PC-PG: Policy Cover Directed Exploration for Provable Policy Gradient Learning

Joint work with Alekh Agarwal, Mikael Henaff, and Sham Kakade









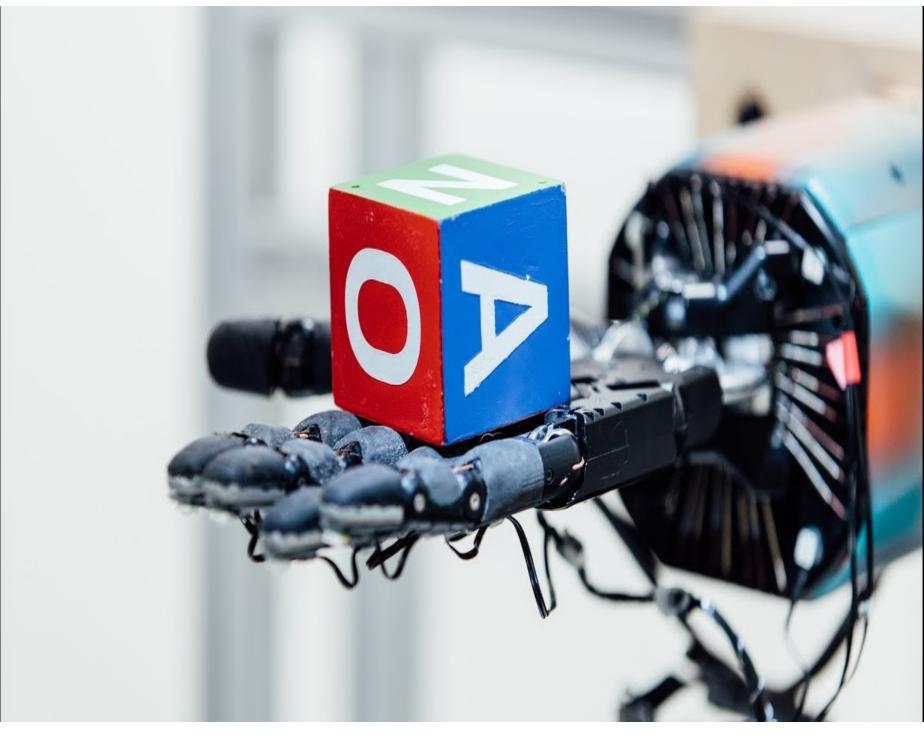




Policy Optimization







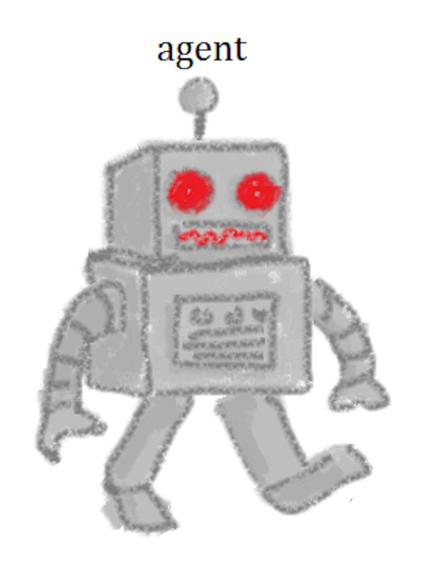
[AlphaZero, Silver et.al, 17]

[OpenAl Five, 18]

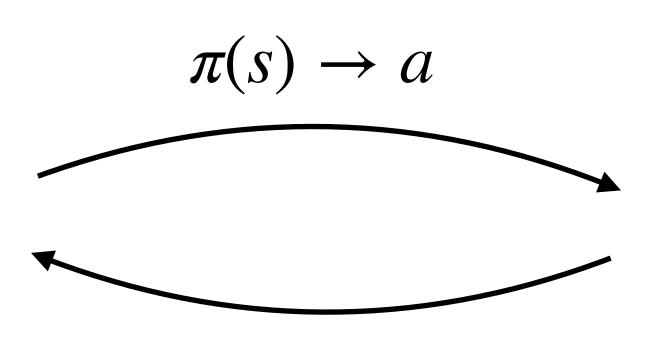
[OpenAI,19]

Can we design Provably Correct Policy Gradient algorithms?

Infinite Horizon Discounted MDPs



Policy: state to action



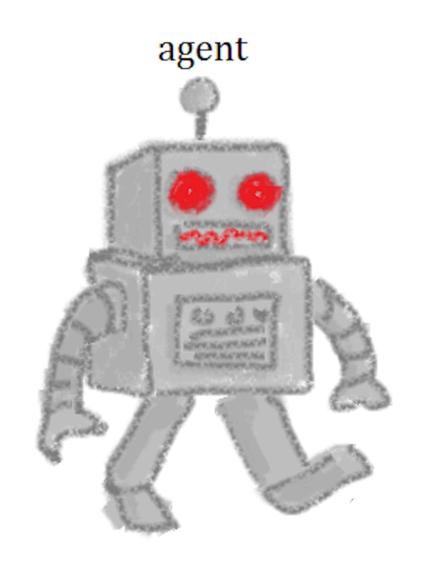


Reward & Next State

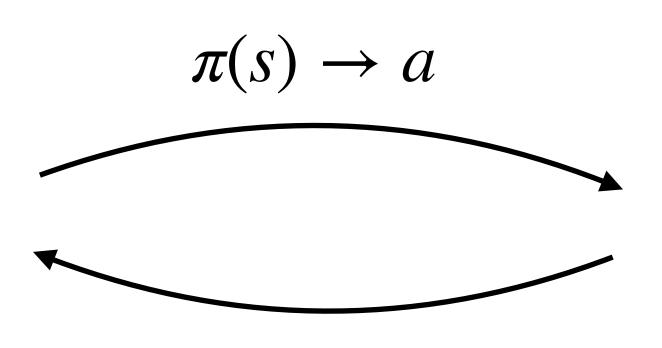
$$r(s,a), s' \sim P(\cdot \mid s,a)$$

Objective:
$$\max_{\pi} \mathbb{E}_{\pi,P} \left[r_0 + \gamma r_1 + \gamma^2 r_2 + \ldots \right]$$

Infinite Horizon Discounted MDPs



Policy: state to action





Reward & Next State

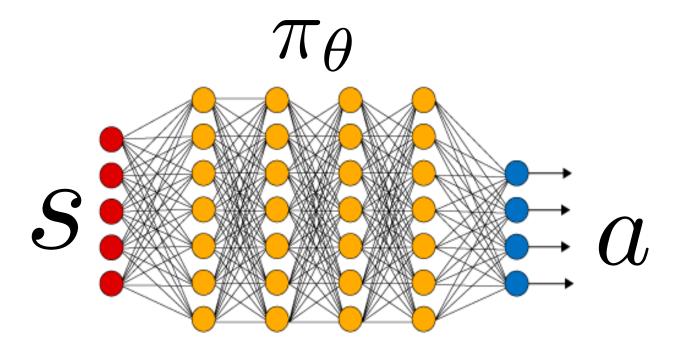
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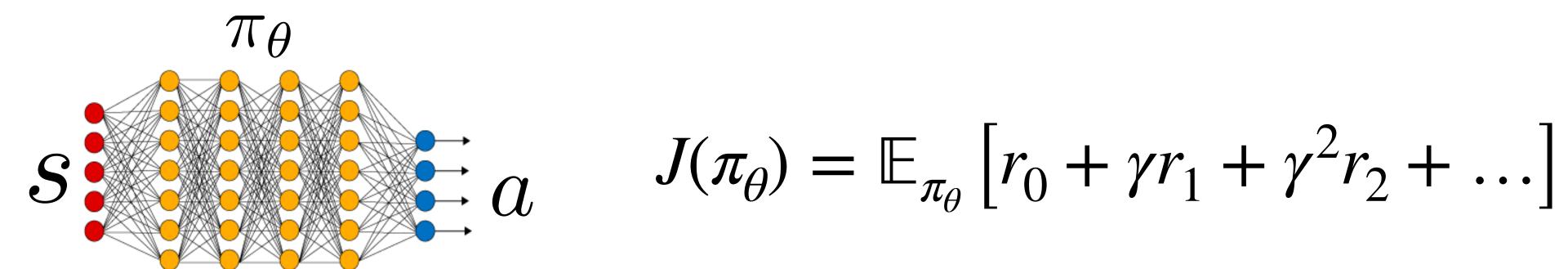
Assume $s_0 \sim \mu_0$ and we can only reset from μ_0

e.g., Reinforce, Natural Policy Gradient, TRPO, PPO:

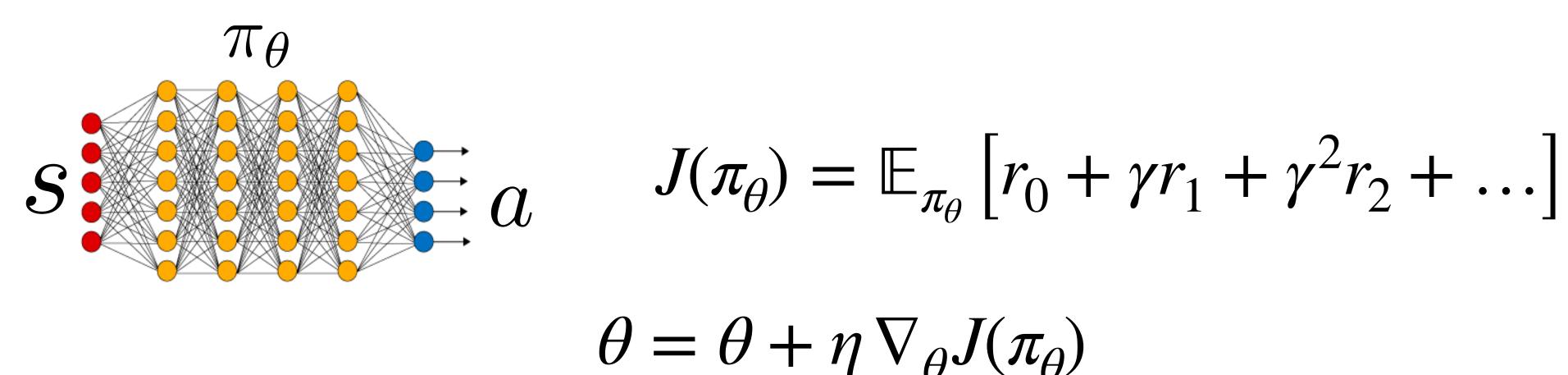
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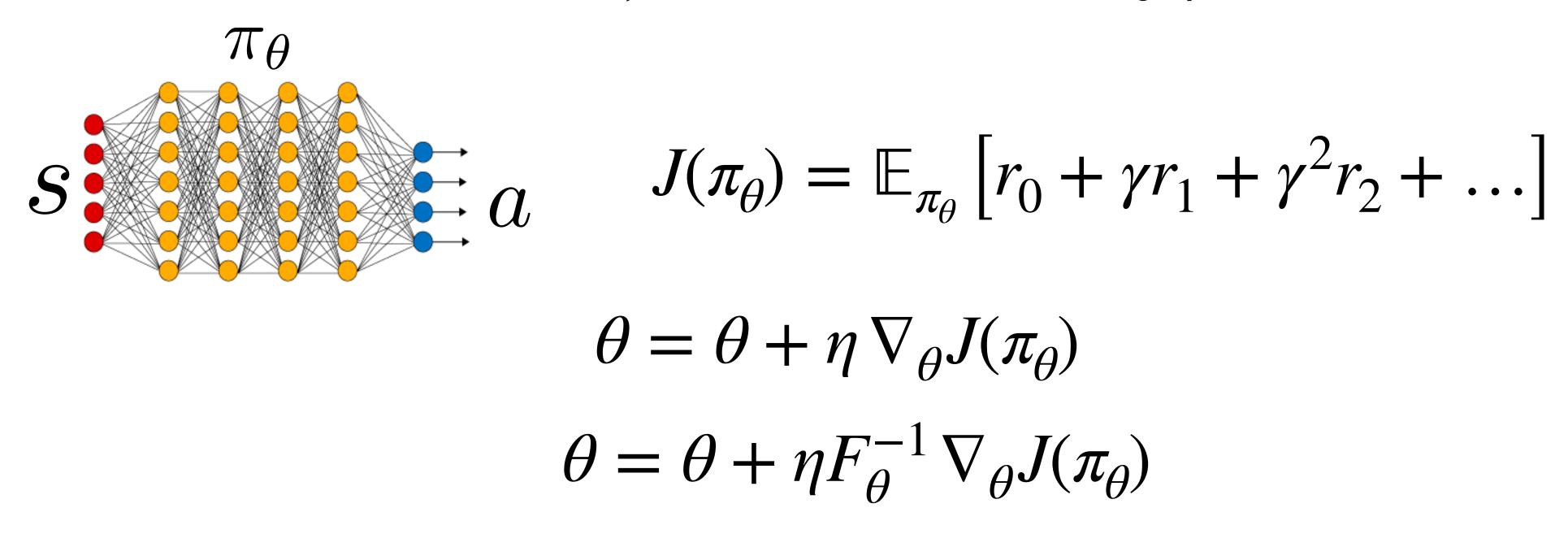
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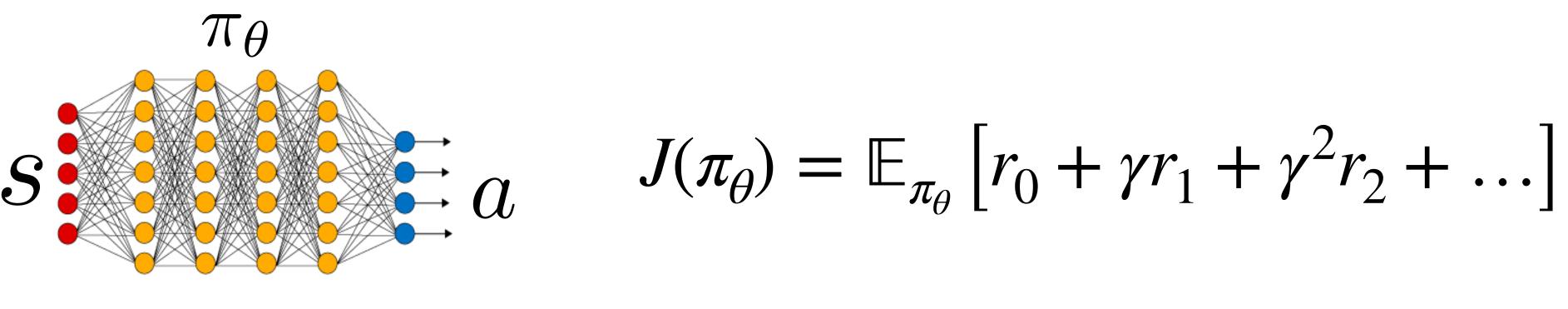


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e.g., Reinforce, Natural Policy Gradient, TRPO, PPO:

(Williams 92, Kakade 02, Schulman et al 15, 17)



$$\theta = \theta + \eta \nabla_{\theta} J(\pi_{\theta})$$

$$\theta = \theta + \eta F_{\theta}^{-1} \nabla_{\theta} J(\pi_{\theta})$$

Preconditioning w/ Fisher Information matrix

(TRPO and PPO are variants of it)

Strong Agnostic guarantee:

Compete to the best policy in the given class: $\widetilde{\pi} \in \Pi$

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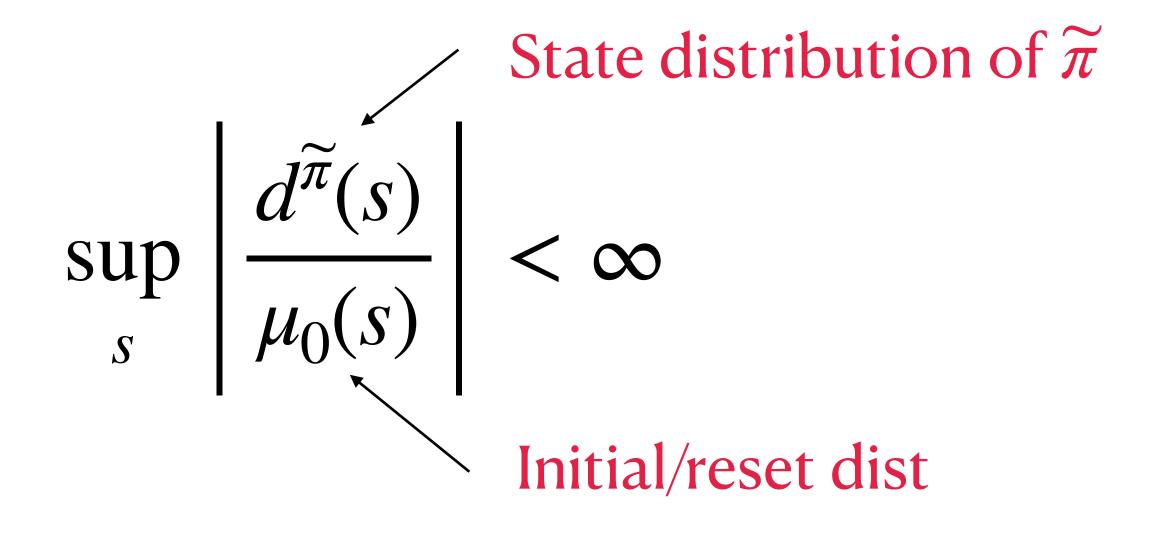
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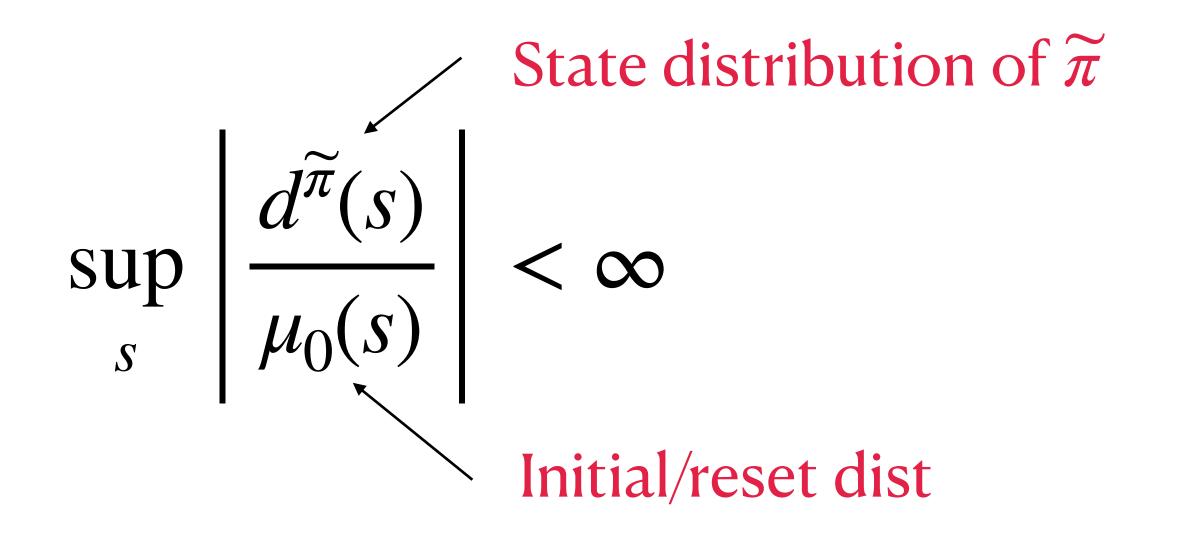
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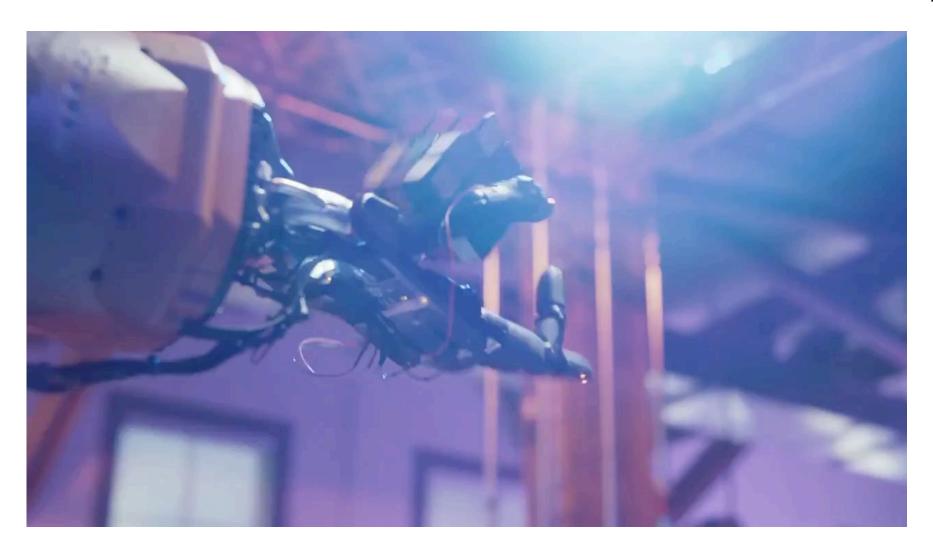
Q-learning, Fitted Q iteration:

Realizability (& Bellman Complete)

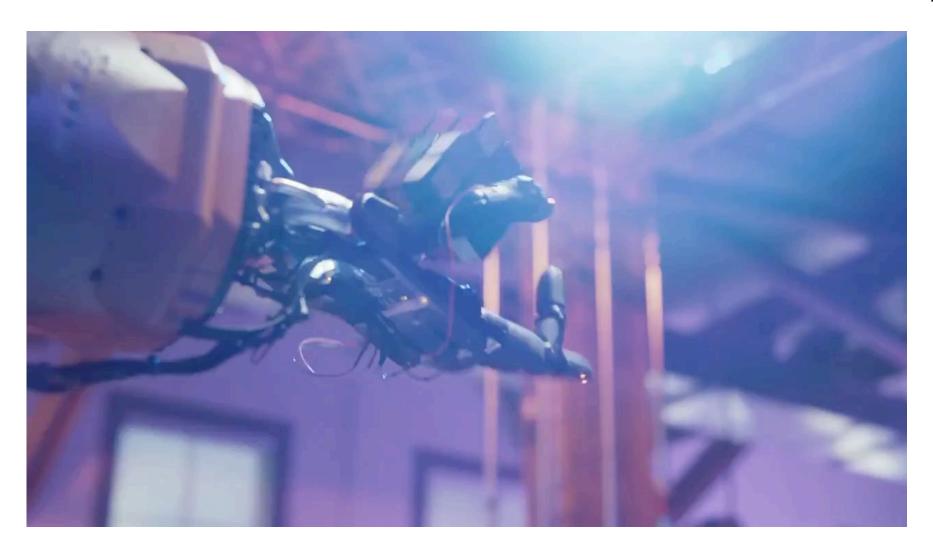
$$Q^{\star} \in \mathcal{Q}$$

Robot hand manipulation (OpenAI, 19)

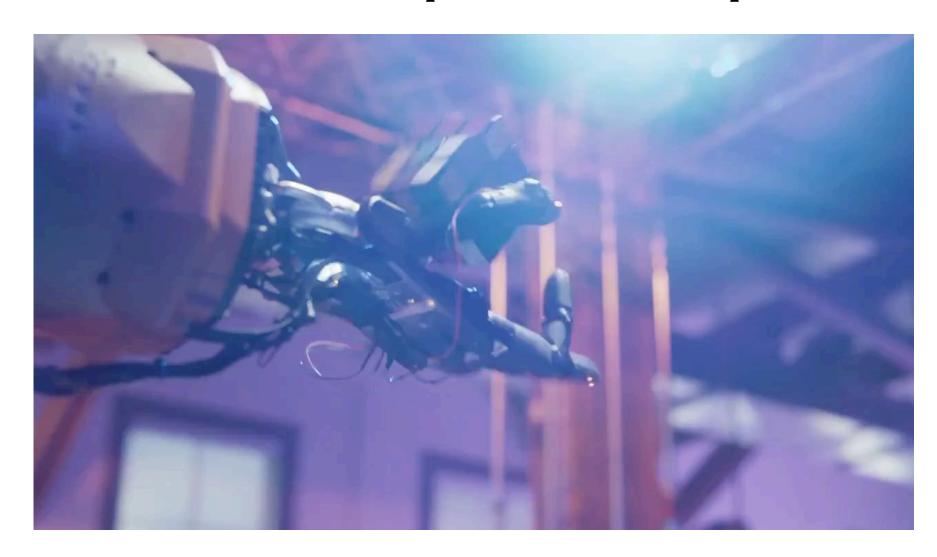
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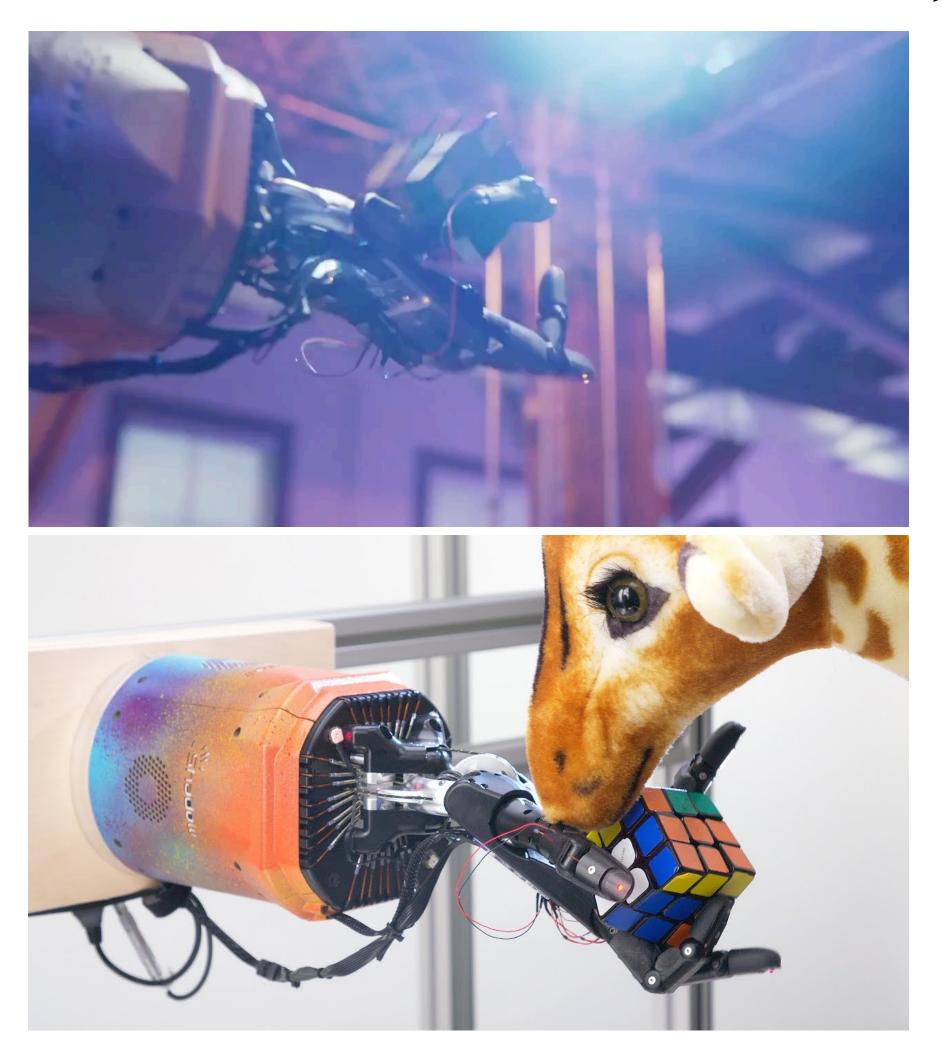
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A notable technique

Domain Randomization:

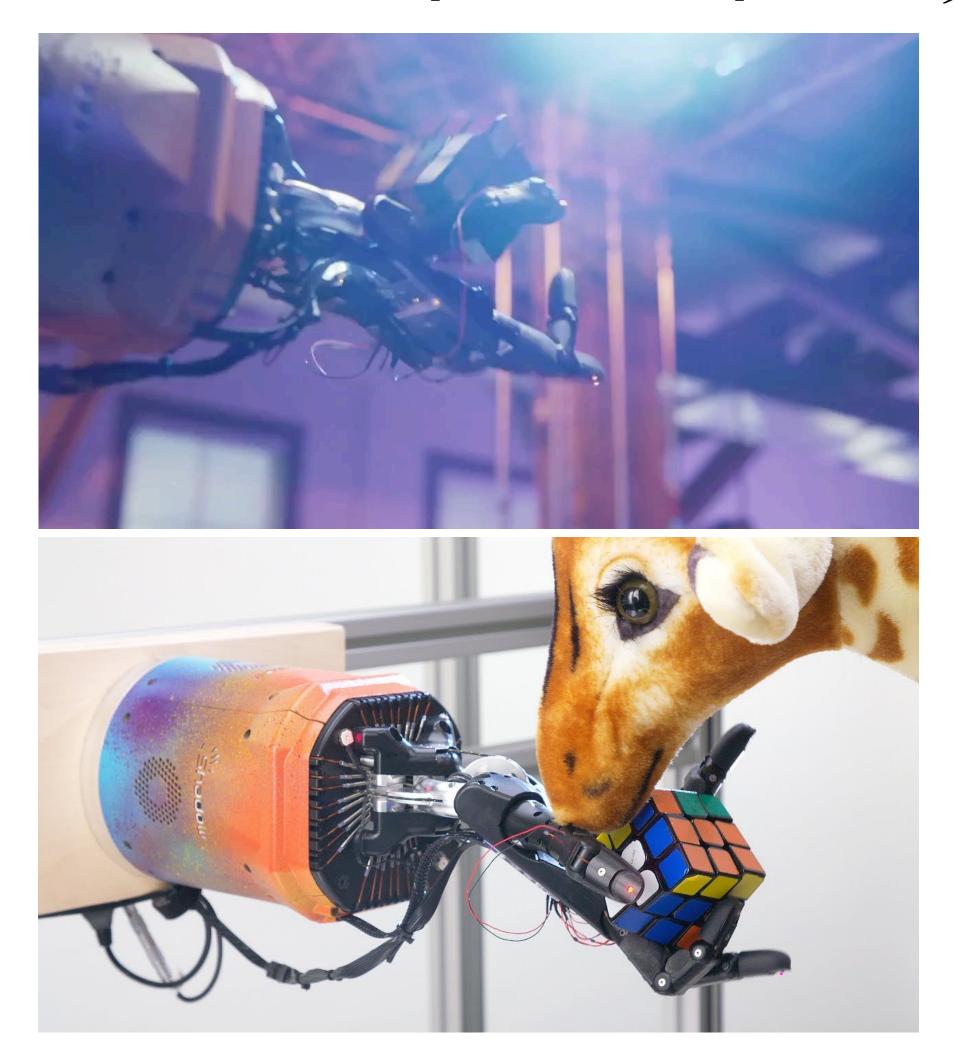
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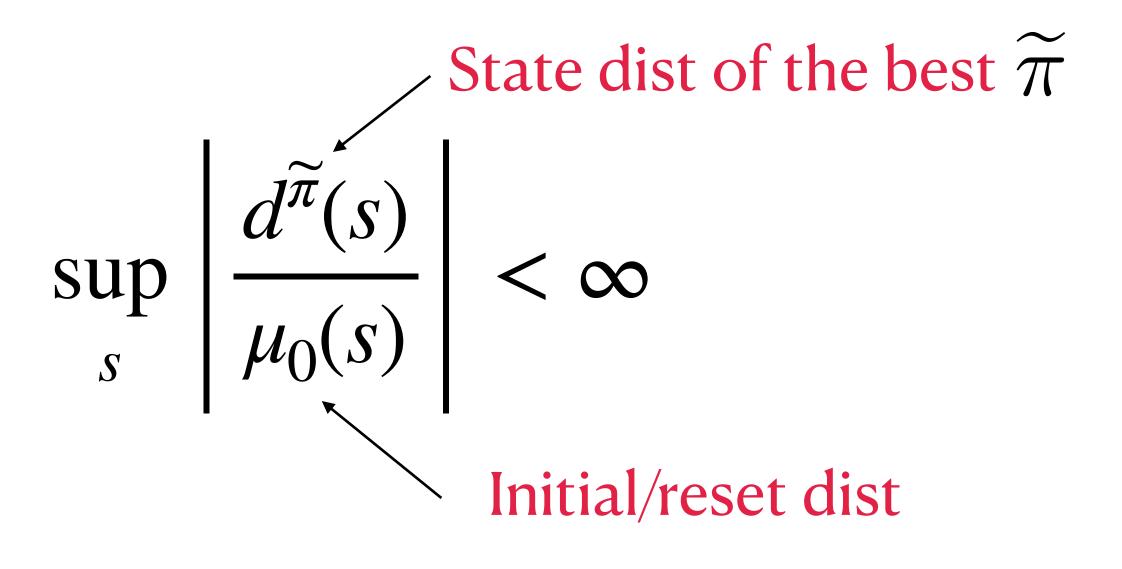
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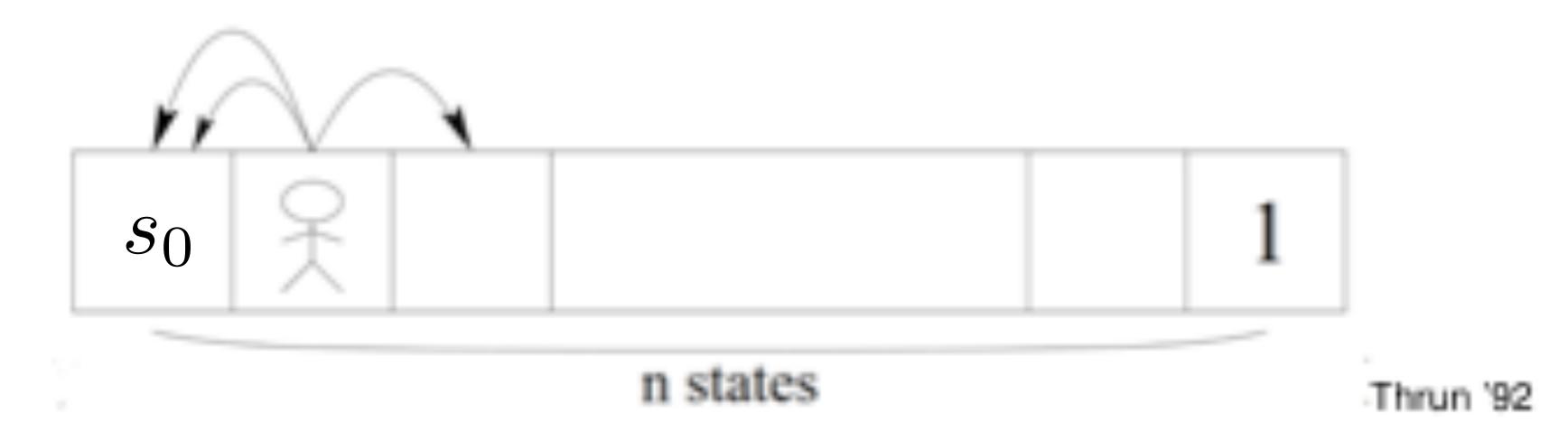
Domain Randomization:



Make μ_0 as "wide" as possible!!

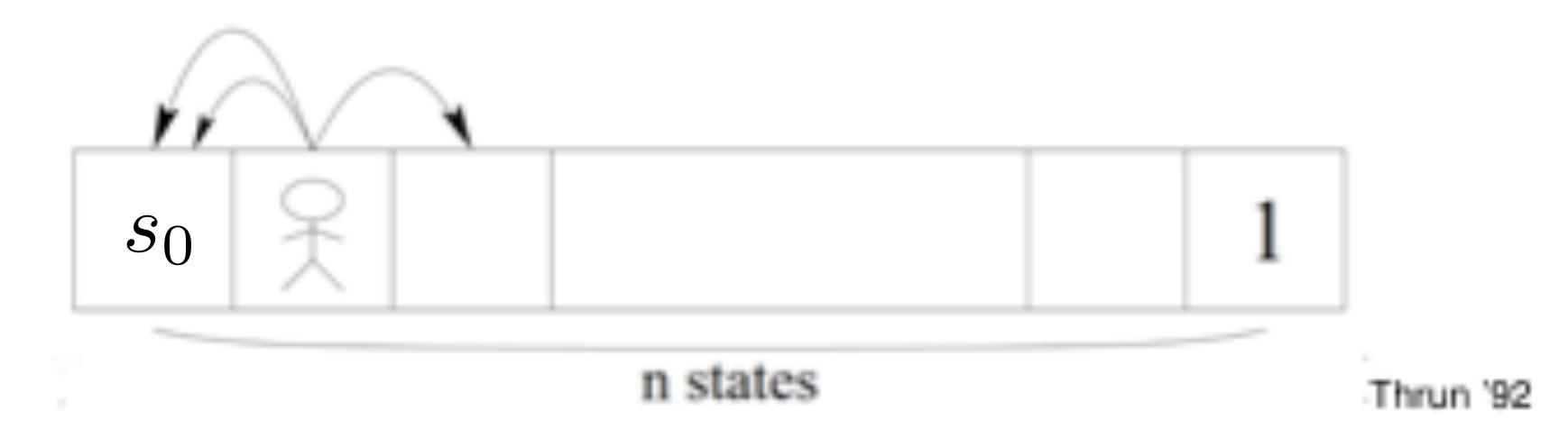
But PG Fails if initial condition does not hold, provably

Initialization: S_0 + random walk



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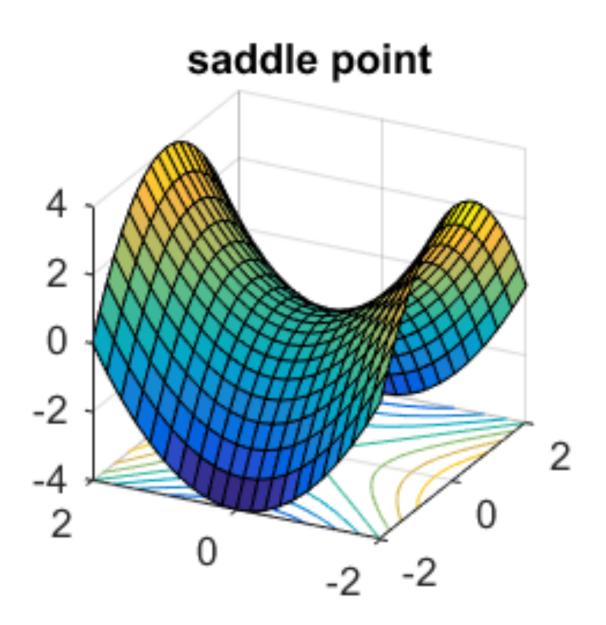
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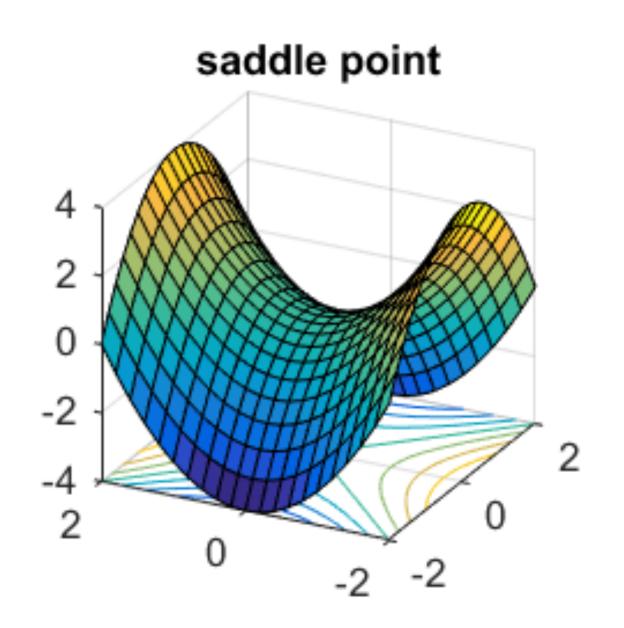
Extremely flatten gradient:

magnitude of gradient is exponentially small (even in higher order): 2^{-H}

(e.g., see CPI from Kadade & Langford 02, and Agarwal et al 19)

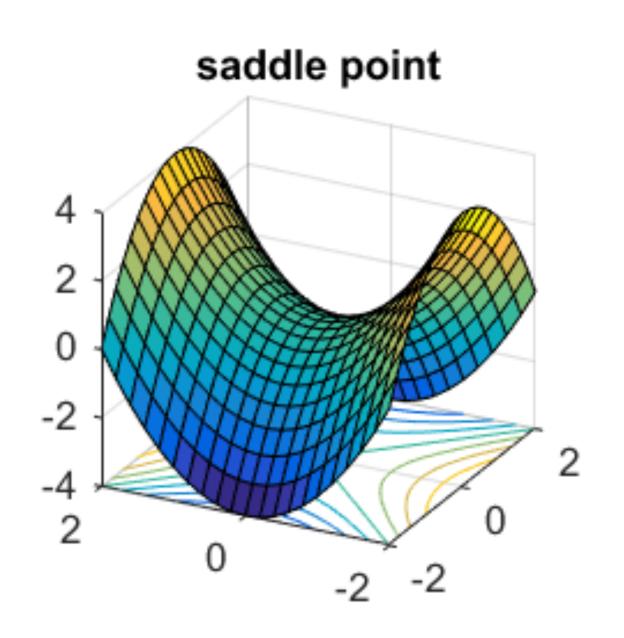


Supervised Learning



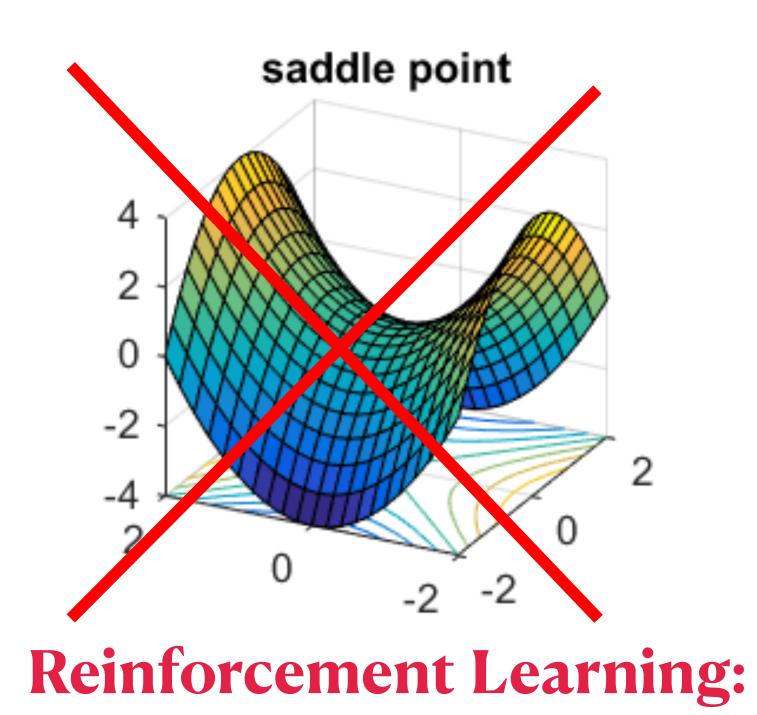
Supervised Learning

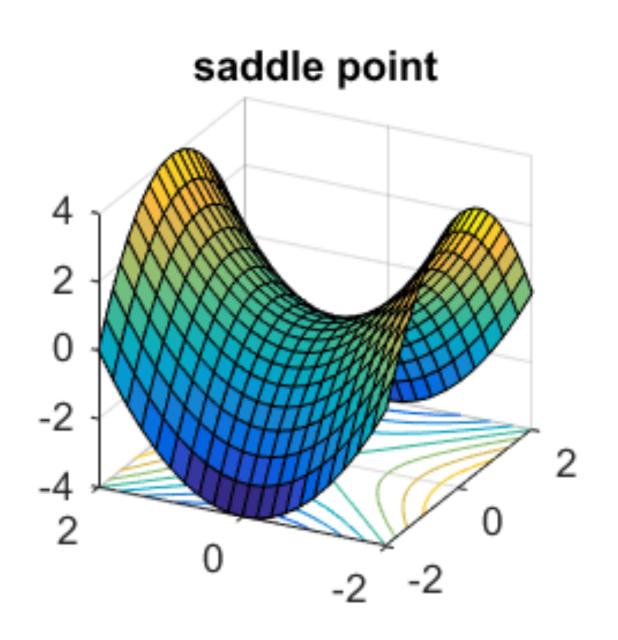
- Gradient descent tends to just work
- Not sensitive to initialization
- Saddle point is not a problem



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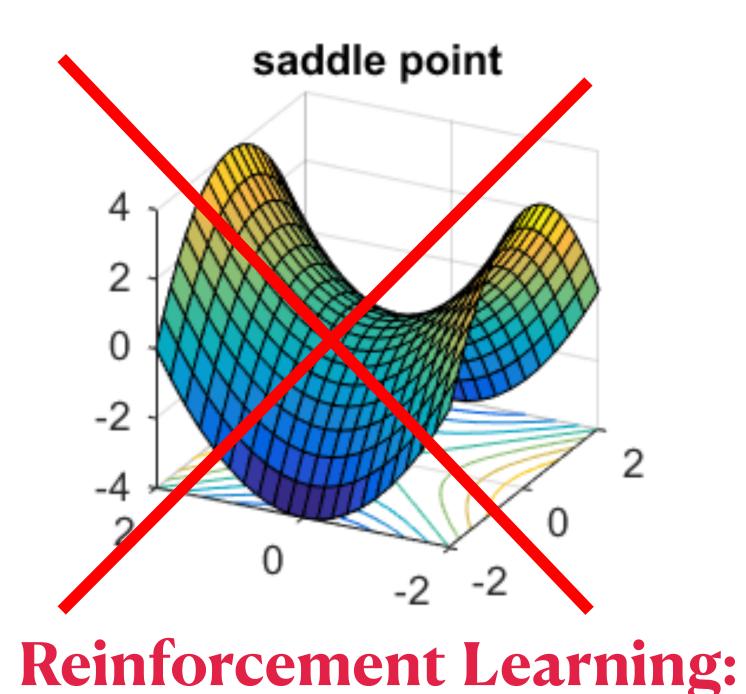
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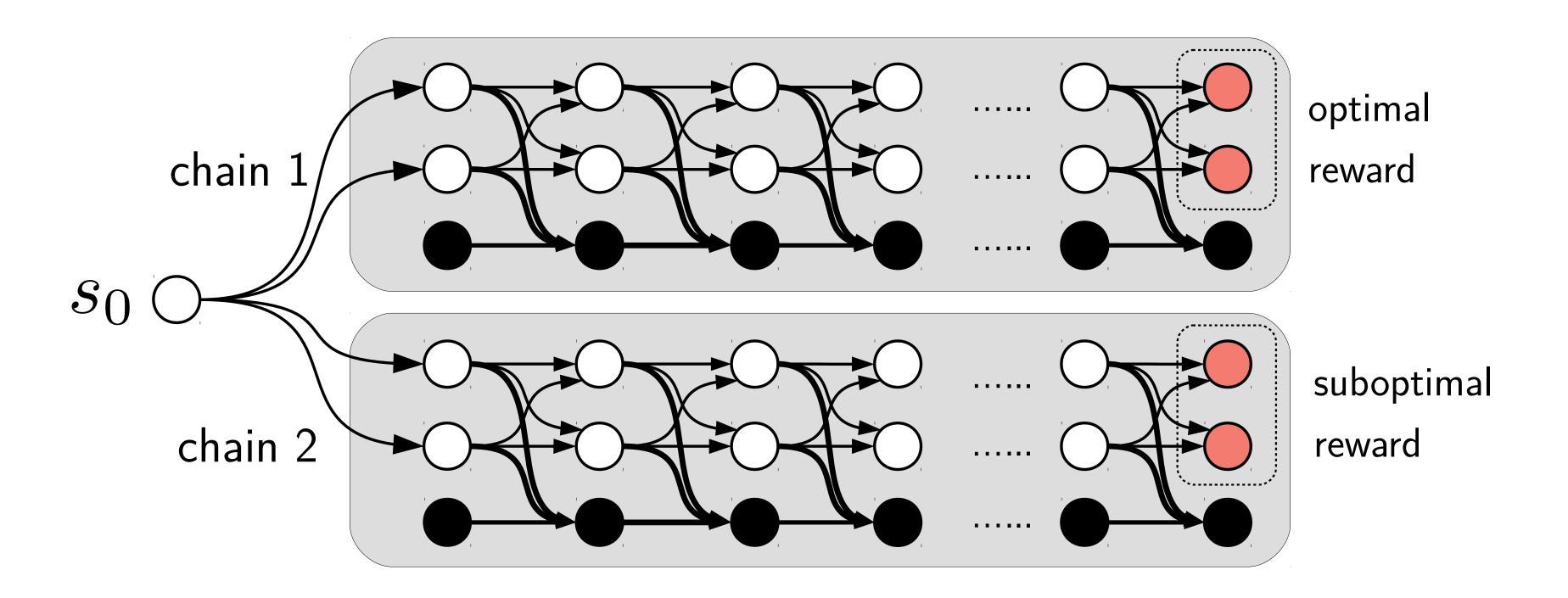


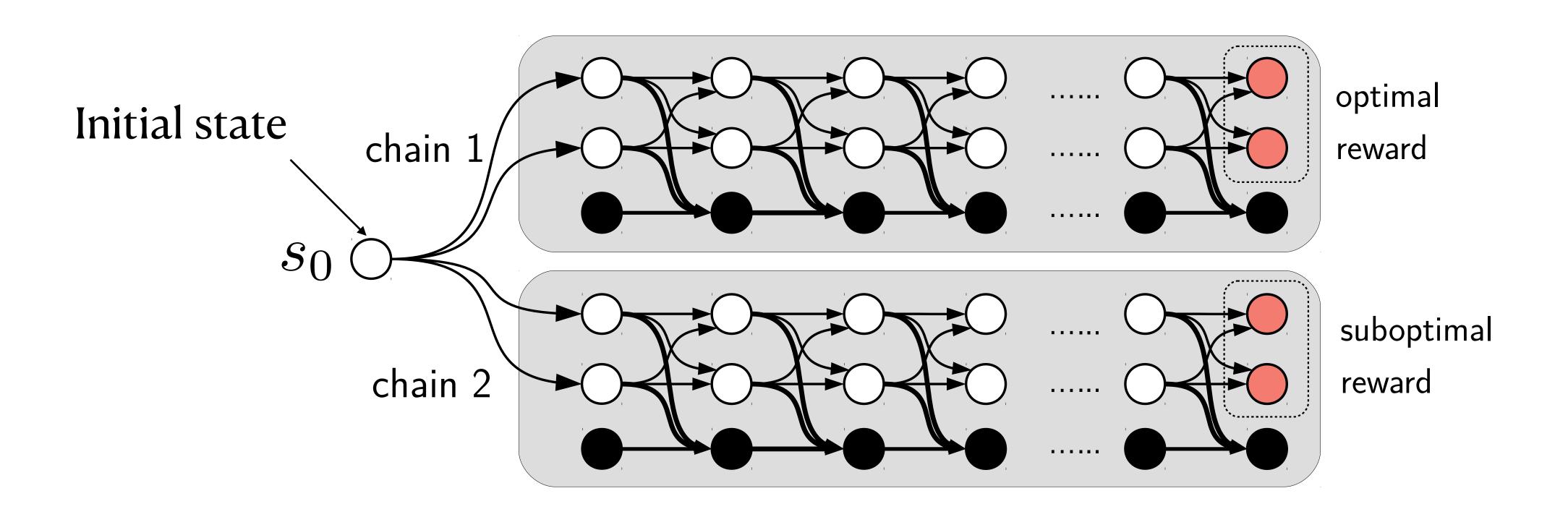
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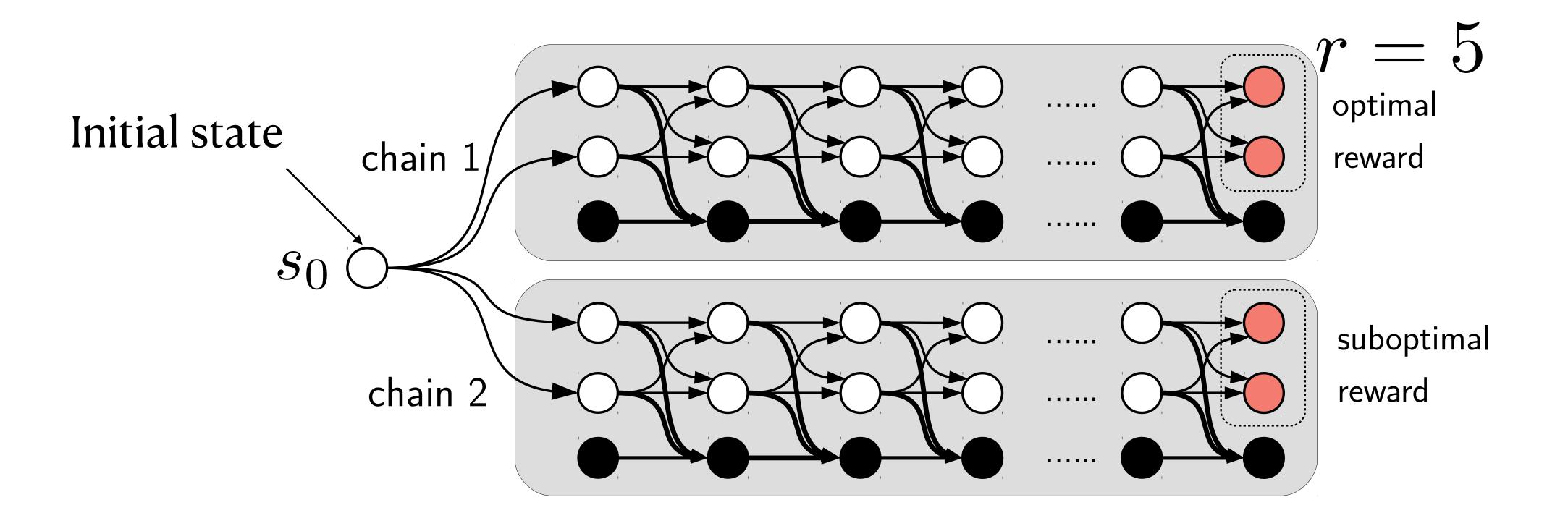
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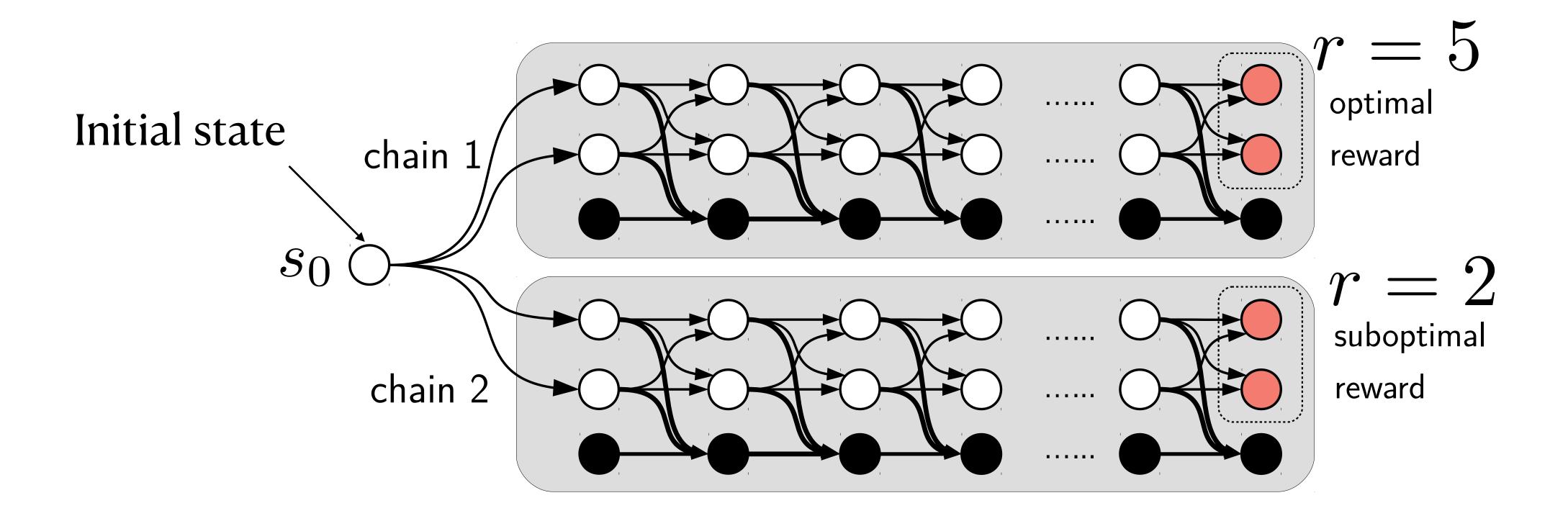


- Extremely flatten region even at initialization
- Due to lack of exploration

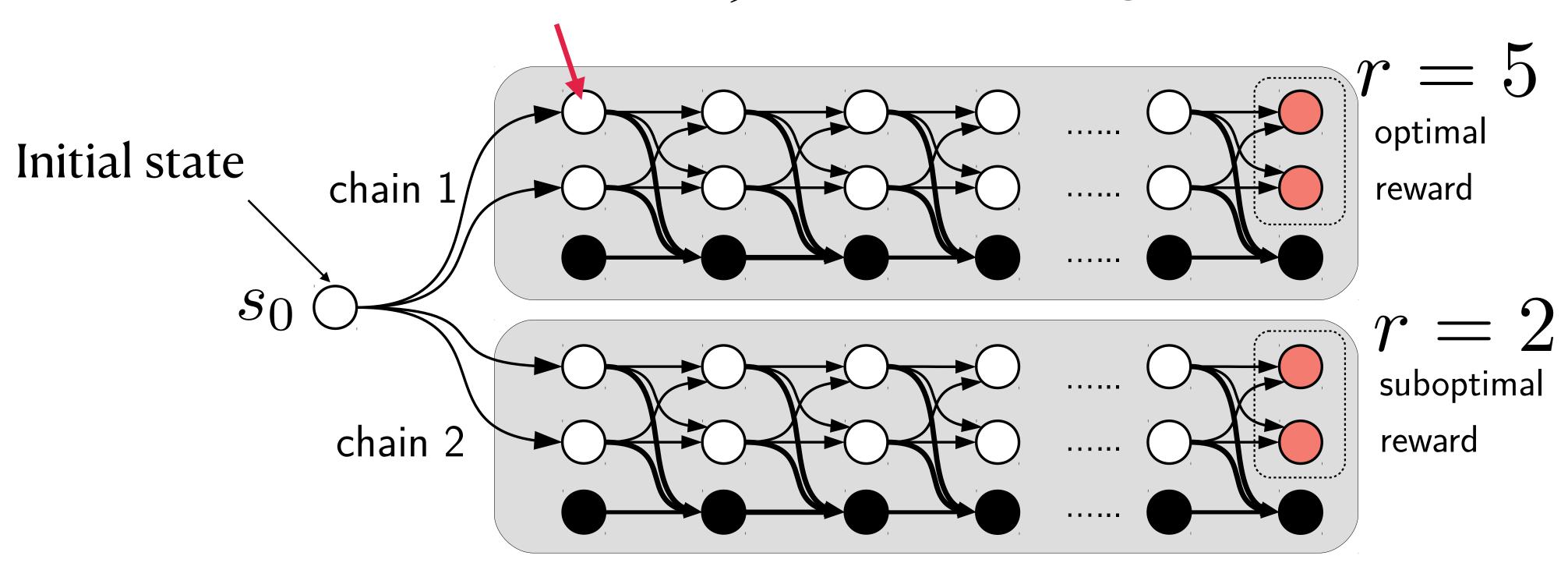




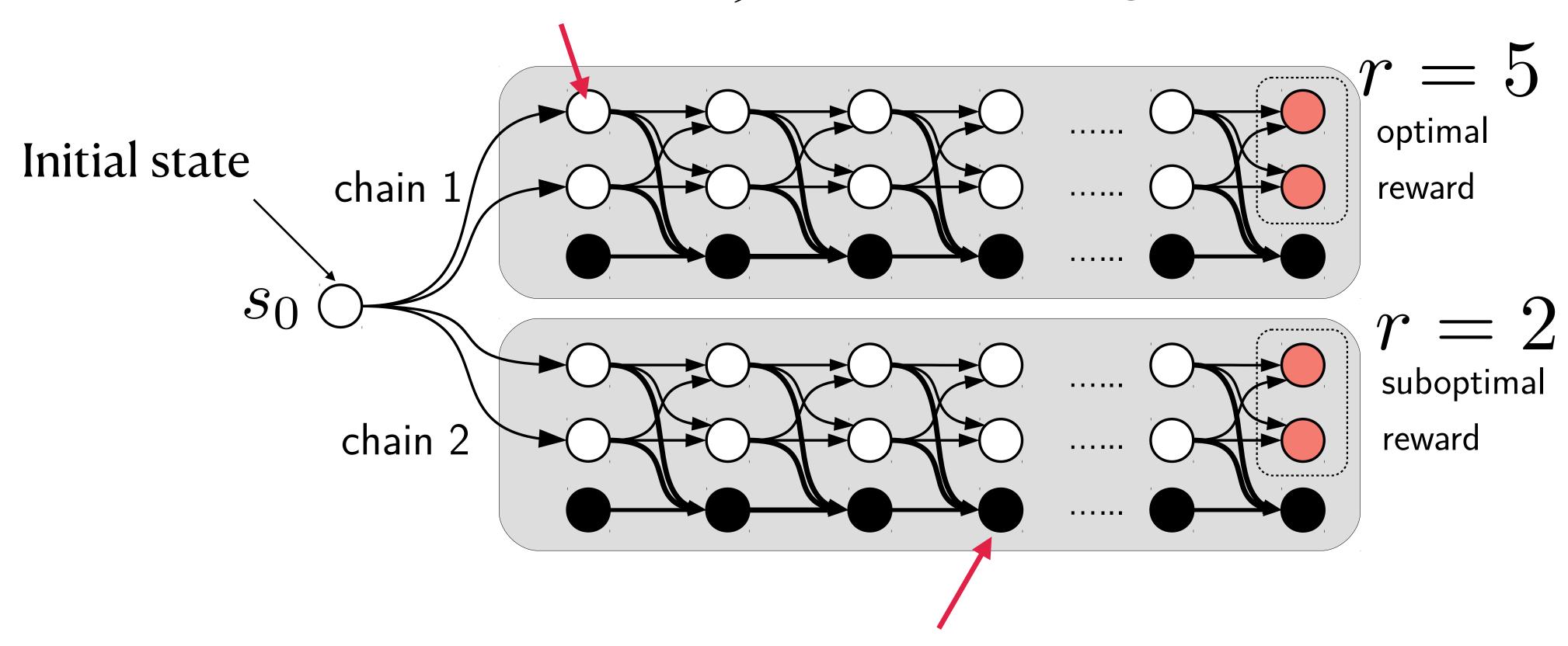




"survived" state (white): 9 out of 10 actions go to bad state (black)



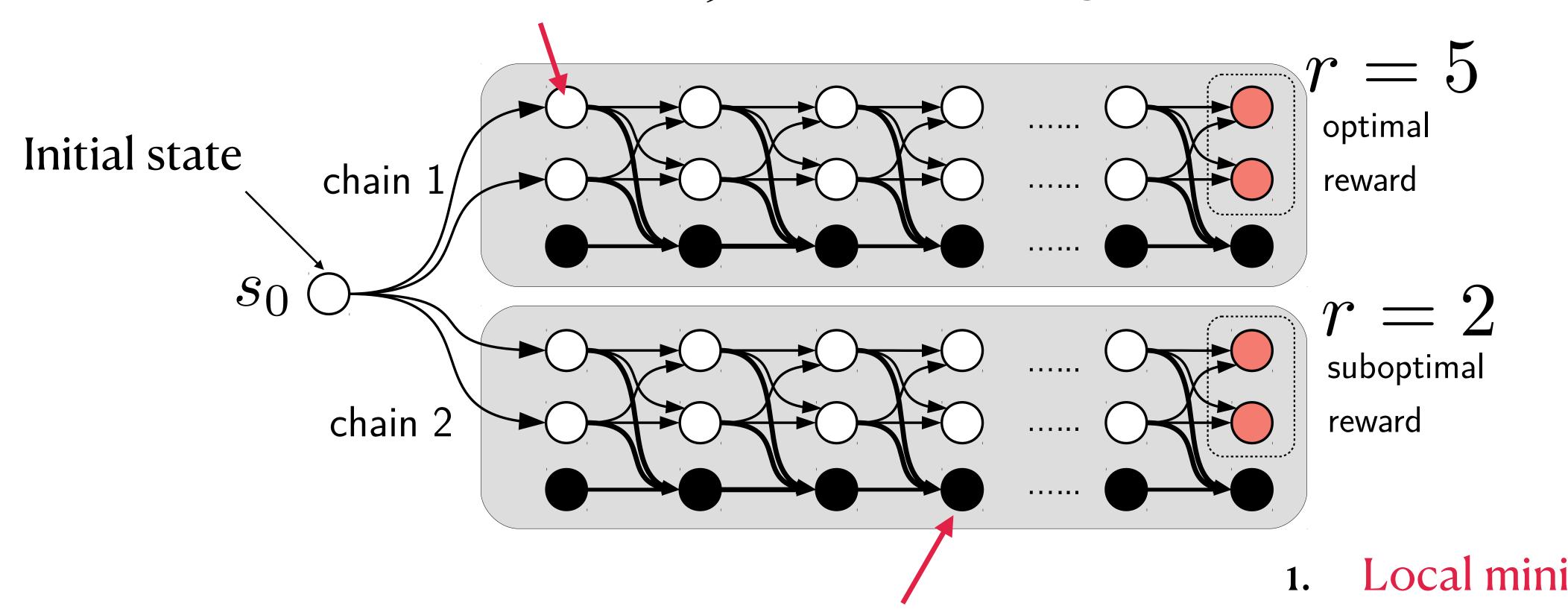
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Bad state (cannot recover) has Anti-shaped reward:

$$r = 1/H$$

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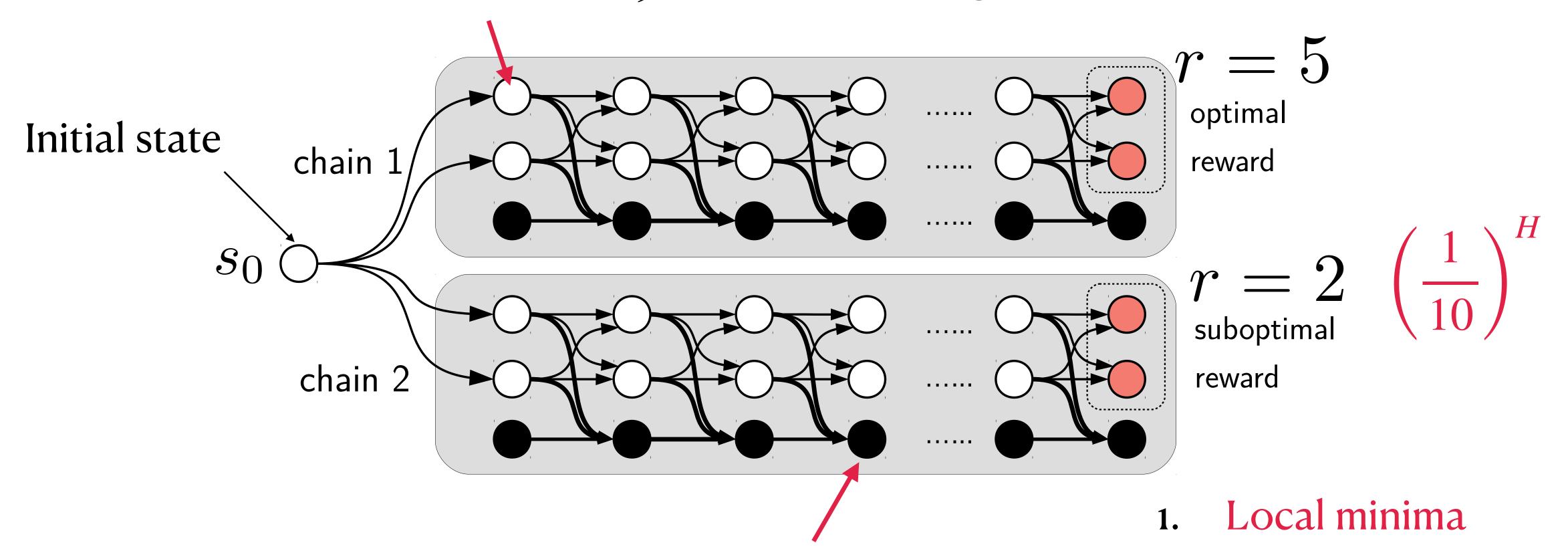


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2. Forgetting (policy becomes deterministic

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Experiments on Bi-directional Comb Lock

Success Rate (visit the better chain):

Algorithm	Horizon			
	2	5	10	15
PPO	1.0	0.0	0.0	0.0
PPO+RND	0.75	0.40	0.50	0.55
PC-PG	?	?	?	?

PPO+RND: Random Network Distillation [Burda et.al, 19]

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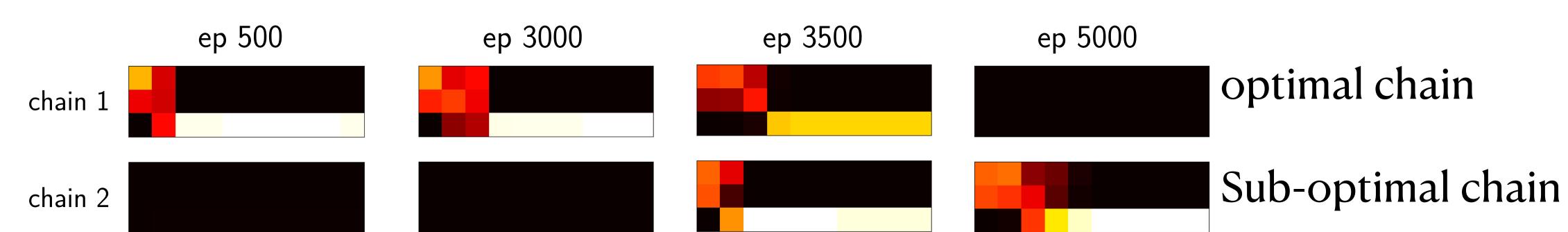
PPO+RND: Random Network Distillation [Burda et.al, 19]

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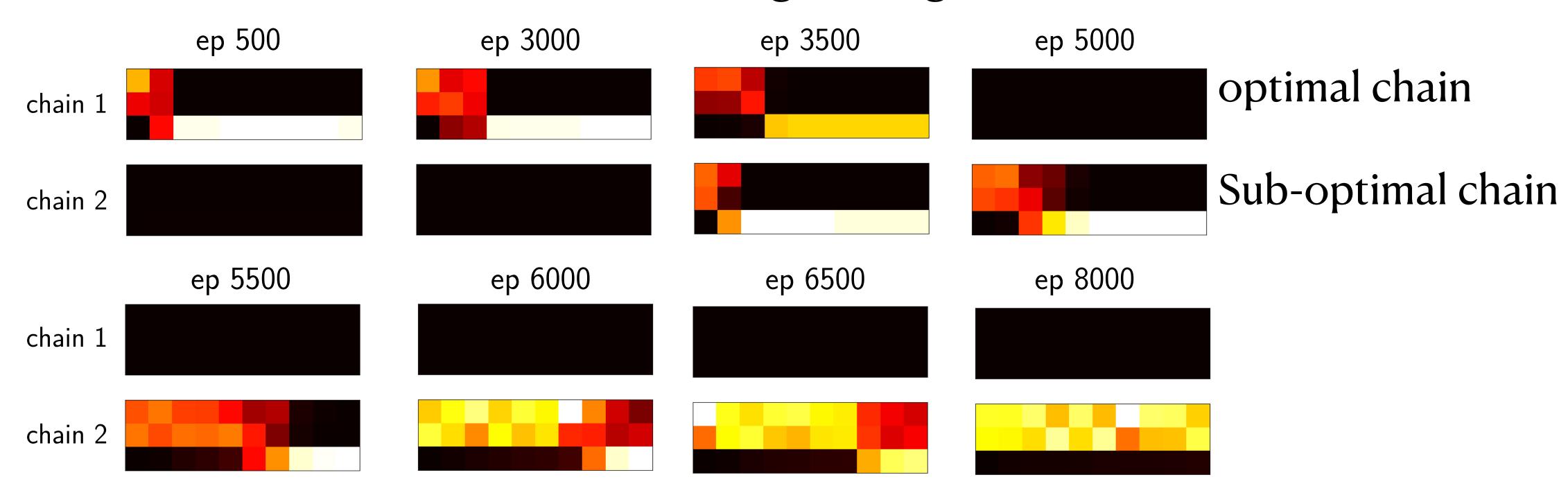
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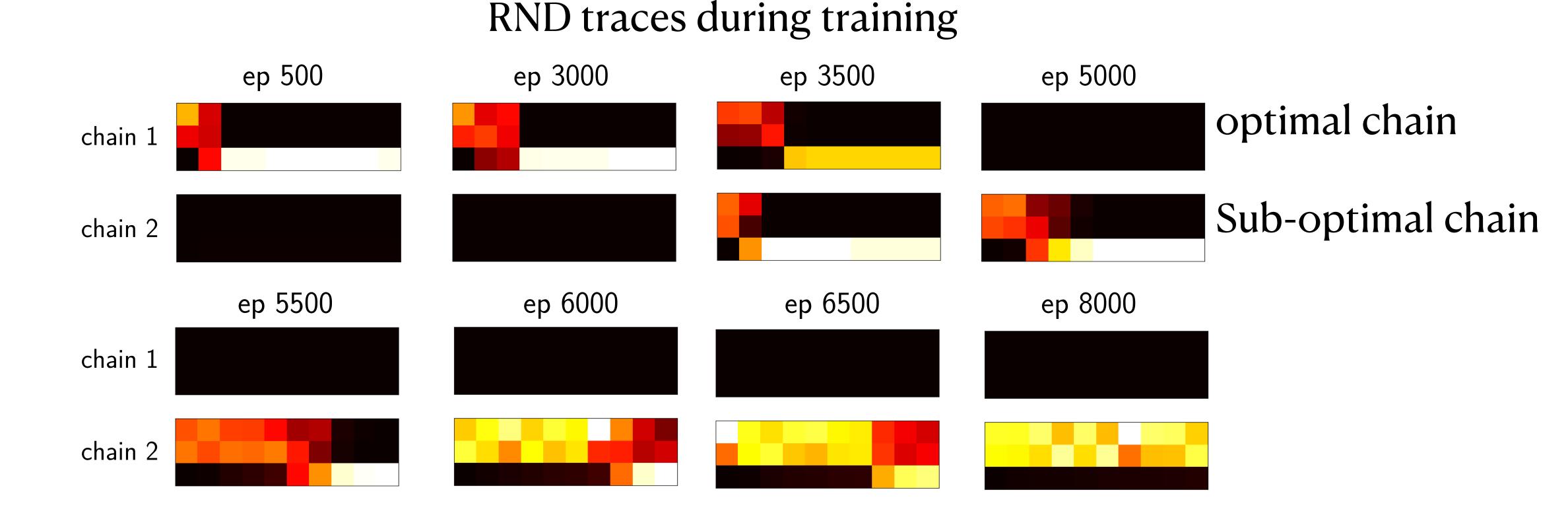
> Forgets to visit the other chain!





RND traces during training





Policy quickly becomes too deterministic and forgets to explore the other (better!) chain

Summary of PG methods' common issues

1. Lack ability to explore

1. Catastrophic forgetting (even w/ reward bonus)

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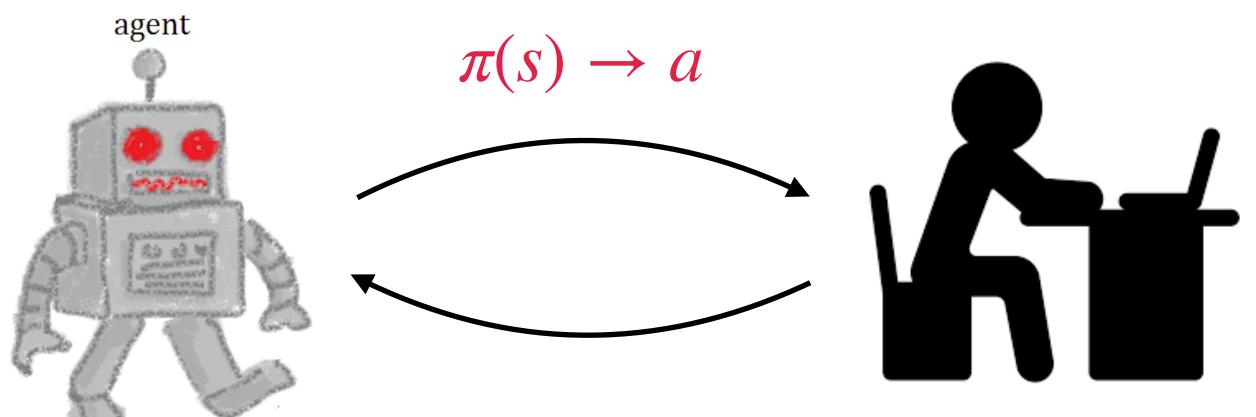
1. Catastrophic forgetting (even w/ reward bonus)

Next:

Our Solution: Policy Cover Policy Gradient (PC-PG)
Policy Ensemble + Reward Bonus

Notations

Policy: state to action



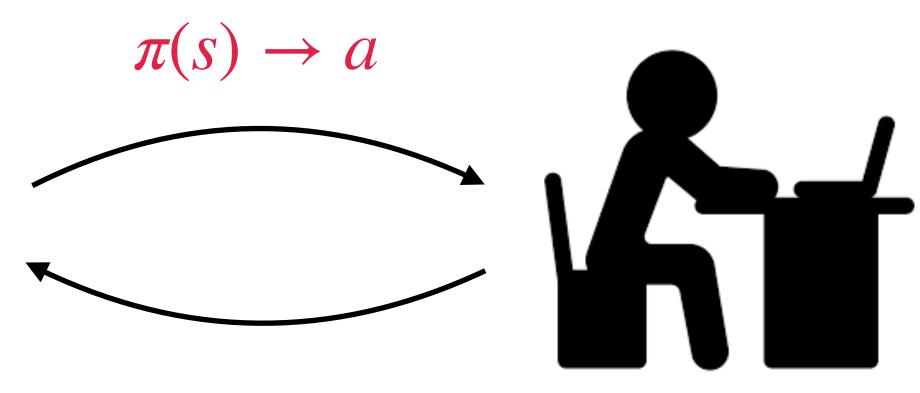
Reward & Next State

$$r(s,a), s' \sim P(\cdot \mid s,a)$$

Notations

Policy: state to action

agent



Value and Q function

$$V^{\pi}(s) = \mathbb{E}\left[r(s_0, a_0) + \gamma r(s_1, a_1) + \dots \mid s_0 = s, a_h \sim \pi(s_h)\right]$$
$$Q^{\pi}(s, a) = r(s, a) + \gamma \mathbb{E}_{s' \sim P(\cdot \mid s, a)} V^{\pi}(s')$$

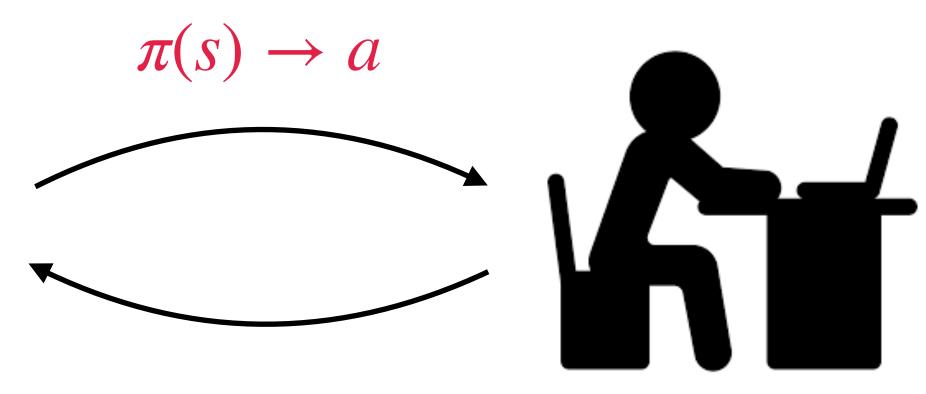
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Reward & Next State

$$r(s,a), s' \sim P(\cdot \mid s,a)$$

Policy's state-action distribution

$$d^{\pi}(s,a) = (1-\gamma) \sum_{h=0}^{\infty} \gamma^h \mathbb{P}^{\pi} \left((s_h, a_h) = (s,a) \right)$$

$$\{\pi_1, \pi_2, \dots, \pi_n\}$$

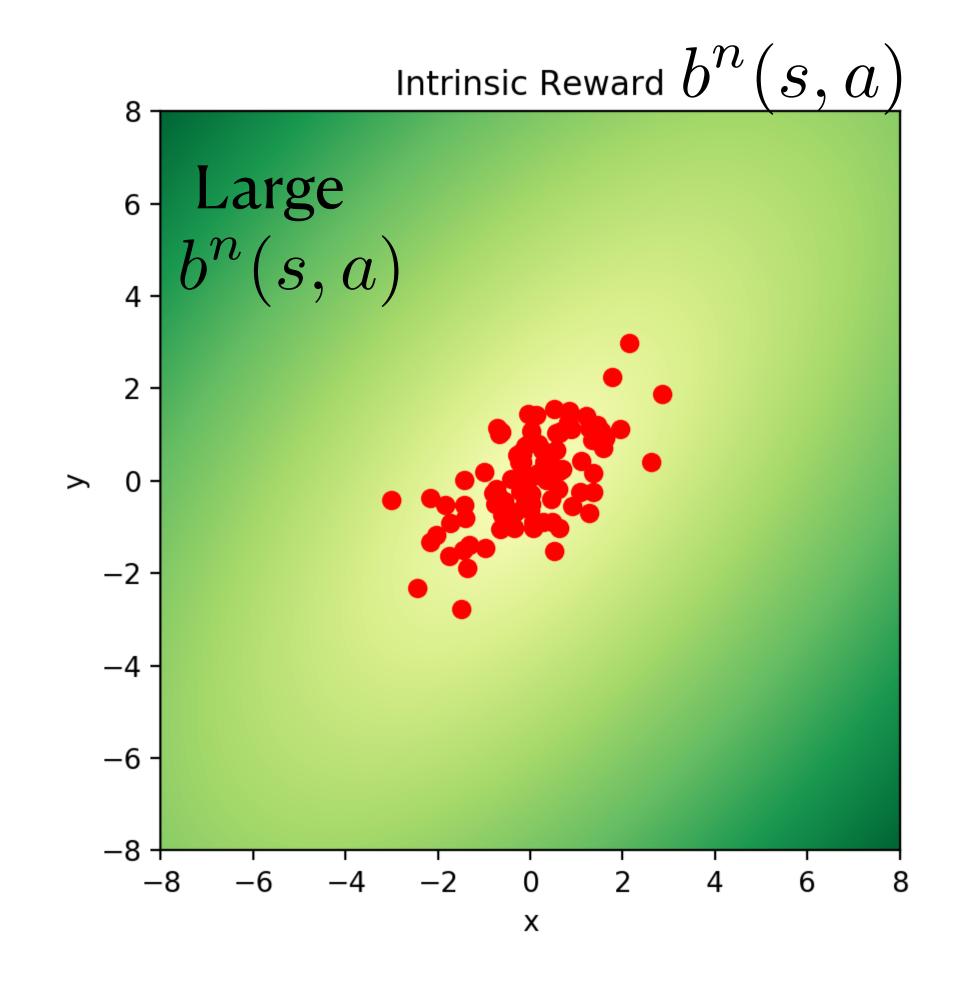
$$\{\pi_1,\pi_2,\ldots,\pi_n\}$$

$$\rho_n := \sum_{i=1}^n d^{\pi^i} / n$$

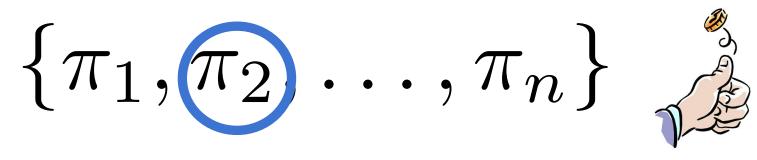
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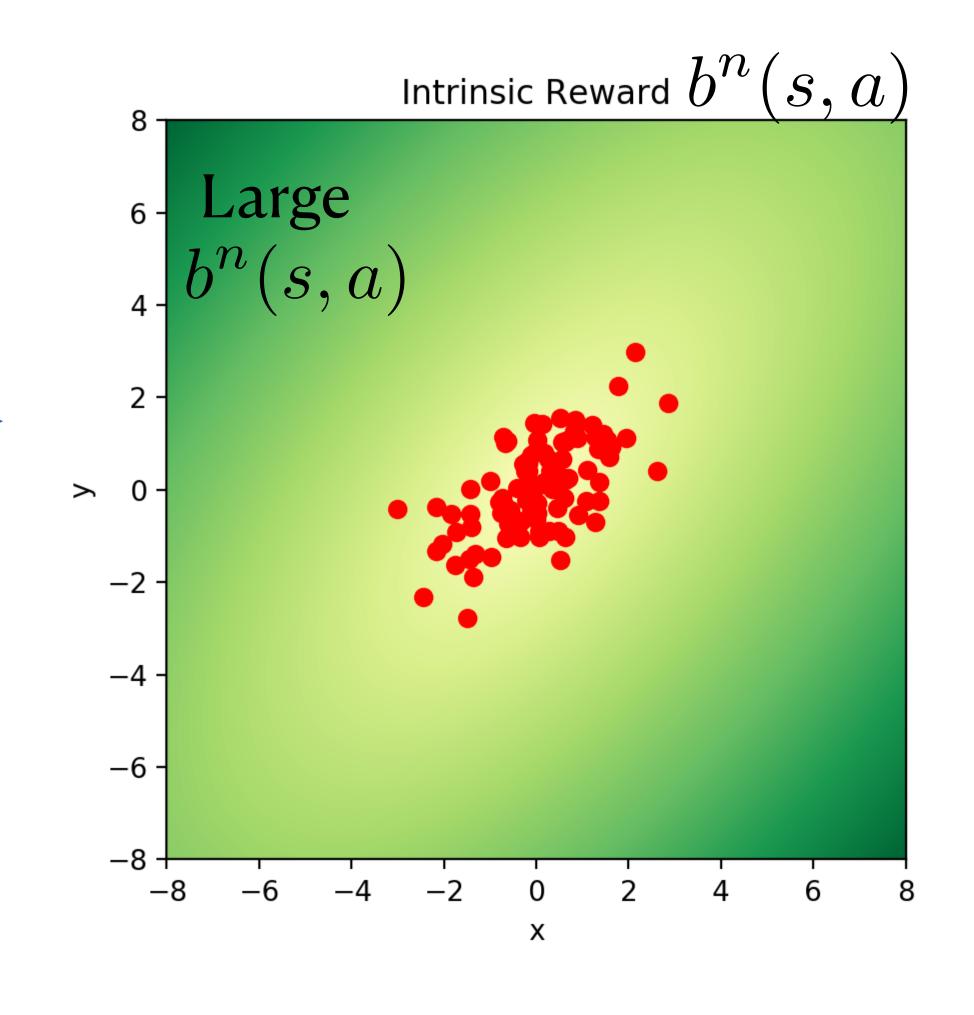


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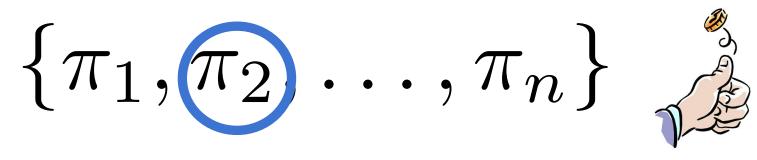




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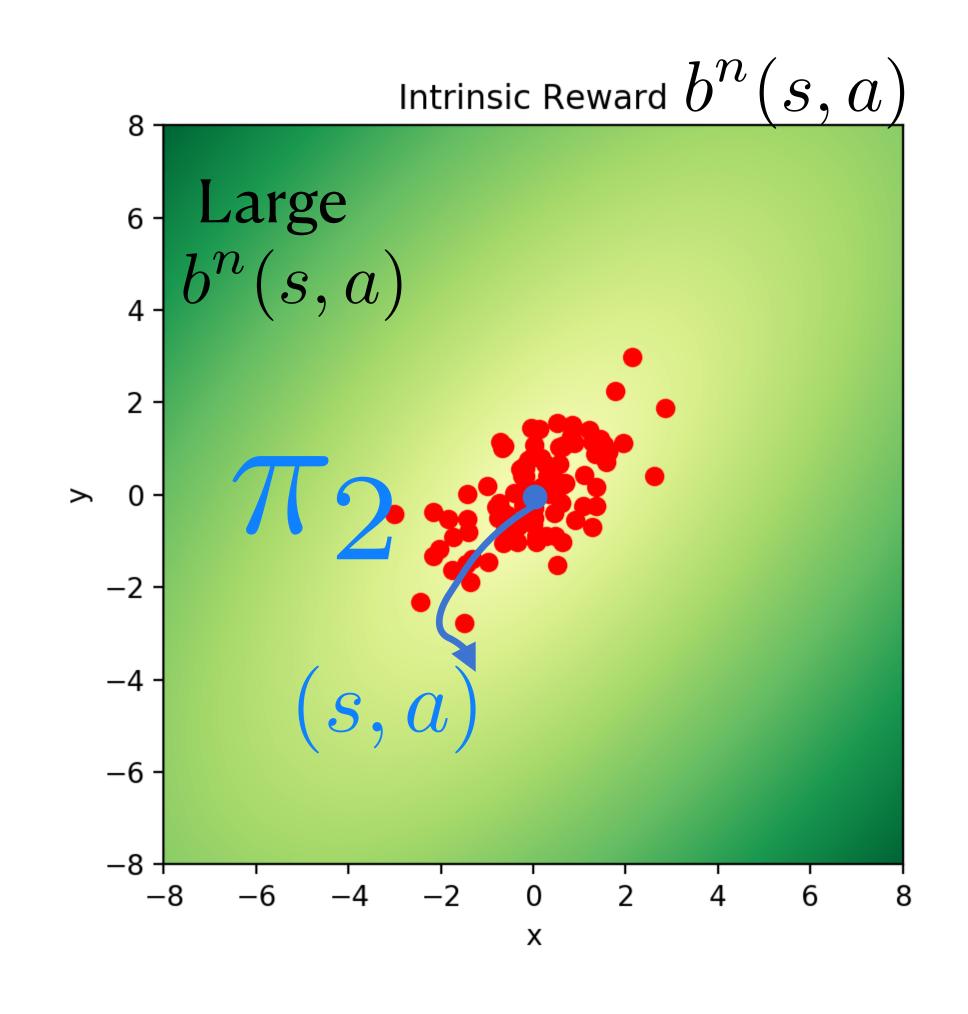


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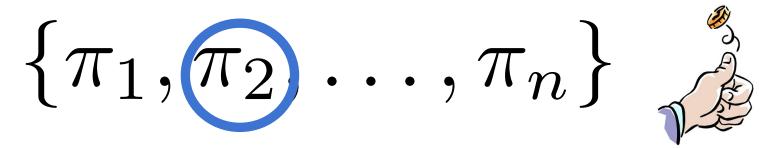




$$\rho_n := \sum_{i=1}^n d^{\pi^i} / r$$

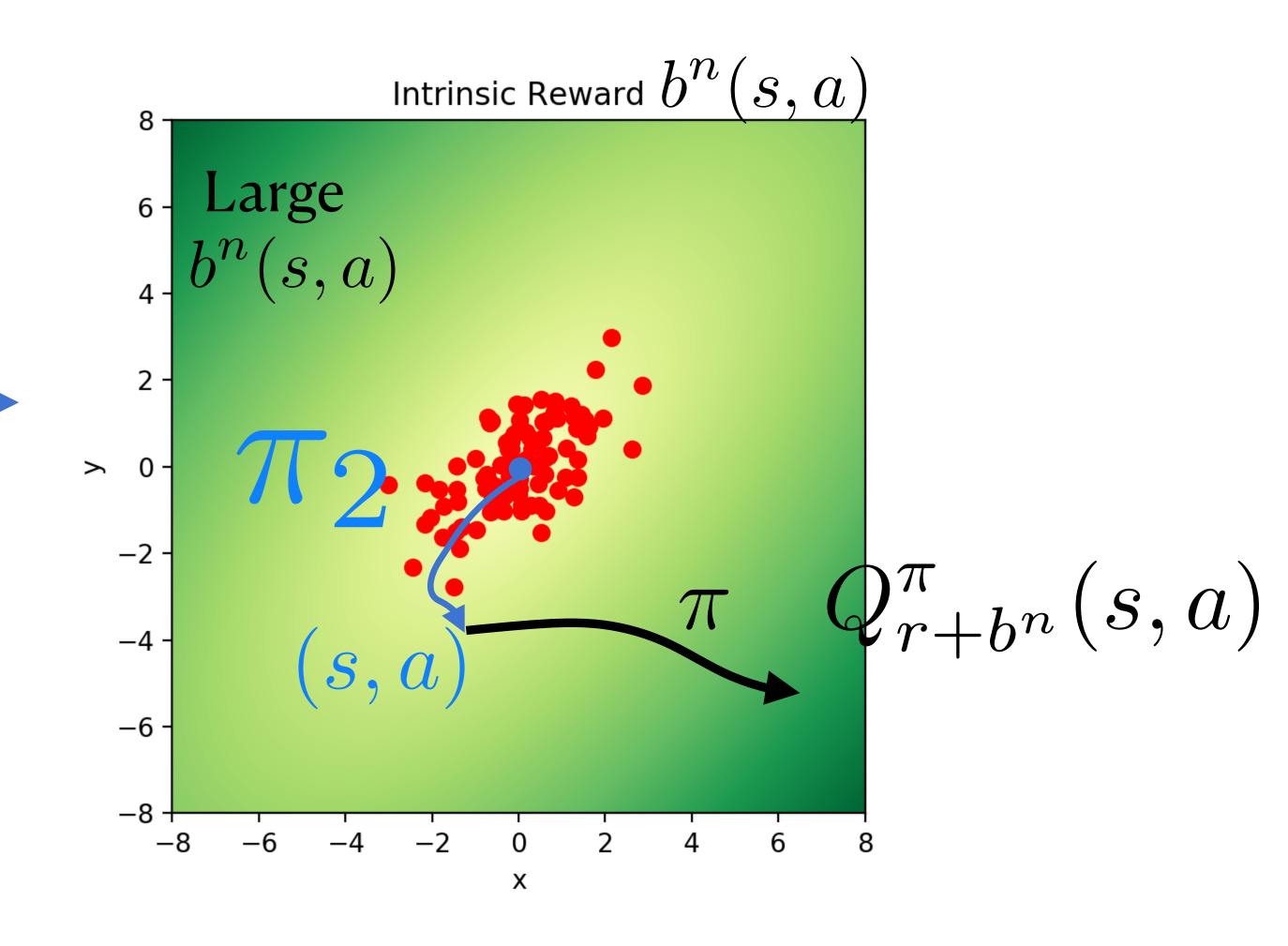


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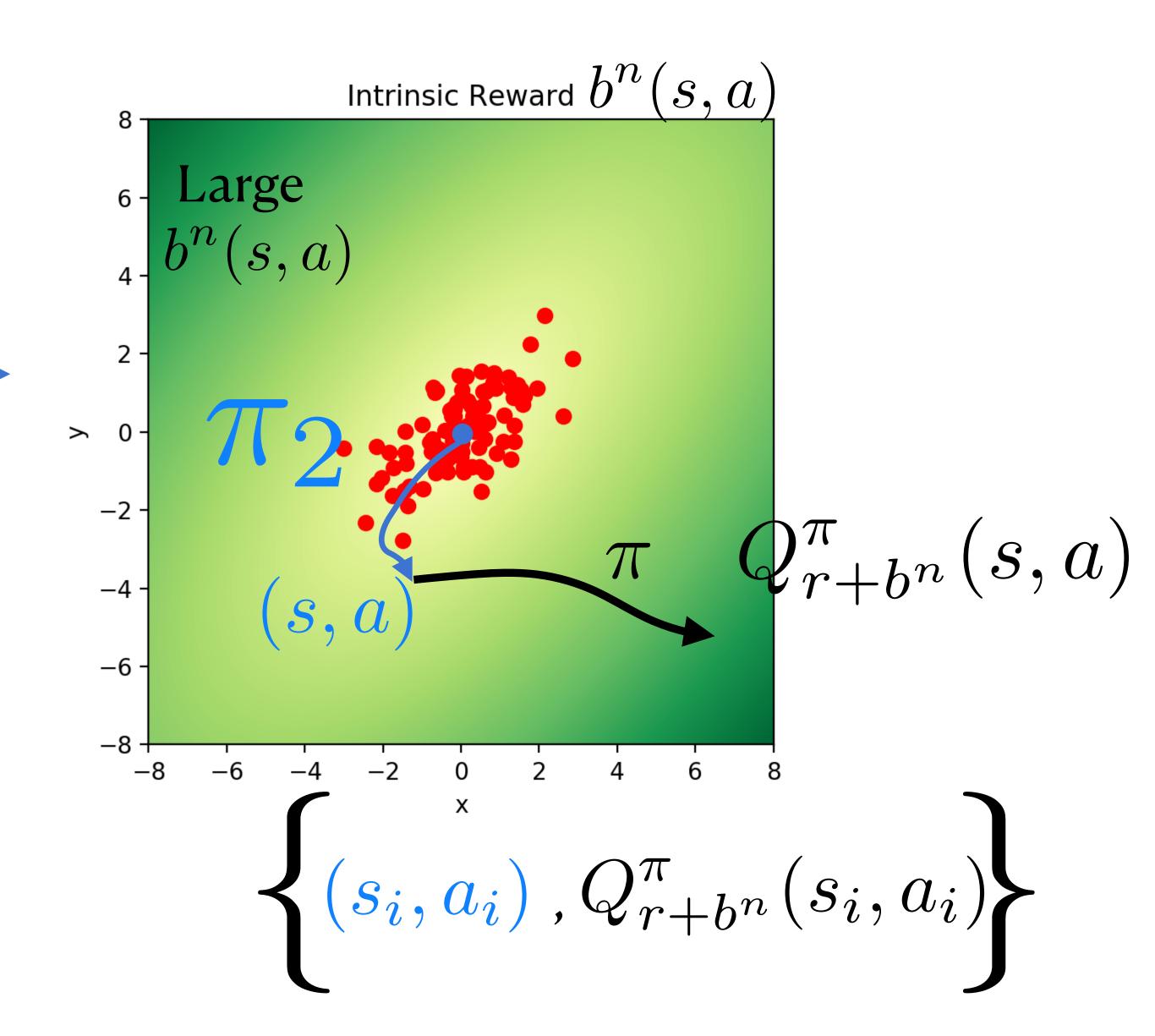


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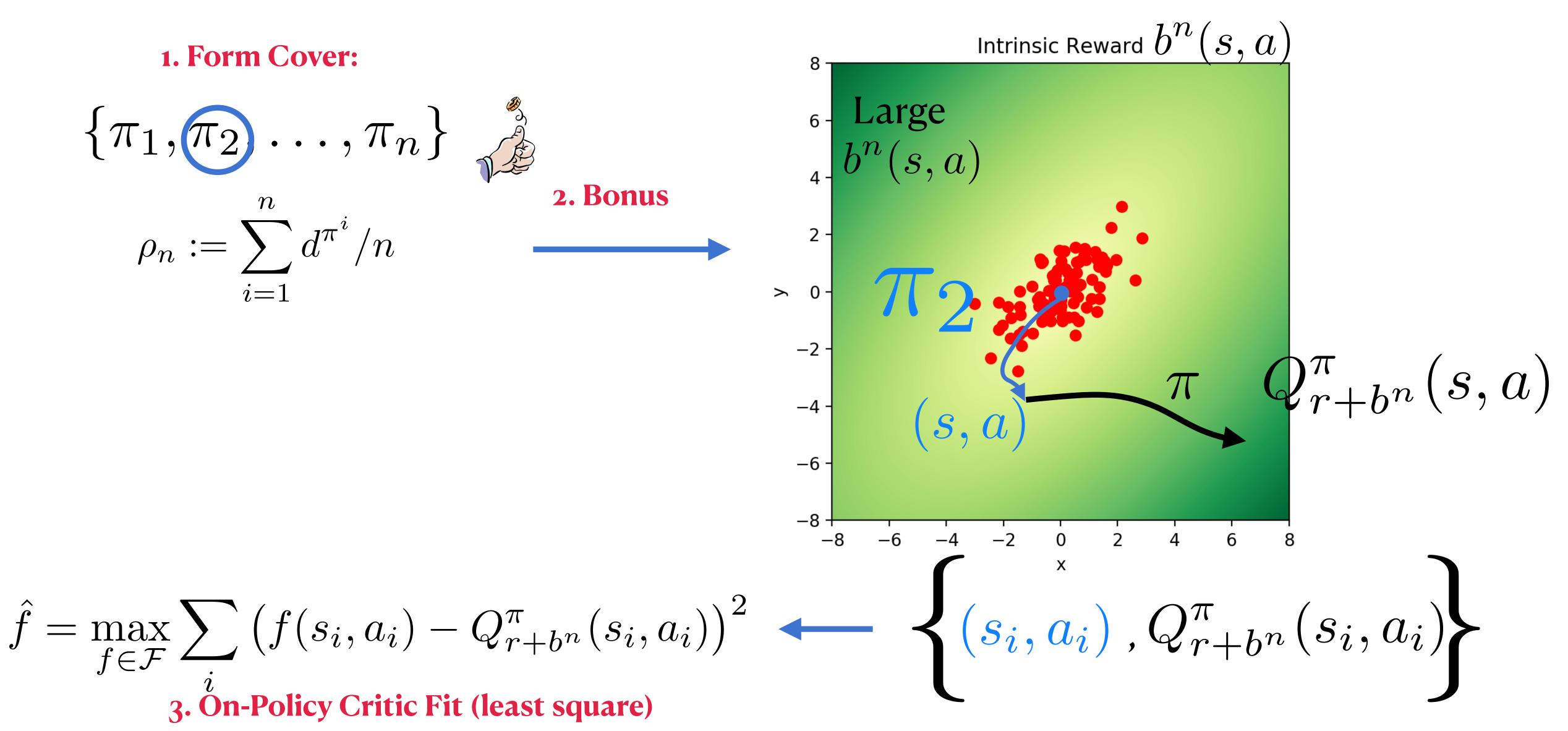


1. Form Cover:

$$\{\pi_1, \pi_2, \dots, \pi_n\}$$



$$\rho_n := \sum_{i=1}^n d^{\pi^i}/n$$



$$\hat{f} = \max_{f \in \mathcal{F}} \sum_{i} (f(s_i, a_i) - Q_{r+b^n}^{\pi}(s_i, a_i))^{\frac{1}{2}}$$
3. On-Policy Critic Fit (least square)

1. Form Cover:

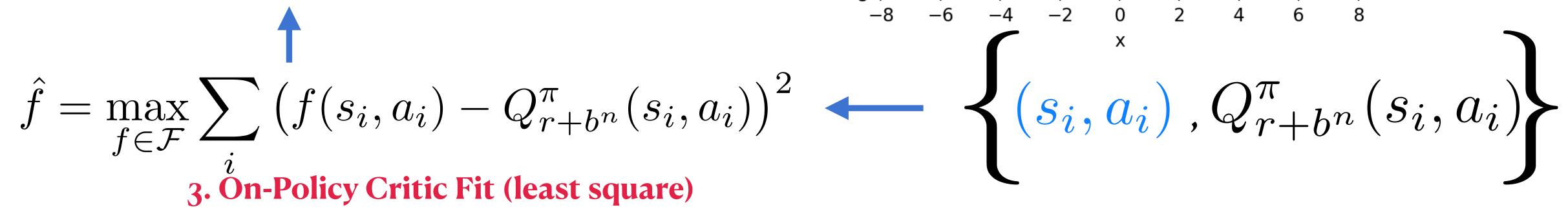
$$\{\pi_1, \pi_2, \dots, \pi_n\}$$

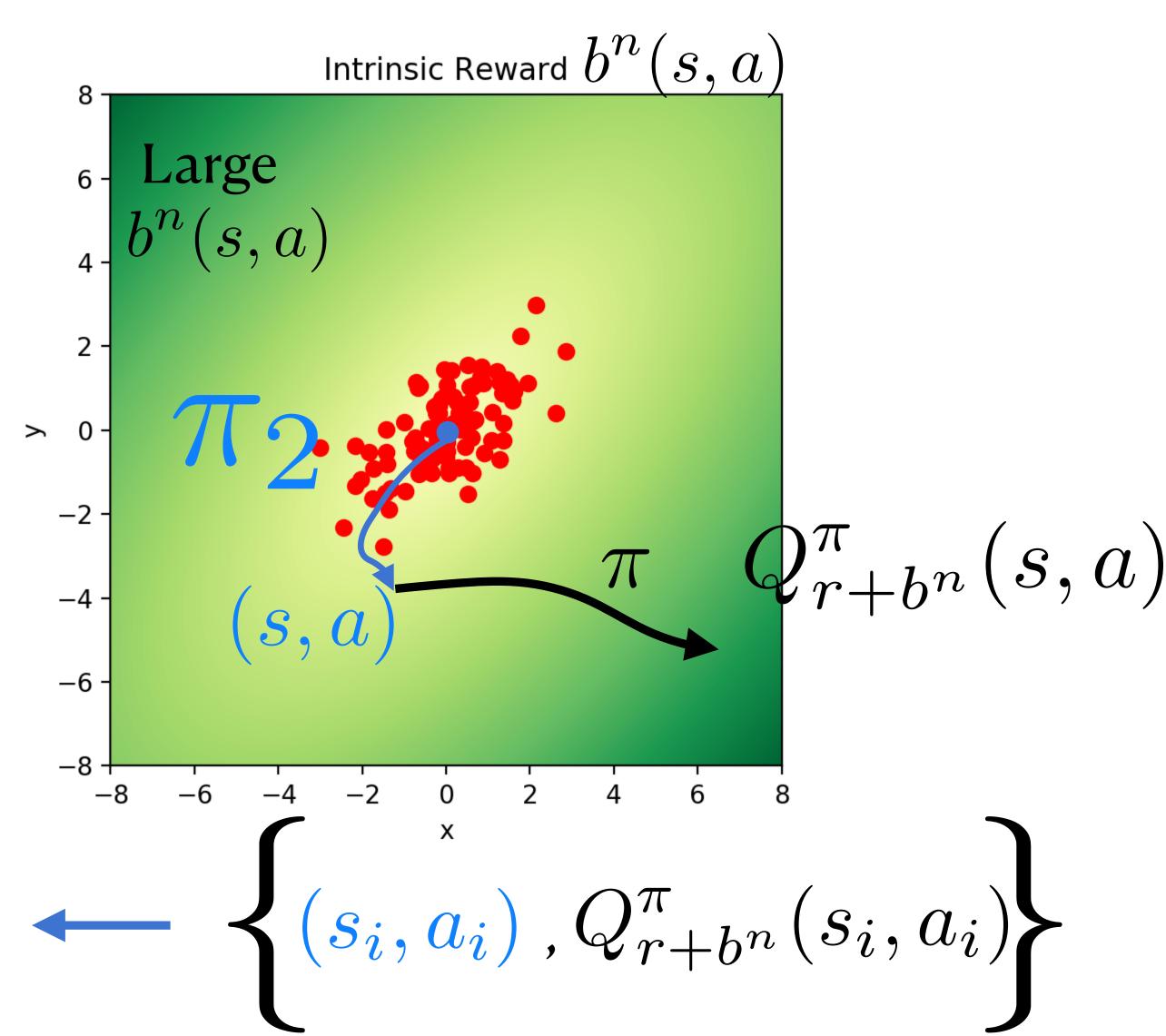
$$\rho_n := \sum_{i=1}^n d^{\pi^i}/n$$

2. Bonus

$$\pi(s, a) \Leftarrow \pi(s, a) \exp(\eta \hat{f}(s, a))$$

4. Actor NPG update (mirror descent)





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$$\{\pi_1, \pi_2, \dots, \pi_n\}$$



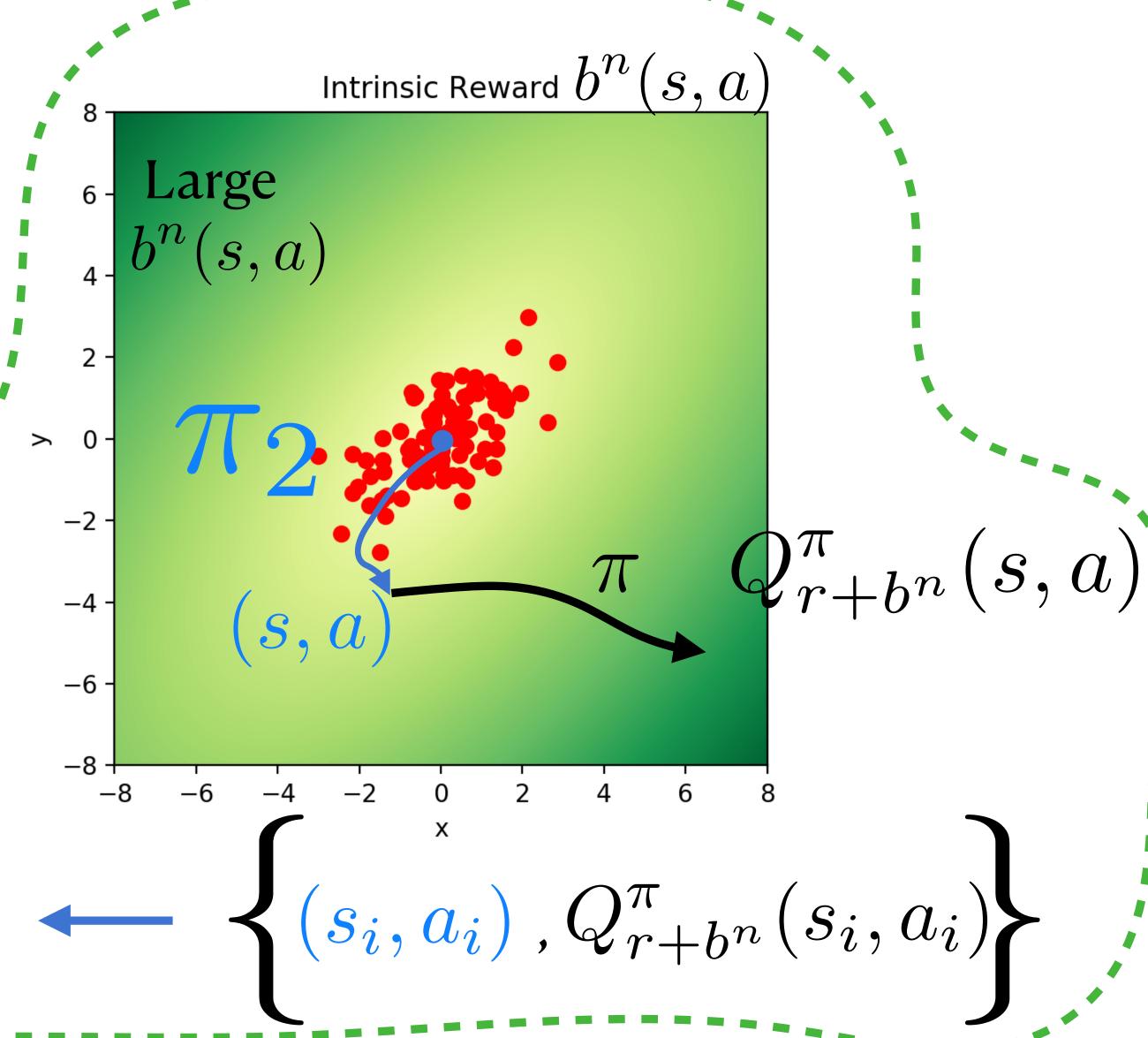
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$$\hat{f} = \max_{f \in \mathcal{F}} \sum_{i} \left(f(s_i, a_i) - Q_{r+b^n}^{\pi}(s_i, a_i) \right)^2 \longleftarrow \left\{ \begin{pmatrix} s_i, a_i \end{pmatrix}, Q_{r+b^n}^{\pi}(s_i, a_i) \right\}$$
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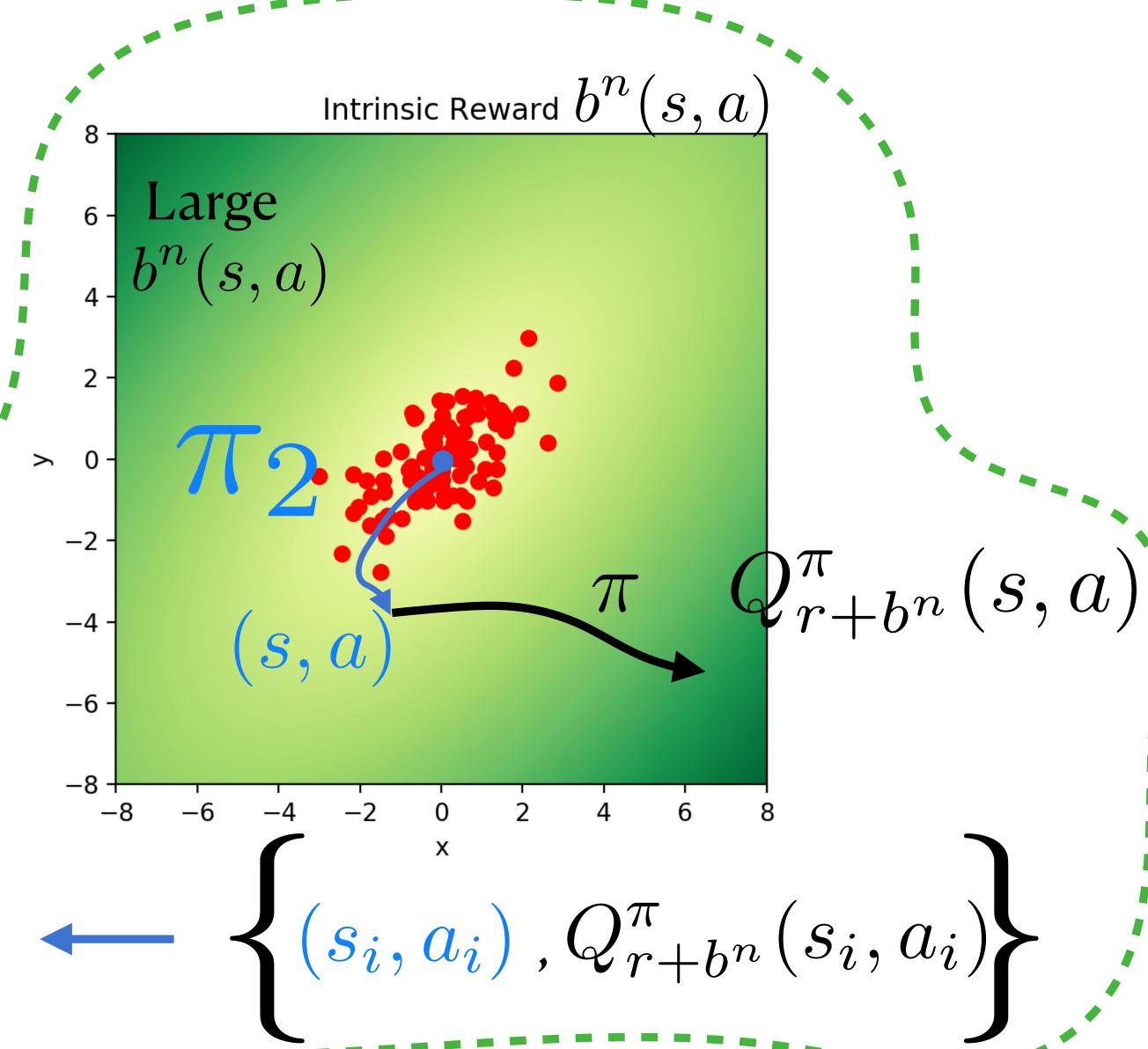
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5. Append

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3. On-Policy Critic Fit (least square)



At episode n: Natural PG is optimizing

$$\mathbb{E}_{s_0,a_0 \sim \rho_n} \left[\sum_{t=0}^{\infty} \gamma^t \left(r(s_t, a_t) + b^n(s_t, a_t) \right) \right]$$

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Use the cover and roll-in via policies in the cover

(note we do not start at μ_0)

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Bonus based on the cover

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No more forgetting!

At episode n: Natural PG is optimizing

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Use the cover and roll-in via policies in the cover

(note we do not start at μ_0)

Bonus based on the cover

No more sparse reward!

No more forgetting!

Use linear function $\theta \cdot \phi(s, a)$ to approximate Q^{π}

$$\{\pi_1, \pi_2, \dots, \pi_n\}$$

$$\Sigma_{\pi_i} = \mathbb{E}_{s, a \sim d_{\pi_i}} \phi(s, a) \phi(s, a)^{\mathsf{T}}$$

$$\Sigma_n = \sum_{i=1}^n \Sigma_{\pi_i} + \lambda I$$

Use linear function $\theta \cdot \phi(s, a)$ to approximate Q^{π}

$$\left\{\pi_{1}, \pi_{2}, \dots, \pi_{n}\right\}$$

$$\Sigma_{\pi_{i}} = \mathbb{E}_{s, a \sim d_{\pi_{i}}} \phi(s, a) \phi(s, a)^{\mathsf{T}} \qquad b^{n}(s, a) = \mathbf{1} \left\{\phi(s, a)^{\mathsf{T}} \Sigma_{n}^{-1} \phi(s, a) \geq \beta\right\} / (1 - \gamma)$$

$$\Sigma_{n} = \sum_{n=1}^{\infty} \Sigma_{\pi_{i}} + \lambda I$$

Use linear function $\theta \cdot \phi(s, a)$ to approximate Q^{π}

$$\left\{\pi_{1}, \pi_{2}, \dots, \pi_{n}\right\}$$

$$\Sigma_{\pi_{i}} = \mathbb{E}_{s, a \sim d_{\pi_{i}}} \phi(s, a) \phi(s, a)^{\top}$$

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$$\Sigma_{n} = \sum_{n=1}^{n} \Sigma_{\pi_{i}} + \lambda I$$
Rewarding (s, a) whose feature $\phi(s, a)$ aligns with small eigenvectors

Use linear function $\theta \cdot \phi(s, a)$ to approximate Q^{π}

1. Form Cover:

$$\{\pi_{1}, \pi_{2}, \dots, \pi_{n}\}$$

$$\Sigma_{\pi_{i}} = \mathbb{E}_{s, a \sim d_{\pi_{i}}} \phi(s, a) \phi(s, a)^{\top}$$

$$\Sigma_{n} = \sum_{n=1}^{\infty} \sum_{\pi_{i}} \lambda_{n} I$$
Reconstruction

2. Bonus

$$b^{n}(s, a) = \mathbf{1} \left\{ \phi(s, a)^{\mathsf{T}} \Sigma_{n}^{-1} \phi(s, a) \ge \beta \right\} / (1 - \gamma)$$

Rewarding (s, a) whose feature $\phi(s, a)$ aligns with small eigenvectors



3. Natural PG:

$$Q_{r+b^n}^{\pi}(s,a) \approx \theta \cdot \phi(s,a) + b^n(s,a)$$
$$\pi \Leftarrow \pi \exp\left(\eta \left(b^n + \theta \cdot \phi\right)\right)$$

Use linear function $\theta \cdot \phi(s, a)$ to approximate Q^{π}

1. Form Cover:

$$\{\pi_1, \pi_2, \dots, \pi_n\}$$

$$\Sigma_{\pi_i} = \mathbb{E}_{s, a \sim d_{\pi_i}} \phi(s, a) \phi(s, a)^{\top}$$

$$\Sigma_n = \sum_{i=1}^n \Sigma_{\pi_i} + \lambda I$$

2. Bonus

$$b^{n}(s, a) = \mathbf{1} \left\{ \phi(s, a)^{\mathsf{T}} \Sigma_{n}^{-1} \phi(s, a) \ge \beta \right\} / (1 - \gamma)$$

Rewarding (s, a) whose feature $\phi(s, a)$ aligns with small eigenvectors



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PC-PG Specialized to Tabular MDPs

One-hot vector: $\phi(s, a) \in \mathbb{R}^{SA}$

$$\rho_n = \sum_{i=1}^n d^{\pi_i}/n$$

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Rewarding state that has low probability of being covered

$$\phi(s,a)^{\mathsf{T}} \Sigma_n^{-1} \phi(s,a) \Leftarrow \frac{1}{\rho_n(s,a)}$$

Well-Specified Setting: Linear MDPs (and Tabular MDPs)

Reward and transition in RKHS:

[RKHS version of the Linear mdp model from Jin et al, 19]

$$r(s,a) = \theta \cdot \phi(s,a), P(\cdot \mid s,a) = \mu \phi(s,a)$$

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with # of samples

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with # of samples
 $(d, \log(A), 1/(1 - \gamma), 1/\epsilon)$

Dim of feature

(extendable to RKHS w/ Information Gain)

[Agarwal et al 19]

A wide initial distribution:

$$\kappa = 1/\sigma_{\min} \left(\mathbb{E}_{s,a \sim \mu_0} \phi(s,a) \phi(s,a)^{\mathsf{T}} \right) < \infty$$

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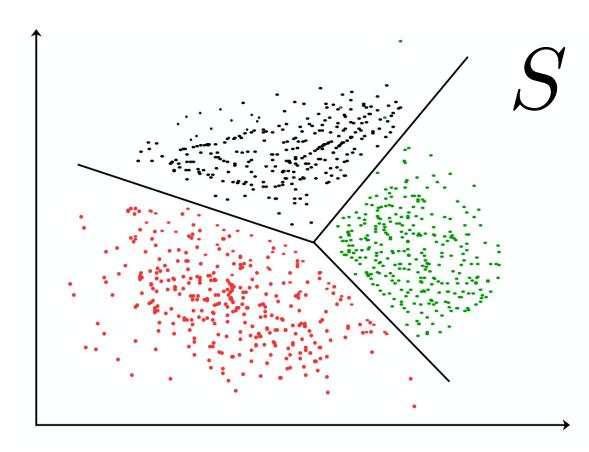


Condition number could be exponential!!

PC-PG eliminates the condition number by actively exploring and building policy cover

Robustness to Model-Misspecification

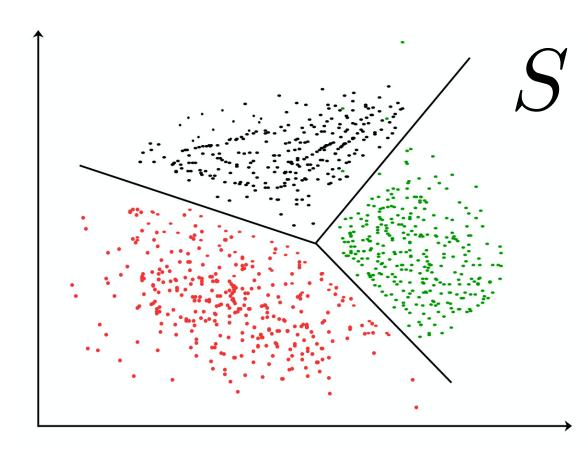
Average VS ℓ_{∞}



 $\phi: S \to Z$

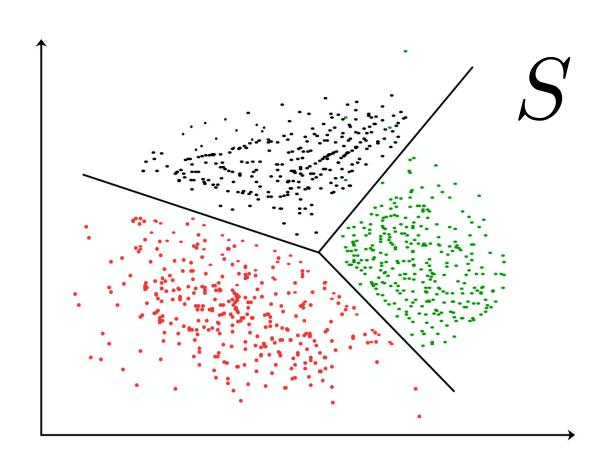
Group "similar" states (s)

into an abstracted state (z)



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 $|Z| \ll |S|$ poly(|Z|)



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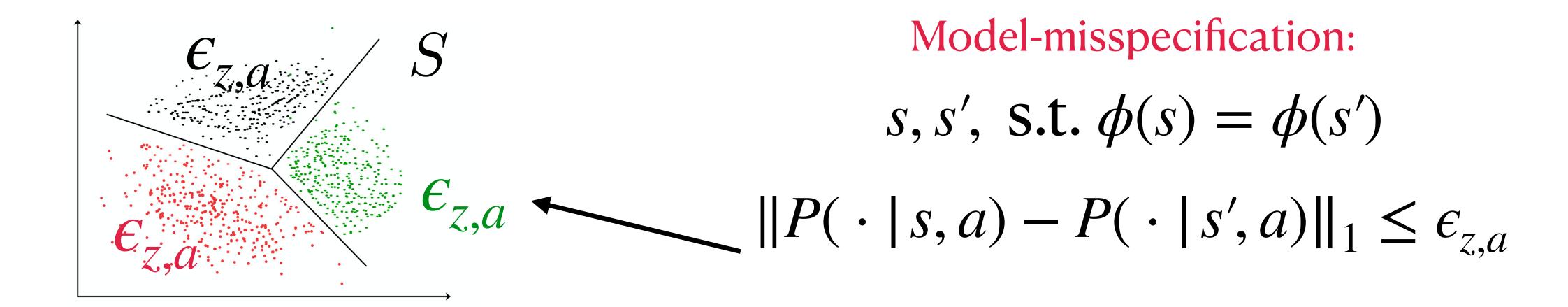
$$|Z| \ll |S|$$

$$poly(|Z|)$$

Model-misspecification:

$$s, s', s.t. \phi(s) = \phi(s')$$

$$||P(\cdot | s, a) - P(\cdot | s', a)||_1 \le \epsilon_{z,a}$$

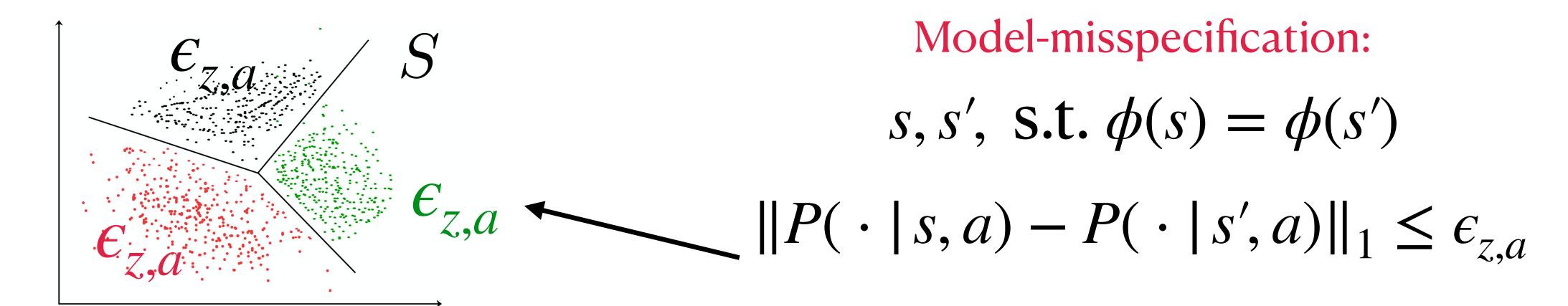


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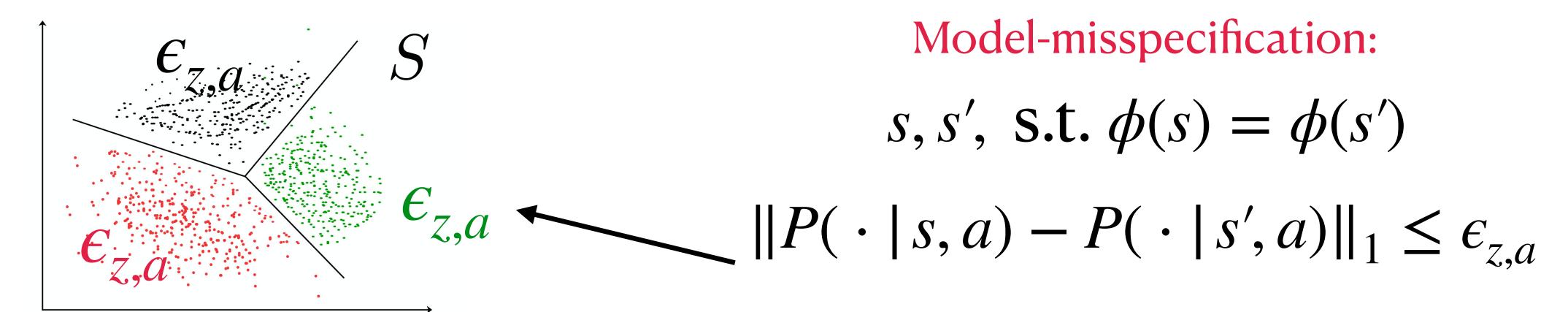


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$$(1/(1-\gamma))$$
 $\left(\max_{z,a} \epsilon_{z,a}\right)$

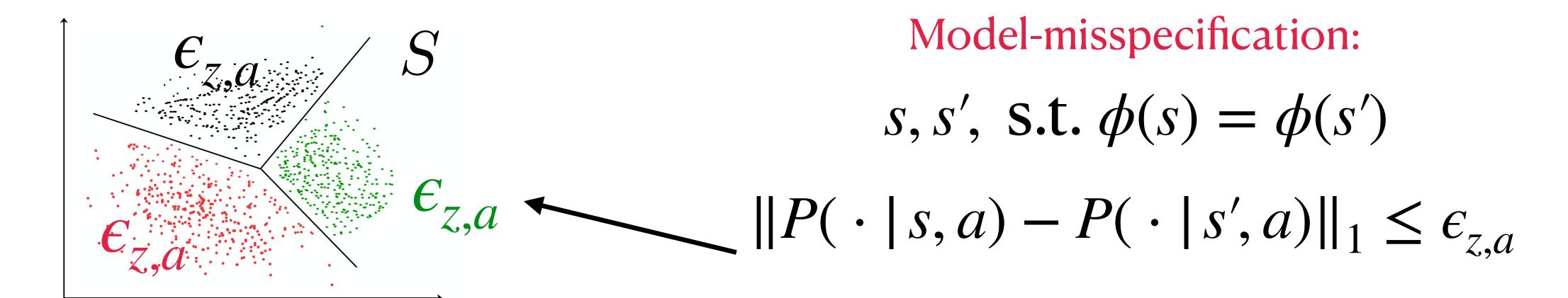


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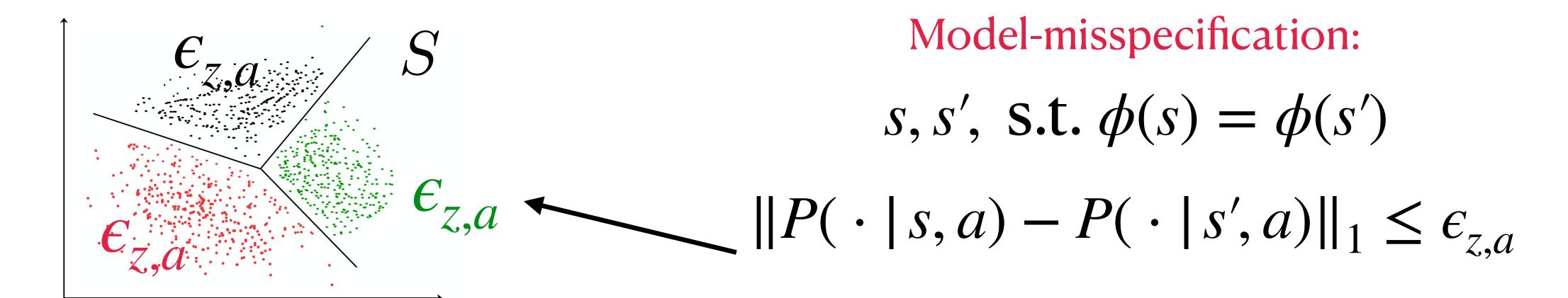
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$$\mathbf{poly}(1/(1-\gamma)) \Big(\mathbb{E}_{z,a\sim d^{\widetilde{\pi}}} \left[\epsilon_{z,a} \right] \Big)$$



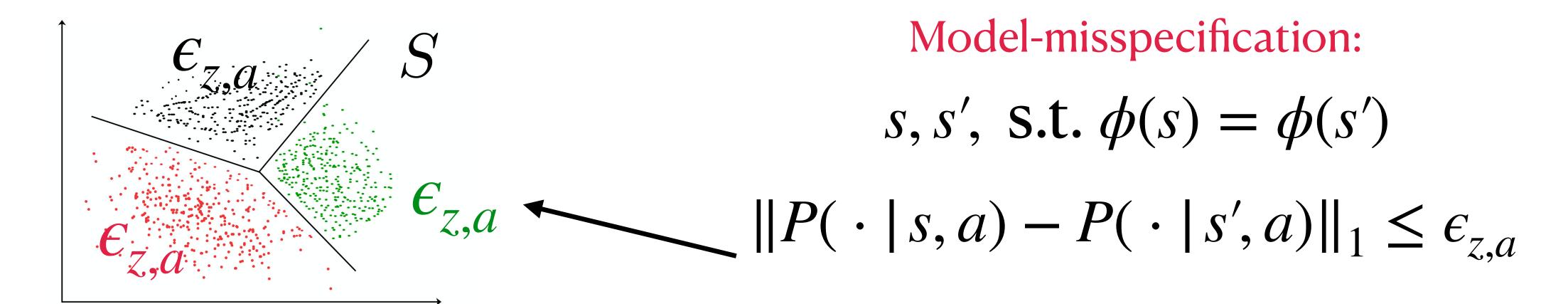
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PC-PG
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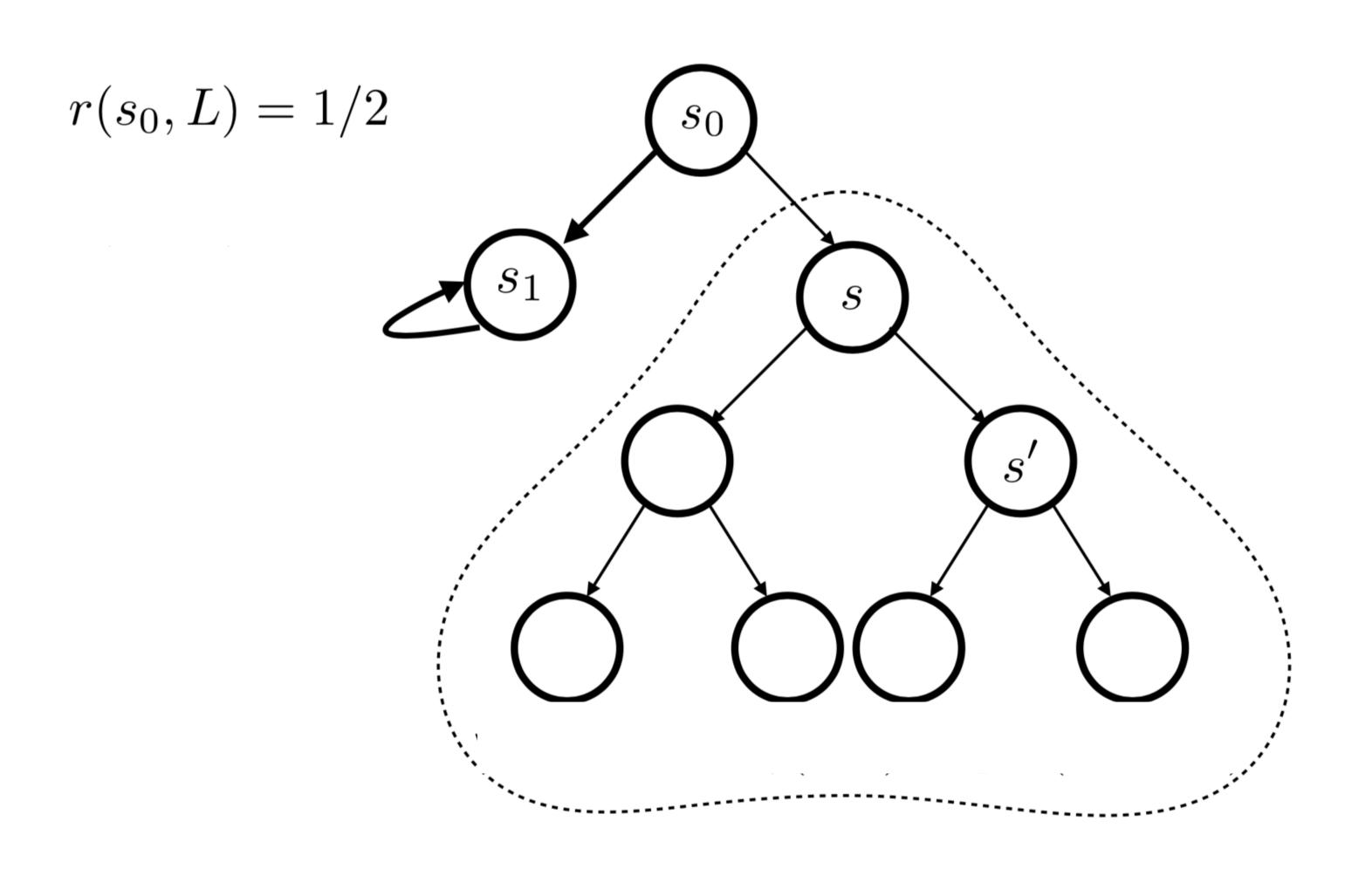
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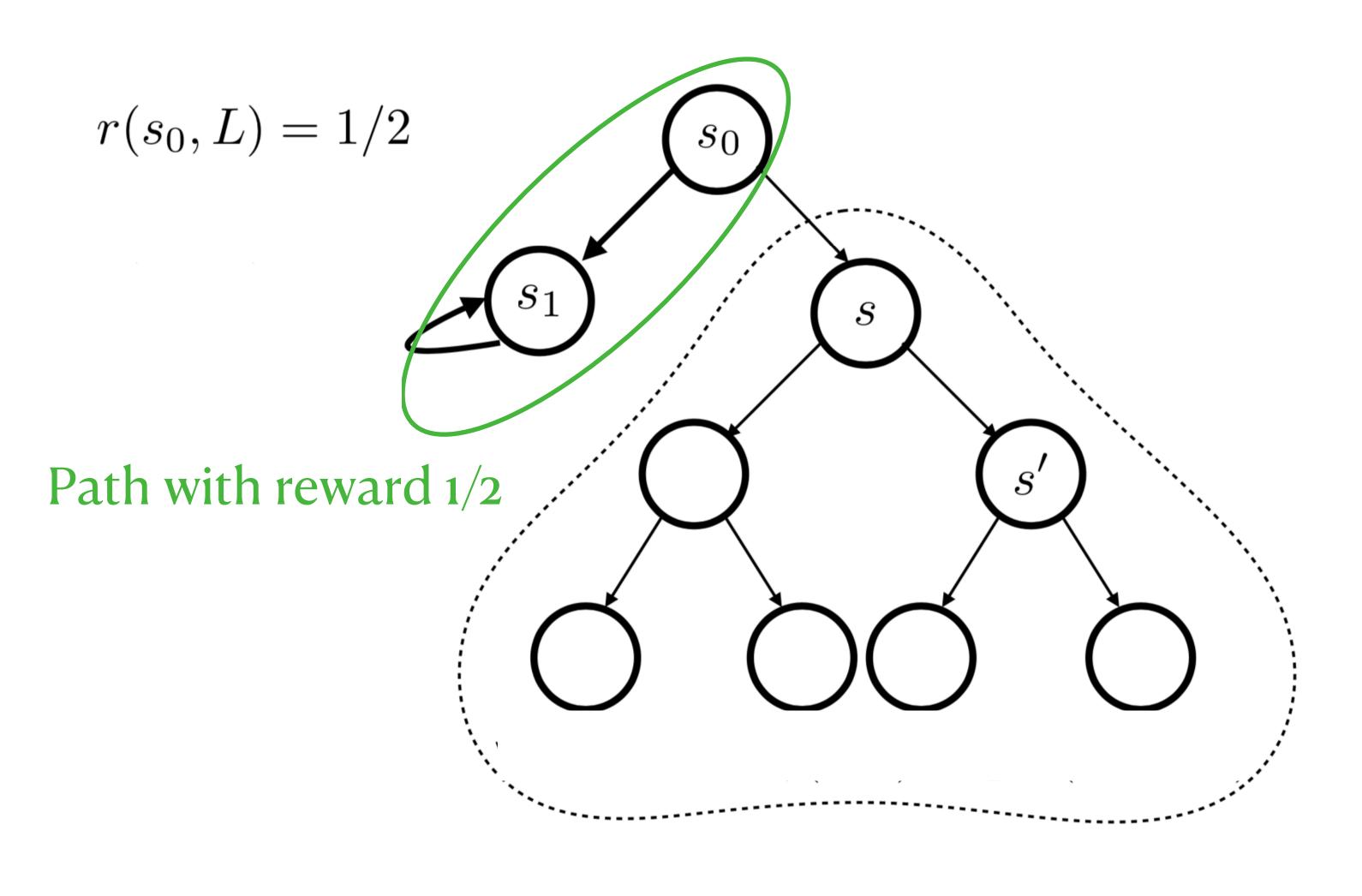
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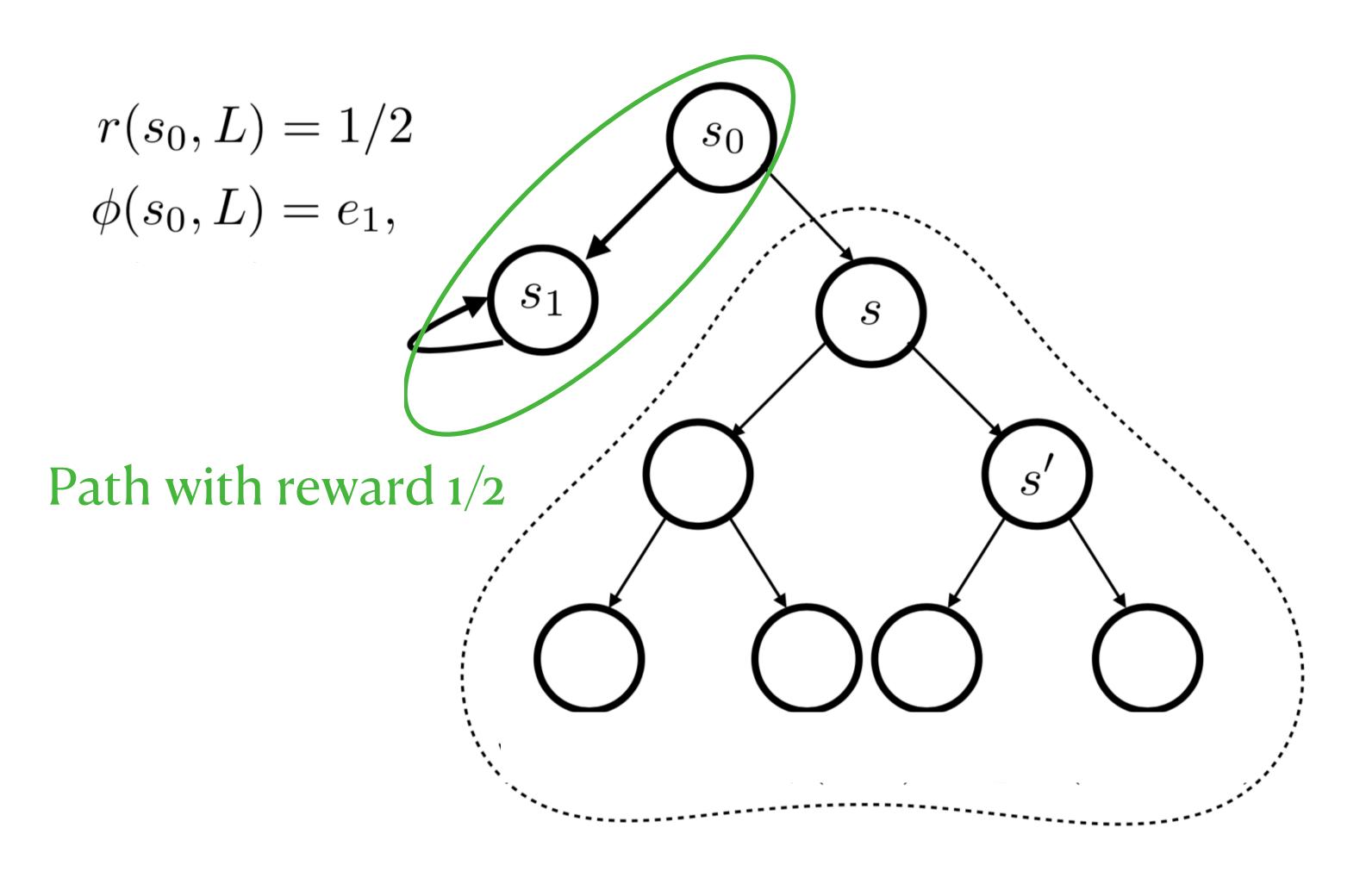
$$poly(|Z|)$$

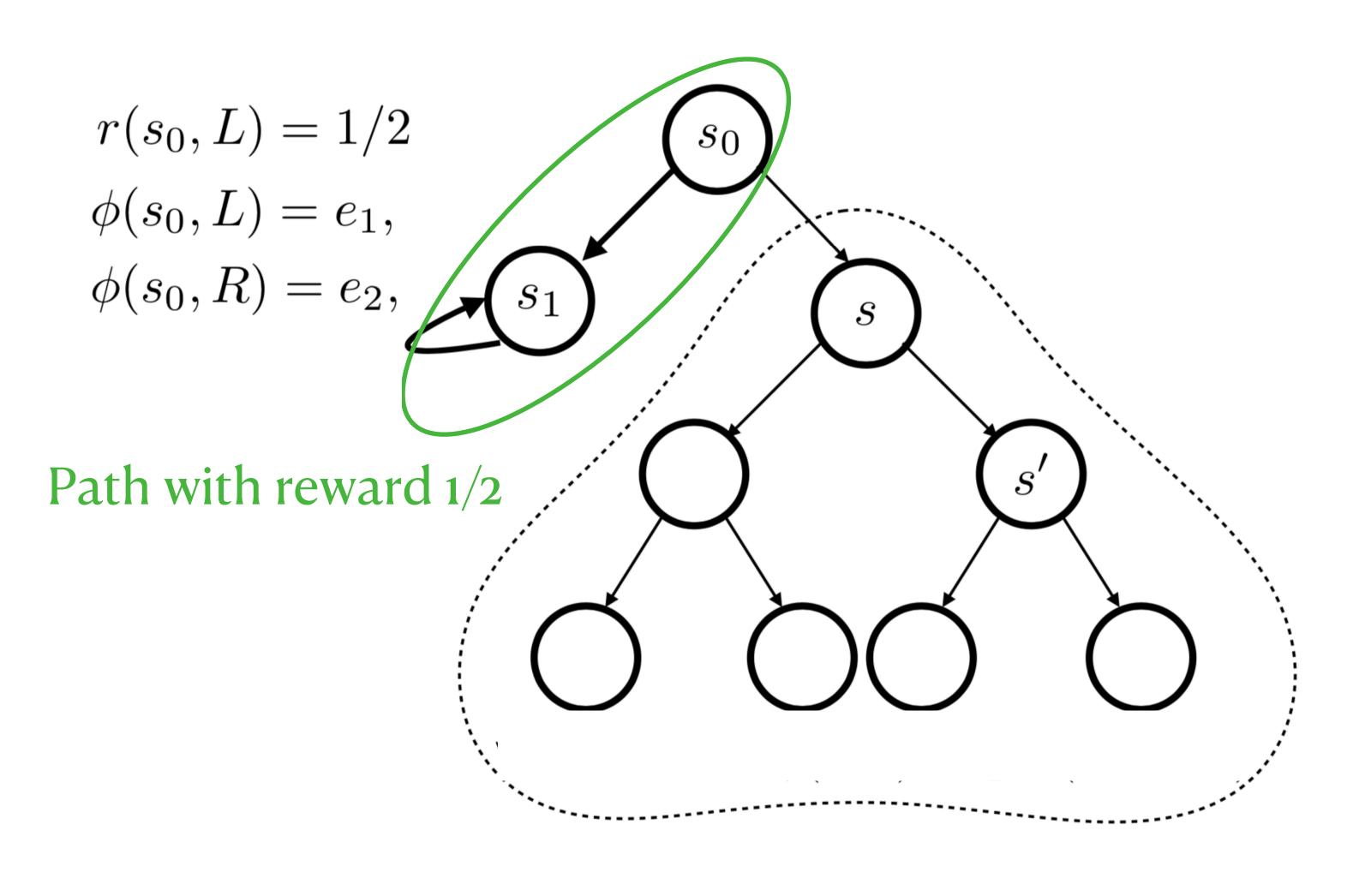
$$\operatorname{poly}\left(1/(1-\gamma)\right)\left(\max_{z,a}\epsilon_{z,a}\right) \leftarrow \ell_{\infty}$$

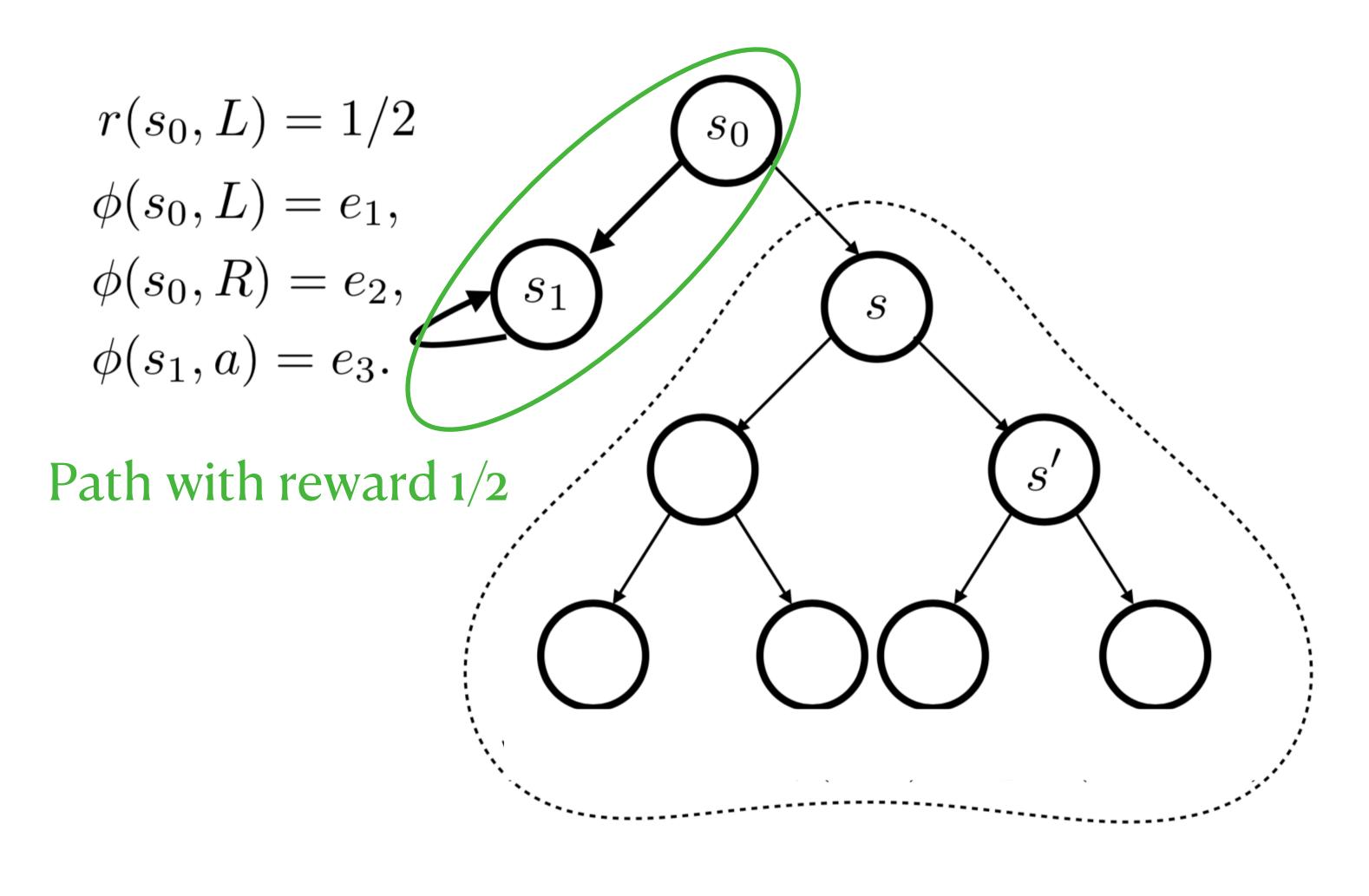
PC-PG Average over poly
$$(1/(1-\gamma))\Big(\mathbb{E}_{z,a\sim d^{\widetilde{\pi}}}\left[\epsilon_{z,a}\right]\Big)$$
 comparator's distribution

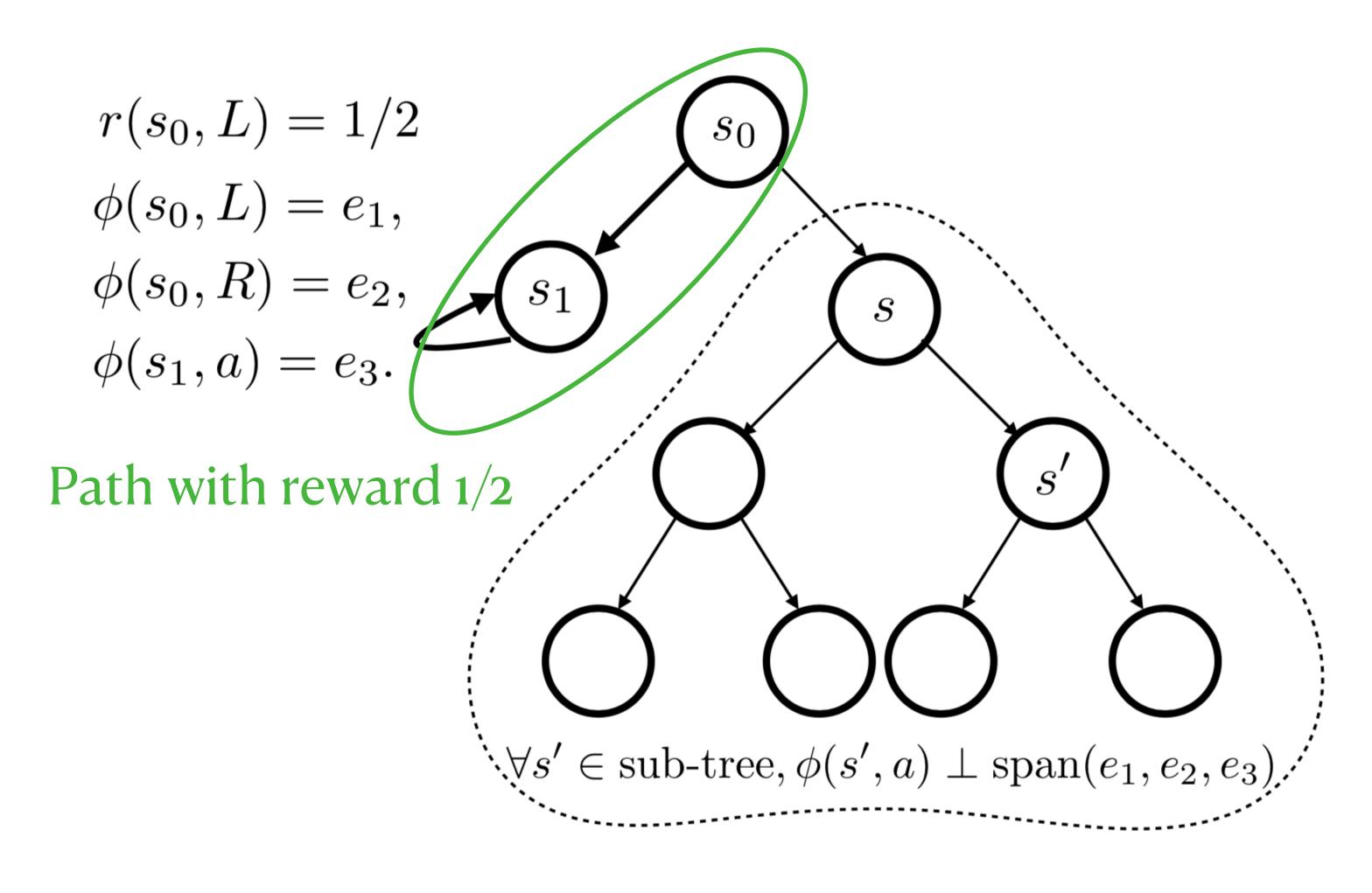


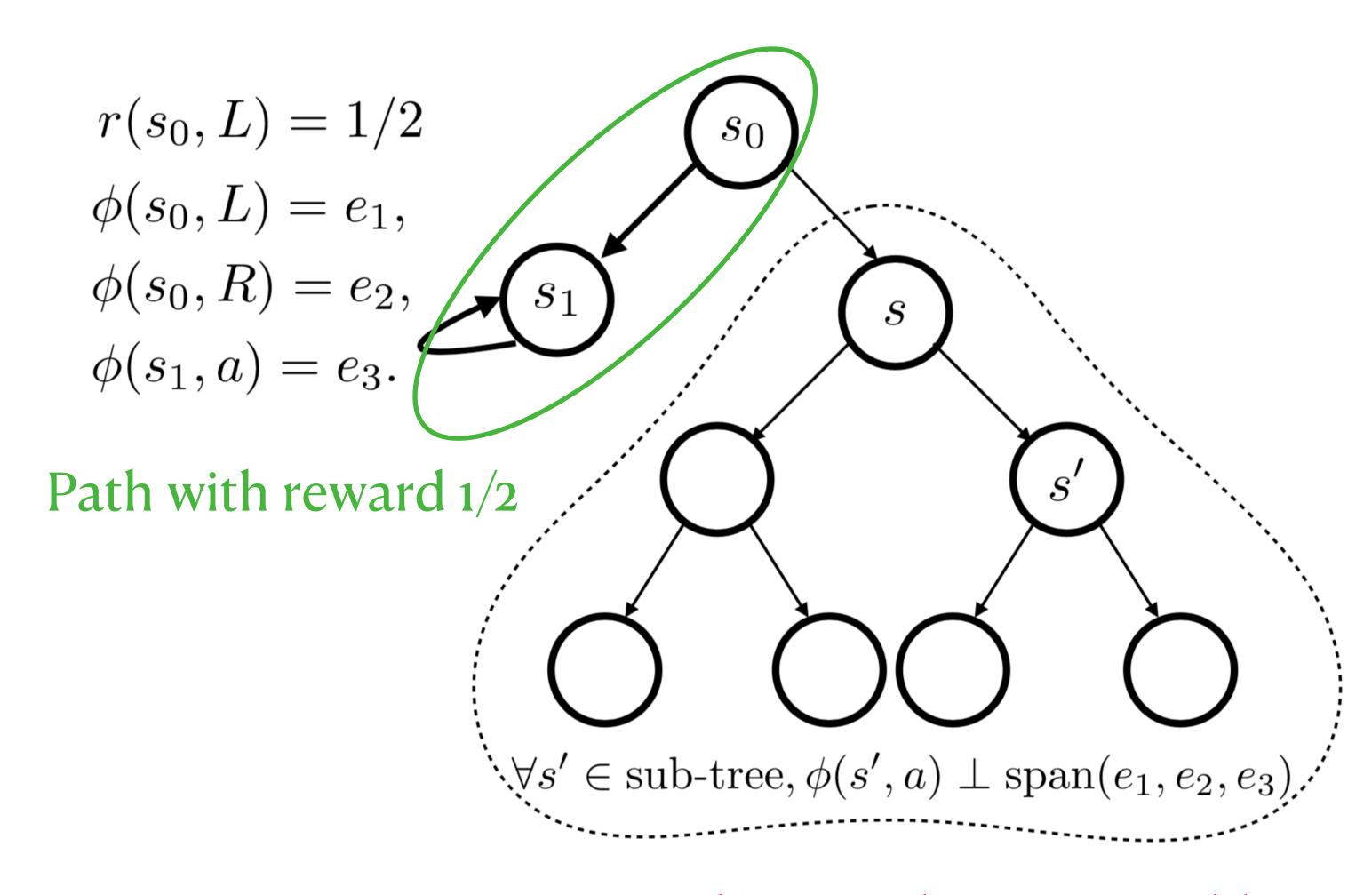




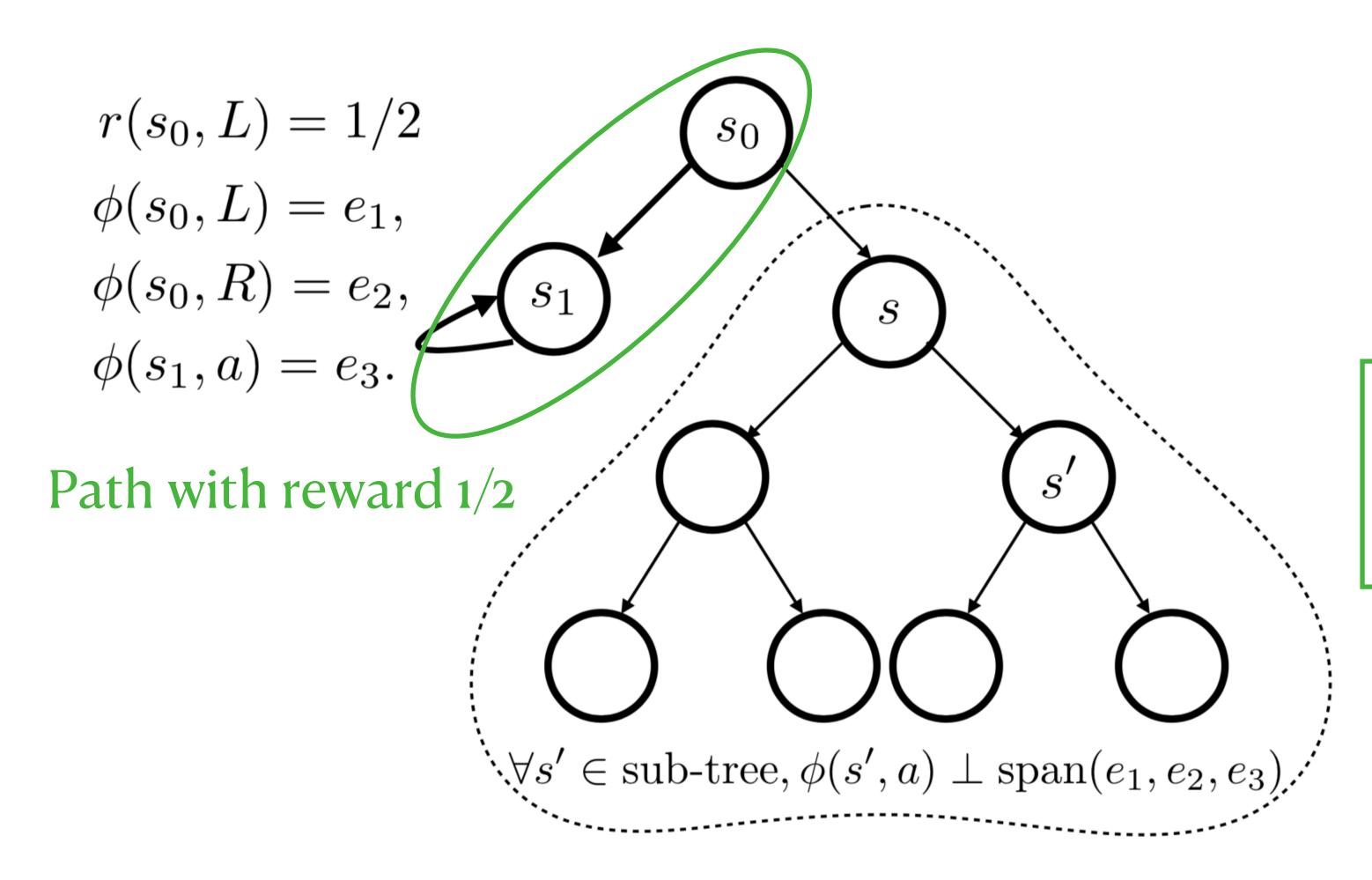








Features is **arbitrary** in the tree, i.e., model-misspecification can be very **serious**.



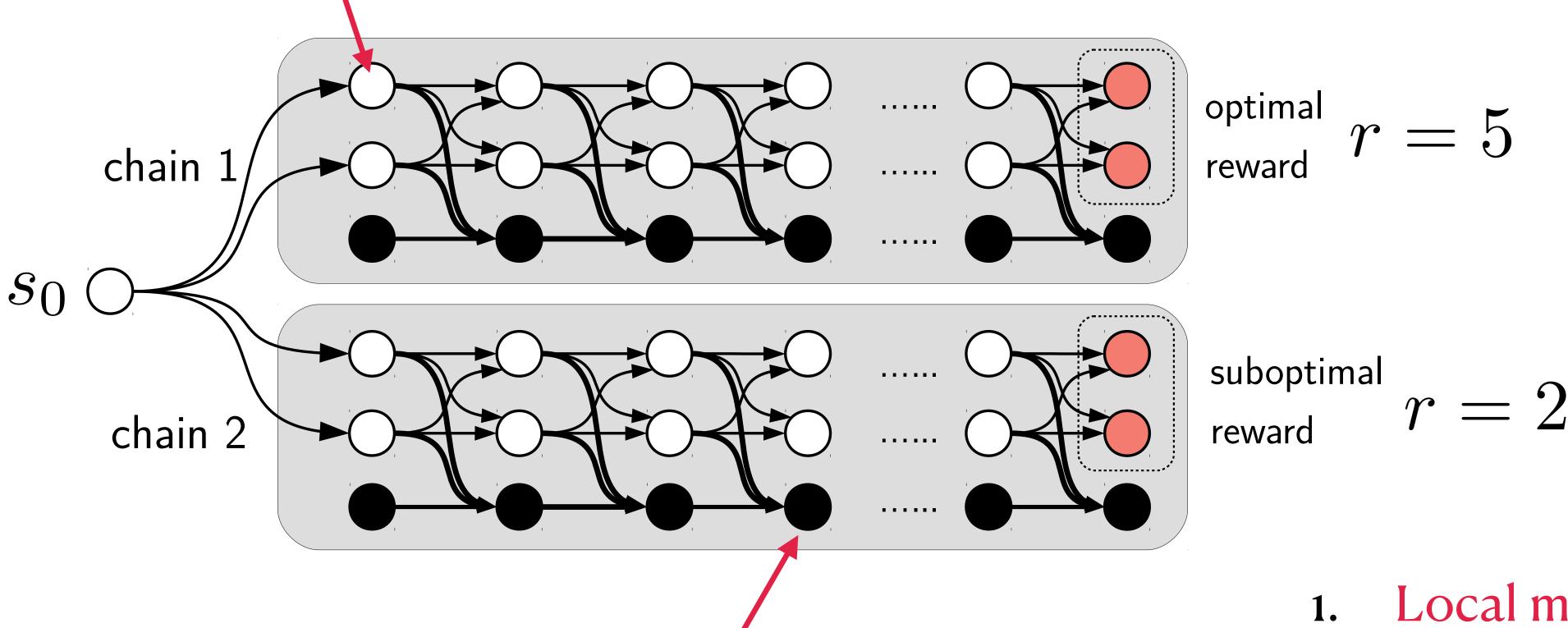
PC-PG is at least as good as the green trajectory

Features is **arbitrary** in the tree, i.e., model-misspecification can be very **serious**.

Experiments

Bidirectional Combination Lock

Good state (white): 9 out of 10 actions go to bad state (black)



Bad state has Anti-shaped reward: r=1/H

- Local minima
- 2. Forgetting

Feature vector: binary vector indicating state-action and time step

Policy Opt procedure: PPO w/ NN policy

Bonus: $\phi^{\top} \Sigma_{n}^{-1} \phi$

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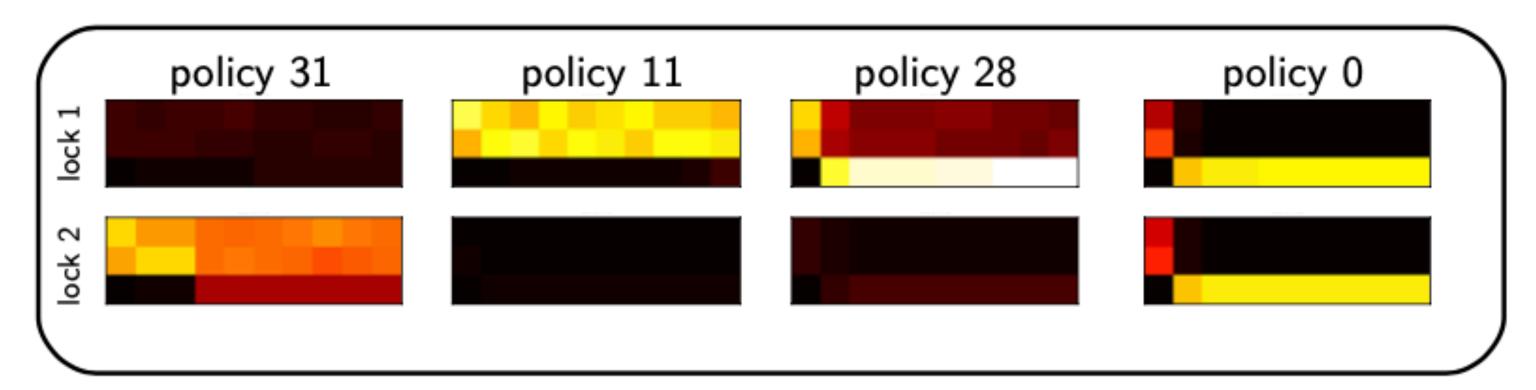
Bonus: $\phi^{\top} \Sigma_{n}^{-1} \phi$

Success Rate (visit two chains):

Algorithm	Horizon			
	2	5	10	15
PPO	1.0	0.0	0.0	0.0
PPO+RND	0.75	0.40	0.50	0.55
PC-PG	1.0	1.0	1.0	1.0

Due to the policy cover PC-PG maintains..

State visitations for top weighted policies in mixture



Due to the policy cover PC-PG maintains..

State visitations for top weighted policies in mixture

visitations for policy mixture

policy 31 policy 11 policy 28 policy 0

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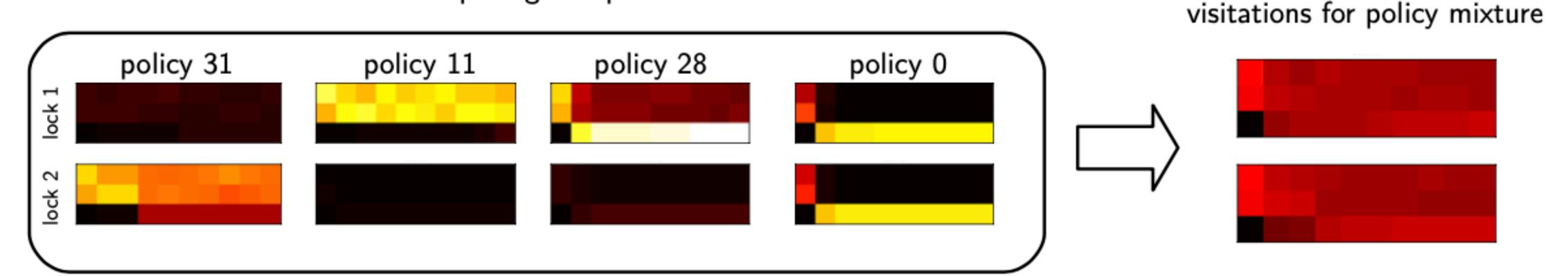
The state visitations for policy mixture

visitations for policy mixture

Cover ρ_n near uniformly cover both chains

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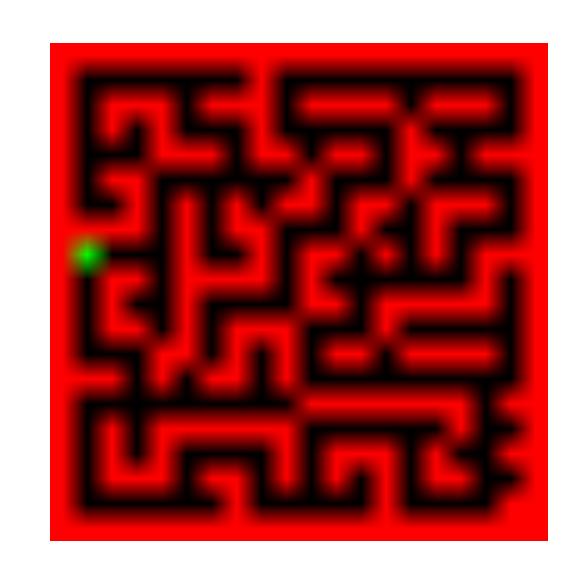
State visitations for top weighted policies in mixture



Cover ρ_n near uniformly cover both chains

PG with ρ_n will succeed!

Reward-Free Explore in Maze



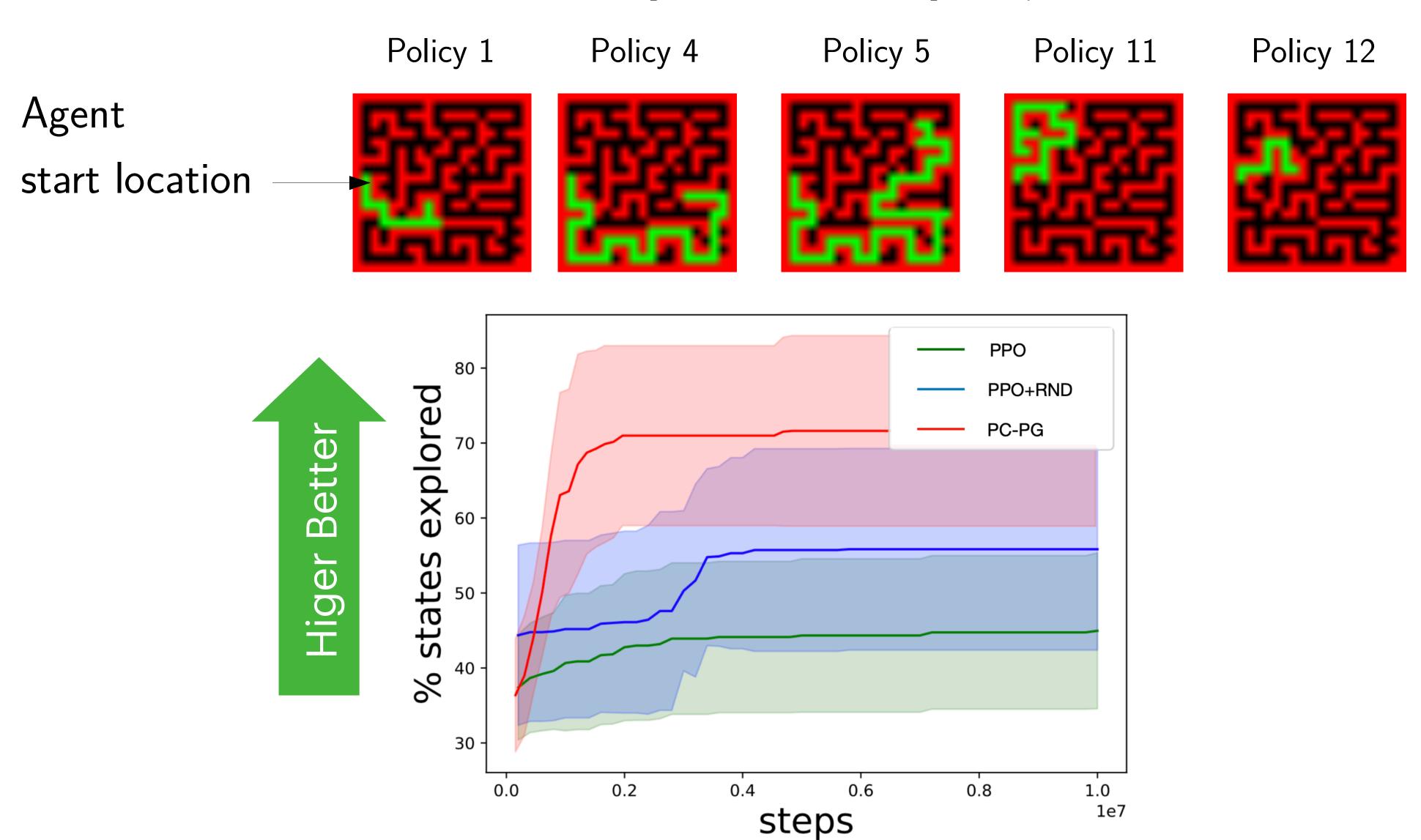
$$r(s,a) = 0$$

 $\phi(s,a)$: Random initialized CovNet

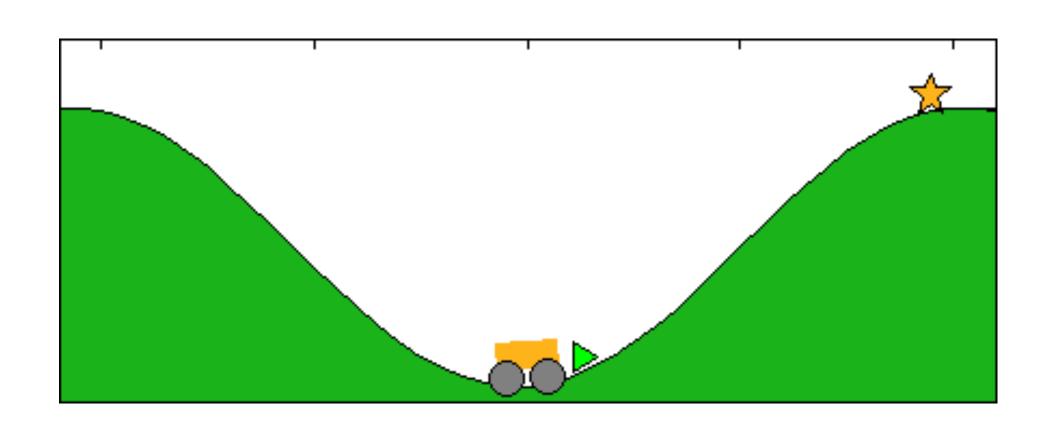
Policy Opt procedure: PPO w/ CovNet-based policy

Reward-Free Explore in Maze

Traces of policies in the policy cover:



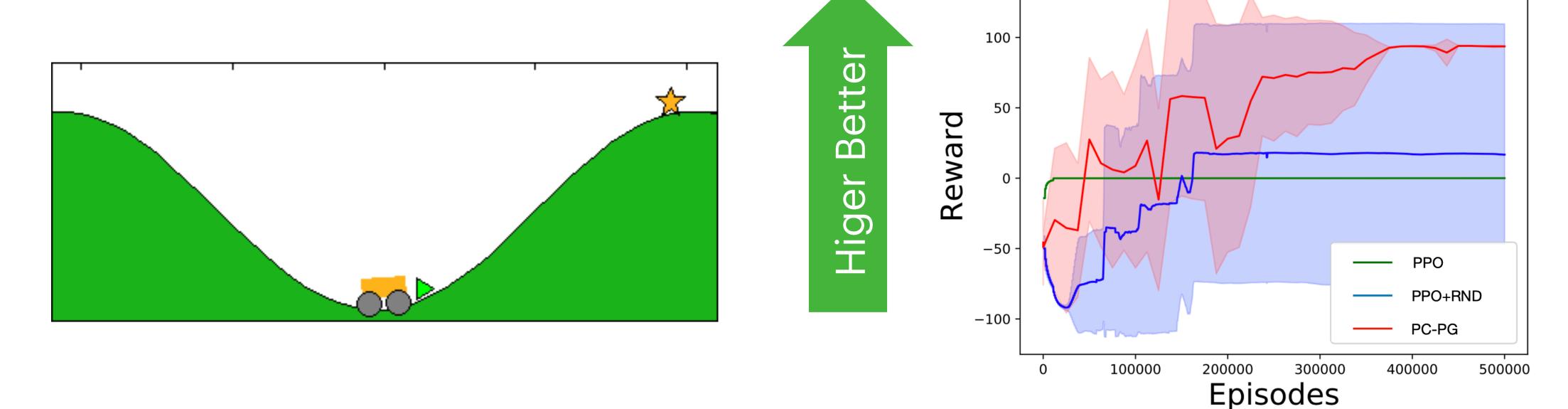
Continuous Control w/ sparse reward



Sparse reward: large reward at the goal;

Anti-shaped reward: penalize control inputs

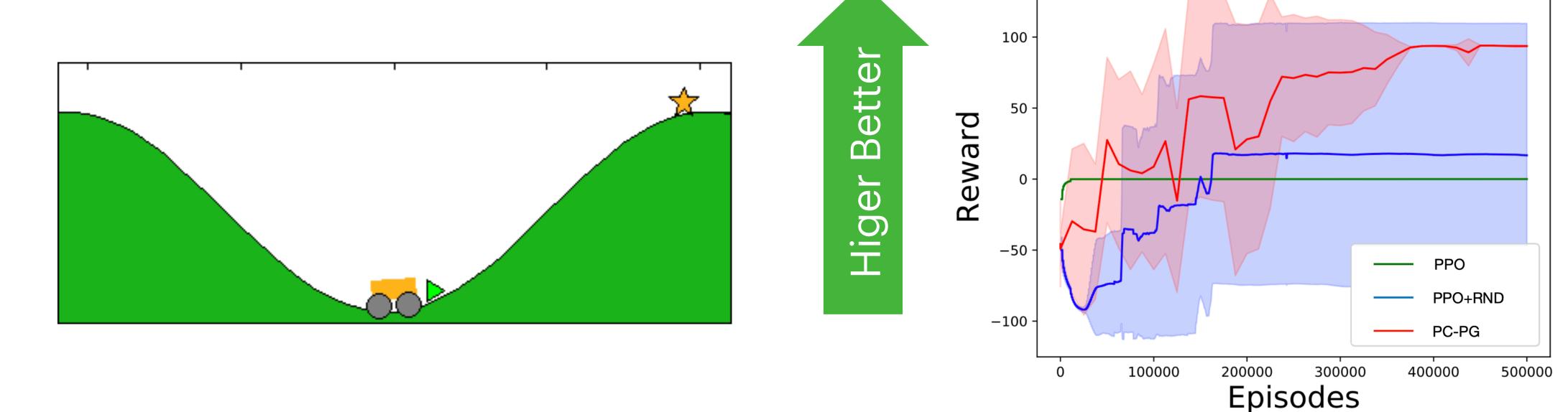
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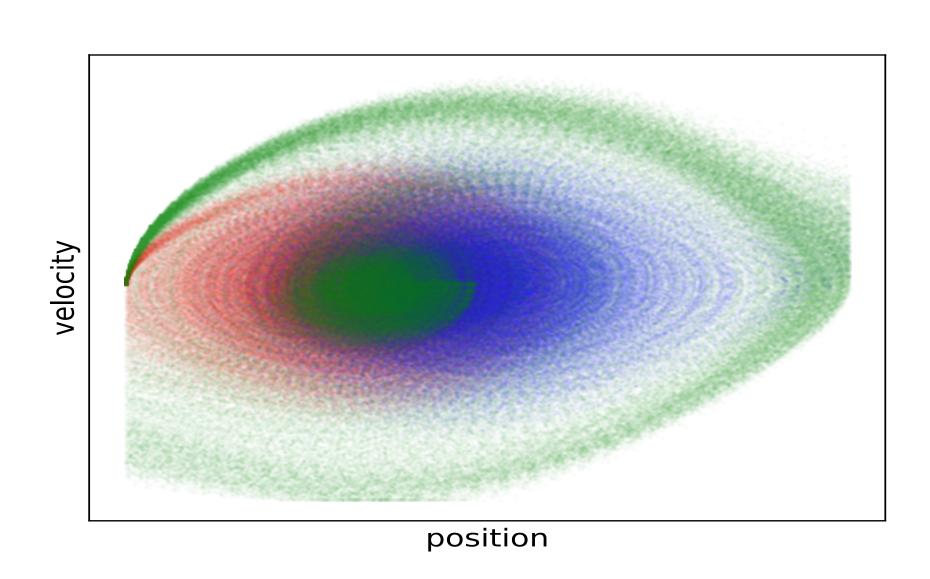
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Average model-misspecification VS ℓ_{∞}

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Polynomial Sample Complexity in well-specified case:

Linear MDPs (RKHS) & Tabular MDPs

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Policy Cover/bonus solve the issue of flatten gradient & Forgetting

Treat policy cover's distribution as the reset distribution for PG

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Flexibility to leverage existing deep learning/RL tools

Vanilla implementation explores 4 to 5 rooms in M-Revenge