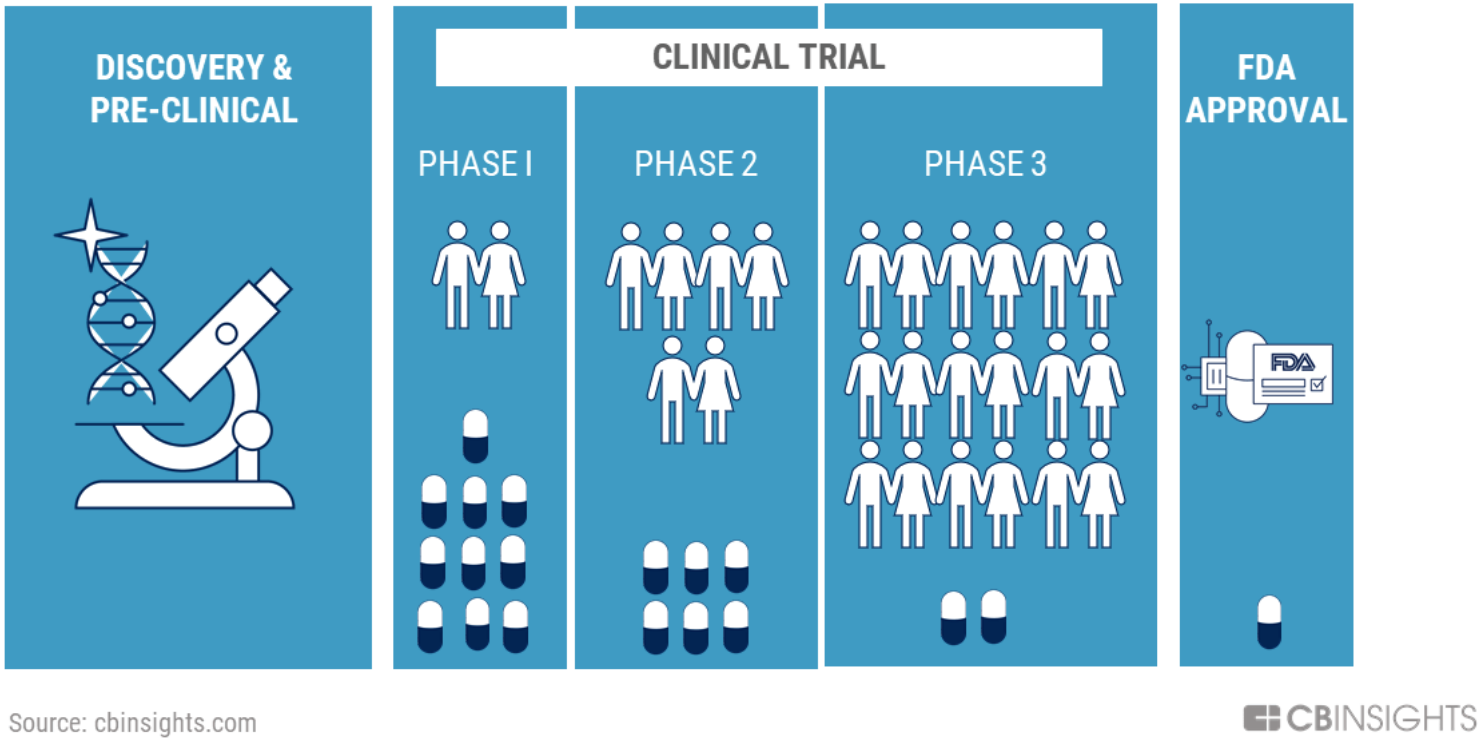


"Recalculating ... recalculating ..."

Challenges of RL

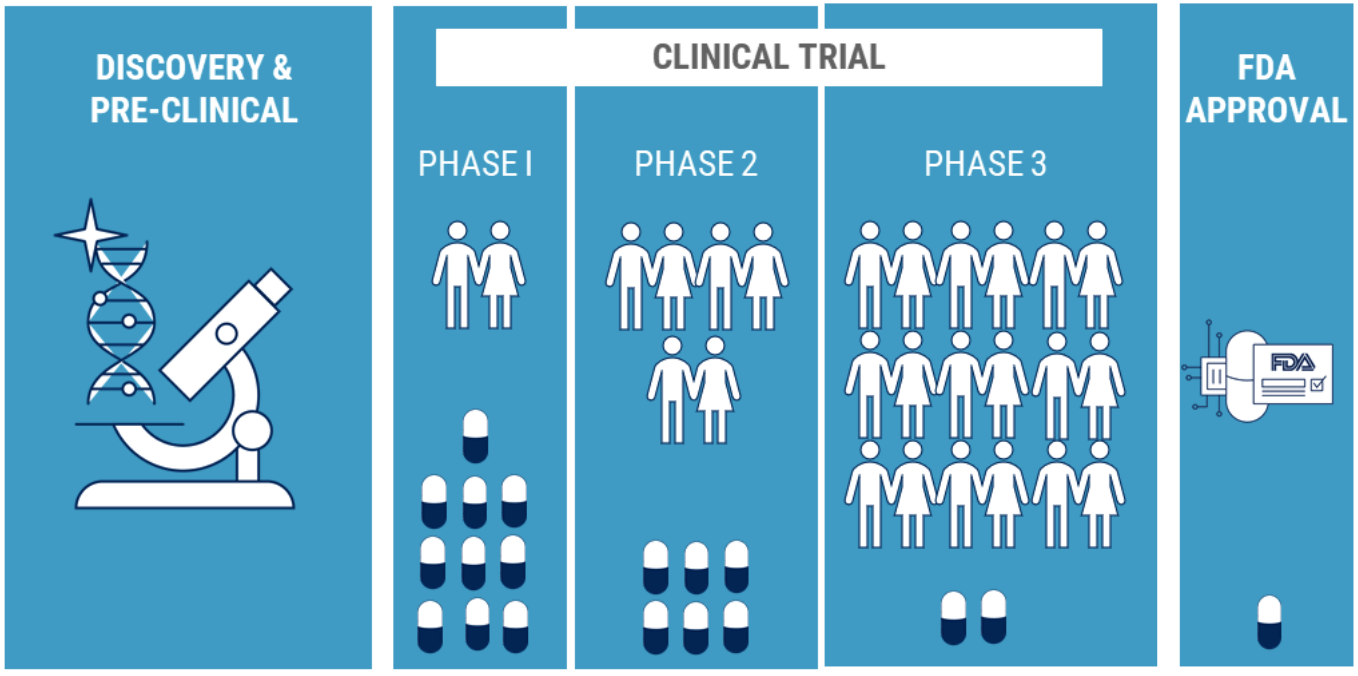
- explore or exploit: unknown or changing environments
- credit assignment problem: delayed rewards or feedback
- enormous state and action space
- nonconvex optimization

Sample efficiency



- prohibitively large state & action space
- collecting data samples can be expensive or time-consuming

Sample efficiency



- prohibitively large state & action space
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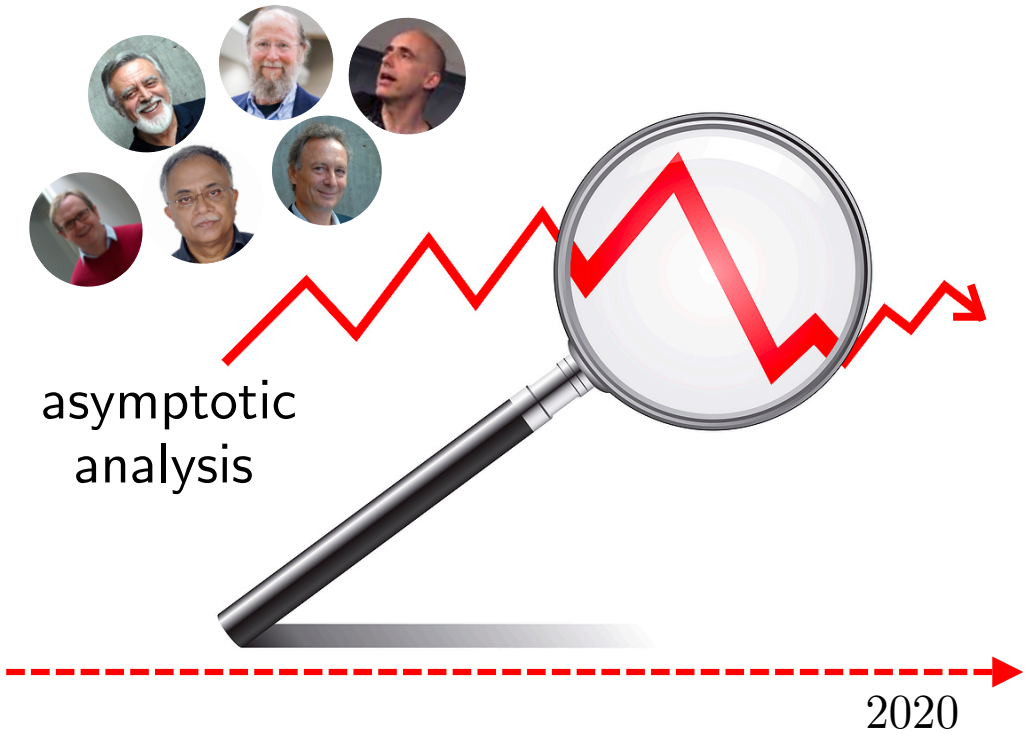
Challenge: how to design sample-efficient RL algorithms?

Statistical foundation of RL



Statistical Science
1986, Vol. 1, No. 2, 276–284

The Contributions of Herbert Robbins to Mathematical Statistics

Tze Leung Lai and David Siegmund

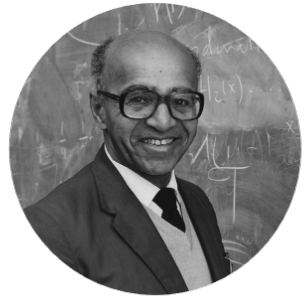
2. STOCHASTIC APPROXIMATION AND ADAPTIVE DESIGN

In 1951, Robbins and his student, Sutton Monro, founded the subject of stochastic approximation with the publication of their celebrated paper [26]. Consider the problem of finding the root θ (assumed unique) of an equation $g(x) = 0$. In the classical

4. SEQUENTIAL EXPERIMENTATION AND OPTIMAL STOPPING

The well known "multiarmed bandit problem" in the statistics and engineering literature, which is prototypical of a wide variety of adaptive control and design problems, was first formulated and studied by Robbins [28]. Let A, B denote two statistical populations with finite means μ_A, μ_B. How should we draw a

Herbert Robbins



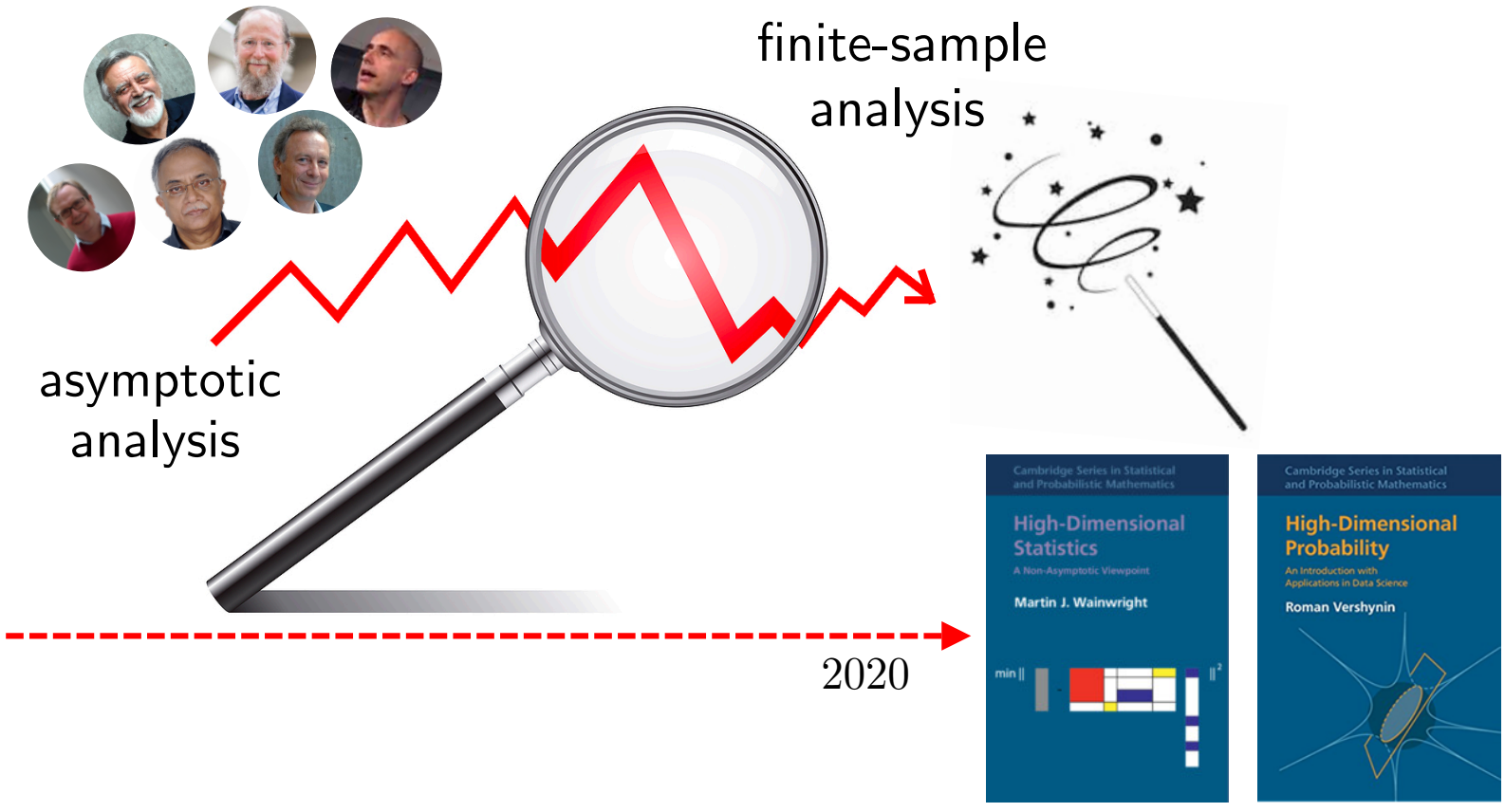
David Blackwell

David Blackwell, 1919–2010: An explorer in mathematics and statistics

Peter J. Bickel[a,1]

Blackwell channel. He also began to work in dynamic programming, which is now called reinforcement learning. In a series of papers, Blackwell gave a rigorous foundation to the theory of dynamic programming, introducing what have become known as Blackwell optimal policies.

Statistical foundation of RL



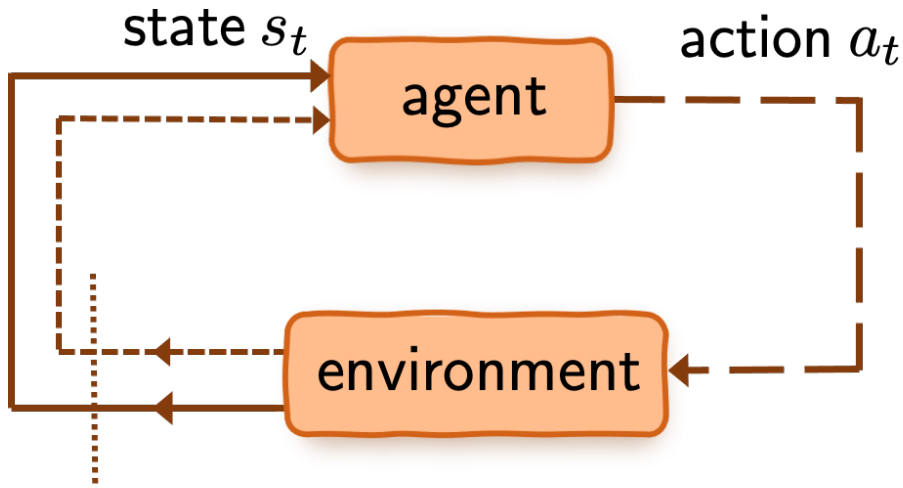
Understanding sample efficiency of RL requires a modern suite of non-asymptotic statistical tools

Outline (Part 1)

- Basics of Markov decision processes
- Basic algorithms for policy evaluation/maximization
- RL with a generative model

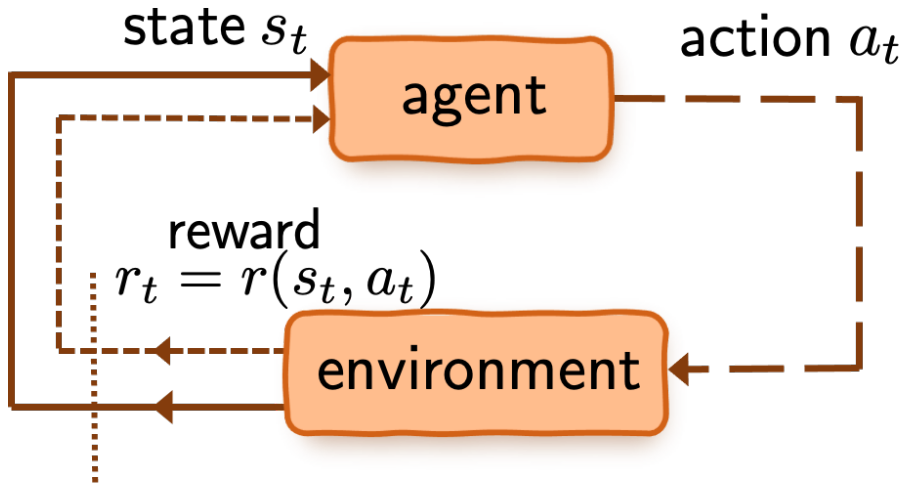
Background: Markov decision processes

Markov decision process (MDP)



- $\mathcal{S}$: state space
- $\mathcal{A}$: action space

Markov decision process (MDP)



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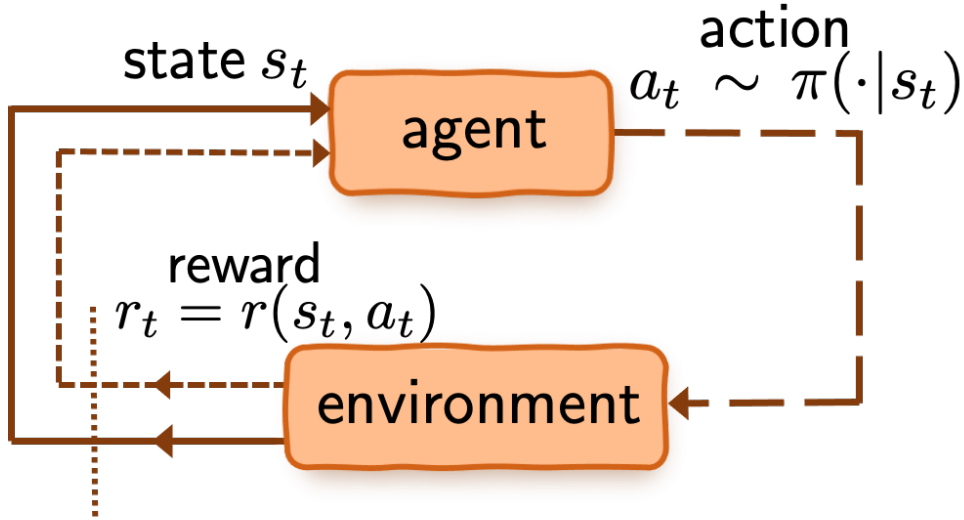

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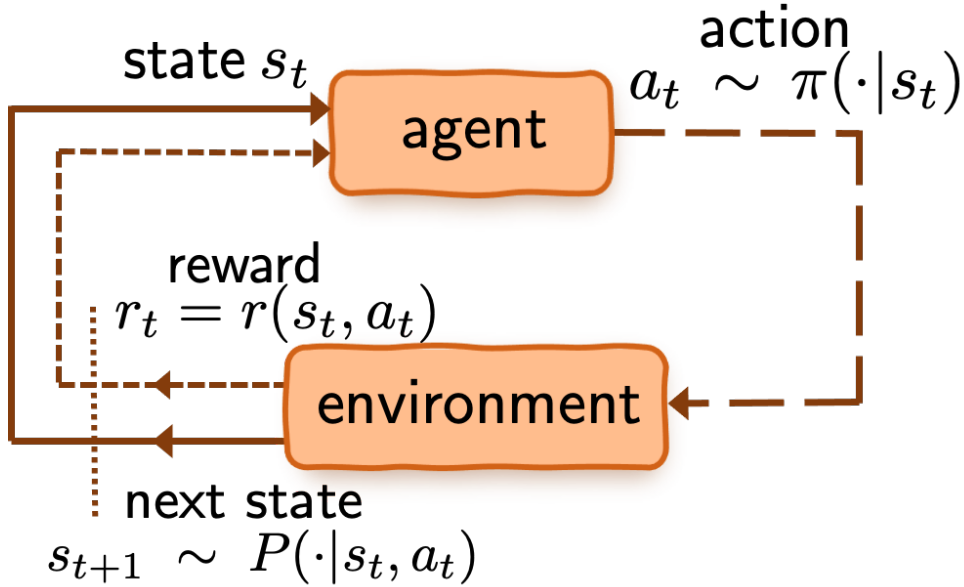

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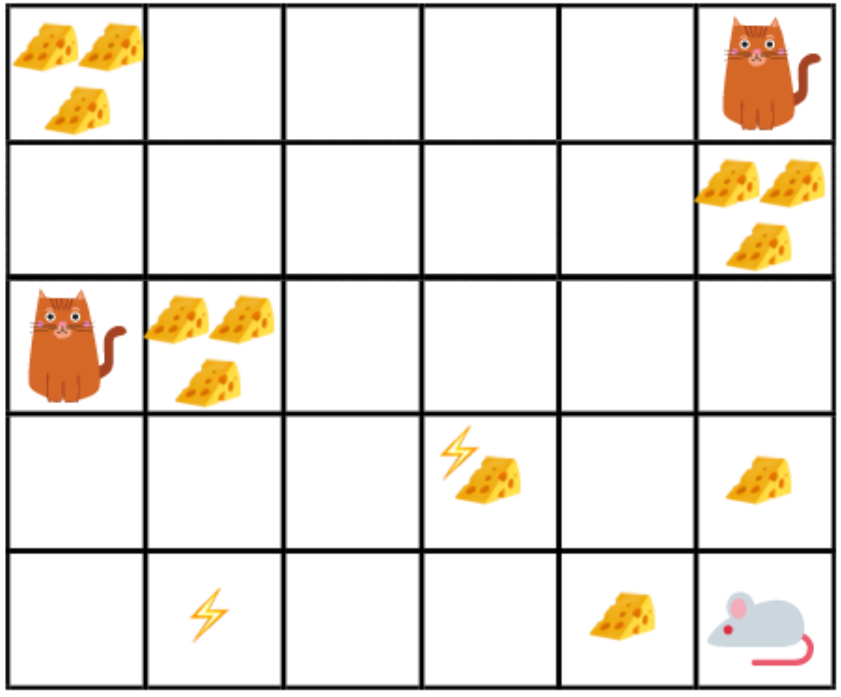
- $P(\cdot|s, a)$: unknown transition probabilities

Help the mouse!



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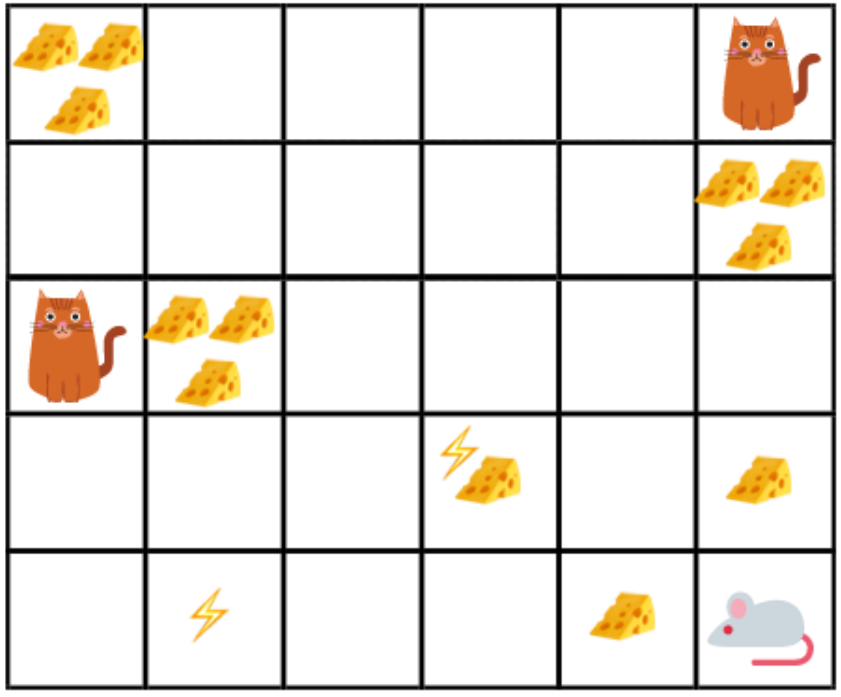
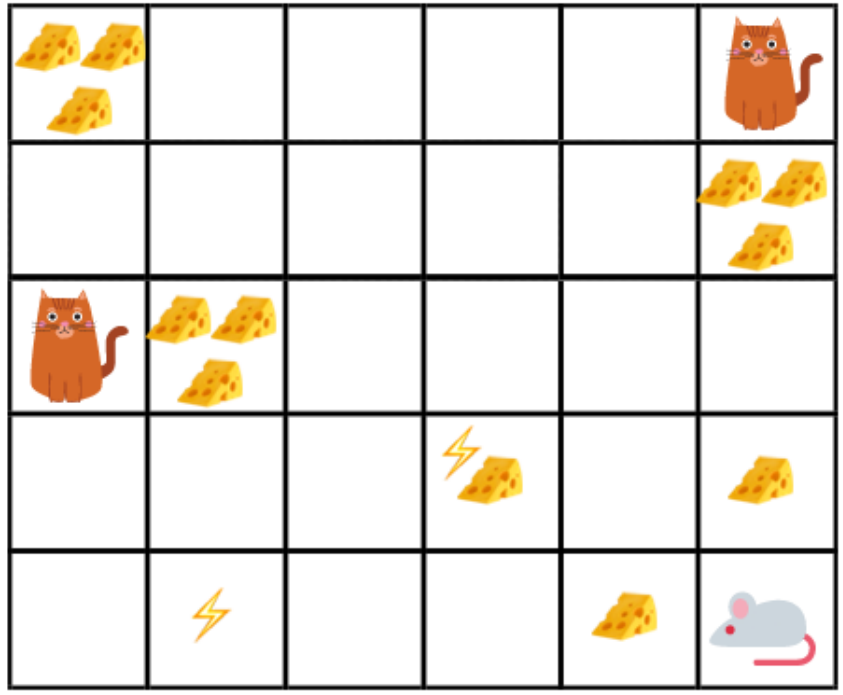


- state space $\mathcal{S}$: positions in the maze

Help the mouse!



- state space $\mathcal{S}$: positions in the maze
- action space $\mathcal{A}$: up, down, left, right

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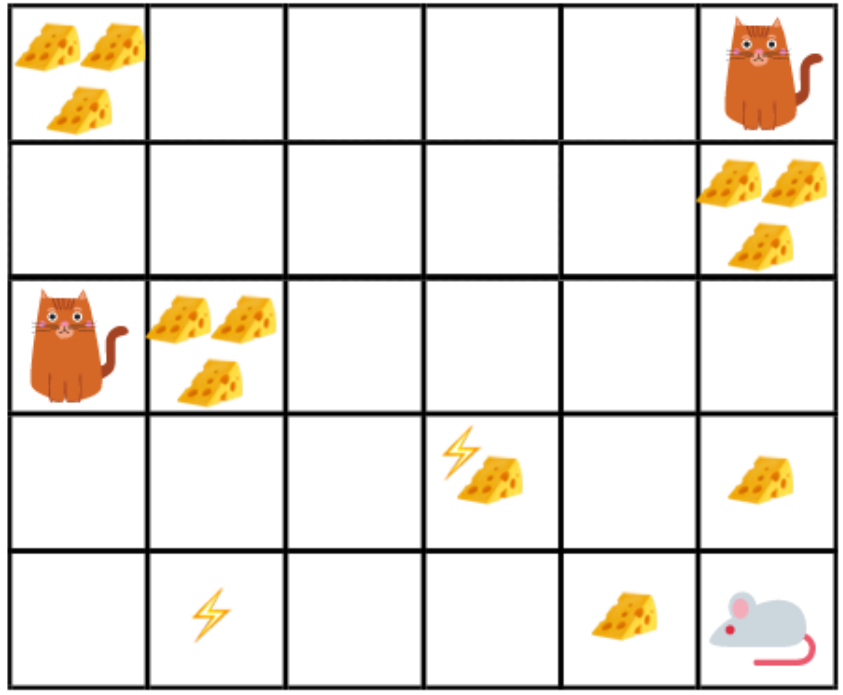

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- immediate reward r: cheese, electricity shocks, cats

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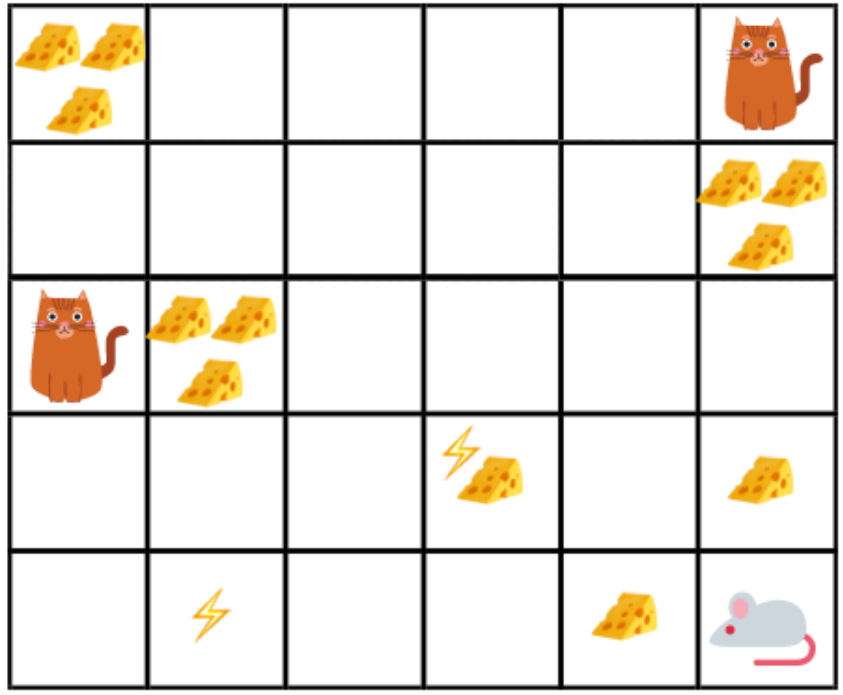
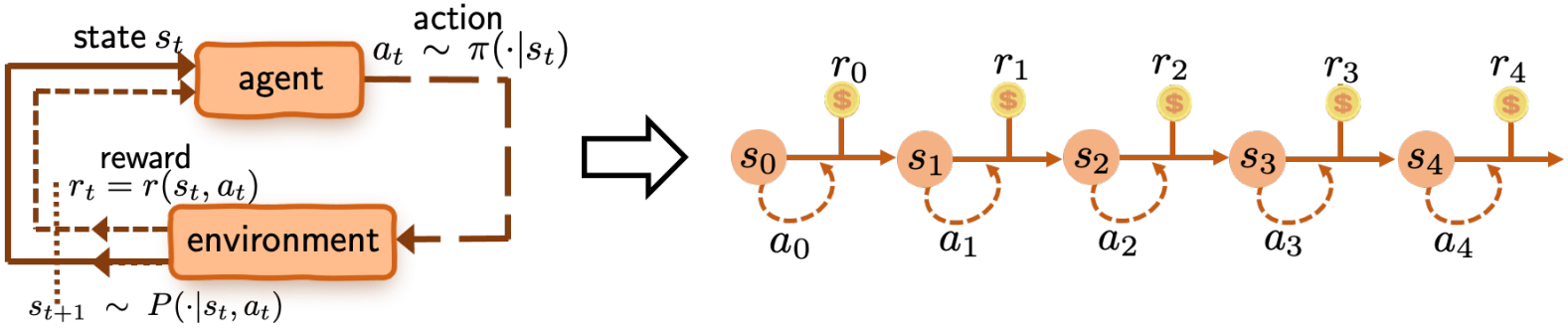


- state space $\mathcal{S}$: positions in the maze
- action space $\mathcal{A}$: up, down, left, right
- immediate reward r: cheese, electricity shocks, cats
- policy $\pi(\cdot|s)$: the way to find cheese

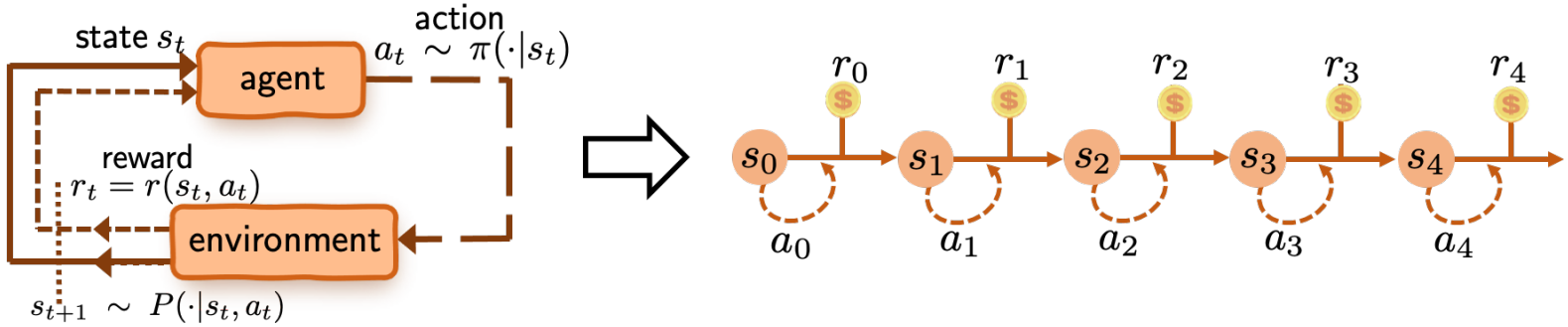
Value function



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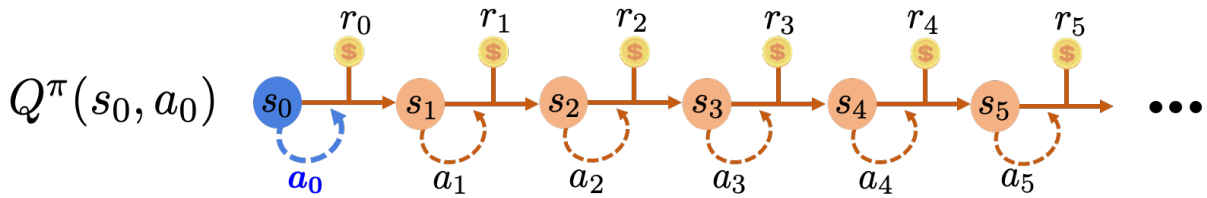
- $\gamma \in [0, 1)$: discount factor
  - take $\gamma \to 1$ to approximate long-horizon MDPs
  - **effective horizon**: $\frac{1}{1-\gamma}$

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

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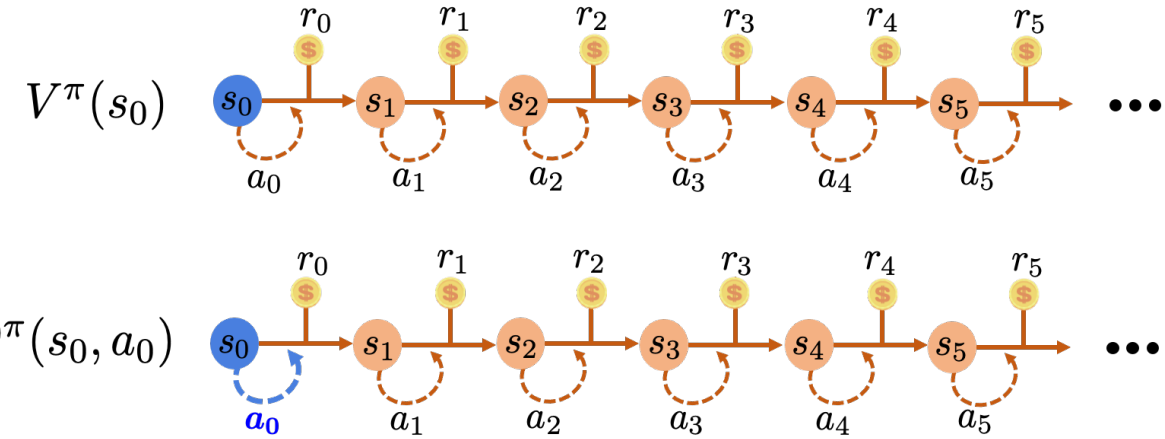

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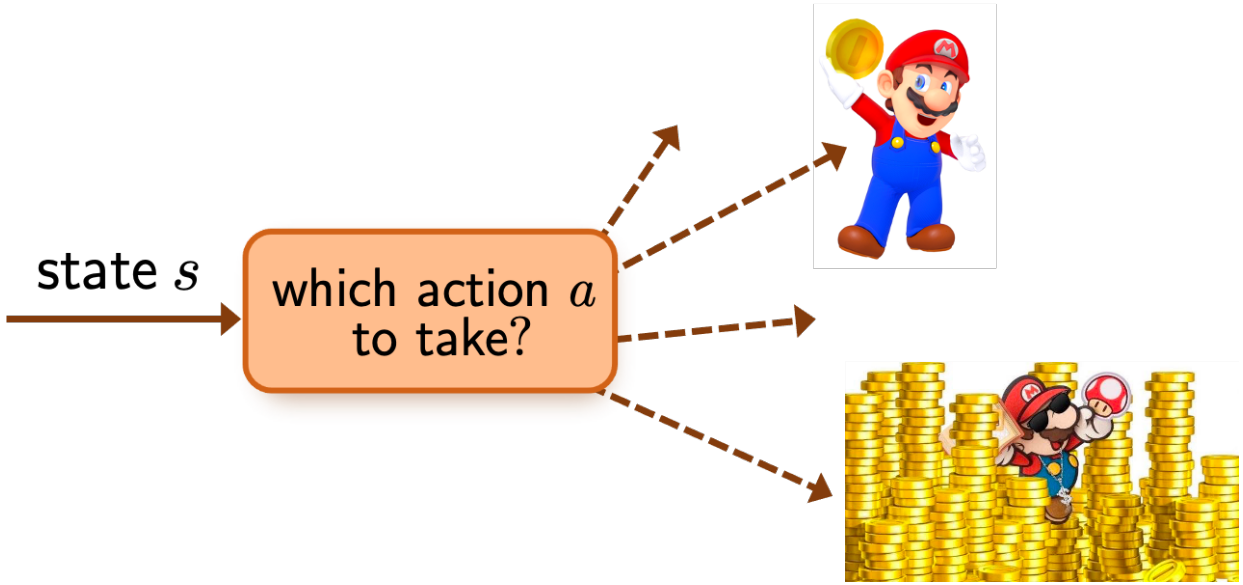
Optimal policy and optimal value



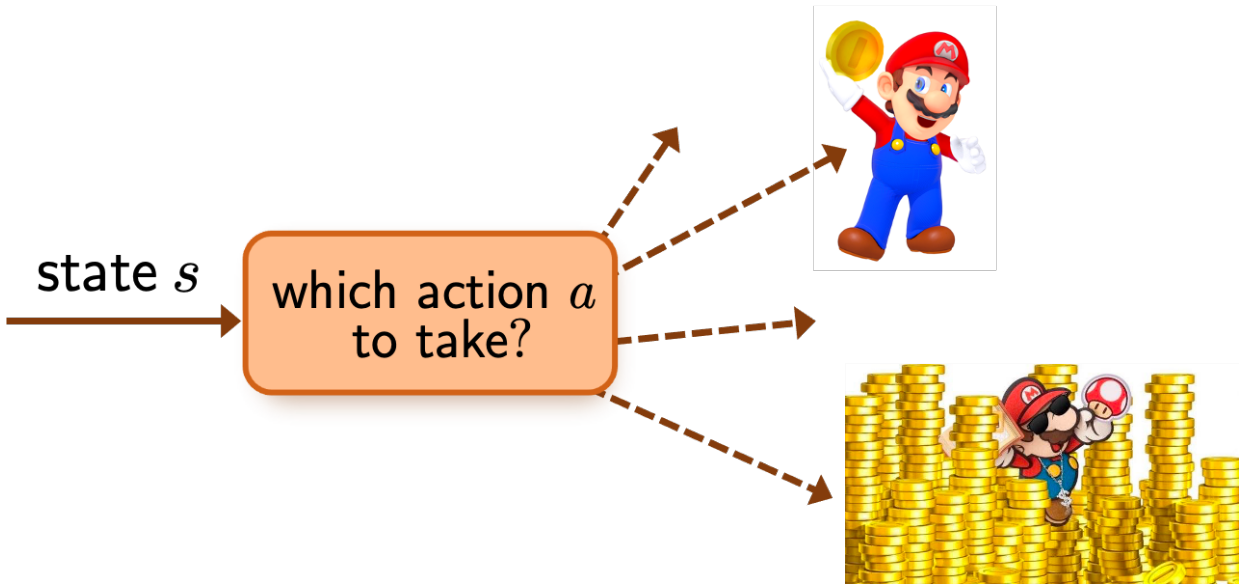
- **optimal policy** $\pi^\star$: maximizing value function $\max_\pi V^\pi(s)$

Theorem 1 (Puterman'94)

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

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

Optimal policy and optimal value



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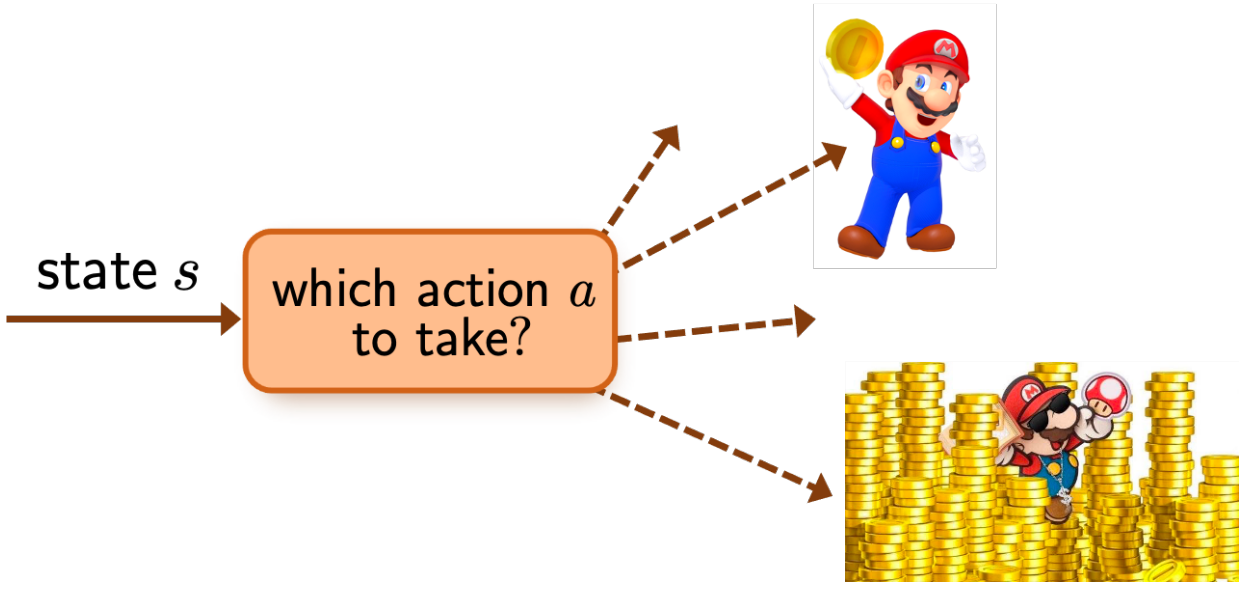
- optimal value / Q function: $V^\star := V^{\pi^\star}$, $Q^\star := Q^{\pi^\star}$

Optimal policy and optimal value



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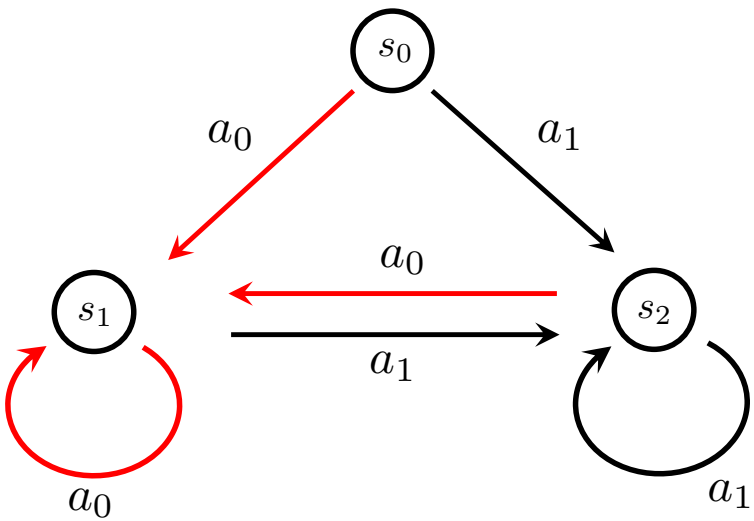
- How to find this $\pi^\star$?

Example

Consider a **deterministic** MDP with 3 states & 2 actions

What is the optimal policy?



Reward: $r(s_1, a_0) = 1, \quad 0$ else where

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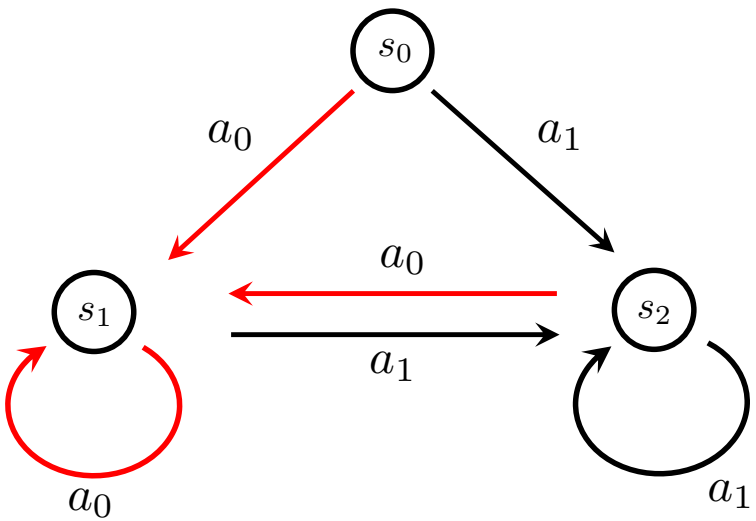

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- $\pi^\star(s) = a_0, \ \forall s$

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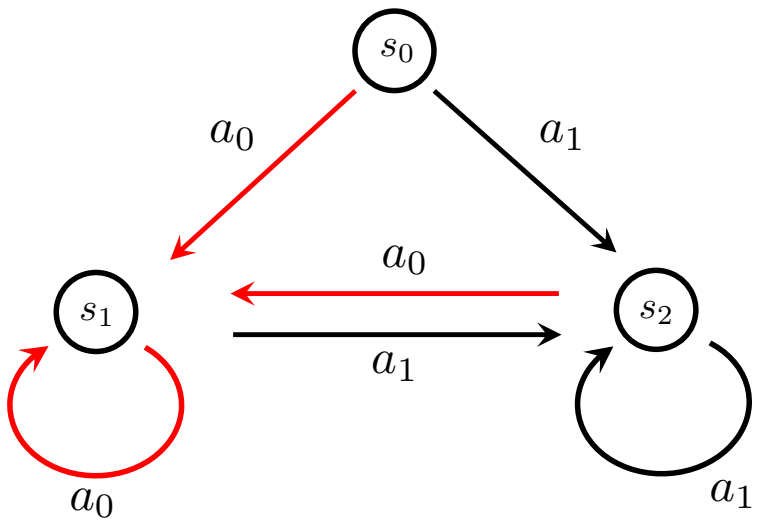

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What is the optimal policy?

- $\pi^\star(s) = a_0, \ \forall s$
- $V^\star(s_0) = \frac{\gamma}{1-\gamma}$,
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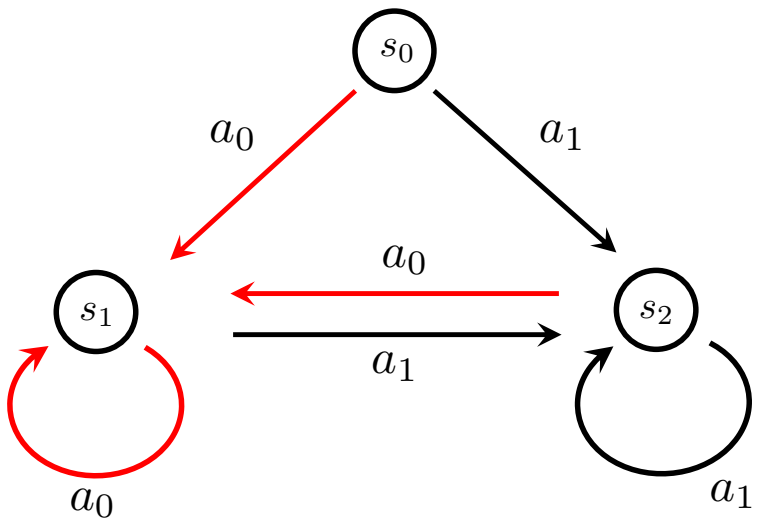

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What is V^π for $\pi(s) = a_1, \ \forall s$?

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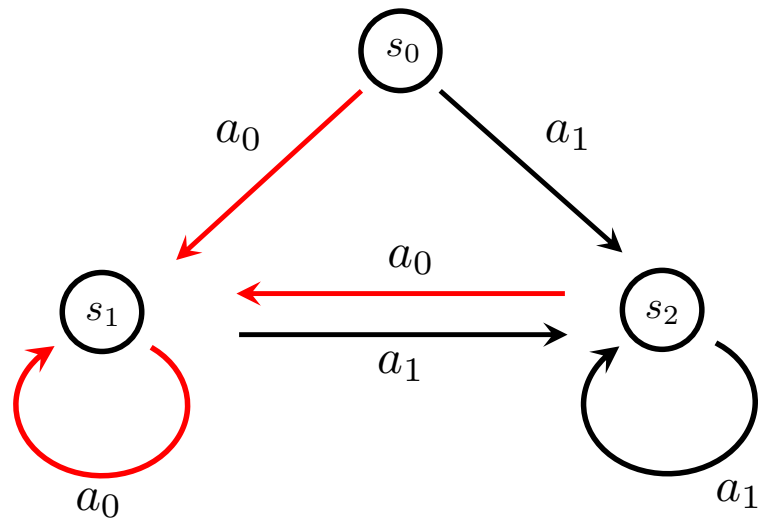

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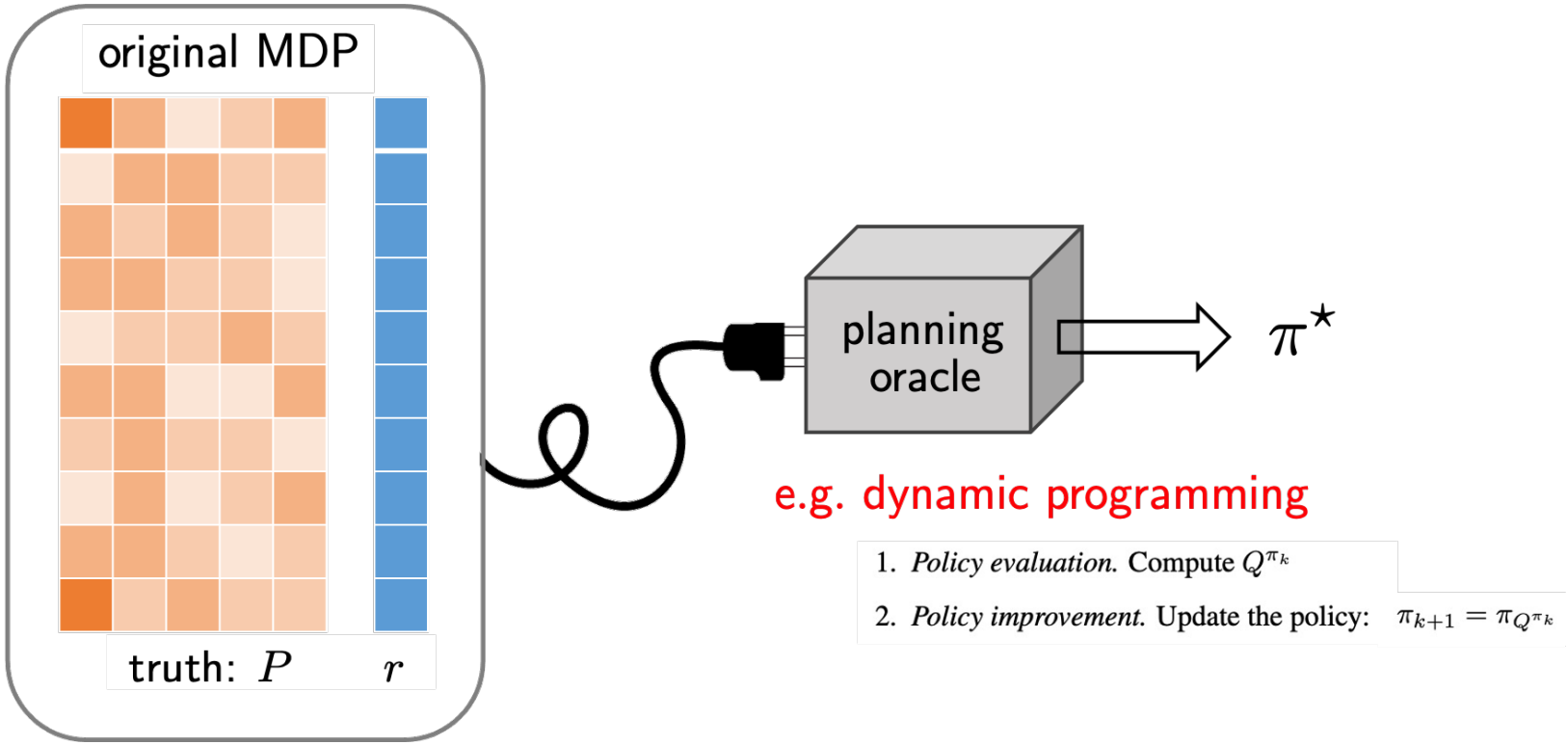
What is V^π for $\pi(s) = a_1, \ \forall s$?

- $V^\pi(s) = 0, \ \forall s$

Background: Basic dynamic programming algorithms

When the model is known . . .



Planning: computing the optimal policy $\pi^\star$ given the MDP specification

Policy evaluation: Given MDP $\mathcal{M} = (\mathcal{S}, \mathcal{A}, r, P, \gamma)$ and policy $\pi : \mathcal{S} \mapsto \mathcal{A}$, how good is π? (i.e., how to compute V^π, $\forall s$?)

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Possible scheme:

- exact policy evaluation for each π
- find the optimal one

Policy evaluation: Bellman's consistency equation

- V^π / Q^π: value / action-value function under policy π

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Bellman's consistency equation

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

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

Richard Bellman

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Richard Bellman

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- one-step look-ahead
- let P^π be the 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

Bellman's optimality principle

Bellman operator

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

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- one-step look-ahead

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

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

γ-contraction of Bellman operator:

$$\|\mathcal{T}(Q_1) - \mathcal{T}(Q_2)\|_\infty \leq \gamma \|Q_1 - Q_2\|_\infty$$

Richard Bellman

Value iteration (VI)

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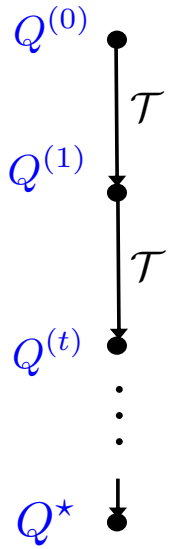
Initialize at $Q = 0$. For $t = 0, 1, \ldots,$

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



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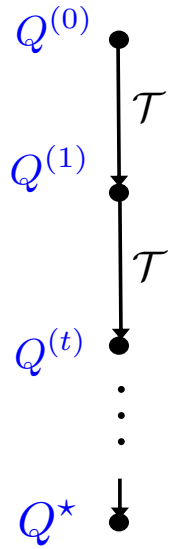


Iterative algorithm for fix-point solution:

Initialize at 0, repeat $x^{t+1} = f(x^t)$. If f is a contraction mapping, then $x^t \to x^\star$.

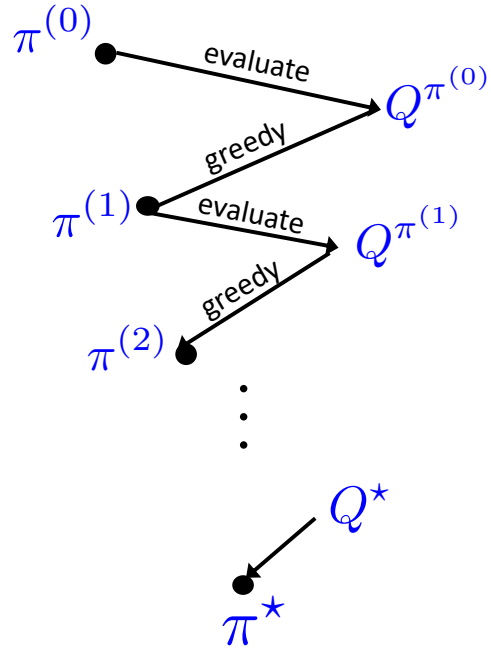
Policy iteration (PI)

Policy iteration (PI)

Initialize at $Q = 0$. For $t = 0, 1, \ldots,$

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

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



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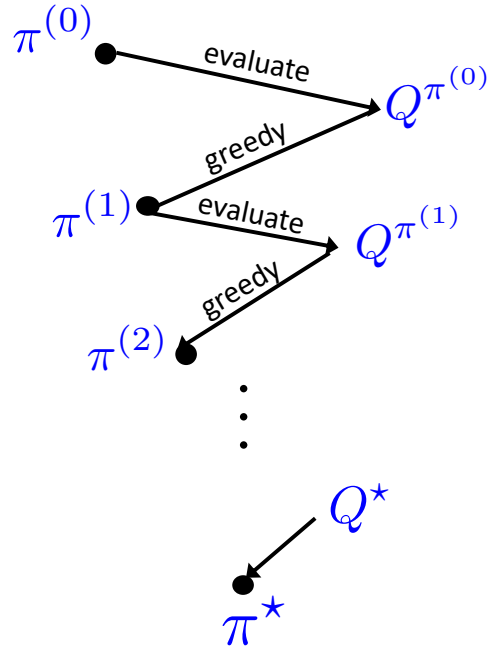

Monotonic improvement:

$$Q^{\pi^{t+1}}(s, a) \geq Q^{\pi^t}(s, a) \qquad \forall (s, a) \in \mathcal{S} \times \mathcal{A}$$

Iteration complexity

Theorem 1 (Linear convergence of policy/value iteration)

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

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

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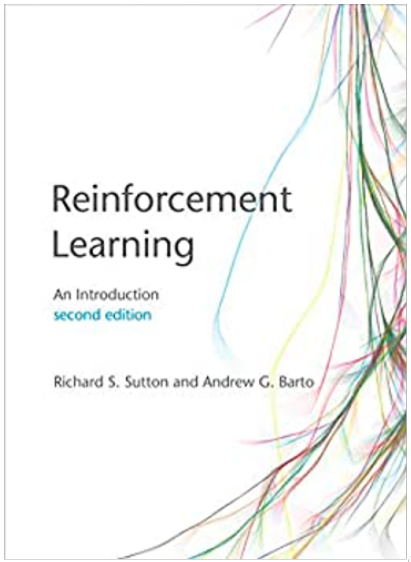
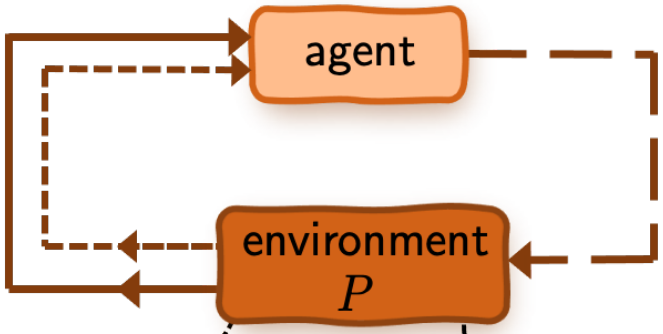
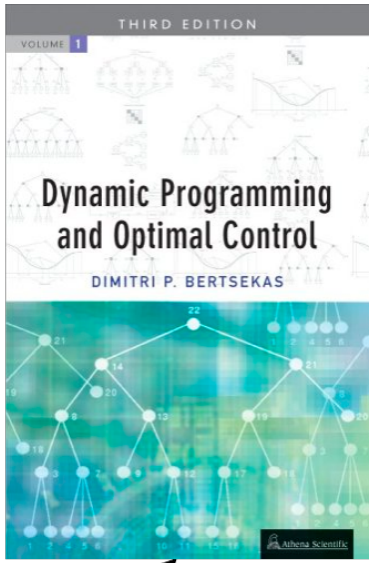
Linear convergence at a **dimension-free** rate!

When the model is unknown . . .







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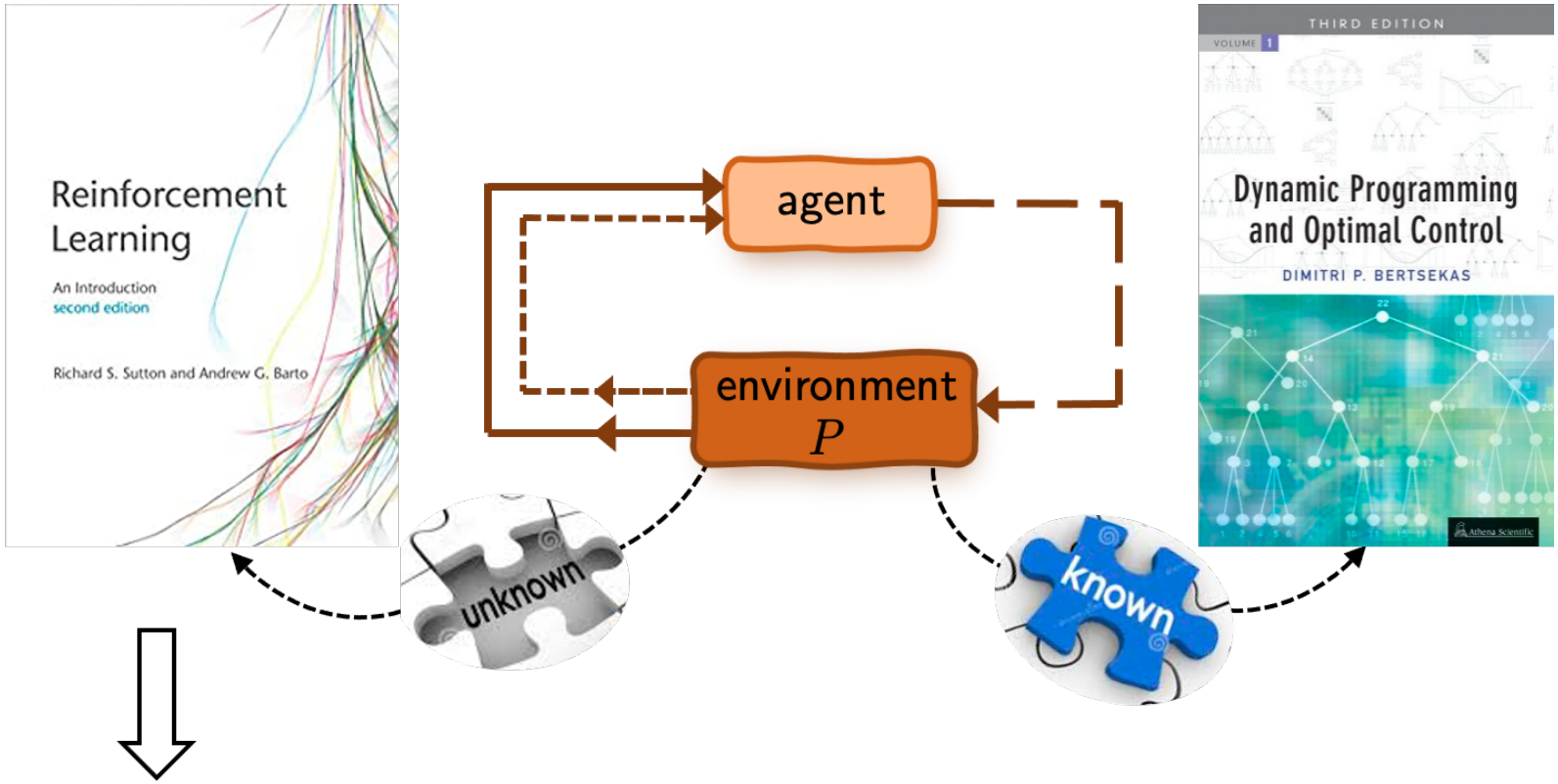
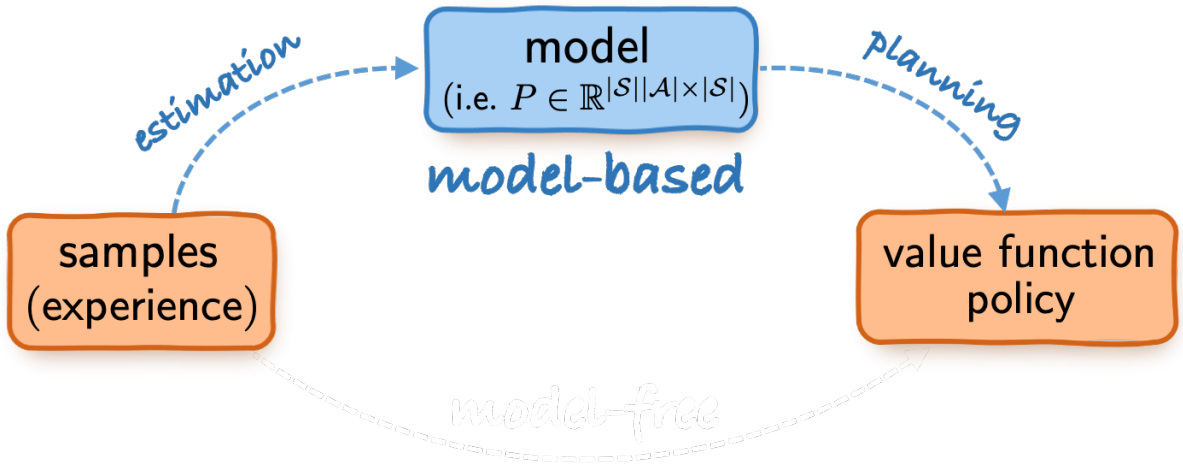


Need to learn optimal policy from samples w/o model specification

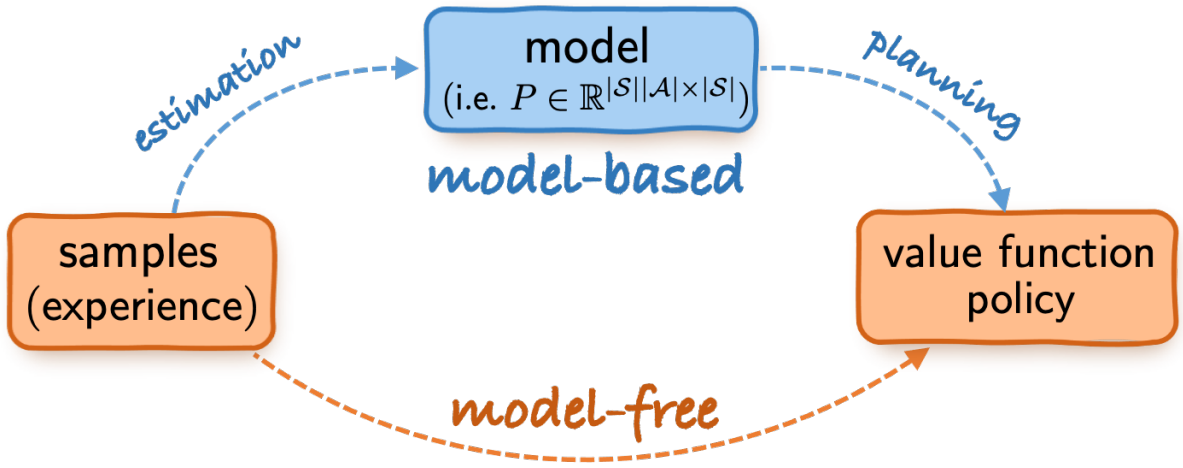
Two approaches



Model-based approach ("plug-in")

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

Two approaches



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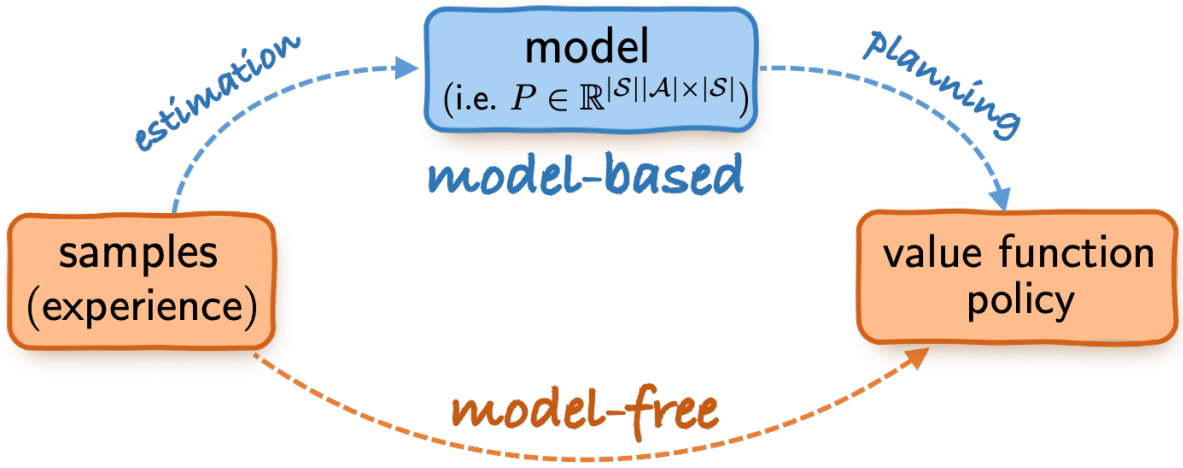
Model-free approach (e.g. Q-learning; part iii)

— learning w/o estimating the model explicitly

Two approaches



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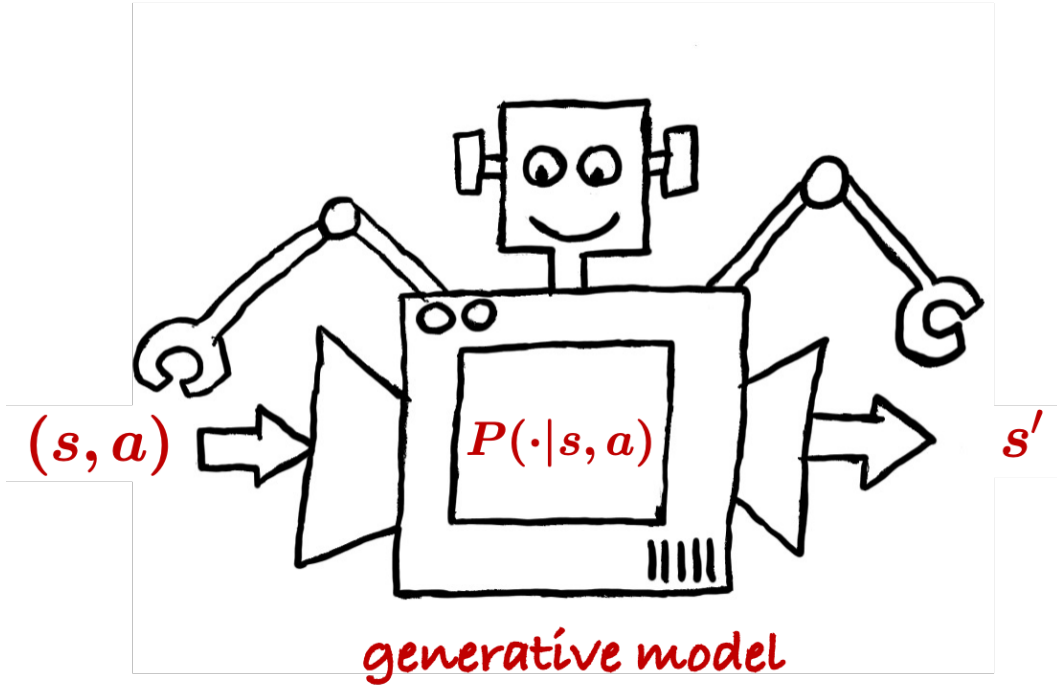
1. Sampling from a generative model (simulator)
2. Offline RL / batch RL

Sampling from a generative model

— *Kearns, Singh '99*



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

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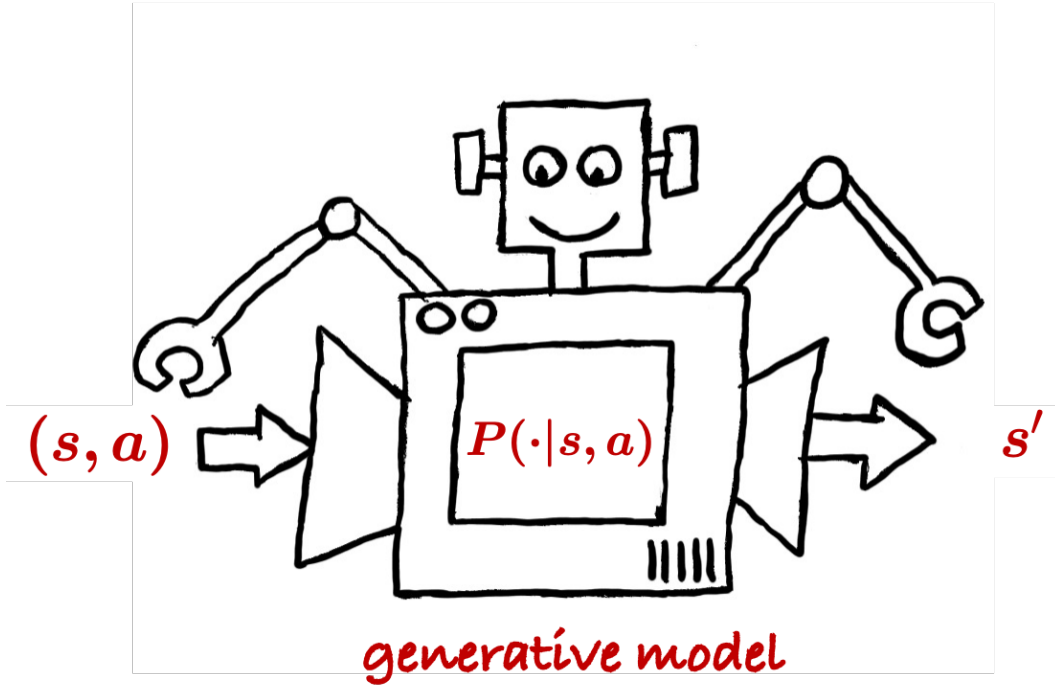


- **Sampling:** for each (s, a), collect N samples $\{(s, a, s'_{(i)})\}_{1 \le i \le N}$
- construct $\widehat{\pi}$ based on samples (in total $|\mathcal{S}||\mathcal{A}| \times N$)

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

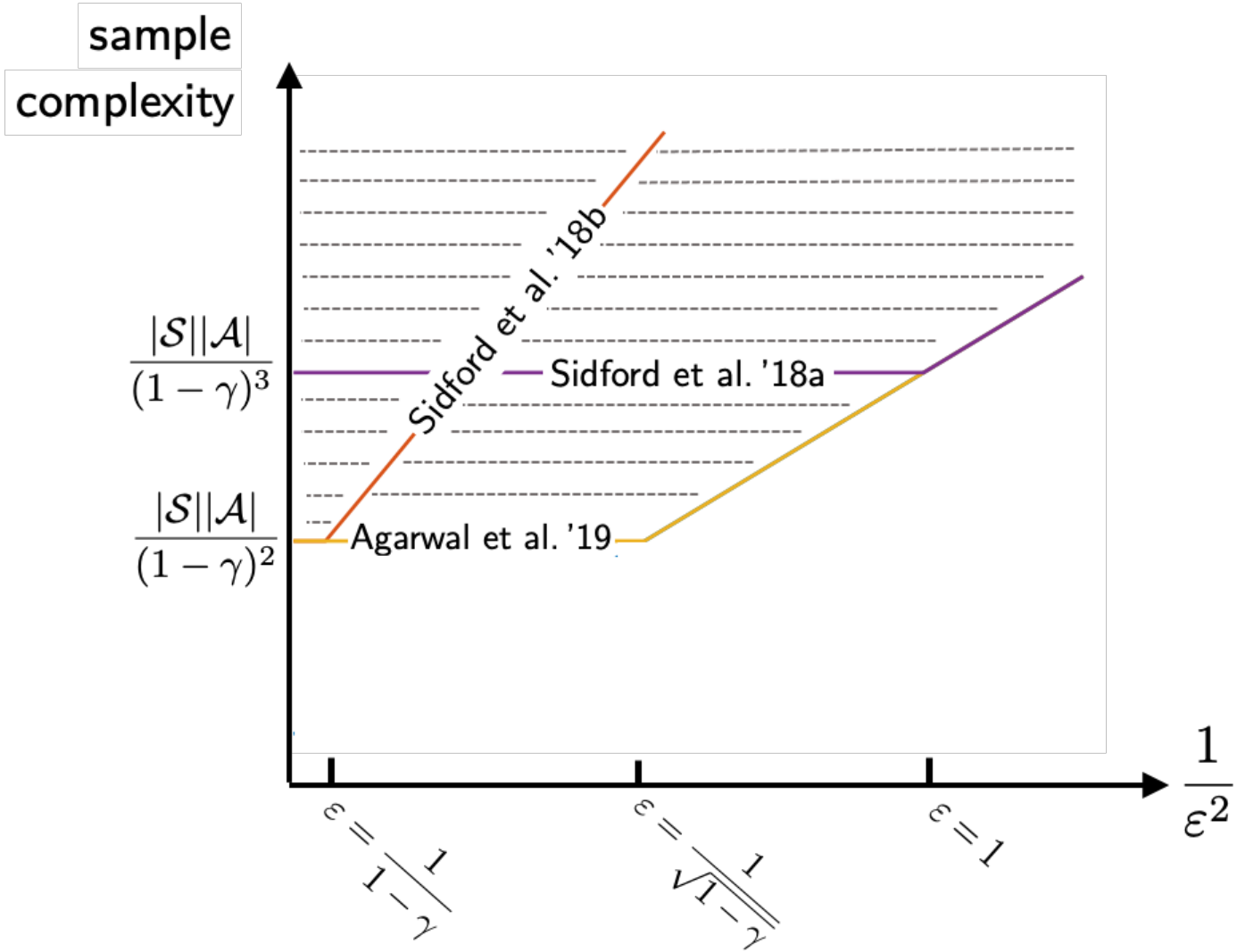
An incomplete list of prior art

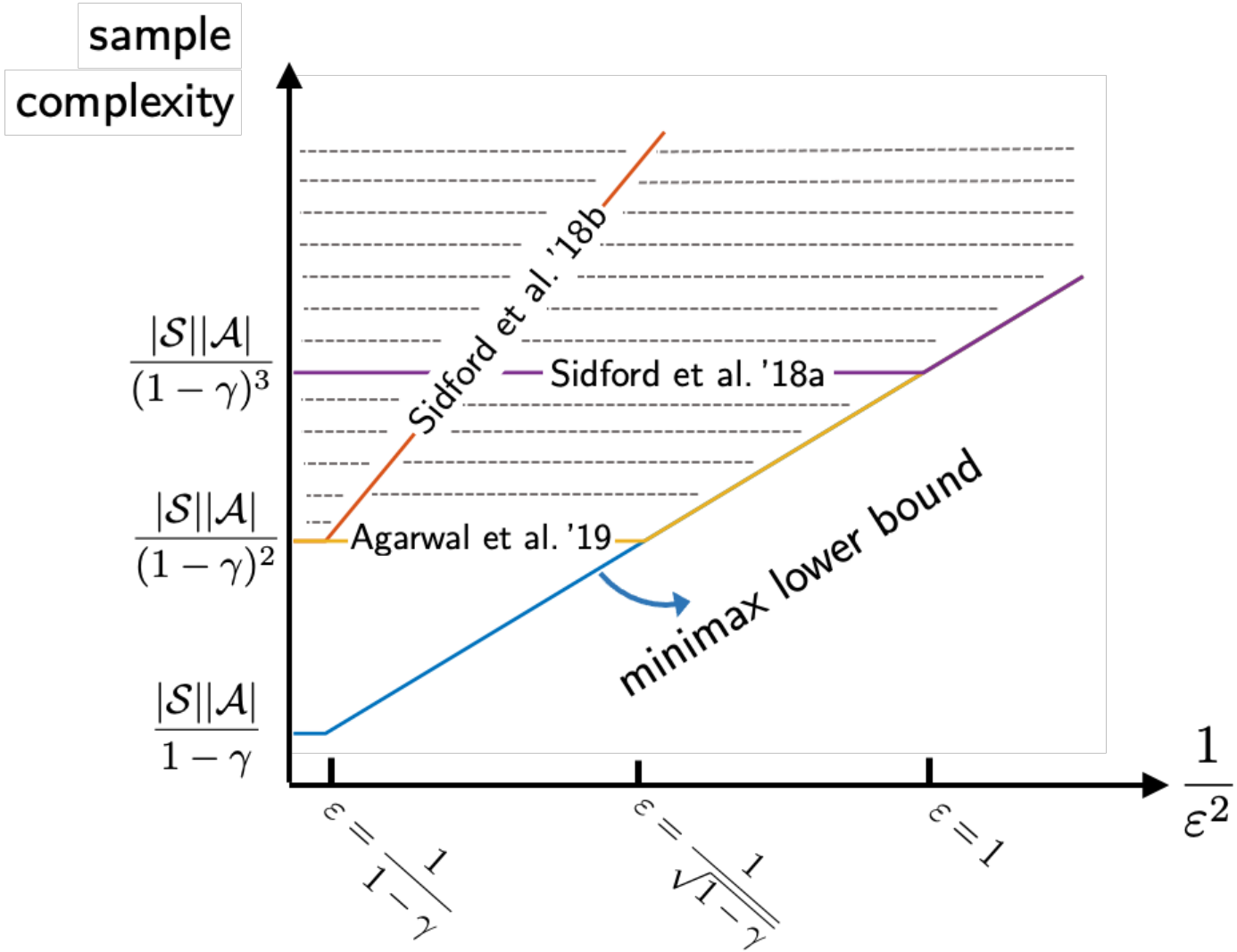
- Kearns & Singh '99
- Kakade '03
- Kearns, Mansour & Ng '02
- Azar, Munos & Kappen '12
- Azar, Munos, Ghavamzadeh & Kappen '13
- Sidford, Wang, Wu, Yang & Ye '18
- Sidford, Wang, Wu & Ye '18
- Wang '17
- Agarwal, Kakade & Yang '19
- Wainwright '19a
- Wainwright '19b
- Pananjady & Wainwright '20
- Yang & Wang '19
- Khamaru, Pananjady, Ruan, Wainwright & Jordan '20
- Mou, Li, Wainwright, Bartlett & Jordan '20
- ...

An even shorter list of prior art

algorithm	sample size range	sample complexity	ε-range
phased Q-learning Kearns and Singh '99	$\left[\frac{\lvert\mathcal{S}\rvert^2\lvert\mathcal{A}\rvert}{(1-\gamma)^5}, \infty\right)$	$\frac{\lvert\mathcal{S}\rvert\lvert\mathcal{A}\rvert}{(1-\gamma)^7\varepsilon^2}$	$(0, \frac{1}{1-\gamma}]$
empirical QVI Azar et al. '13	$\left[\frac{\lvert\mathcal{S}\rvert^2\lvert\mathcal{A}\rvert}{(1-\gamma)^2}, \infty\right)$	$\frac{\lvert\mathcal{S}\rvert\lvert\mathcal{A}\rvert}{(1-\gamma)^3\varepsilon^2}$	$(0, \frac{1}{\sqrt{(1-\gamma)\lvert\mathcal{S}\rvert}}]$
sublinear randomized VI Sidford et al. '18a	$\left[\frac{\lvert\mathcal{S}\rvert\lvert\mathcal{A}\rvert}{(1-\gamma)^2}, \infty\right)$	$\frac{\lvert\mathcal{S}\rvert\lvert\mathcal{A}\rvert}{(1-\gamma)^4\varepsilon^2}$	$\left(0, \frac{1}{1-\gamma}\right]$
variance-reduced QVI Sidford et al. '18b	$\left[\frac{\lvert\mathcal{S}\rvert\lvert\mathcal{A}\rvert}{(1-\gamma)^3}, \infty\right)$	$\frac{\lvert\mathcal{S}\rvert\lvert\mathcal{A}\rvert}{(1-\gamma)^3\varepsilon^2}$	$(0, 1]$
empirical MDP + planning Agarwal et al. '19	$\left[\frac{\lvert\mathcal{S}\rvert\lvert\mathcal{A}\rvert}{(1-\gamma)^2}, \infty\right)$	$\frac{\lvert\mathcal{S}\rvert\lvert\mathcal{A}\rvert}{(1-\gamma)^3\varepsilon^2}$	$(0, \frac{1}{\sqrt{1-\gamma}}]$

— see also Wainwright '19a '19b (for estimating optimal values)


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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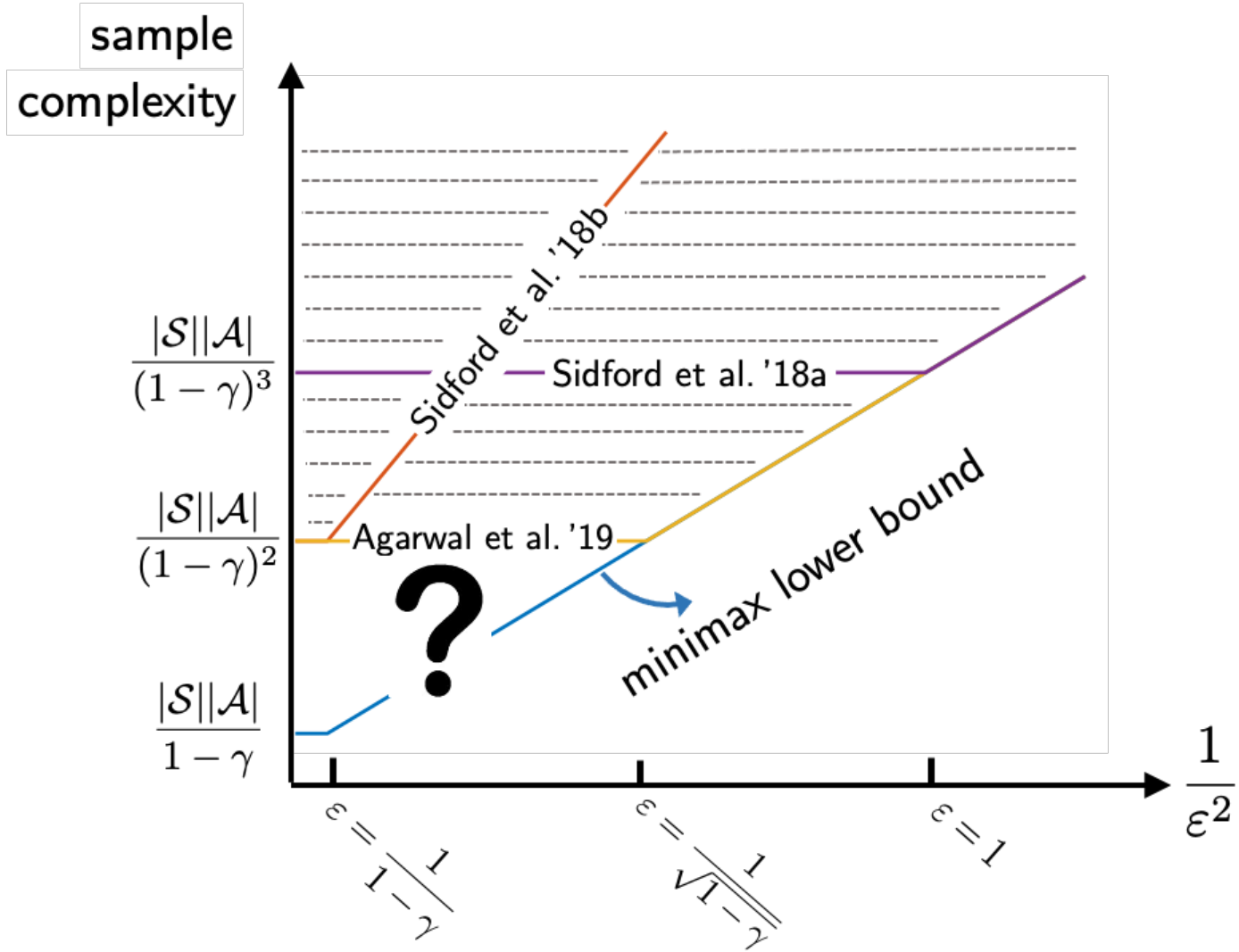
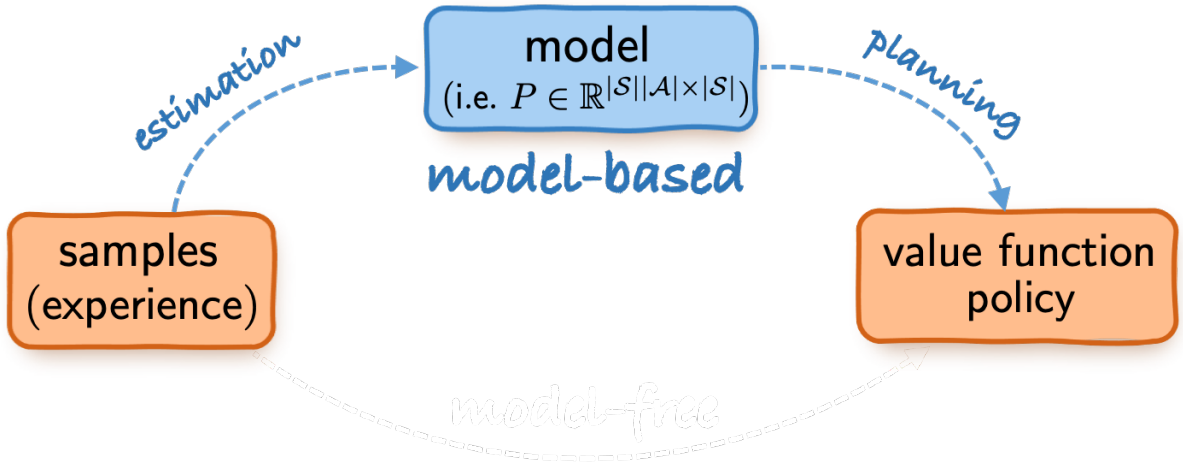


All prior theory requires sample size $> \underbrace{\frac{|\mathcal{S}||\mathcal{A}|}{(1-\gamma)^2}}_{\text{sample size barrier}}$

Our algorithm: model-based RL



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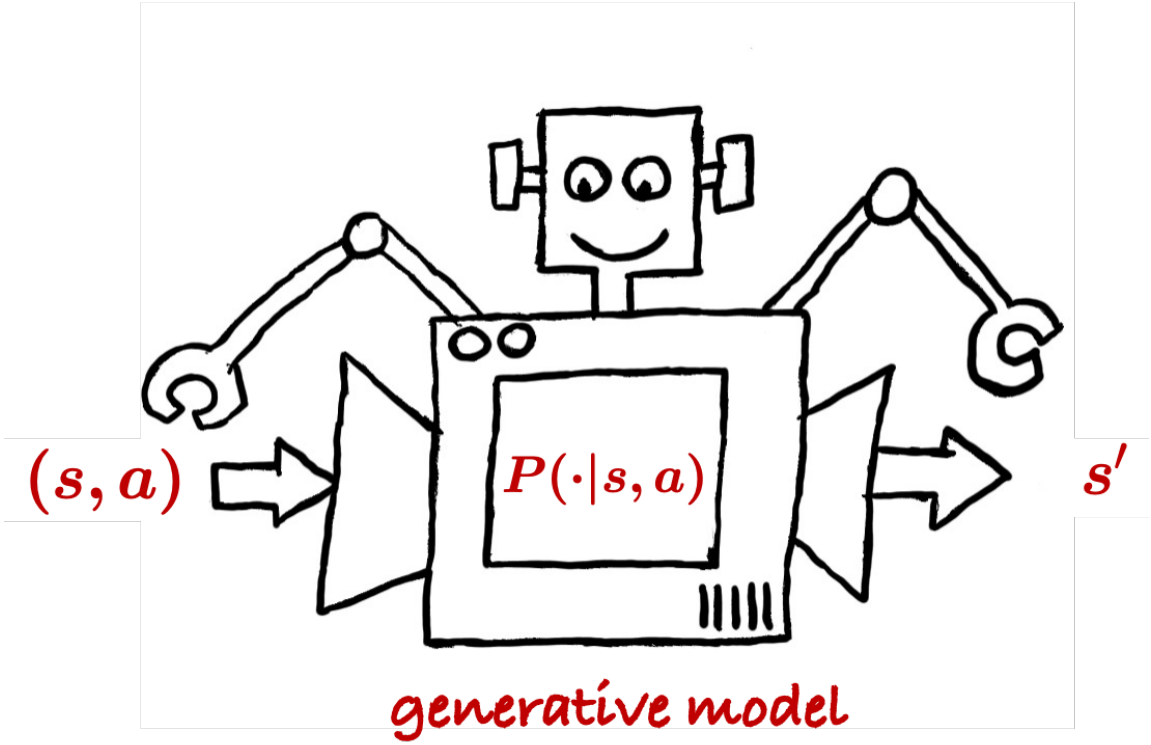
1. build an empirical estimate $\widehat{P}$ for P
2. planning based on empirical $\widehat{P}$

Model estimation



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

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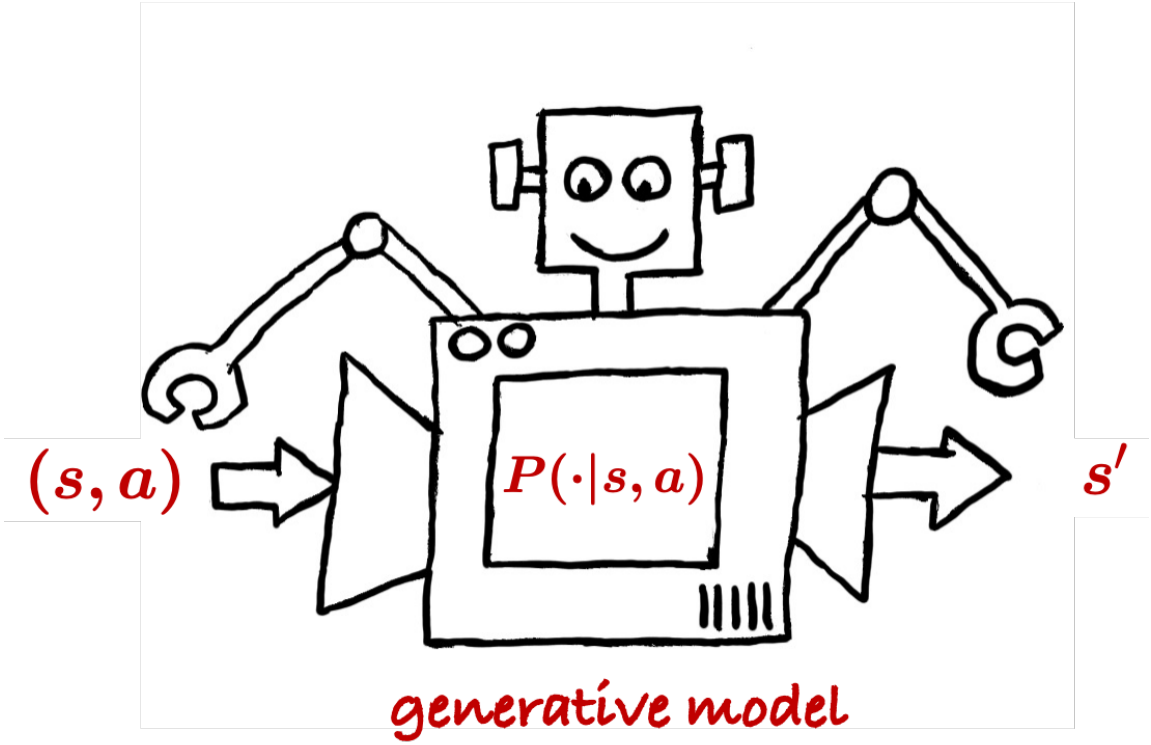
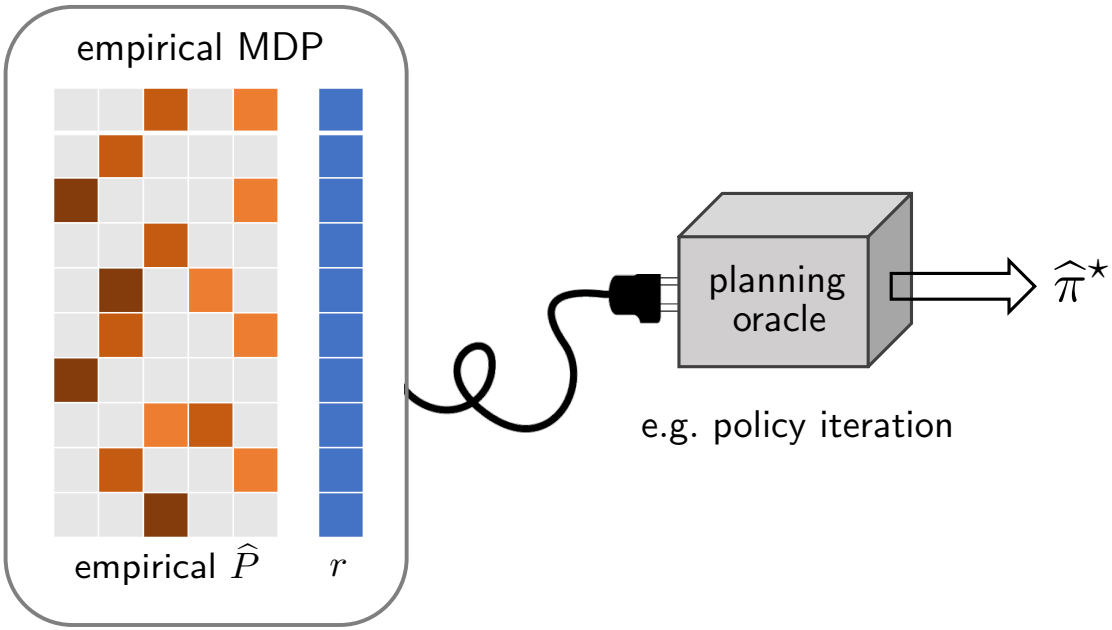


Sampling: for each (s, a), collect N ind. samples $\{(s, a, s'_{(i)})\}_{1 \le i \le N}$

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

Model-based (plug-in) estimator

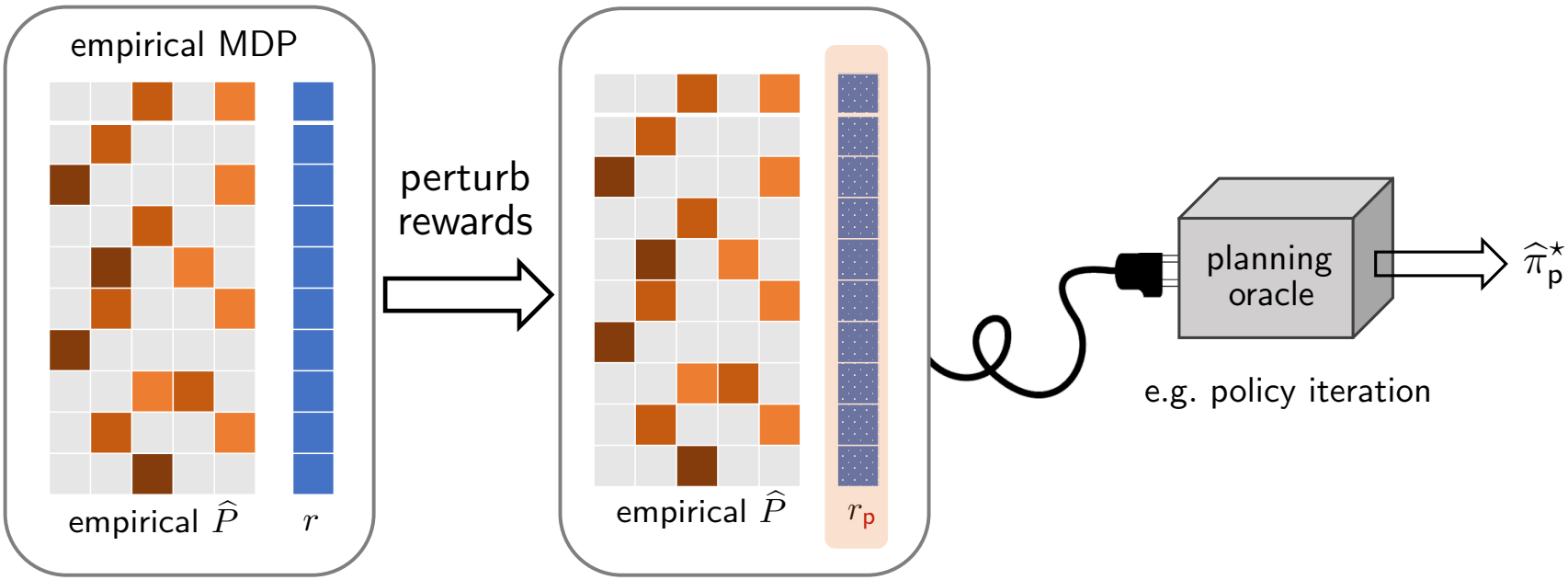
— *Azar et al. '13, Agarwal et al. '19, Pananjady et al. '20*



Planning based on the *empirical* MDP with *slightly perturbed rewards*

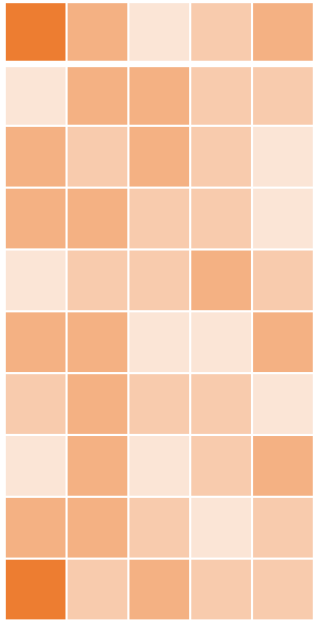
Our method: plug-in estimator + perturbation

— Li, Wei, Chi, Gu, Chen '20

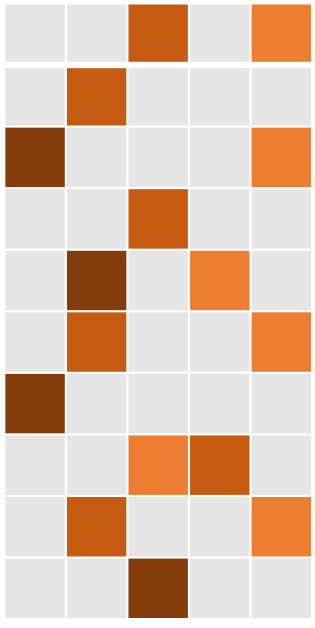


Run planning algorithms based on the *empirical* MDP

Challenges in the sample-starved regime



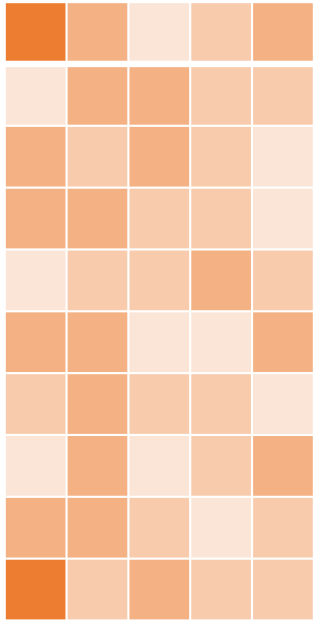
truth:
$P \in \mathbb{R}^{|\mathcal{S}||\mathcal{A}| \times |\mathcal{S}|}$



empirical estimate:
$\widehat{P}$

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

Challenges in the sample-starved regime



truth:
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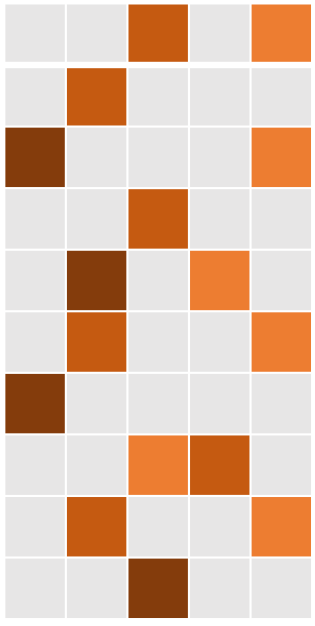

empirical estimate:
$\widehat{P}$

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

Main result

Theorem 2 (Li, Wei, Chi, Gu, Chen '20)

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

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

with high prob., with sample complexity at most

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

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- $\widehat{\pi}_{\mathrm{p}}^{\star}$: obtained by empirical QVI or PI within $\widetilde{O}(\frac{1}{1-\gamma})$ iterations

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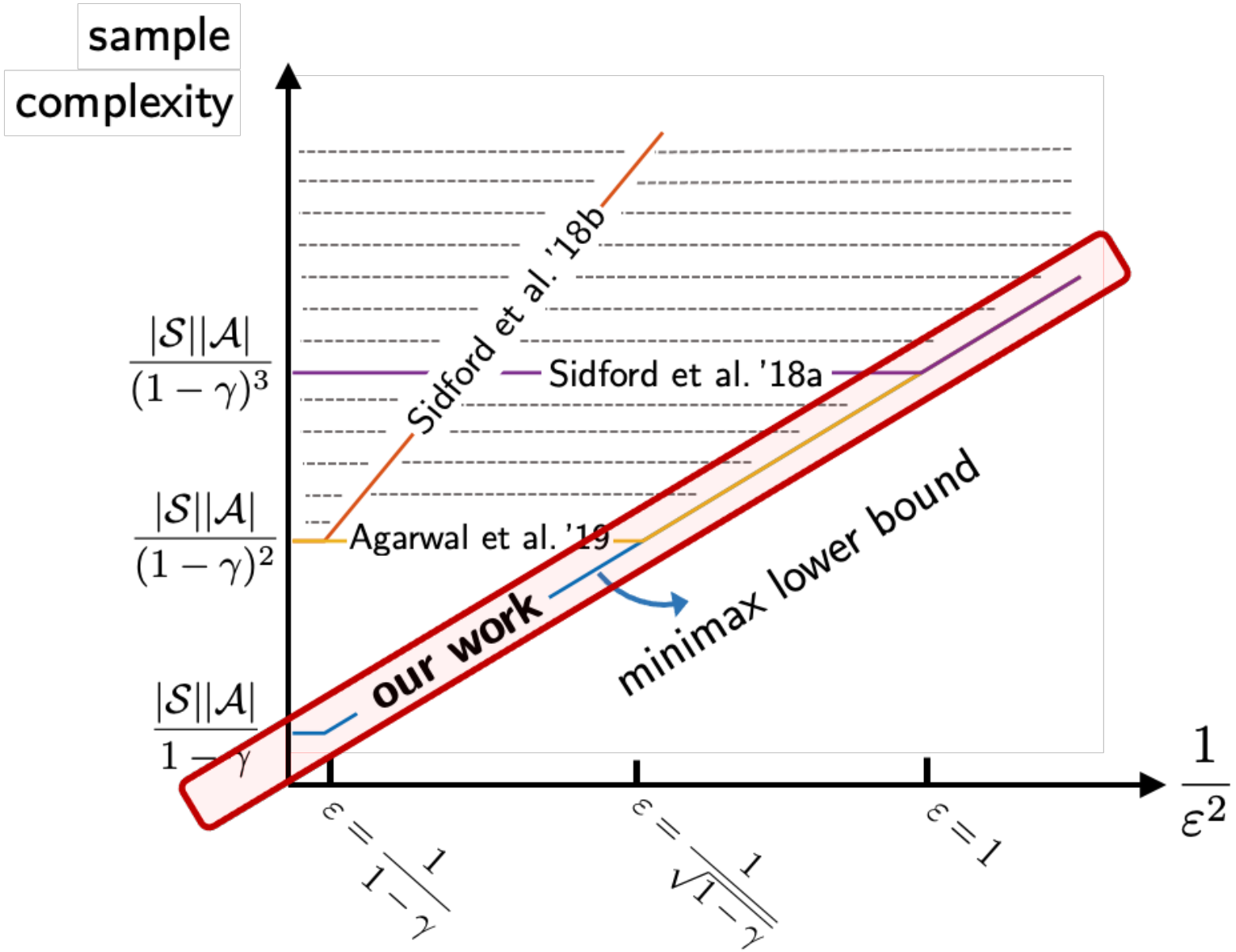
- $\widehat{\pi}_{\mathrm{p}}^{\star}$: obtained by empirical QVI or PI within $\widetilde{O}(\frac{1}{1-\gamma})$ iterations
- **Minimax lower bound:** $\widetilde{\Omega}(\frac{|\mathcal{S}||\mathcal{A}|}{(1-\gamma)^3\varepsilon^2})$ (Azar et al. '13)


sample
complexity
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Sidford et al. '18b
Sidford et al. '18a
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our work
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$\varepsilon = \frac{1}{1-\gamma}$
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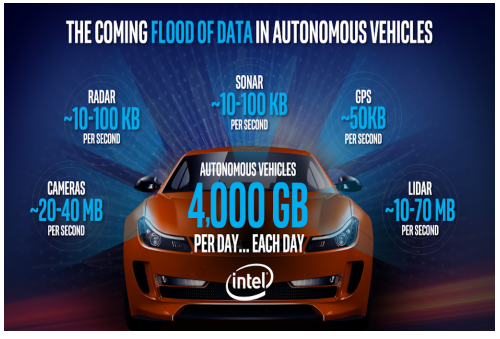
Model-based RL (a "plug-in" approach)

1. Sampling from a generative model (simulator)
2. Offline RL / batch RL

Offline RL / Batch RL

- Collecting new data might be expensive or time-consuming
- Having stored tons of historical data

medical records



data of self-driving

clicking times of ads

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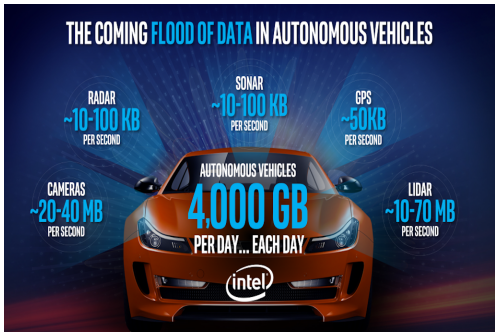


data of self-driving

clicking times of ads

Can we design algorithms based solely on historical data?

Offline RL / Batch RL

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

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

for some state distribution ρ^{b} and behavior policy π^{b}

Offline RL / Batch RL

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

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

for some state distribution ρ^{b} and behavior policy π^{b}

Goal: given some test distribution ρ and accuracy level ε, find an ε-optimal policy $\widehat{\pi}$ based on $\mathcal{D}$ obeying

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

— in a sample-efficient manner

Challenges of offline RL

- **Distribution shift**:

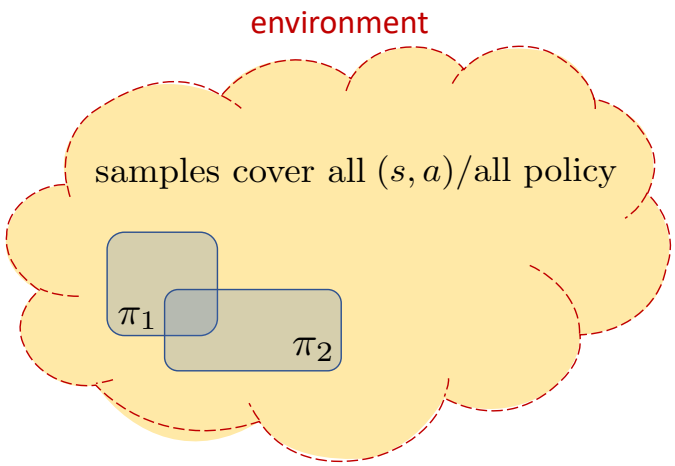
$$\text{distribution}(\mathcal{D}) \;\neq\; \text{distribution under } \pi^\star$$

Challenges of offline RL

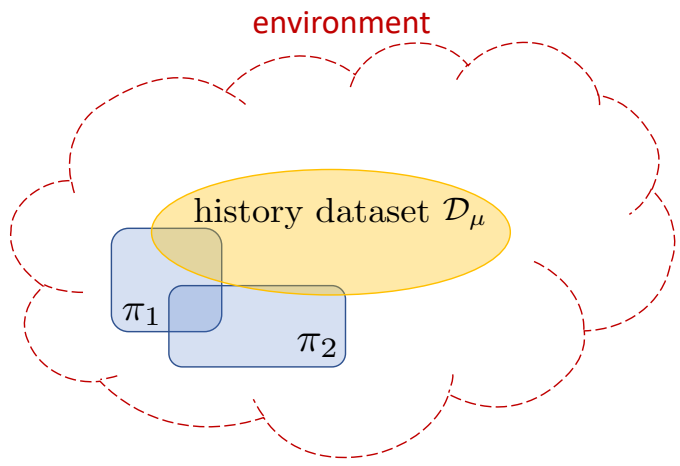
- **Distribution shift**:

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

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



Online/Vanilla Offline: Uniform coverage



Offline RL with partial coverage

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

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

$$C^\star := \max_{s,a} \frac{d^{\pi^\star}(s,a)}{d^{\pi^{\mathsf{b}}}(s,a)}$$

where $d^\pi(s,a) = (1-\gamma)\sum_{t=0}^{\infty} \gamma^t \mathbb{P}\big((s^t,a^t) = (s,a) \,|\, \pi\big)$

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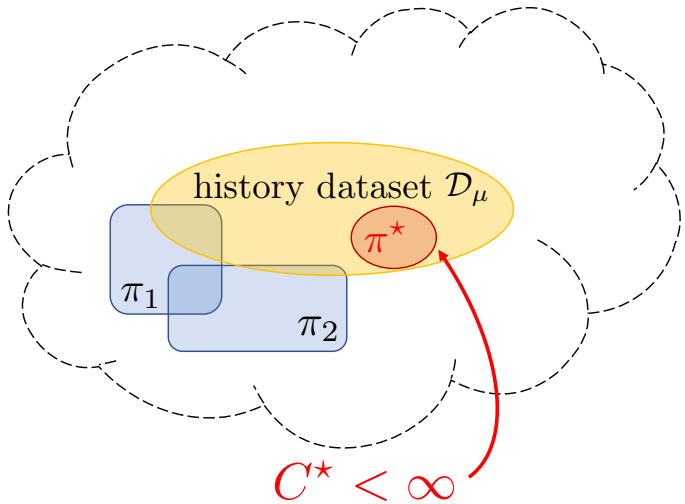
Single-policy concentrability coefficient (Rashidinejad et al. '21)

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

where $d^\pi(s,a) = (1-\gamma)\sum_{t=0}^{\infty} \gamma^t \mathbb{P}\big((s^t,a^t)=(s,a) \,|\, \pi\big)$

- captures distributional shift
- allows for partial coverage



A model-based offline algorithm: VI-LCB

Pessimism in the face of uncertainty: penalize value estimate of those (s, a) pairs that were poorly visited

A model-based offline algorithm: VI-LCB

Pessimism in the face of uncertainty: penalize value estimate of those (s, a) pairs that were poorly visited

Algorithm: value iteration w/ lower confidence bounds

- compute empirical estimate $\widehat{P}$ of P
- initialize $\widehat{Q} = 0$, and repeat

$$\widehat{Q}(s,a) \;\leftarrow\; \max\Big\{r(s,a) + \gamma\langle \widehat{P}(\cdot \,|\, s,a), \widehat{V}\rangle - \underbrace{b(s,a;\widehat{V})}_{\text{Bernstein-style confidence bound}} \;,\; 0\Big\}$$

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

Minimax optimality of model-based offline RL

Theorem 3 (Li, Shi, Chen, Chi, Wei '22)

For any $0 < \varepsilon \leq \frac{1}{1-\gamma}$, *the policy* $\widehat{\pi}$ *returned by VI-LCB 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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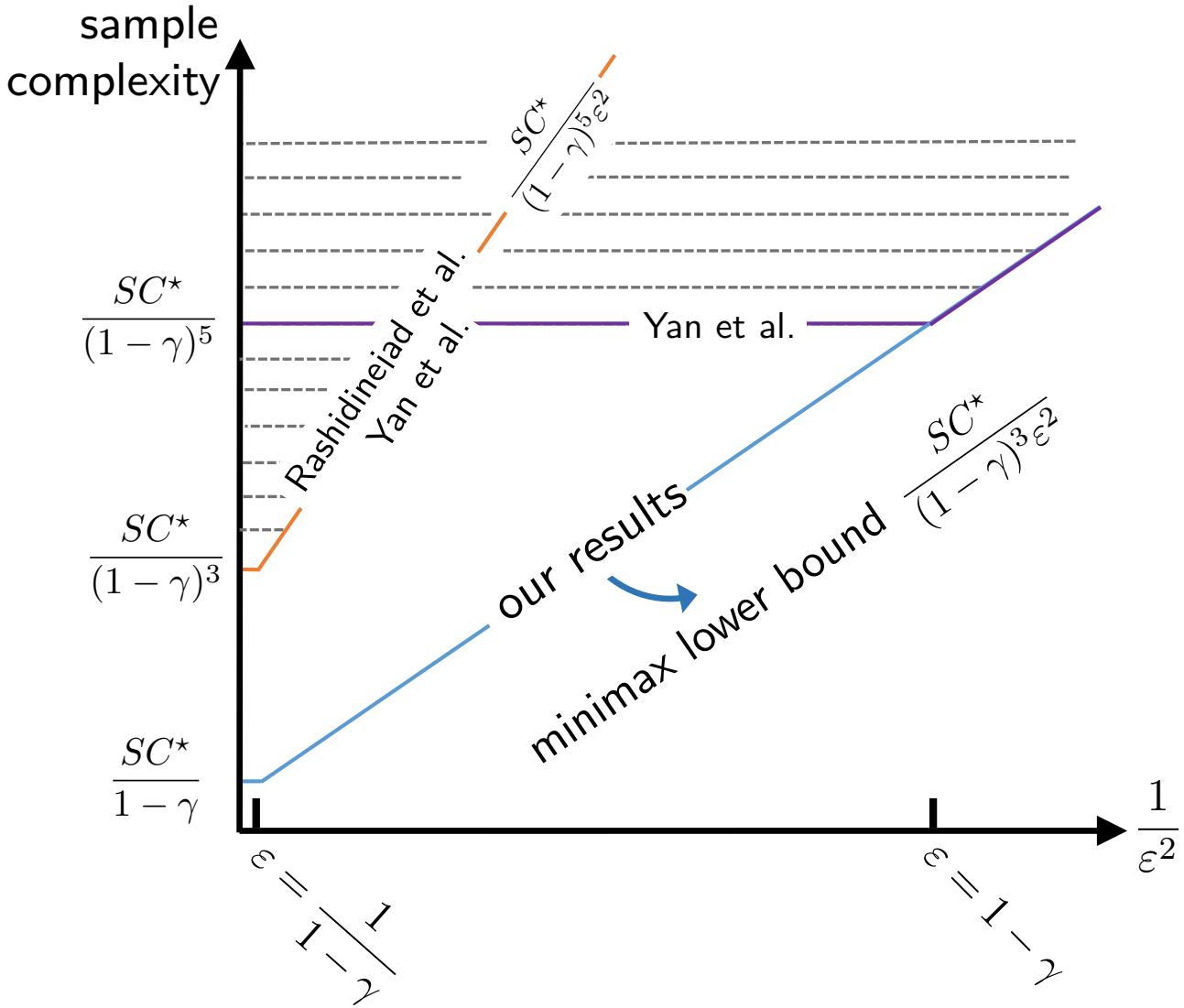
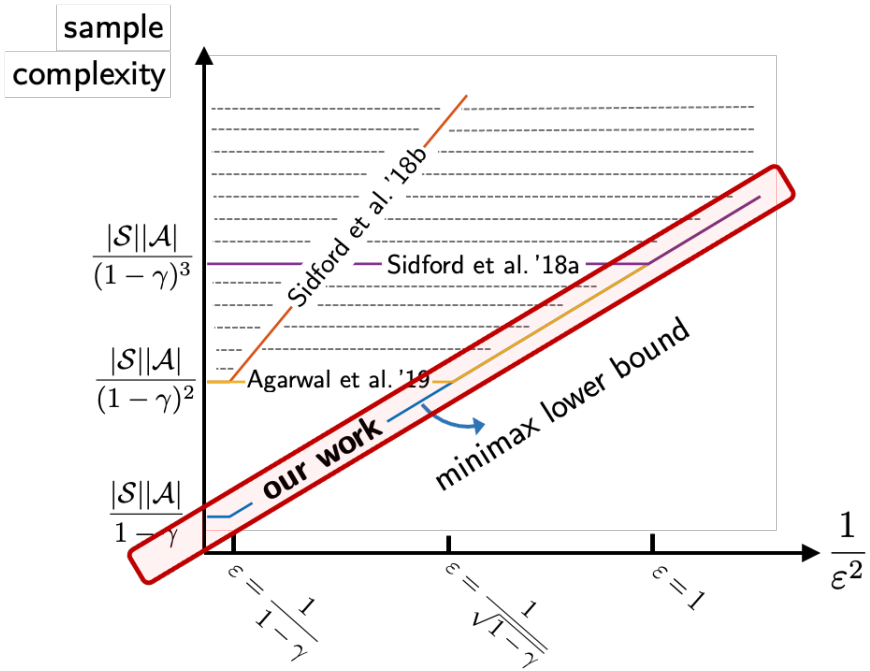
- matches minimax lower bound: $\widetilde{\Omega}(\frac{SC^{\star}}{(1-\gamma)^3\varepsilon^2})$ (Rashidinejad et al. '21)
- depends on distribution shift (as reflected by $C^{\star}$)
- full ε-range (no burn-in cost)

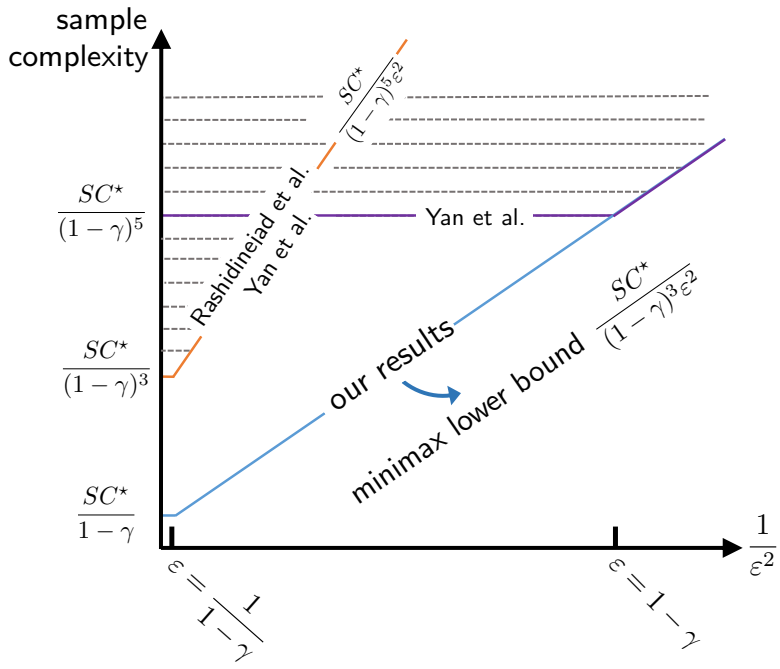
Comparisons with prior art



Summary of this part



generative model



offline RL

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

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