Towards a Theory of Generalization in Reinforcement Learning

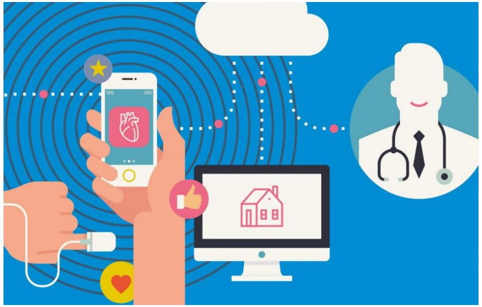
Sham M. Kakade

University of Washington & Microsoft Research

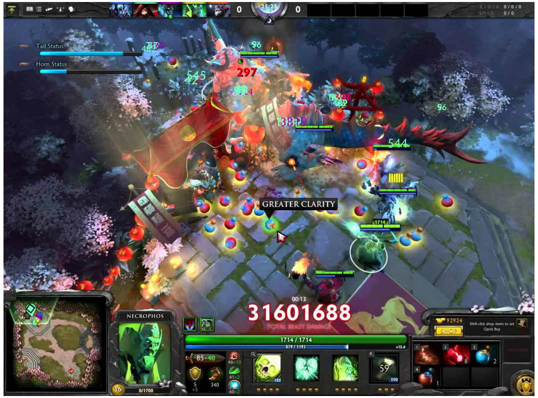
Hello Harvard

(& MIT) !

Progress of RL in Practice

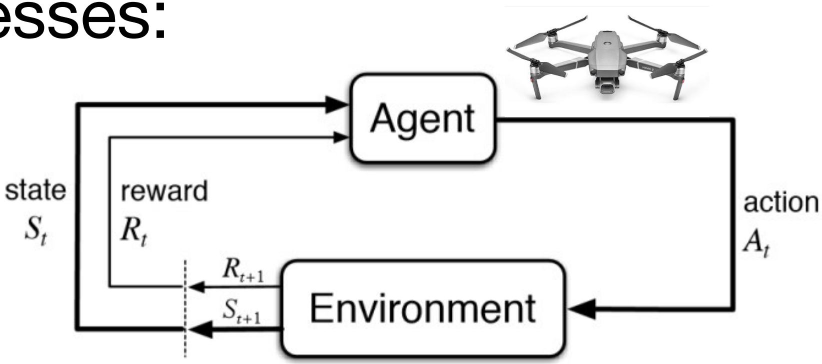


[AlphaZero, Silver et.al, 17]



[OpenAI Five, 18]

Markov Decision Processes:
a framework for RL



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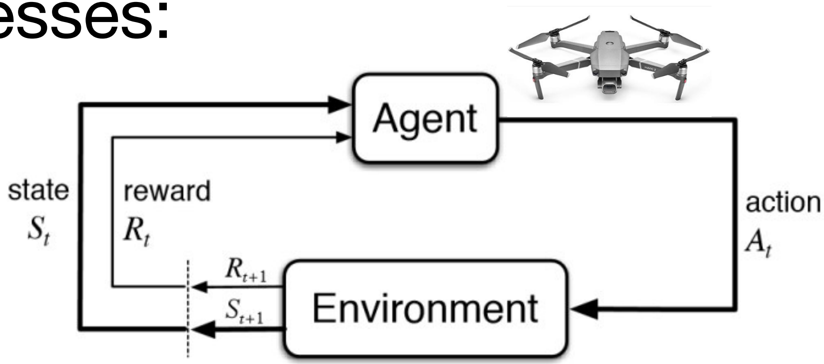
a framework for RL

- A policy:
  π : States $\rightarrow$ Actions



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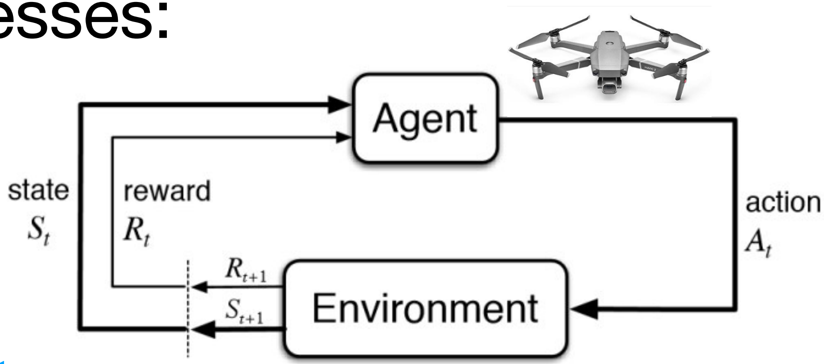

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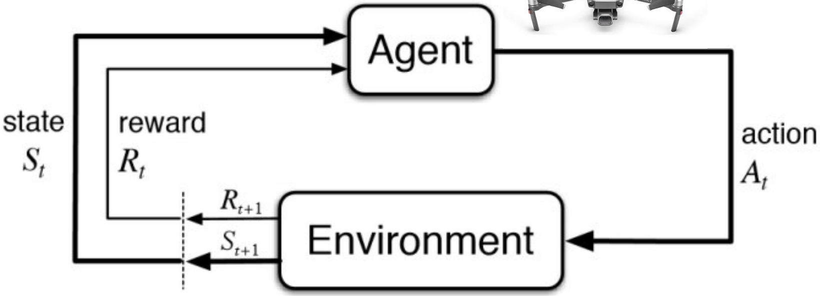

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- Cumulative H-step reward:

state-action value

$$V_H^\pi(s) = \mathbb{E}_\pi \left[\sum_{t=0}^{H-1} r_t \middle| s_0 = s \right], \quad Q_H^\pi(s,a) = \mathbb{E}_\pi \left[\sum_{t=0}^{H-1} r_t \middle| s_0 = s, a_0 = a \right]$$

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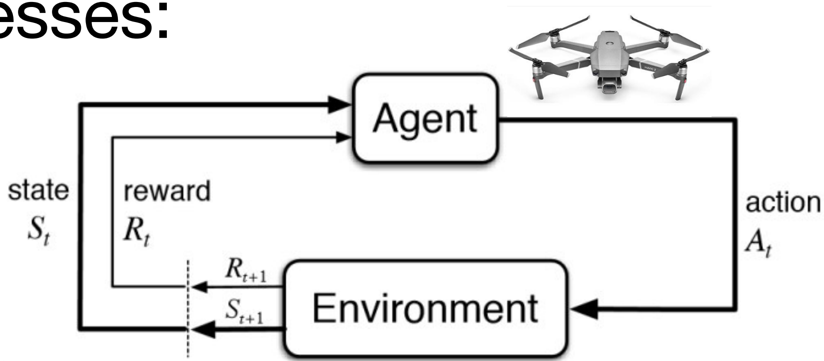

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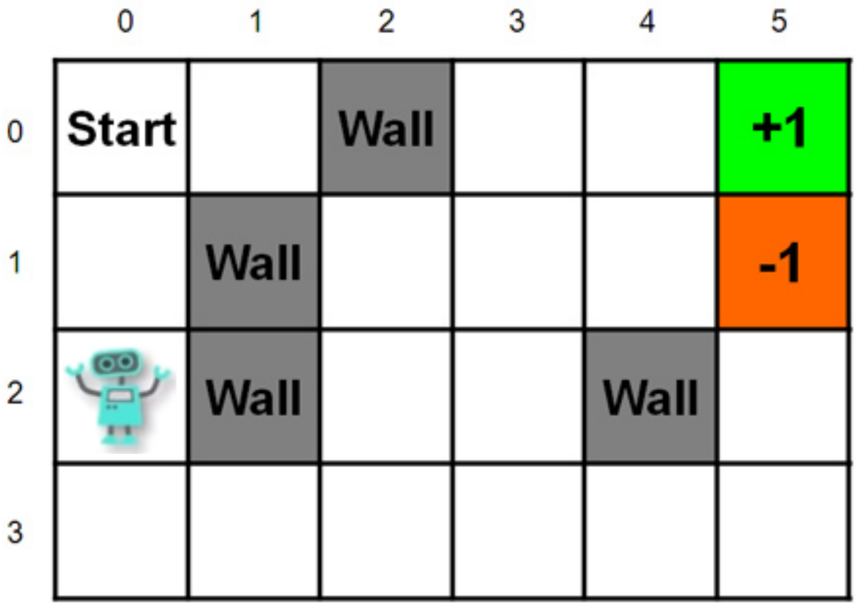
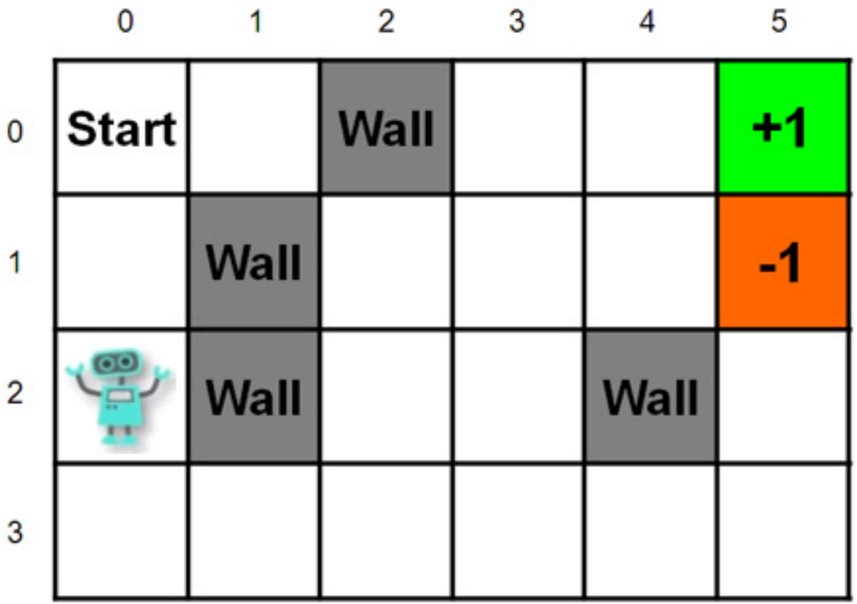
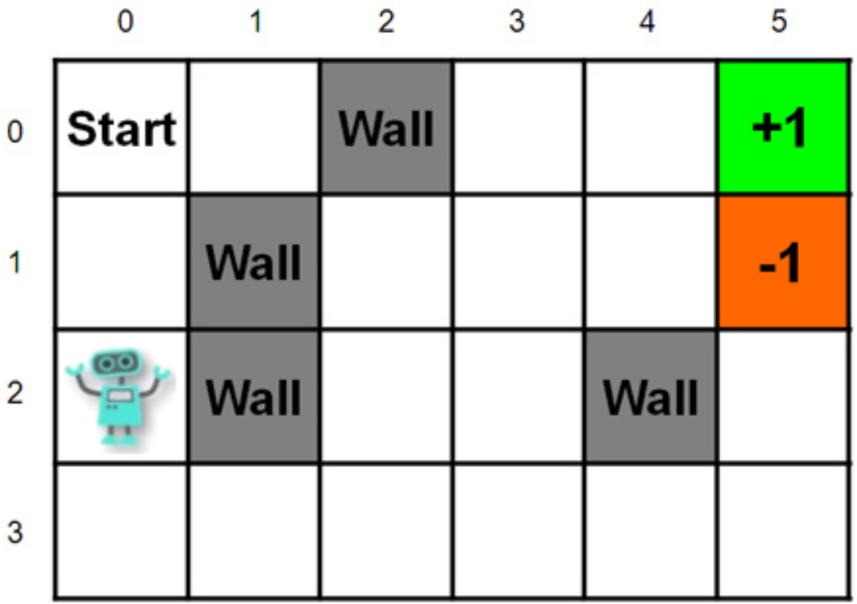
- Goal: Find a policy π that maximizes our value $V^{\pi}(s_0)$ from s_0.

  Episodic setting: We start at s_0; act for H steps; repeat…


0
1
2
3
4
5
0
Start
Wall
+1
1
Wall
-1
2
Wall
Wall
3

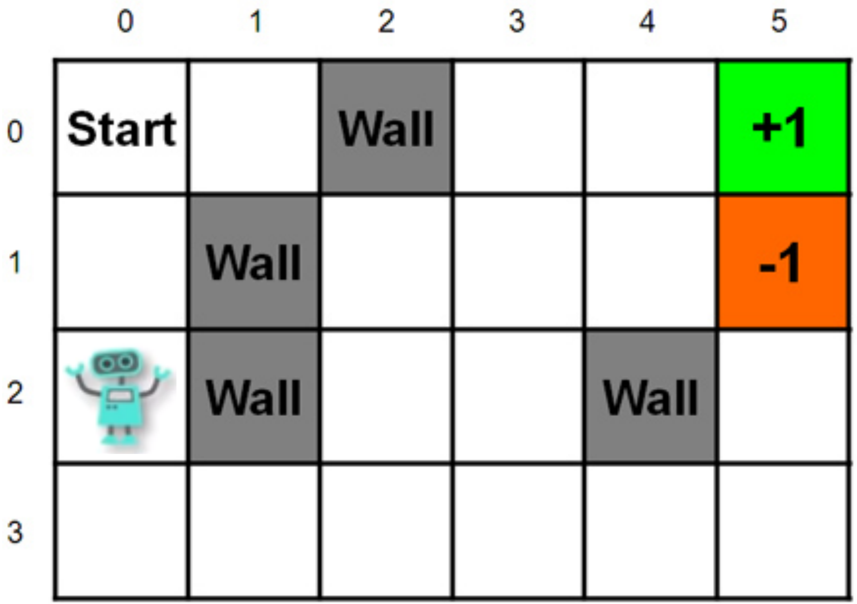


Challenges in RL



Challenges in RL

1. Exploration
   (the environment may be unknown)



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2. Credit assignment problem
(due to delayed rewards)

Dexterous Robotic Hand Manipulation
OpenAI, ‘19

Challenges in RL

1. Exploration
   (the environment may be unknown)

2. Credit assignment problem
   (due to delayed rewards)

3. Large state/action spaces:
   hand state: joint angles/velocities
   cube state: configuration
   actions: forces applied to actuators

<u>Part-0:</u>

A Whirlwind Tour of Generalization

from Supervised Learning to RL

Provable Generalization in Supervised Learning (SL)

Generalization is possible in the IID supervised learning setting!

To get ϵ-close to best in hypothesis class $\mathscr{F}$, we need # of samples that is:

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To get ϵ-close to best in hypothesis class $\mathscr{F}$, we need # of samples that is:

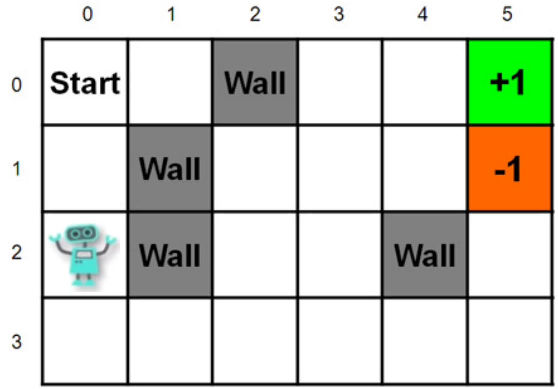
- "Occam's Razor" Bound (finite hypothesis class): need $O(\log|\mathscr{F}|/\epsilon^2)$
- Various Improvements:
  - VC dim $O(\mathrm{VC}(\mathscr{F})/\epsilon^2)$; Classification (margin bounds): $O(\mathrm{margin})/\epsilon^2)$;

    Linear regression: $O(\mathrm{dimension}/\epsilon^2)$
  - Deep Learning: the algorithm also determines the complexity control

The key idea in SL: data reuse

With a training set, we can simultaneously evaluate the loss of all hypotheses in our class!

Sample Efficient RL in the Tabular Case (no generalization here)



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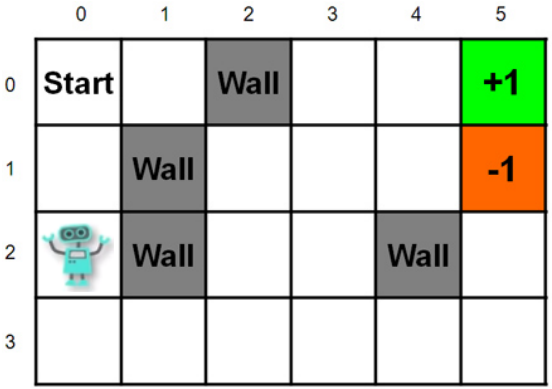
small

- S = #states, A = #actions, H = #horizon
- We have an (unknown) MDP.



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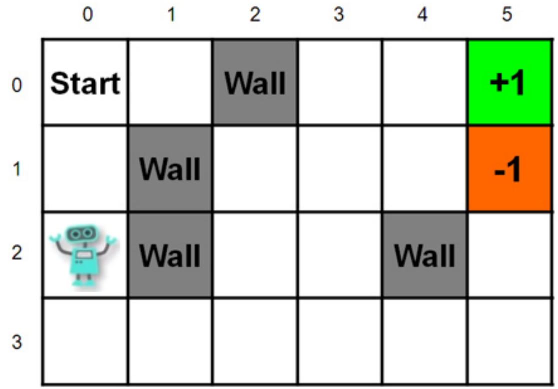

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- We have an (unknown) MDP.
- Thm: [Kearns & Singh '98] In the episodic setting, E^3
  $poly(S, A, H, 1/\epsilon)$ samples suffice to find an ϵ-opt policy.
  Key idea: $\underbrace{\text{optimism}}$ + dynamic programming ← plan to explore

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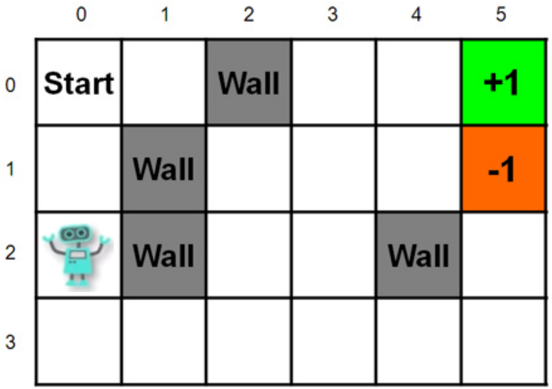

goal: find π $\quad V_H^{\pi}(s_0) \geq V_H^{*}(s_0) - \varepsilon$

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  "model based"

  Key idea: optimism + dynamic programming

  Watkins '90

  asym.

- Lots improvements on the rate:
  [Brafman& Tennenholtz '02][K. '03][Auer+ '09] [Agrawal, Jia '17]
  [Azar+ '13],[Dann & Brunskill '15] minmax optimal
- Provable Q-learning (+bonus):
  [Strehl+ (2006)], [Szita & Szepesvari '10],[Jin+ '18] "model free"

I: Provable Generalization in RL

Q1: Can we find an ϵ-opt policy with no S dependence?

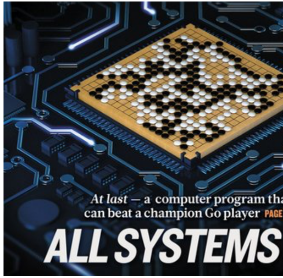
on value

- How can we reuse data to estimate the value of all policies in a policy class $\mathscr{F}$?

  Idea: Trajectory tree algo

  dataset collection: uniformly at random choose actions for all H steps in an episode.

  estimation: uses importance sampling to evaluate every $f \in \mathscr{F}$



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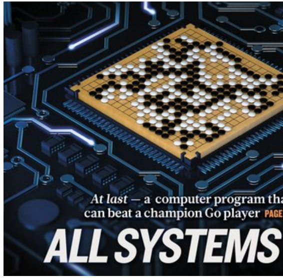

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"classic gen" because the MDP is stoch.

- Thm:[Kearns, Mansour, & Ng '00]
  To find an ϵ-best in class policy, the trajectory tree algo uses $O(A^H \log(|\mathscr{F}|/\epsilon^2))$ samples

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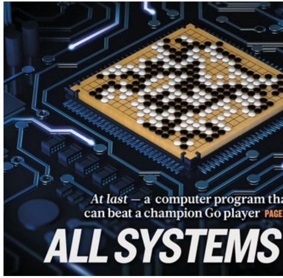

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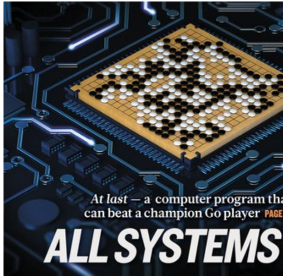
- Thm:[Kearns, Mansour, & Ng '00] "agnostic" with no assumptions on MDP.
  To find an ϵ-best in class policy, the trajectory tree algo uses $O(A^H \log(|\mathscr{F}|/\epsilon^2))$ samples
  - Only $\log(|\mathscr{F}|)$ dependence on hypothesis class size.
  - There are VC analogues as well.

  $A = 2$

  A^H

- Can we avoid the $\cancel{2^H}$ dependence to find an an ϵ-best-in-class policy?
  Agnostically, **NO**!
  Proof: Consider a binary tree with 2^H-policies and a sparse reward at a leaf node.

II: Provable Generalization in RL



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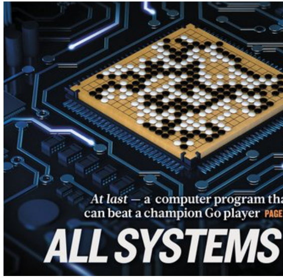

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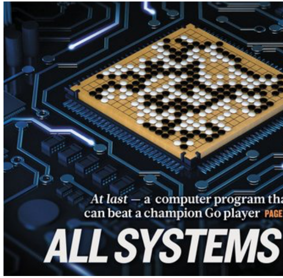

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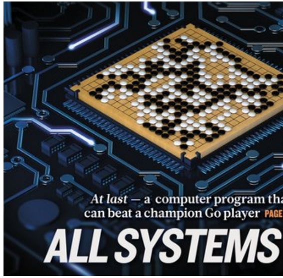

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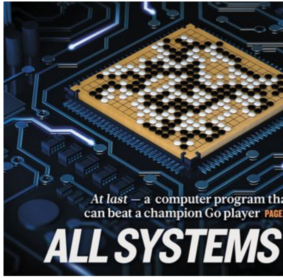

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What is the nature of the assumptions under which generalization in RL is possible?
(what is necessary? what is sufficient?)

Today's Lecture

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  Is RL possible?

- Part III: Upper bounds:
  Are there unifying conditions that are sufficient?

<u>Part-I:</u>

Bandits (the $H = 1$ case)

(Let’s set the stage for RL!)

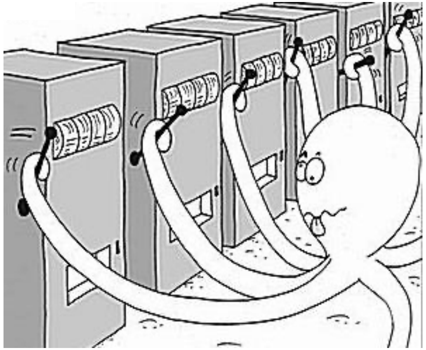
Multi-armed bandits

How should we allocate

T tokens to A "arms"

to maximize our return?

[Robins '52, Gittins'79, Lai & Robbins '85 …]



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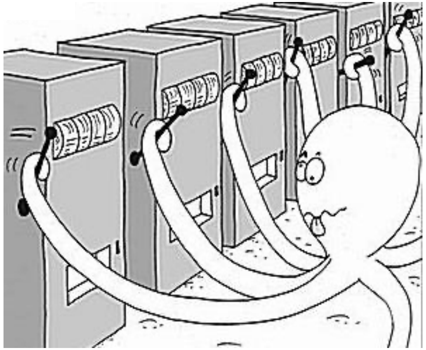
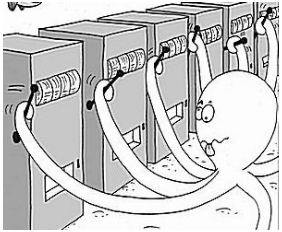


- Very successful algo when A is small.
- What can we do when the number or arms A is large?

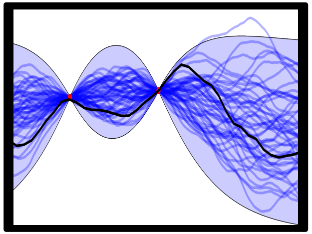
Dealing with the large action case

Bandits



- decision: pull an arm

Linear (RKHS) Bandits



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- e.g. $x \in R$

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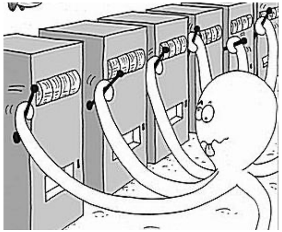
Bandits



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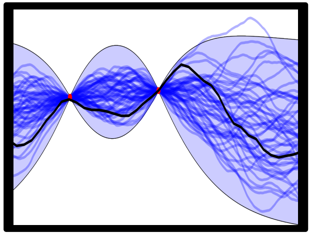

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  successful in many applications: scheduling, ads…

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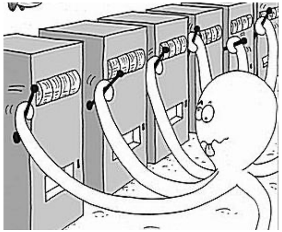

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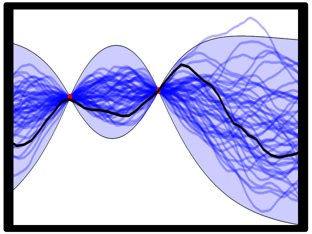

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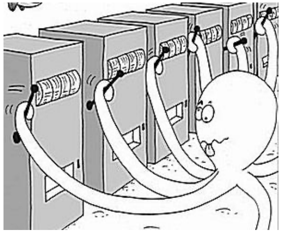

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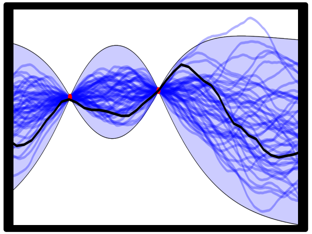

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- Hypothesis class $\mathcal{F}$ is set of linear/RKHS functions

Linear-UCB/GP-UCB:

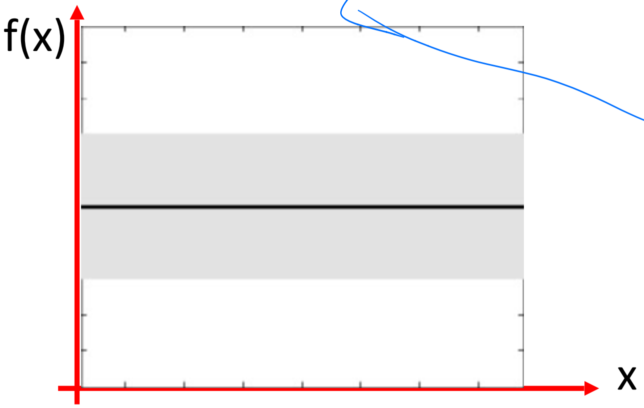
Algorithmic Principle: Optimism in the face of uncertainty

Pick input that maximizes upper confidence bound:

$$\boxed{x_t = \arg\max_{x \in D} \mu_{t-1}(x) + \beta_t \sigma_{t-1}(x)}$$

uncertainty of the function

our "mean" estimate of "f"



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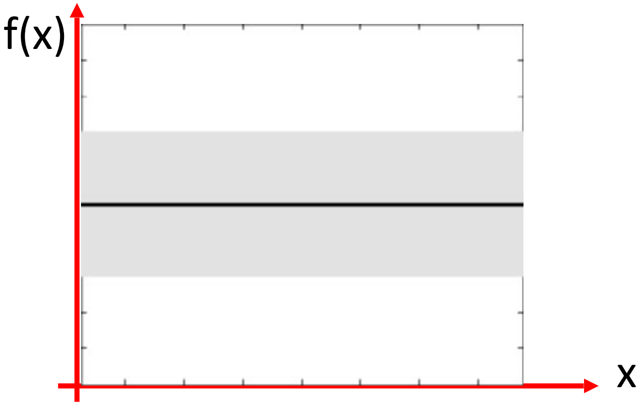

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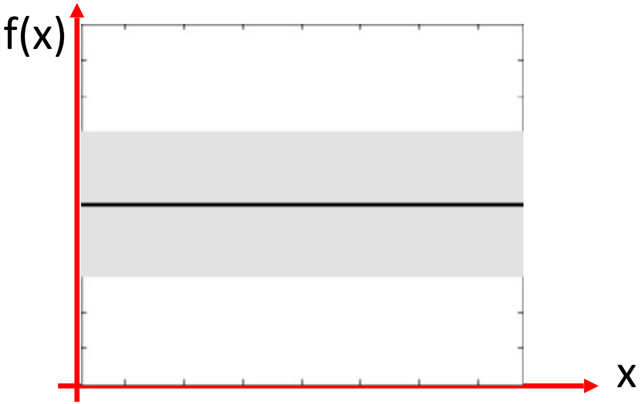

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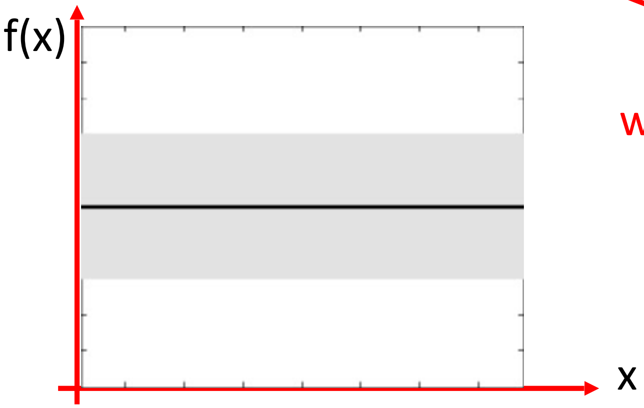

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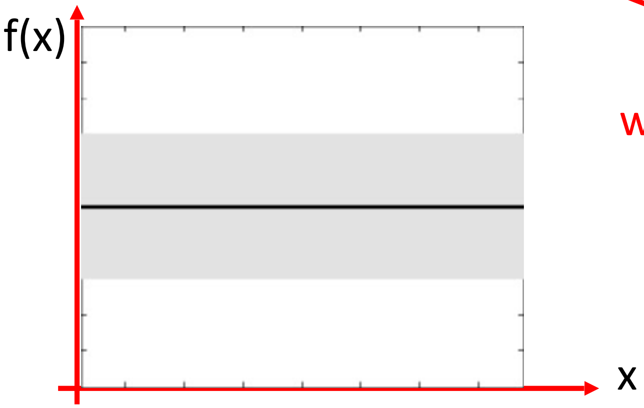

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Regret of Lin-UCB/GP-UCB

(generalization in action space)

Theorem: [Dani, Hayes, & K. ’08], [Srinivas, Krause, K. & Seeger '10]

Assuming $\mathscr{F}$ is an RKHS (with bounded norm), if we choose β_t “correctly”,

$$\frac{1}{T}\sum_{t=1}^{T}[f(x^*) - f(x_t)] = \mathcal{O}^*\left(\sqrt{\frac{\gamma_T}{T}}\right)$$

where $\gamma_T := \max_{x_0 \ldots x_{T-1} \in \mathcal{X}} \log\det\left(I + \sum_{t=0}^{T-1} \phi(x_t)\phi(x_t)^\top\right)$

$f \in$ linear in ϕ

Regret of Lin-UCB/GP-UCB

(generalization in action space)

Theorem: [Dani, Hayes, & K. '08], [Srinivas, Krause, K. & Seeger '10]

Assuming $\mathscr{F}$ is an RKHS (with bounded norm), if we choose β_t "correctly",

$$\frac{1}{T}\sum_{t=1}^{T}[f(x^*) - f(x_t)] = \mathcal{O}^*\left(\sqrt{\frac{\gamma_T}{T}}\right) \quad c\sqrt{\frac{d}{T}}$$

where $\gamma_T := \max_{x_0 \ldots x_{T-1} \in \mathscr{X}} \log\det\left(I + \sum_{t=0}^{T-1} \phi(x_t)\phi(x_t)^\top\right)$

- Key complexity concept: "*maximum information gain*" γ_T determines the regret
  - $\gamma_T \approx d \log T$ for ϕ in d-dimensions
  - Think of γ_T as the "effective dimension"
- Easy to incorporate context
- Also: [Auer+ '02; Abbasi-Yadkori+ '11]

Switch
(LinUCB analysis)

Part-2: RL

What are necessary conditions?

Let’s look at the most natural assumptions.

Approx. Dynamic Programming with Linear Function Approximation

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Basic idea: approximate the $Q(s, a)$ values with linear basis functions $\phi_1(s, a), \ldots \phi_d(s, a)$. (where $d \ll$ #states, #actions)

$\vec{\phi} \in \mathbb{R}^d$

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- Lots of work on this approach, e.g.
  [Tesauro, ’95], [de Farias & Van Roy ’03], [Wen & Van Roy ’13]

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$E[r_t \mid a_t] = w^{*} \cdot \phi(a_t)$

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- Let’s look at the most basic question with “linearly realizable Q*”

RL with Linearly Realizable Q*-Function Approximation

(Does there exist a sample efficient algo?)

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$$E\left[\sum_{\tau=H-h}^{H} r_\tau \,\middle|\, \pi\right] \approx \quad Q_h^\star(s,a) = w_h^\star \cdot \phi(s,a)$$

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

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  - The LP is not general because it encodes the Bellman optimality constraints.
  - We have sampling access (in the episodic setting).

Linearly Realizability is Not Sufficient for RL

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- [Weisz, Amortila, Szepesvári '21]:
  There exists an MDP and a ϕ satisfying A1 s.t any online RL algorithm (with knowledge of ϕ) requires $\Omega(\min(2^d, 2^H))$ samples to output the value $V^\star(s_0)$ up to constant additive error (with prob. ≥ 0.9).

0.1 close

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  A2 (Large Suboptimality Gap): for all $a \neq \pi^\star(s)$, $V_h^\star(s) - Q_h^\star(s, a) \geq 1/16.$
  The lower bound holds even with **both** A1 and A2.

orig'

min { 2^A, 2^H, 2^d }

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~~xxx~~ Not possible

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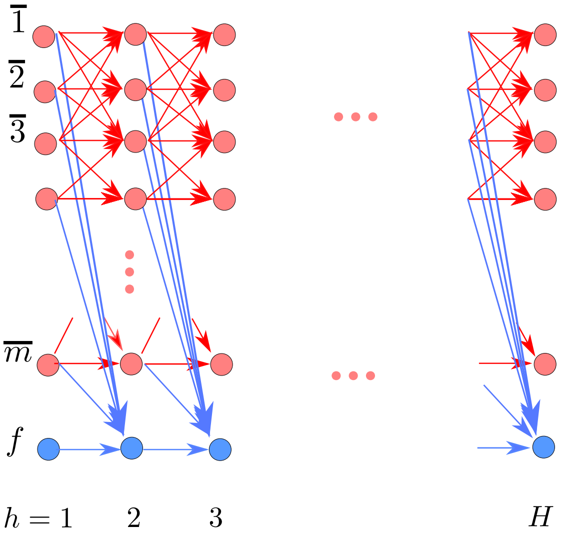
Comments: An exponential separation between online RL vs simulation access.

[Du, K., Wang, Yang '20]: A1+A2+simulator access (input: any s, a; output: $s' \sim P(\cdot \mid s, a), r(s, a)$)

$\Longrightarrow$ there is sample efficient approach to find an ϵ-opt policy.

Construction Sketch: a Hard MDP Family

(A ``leaking complete graph'')



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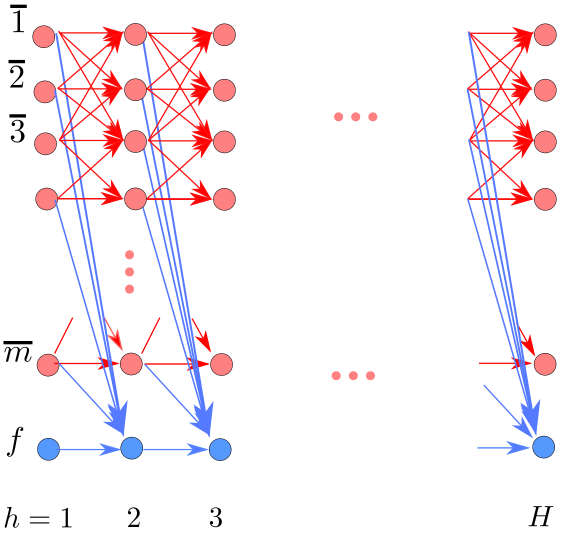

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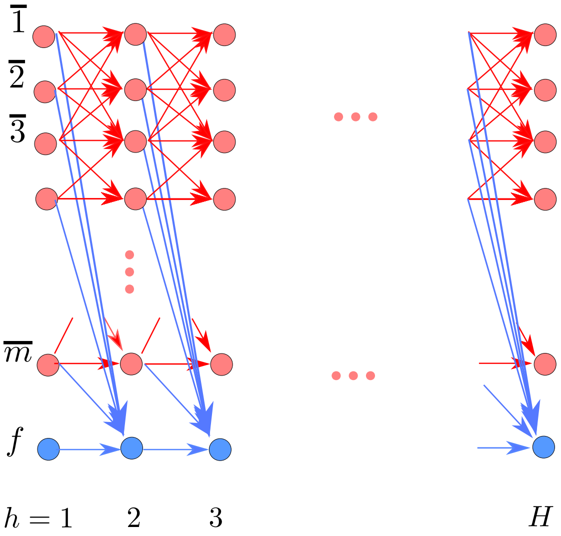

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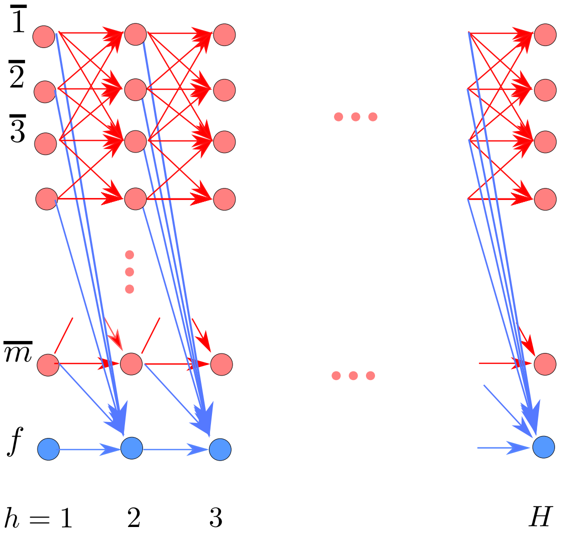

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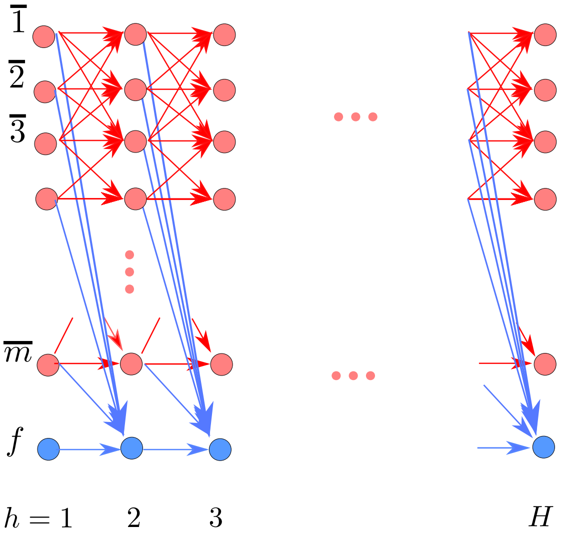

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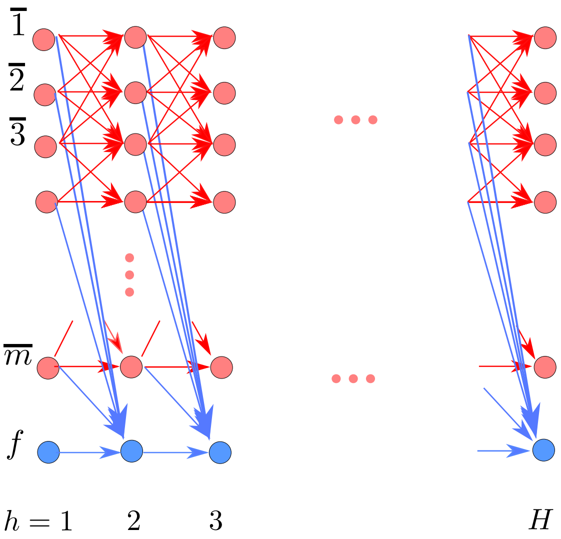

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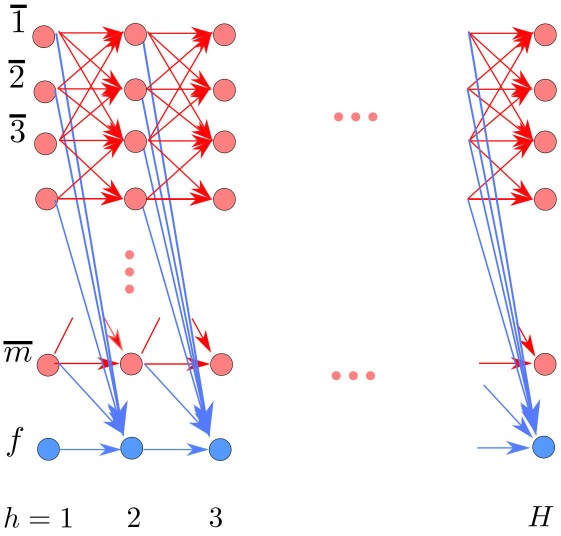

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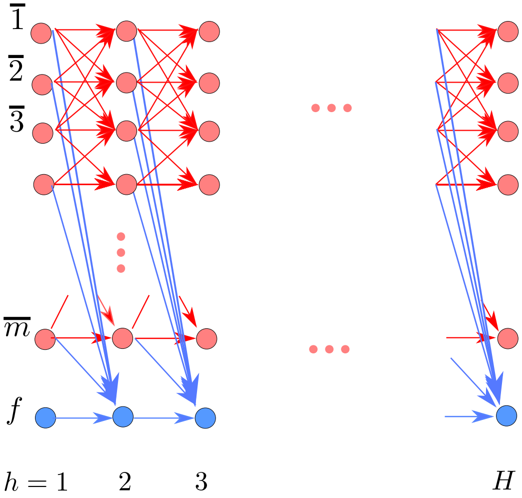
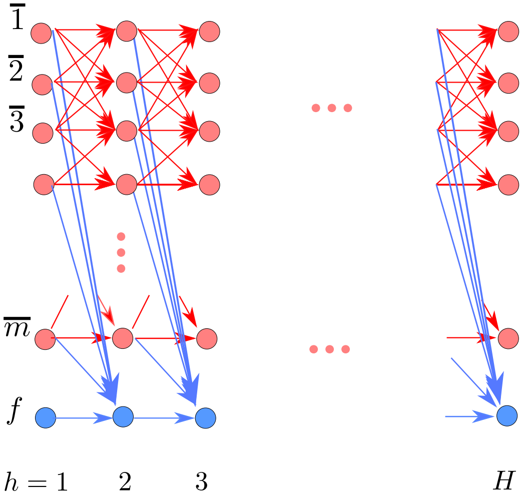
Lemma: For any $\gamma > 0$, there exist $m = \lfloor \exp(\frac{1}{8}\gamma^2 d) \rfloor$ unit vectors $\{v_1, \cdots, v_m\}$ in R^d s.t. $\forall i, j \in [m]$ and $i \neq j$, $|\langle v_i, v_j \rangle| \leq \gamma$.

We will set $\gamma = 1/4$.

(proof: Johnson-Lindenstrauss)

The construction, continued





The construction, continued

Pr(next state | curr. state, false a)

- Transitions: $s_0 \sim \text{Uniform}([m])$.
  $\Pr[f \,|\, \overline{a_1}, a^*] = 1$,

$$\Pr[\,\cdot\,|\,\overline{a_1}, a_2] = \begin{cases} \overline{a_2} : \left\langle v(a_1), v(a_2) \right\rangle + 2\gamma \\ f : 1 - \left\langle v(a_1), v(a_2) \right\rangle - 2\gamma \end{cases}, (a_2 \neq a^*, a_2 \neq a_1)$$

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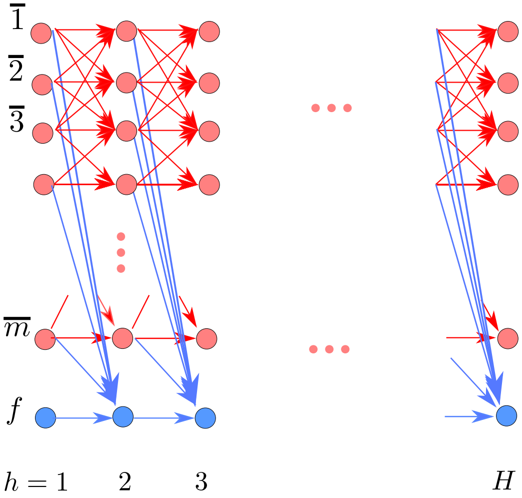

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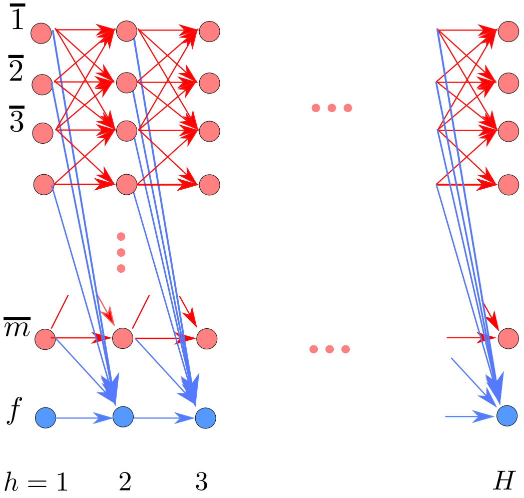

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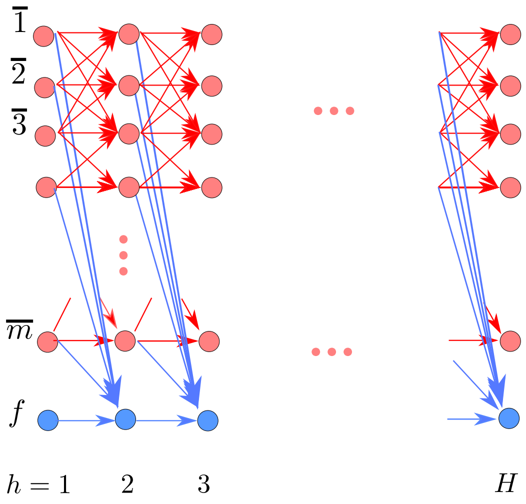

γ $(i \neq j)$ γ

$-\frac{1}{4} \le \langle v_i, v_j \rangle \le \frac{1}{4}$

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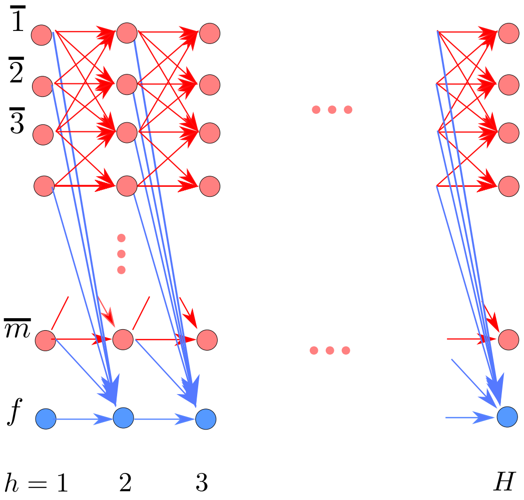
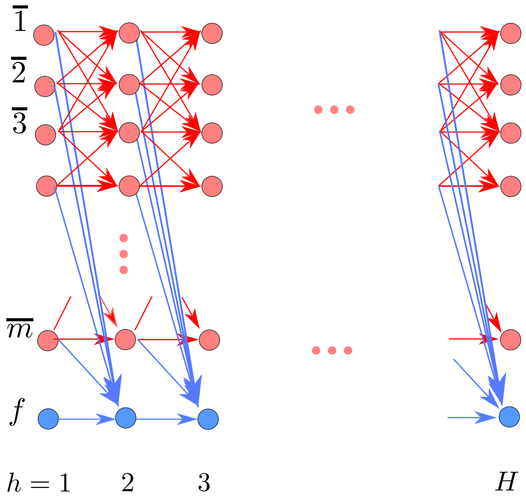
- The transition probabilities are indeed valid, because
  $$0 < \gamma \le \left\langle v(a_1), v(a_2) \right\rangle + 2\gamma \le 3\gamma < 1.$$

The construction, continued





The construction, continued

- Features: of dimension d defined as:

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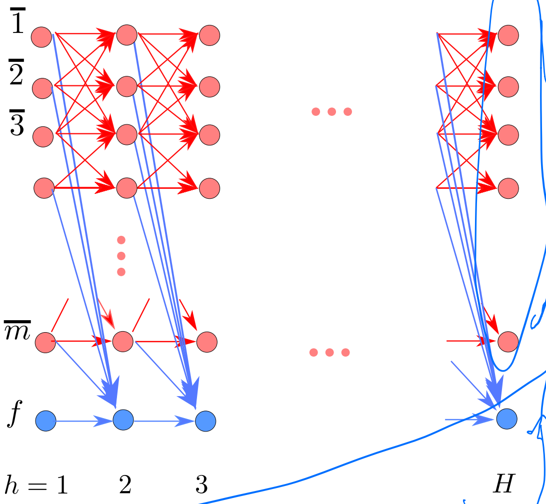
$$\phi(f, \cdot\ ) := \mathbf{0}$$

note: the feature map does not depend of a^*.



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- Rewards: $\frac{1}{4} = \gamma \leq$

for $1 \leq h < H$,

$$R_h(\overline{a_1}, a^*) := \left\langle v(a_1), v(a^*) \right\rangle + 2\gamma,$$

$\leq 3\gamma = 3/4$

$$R_h(\overline{a_1}, a_2) := -2\gamma \left[\left\langle v(a_1), v(a_2) \right\rangle + 2\gamma \right], \quad a_2 \neq a^*, a_2 \neq a$$

$\leq -2\gamma^2 \approx -\frac{1}{8}$

$$R_h(f, \cdot) := 0.$$

for $h = H$,

$$r_H(s, a) := \langle \phi(s, a), v(a^*) \rangle$$

critical

we don't get to quickly

depends on a^*

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$\phi(s, a)$

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$\implies$ π is optimal

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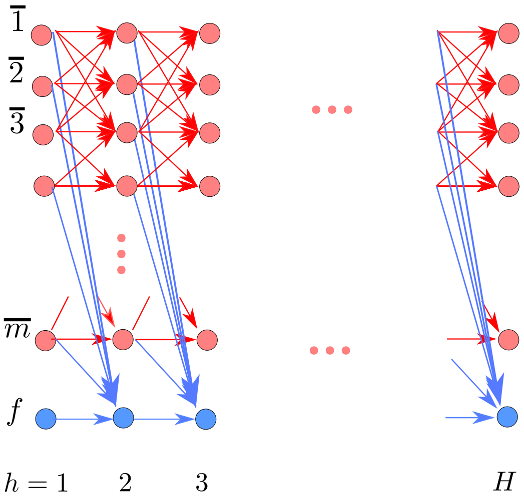
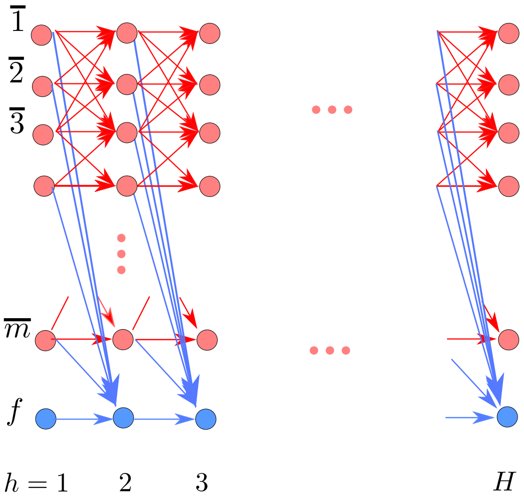
- Proving the large gap: for $a_2 \neq a^*$

$$V_h^*(\overline{a_1}) - Q_h^*(\overline{a_1}, a_2) = Q_h^\pi(\overline{a_1}, a^*) - Q_h^\pi(\overline{a_1}, a_2) > \gamma - 3\gamma^2 \geq \frac{1}{4}\gamma\,.$$

The information theoretic proof:





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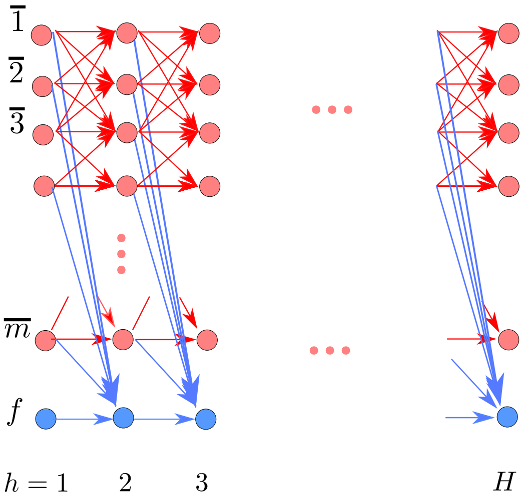
Proof: When is info revealed about $\mathscr{M}_{a^*}$, indexed by a^*?



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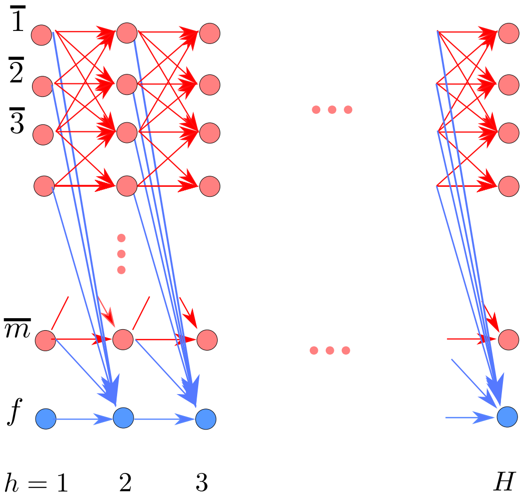

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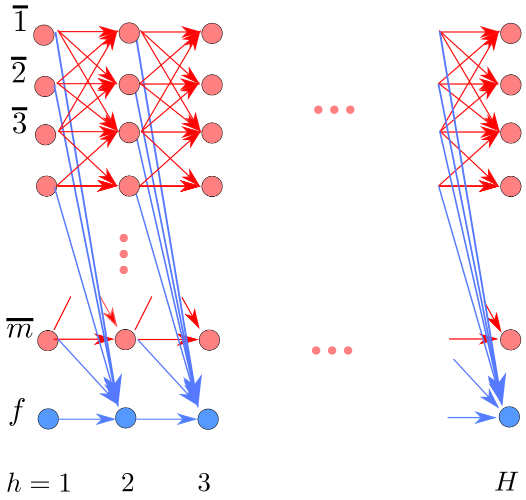

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  (2) also, if we terminate at $s_H \neq f$, then the reward r_H leaks info about on a^*

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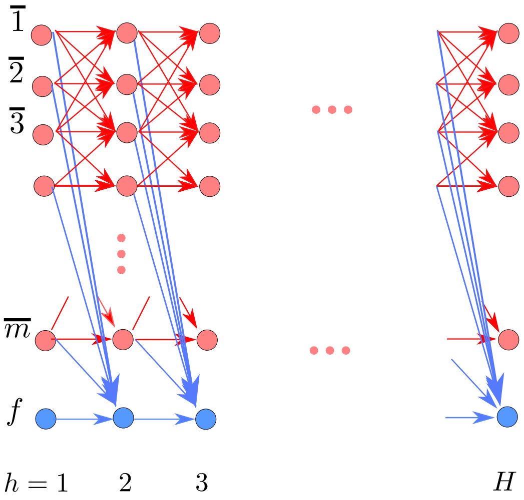

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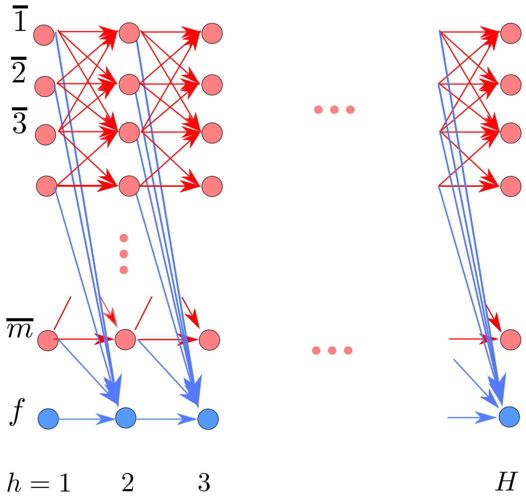

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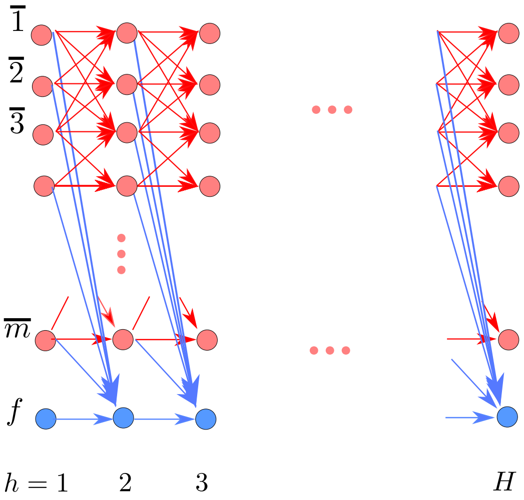

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Open Problem: Can we prove a lower bound with $A = 2$ actions?

Interlude:

Are these issues relevant in practice?

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(related concepts: distribution shift, “the deadly triad”, offline RL)

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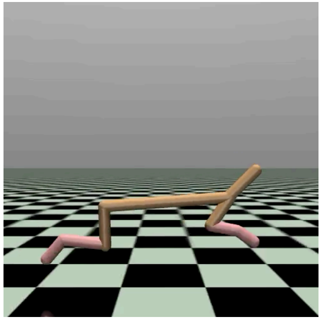
Practice: [Wang, Wu, Salakhutdinov, K., 2021]:

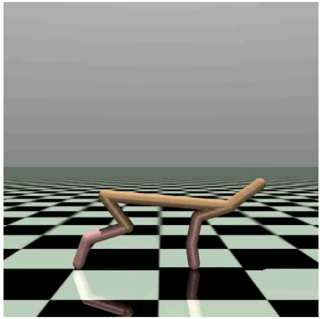
Does it matter in practice? Say given good ""deep-pre-trained- features"? YES!

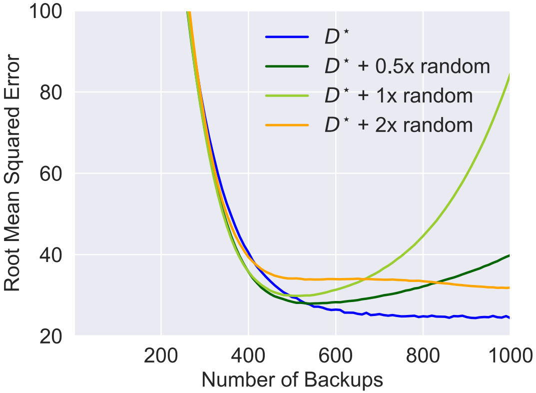
Offline dataset is a mix of two sources:
running & random

Use SL to evaluate the running policy with "deep-pre-trained- features"

Massive error amplification even with 50/50% mixed offline data







Part-3:
What are sufficient conditions?

Is there a common theme to positive results?

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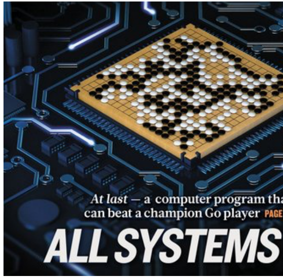

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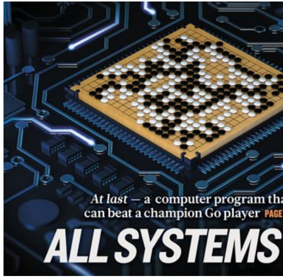

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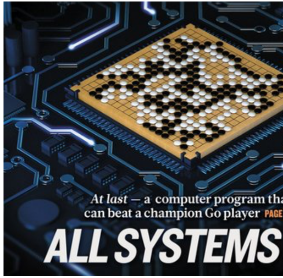

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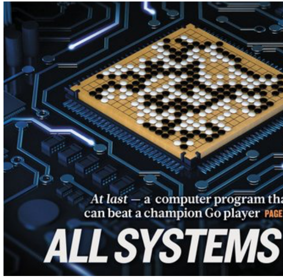

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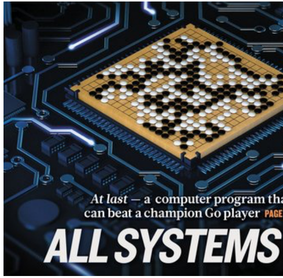

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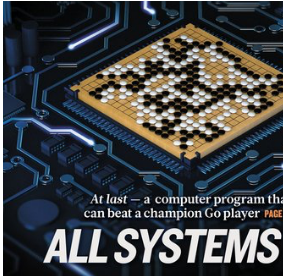

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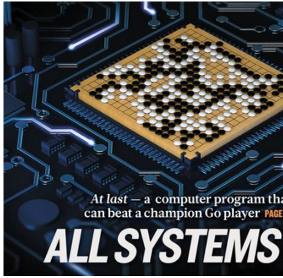

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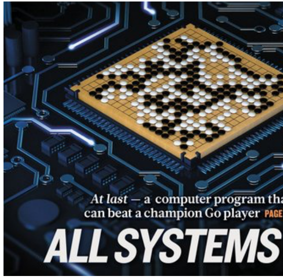

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(back to $H = 1$ RL problem)

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$\mathcal{T}(Q)$ Bellman backup operator.

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- (recall) Bellman optimality: suppose $Q^\star - \mathcal{T}(Q^\star) = 0$

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- Data reuse: there is function $\ell_f(s, a, s', g)$ s.t.

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- The framework easily leads to new models (see paper).

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- return: the best policy π_f found

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- The proof is "elementary" using the elliptical potential function.
  [Dani, Hayes, K. '08]

Thanks!

- A generalization theory in RL is possible and different from SL!
  - necessary: linear realizability insufficient. need much stronger assumptions.
  - sufficient: lin. bandit theory → RL theory (bilinear classes) is rich.
    - covers known cases and new cases
    - FLAMBE: [Agarwal+ '20] feature learning possible in this framework.
  - practice: these issues are relevant ("deadly triad"/RL can be unstable)

See https://rltheorybook.github.io/ for forthcoming book!