

# **Statistical Limits of Generalization**

## **Part II: Linear Realizability**

**Sham Kakade and Wen Sun**

**CS 6789: Foundations of Reinforcement Learning**

# Announcements

- HW1 will be posted tonight
  - Tentatively: due Sept 28 (check ED posting)
- Chapters 1-5 substantially updated.
  - Feedback/questions/finding typos appreciated!

Today:

# Today:

- Recap: lower bounds for generalization
  - agnostic learning is not possible in RL  
(unless we pay an exponential in  $H$  dependence)
  - Linear realizability of  $Q^*$  is still statistically hard

# Today:

- Recap: lower bounds for generalization
  - agnostic learning is not possible in RL  
(unless we pay an exponential in  $H$  dependence)
  - Linear realizability of  $Q^*$  is still statistically hard
- Today:
  - Finish up lower bound when we know  $Q^*$  is linearly realizable.
  - New: linear Bellman completeness.

# Part-2: Linear Realizability

What if we impose linearity assumptions?

Let's look at the most natural assumptions.

# RL with Linearly Realizable $Q^*$ -Function Approximation

(Does there exist a sample efficient algo?)

## RL with Linearly Realizable $Q^*$ -Function Approximation

(Does there exist a sample efficient algo?)

- Suppose we have a feature map:  $\vec{\phi}(s, a) \in R^d$ .



# RL with Linearly Realizable $Q^*$ -Function Approximation

(Does there exist a sample efficient algo?)

$d \ll \ll \# \text{ states}$   
 $\# \text{ actions}$

- Suppose we have a feature map:  $\vec{\phi}(s, a) \in R^d$ .
- (A1: Linearly Realizable  $Q^*$ ): Assume for all  $s, a, h \in [H]$ , there exists  $w_1^*, \dots, w_H^* \in R^d$  s.t.

$$Q_h^*(s, a) = w_h^* \cdot \phi(s, a)$$

# RL with Linearly Realizable $Q^*$ -Function Approximation

(Does there exist a sample efficient algo?)

- Suppose we have a feature map:  $\vec{\phi}(s, a) \in R^d$ .
- (A1: Linearly Realizable  $Q^*$ ): Assume for all  $s, a, h \in [H]$ , there exists  $w_1^*, \dots, w_H^* \in R^d$  s.t.

$$Q_h^*(s, a) = w_h^* \cdot \phi(s, a)$$

- (A2: Large Suboptimality Gap): for all  $a \neq \pi^*(s)$ ,

$$V_h^*(s) - Q_h^*(s, a) \geq \text{constant}$$

$\Downarrow$

$$Q_h^*(s, \pi^*(s))$$

# Linearly Realizability is Not Sufficient for RL

# Linearly Realizability is Not Sufficient for RL

Theorem:

# Linearly Realizability is Not Sufficient for RL

## Theorem:

- [Weisz, Amortila, Szepesvári '21]:

There exists an MDP and a  $\phi$  satisfying A1 s.t any online RL algorithm (with knowledge of  $\phi$ ) requires  $\Omega(\min(2^d, 2^H))$  samples to output the value  $V^*(s_0)$  up to constant additive error (with prob.  $\geq 0.9$ ).

# Linearly Realizability is Not Sufficient for RL

## Theorem:

- [Weisz, Amortila, Szepesvári '21]:

There exists an MDP and a  $\phi$  satisfying **A1** s.t any online RL algorithm (with knowledge of  $\phi$ ) requires  $\Omega(\min(2^d, 2^H))$  samples to output the value  $V^*(s_0)$  up to constant additive error (with prob.  $\geq 0.9$ ).

- [Wang, Wang, K. '21]:

Let's make the problem even easier, where we also assume **A2 (large gap)**  
The lower bound holds even with **both A1 and A2**.

# Linearly Realizability is Not Sufficient for RL

holds with

gen  
model

## Theorem:

- [Weisz, Amortila, Szepesvári '21]:

There exists an MDP and a  $\phi$  satisfying **A1** s.t any online RL algorithm (with knowledge of  $\phi$ ) requires  $\Omega(\min(2^d, 2^H))$  samples to output the value  $V^*(s_0)$  up to constant additive error (with prob.  $\geq 0.9$ ).

- [Wang, Wang, K. '21]:

Let's make the problem even easier, where we also assume **A2 (large gap)**

The lower bound holds even with **both A1 and A2**.

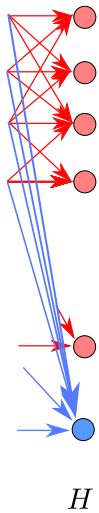
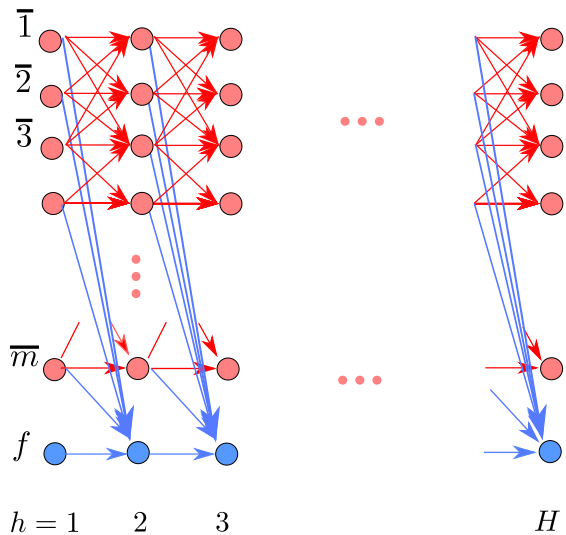
holds only in  
the episodic setting

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

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

$\implies$  there is sample efficient approach to find an  $\epsilon$ -opt policy.

# Construction Sketch: a Hard MDP Family (A "leaking complete graph")

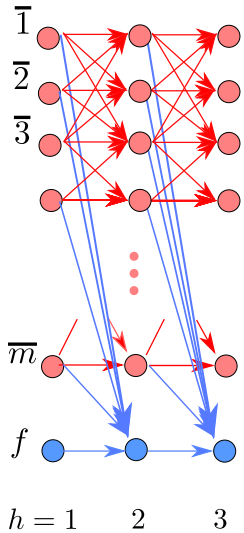




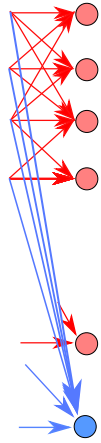
# Construction Sketch: a Hard MDP Family

(A "leaking complete graph")

- $m$  is an integer (we will set  $m \approx 2^d$ )



...



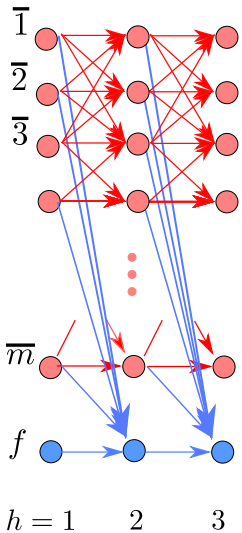
...

$H$

# Construction Sketch: a Hard MDP Family

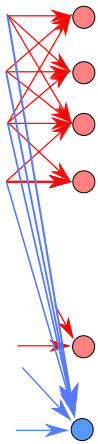
(A "leaking complete graph")

- $m$  is an integer (we will set  $m \approx 2^d$ )
- the state space:  $\{\bar{1}, \dots, \bar{m}, f\}$



...

...

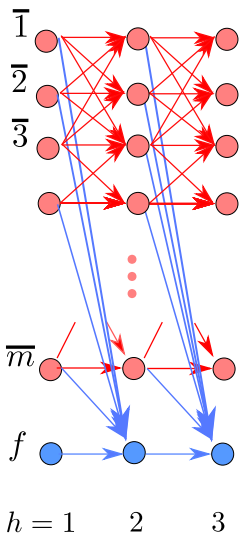


$H$

# Construction Sketch: a Hard MDP Family

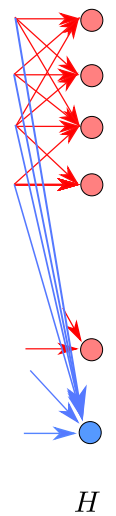
(A “leaking complete graph”)

- $m$  is an integer (we will set  $m \approx 2^d$ )
- the state space:  $\{\bar{1}, \dots, \bar{m}, f\}$
- call the special state  $f$  a “terminal state”.



...

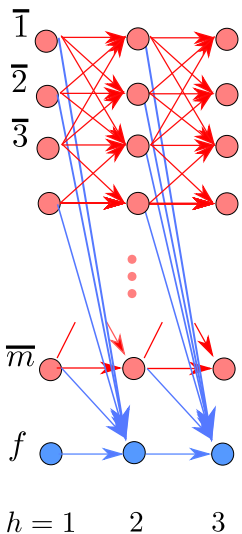
...



# Construction Sketch: a Hard MDP Family

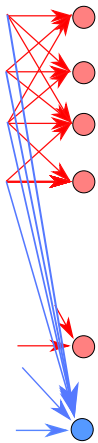
(A “leaking complete graph”)

- $m$  is an integer (we will set  $m \approx 2^d$ )
- the state space:  $\{\bar{1}, \dots, \bar{m}, f\}$
- call the special state  $f$  a “terminal state”.
- at state  $\bar{i}$ , the feasible actions set is  $[m] \setminus \{i\}$
- at  $f$ , the feasible action set is  $[m - 1]$ .  
i.e. there are  $m - 1$  feasible actions at each state.



...

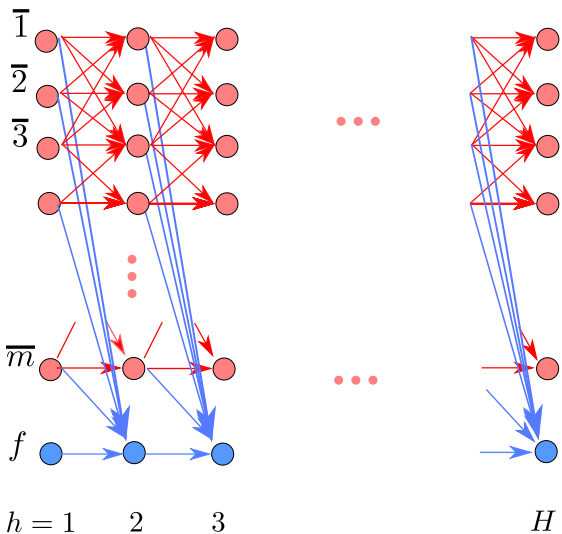
...



H

# Construction Sketch: a Hard MDP Family

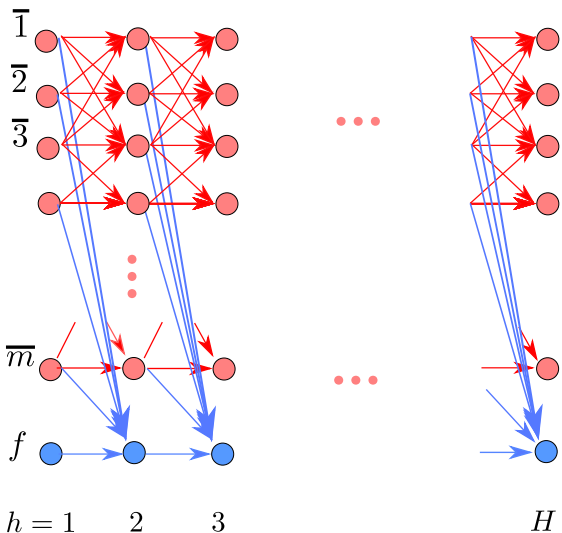
(A "leaking complete graph")



- $m$  is an integer (we will set  $m \approx 2^d$ )
- the state space:  $\{\bar{1}, \dots, \bar{m}, f\}$
- call the special state  $f$  a "terminal state".
- at state  $\bar{i}$ , the feasible actions set is  $[m] \setminus \{i\}$   
i.e. there are  $m - 1$  feasible actions at each state.
- each MDP in this family is specified by an index  $a^* \in [m]$  and denoted by  $\mathcal{M}_{a^*}$ .  
i.e. there are  $m$  MDPs in this family.

# Construction Sketch: a Hard MDP Family

(A “leaking complete graph”)



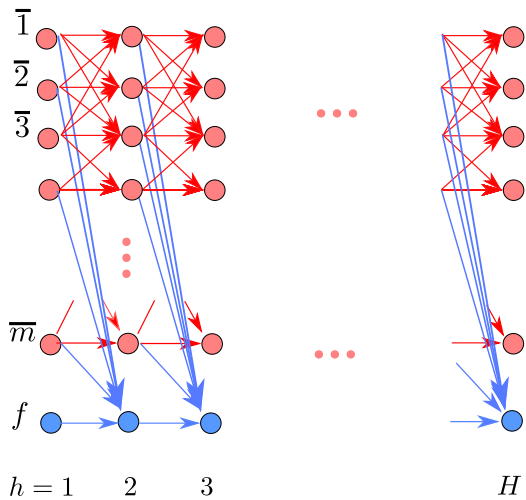
- $m$  is an integer (we will set  $m \approx 2^d$ )
- the state space:  $\{\bar{1}, \dots, \bar{m}, f\}$
- call the special state  $f$  a “terminal state”.
- at state  $\bar{i}$ , the feasible actions set is  $[m] \setminus \{i\}$   
at  $f$ , the feasible action set is  $[m - 1]$ .  
i.e. there are  $m - 1$  feasible actions at each state.
- each MDP in this family is specified by an index  $a^* \in [m]$  and denoted by  $\mathcal{M}_{a^*}$ .  
i.e. there are  $m$  MDPs in this family.

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

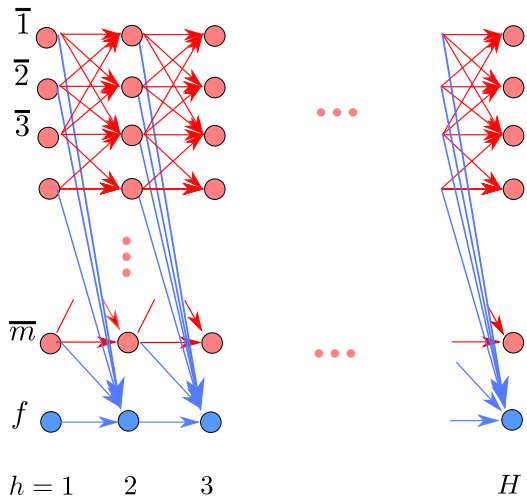
**We will set  $\gamma = 1/4$ .**

(proof: Johnson-Lindenstrauss)

# The construction, continued



## The construction, continued



- **Transitions:**  $s_0 \sim \text{Uniform}([m])$ .

$$\Pr[f | \bar{a}_1, a^*] = 1$$

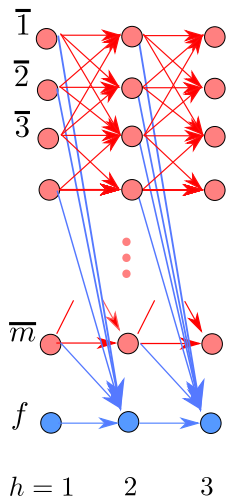
*depends on  $\bar{a}$*

$$\Pr[\cdot | \bar{a}_1, a_2] = \begin{cases} \bar{a}_2 : \langle v(a_1), v(a_2) \rangle + 2\gamma \\ f : 1 - \langle v(a_1), v(a_2) \rangle - 2\gamma \end{cases}, (a_2 \neq a^*, a_2 \neq a_1)$$

$$\Pr[f | f, \cdot] = 1.$$

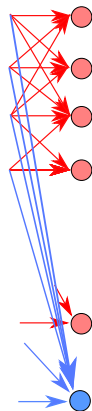
$\delta \leq \Pr(\bar{5} | \bar{3}, 5) \leq 3\delta$   
 $\leq \Pr(\delta | \bar{3}, 5) \leq 1 - \delta$   
 $\frac{1-3\delta}{4} \qquad \frac{3}{4}$





...

...



H

## The construction, continued

- **Transitions:**  $s_0 \sim \text{Uniform}([m])$ .

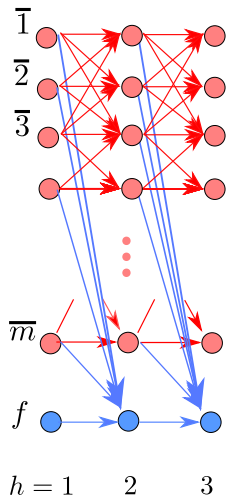
$$\Pr[f | \bar{a}_1, a^*] = 1$$

$$\Pr[\cdot | \bar{a}_1, a_2] = \begin{cases} \bar{a}_2 : \langle v(a_1), v(a_2) \rangle + 2\gamma \\ f : 1 - \langle v(a_1), v(a_2) \rangle - 2\gamma \end{cases}, (a_2 \neq a^*, a_2 \neq a_1)$$

$$\Pr[f | f, \cdot] = 1.$$

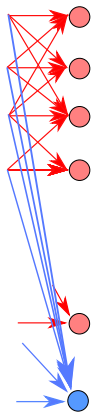
- After taking action  $a_2$ , the next state is either  $\bar{a}_2$  or  $f$ . This MDP looks like a "leaking complete graph"

## The construction, continued



...

...



$H$

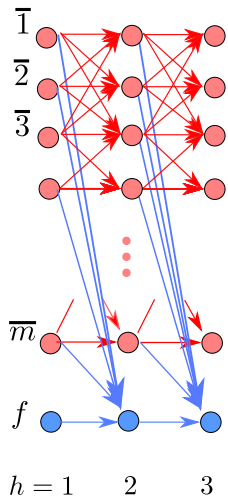
- **Transitions:**  $s_0 \sim \text{Uniform}([m])$ .

$$\Pr[f | \bar{a}_1, a^*] = 1$$

$$\Pr[\cdot | \bar{a}_1, a_2] = \begin{cases} \bar{a}_2 : \langle v(a_1), v(a_2) \rangle + 2\gamma \\ f : 1 - \langle v(a_1), v(a_2) \rangle - 2\gamma \end{cases}, (a_2 \neq a^*, a_2 \neq a_1)$$

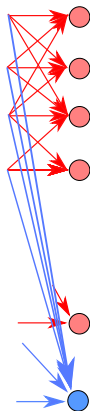
$$\Pr[f | f, \cdot] = 1.$$

- After taking action  $a_2$ , the next state is either  $\bar{a}_2$  or  $f$ . This MDP looks like a "leaking complete graph"
- It is possible to visit any other state (except for  $\bar{a}^*$ ); **however**, there is at least  $1 - 3\gamma = 1/4$  probability of going to the terminal state  $f$ .



...

...



H

## The construction, continued

- **Transitions:**  $s_0 \sim \text{Uniform}([m])$ .

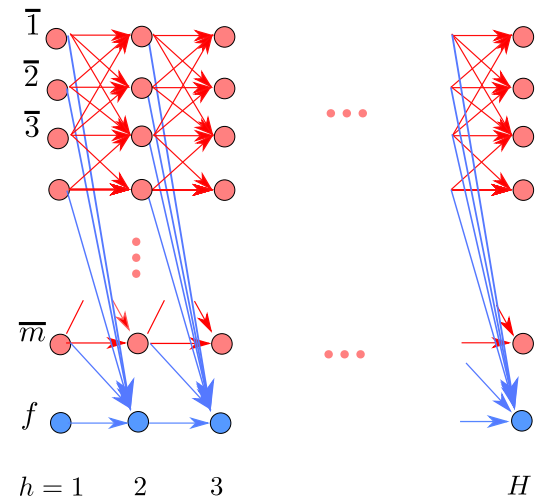
$$\Pr[f | \bar{a}_1, a^*] = 1$$

$$\Pr[\cdot | \bar{a}_1, a_2] = \begin{cases} \bar{a}_2 : \langle v(a_1), v(a_2) \rangle + 2\gamma \\ f : 1 - \langle v(a_1), v(a_2) \rangle - 2\gamma \end{cases}, (a_2 \neq a^*, a_2 \neq a_1)$$

$$\Pr[f | f, \cdot] = 1.$$

- After taking action  $a_2$ , the next state is either  $\bar{a}_2$  or  $f$ . This MDP looks like a "leaking complete graph"
- It is possible to visit any other state (except for  $\bar{a}^*$ ); **however**, there is at least  $1 - 3\gamma = 1/4$  probability of going to the terminal state  $f$ .
- The transition probabilities are indeed valid, because  $0 < \gamma \leq \langle v(a_1), v(a_2) \rangle + 2\gamma \leq 3\gamma < 1$ .

# The construction, continued



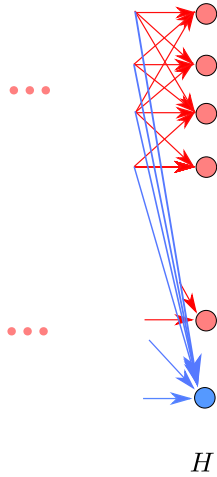
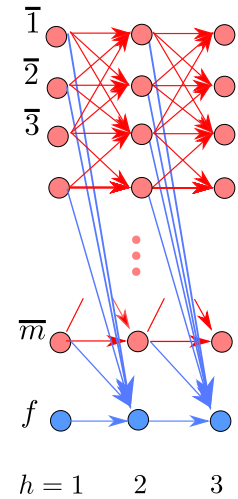
## The construction, continued

- **Features:** of dimension  $d$  defined as:

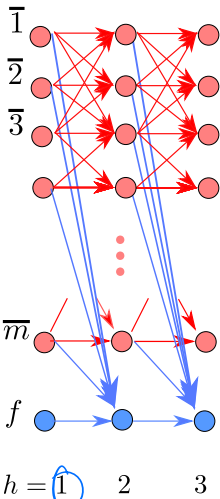
$$\phi(\bar{a}_1, a_2) := \left( \langle v(a_1), v(a_2) \rangle + 2\gamma \right) \cdot v(a_2), \quad \forall a_1 \neq a_2$$

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

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

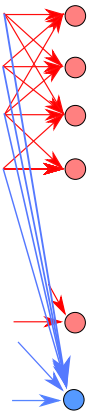


# The construction, continued



...

...



- **Features:** of dimension  $d$  defined as:

$$\phi(\bar{a}_1, a_2) := \left( \langle v(a_1), v(a_2) \rangle + 2\gamma \right) \cdot v(a_2), \quad \forall a_1 \neq a_2$$

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

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

- **Rewards:**  $H-1 \leq \leq 3$   
for  $1 \leq h < H$ ,

$$R_h(\bar{a}_1, a^*) := \langle v(a_1), v(a^*) \rangle + 2\gamma,$$

$$R_h(\bar{a}_1, a_2) := -2\gamma \left[ \langle v(a_1), v(a_2) \rangle + 2\gamma \right], \quad a_2 \neq a^*, a_2 \neq a_1$$

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

for  $h = H-1$

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

we will choose  $a^* = v(a^*)$

$$-6\gamma^2 \leq \leq -2\gamma^2$$

# Verifying the Assumptions: Realizability and the Large Gap

## Verifying the Assumptions: Realizability and the Large Gap

**Lemma:** For all  $(s, a)$ , we have  $Q_h^*(s, a) = \langle \phi(s, a), v(a^*) \rangle$  and the “gap” is  $\geq \gamma/4$ .



## Verifying the Assumptions: Realizability and the Large Gap

**Lemma:** For all  $(s, a)$ , we have  $Q_h^*(s, a) = \langle \phi(s, a), v(a^*) \rangle$  and the “gap” is  $\geq \gamma/4$ .

**Proof:** throughout  $a_2 \neq a^*$

## Verifying the Assumptions: Realizability and the Large Gap

**Lemma:** For all  $(s, a)$ , we have  $Q_h^*(s, a) = \langle \phi(s, a), v(a^*) \rangle$  and the “gap” is  $\geq \gamma/4$ .

**Proof:** throughout  $a_2 \neq a^*$

- First, let's verify  $Q_h^\pi(s, a) = \langle \phi(s, a), v(a^*) \rangle$  is the value of the policy  $\pi(\bar{a}) = a^*$ .  
By induction, we can show:

$$Q_h^\pi(\bar{a}_1, a_2) = \left( \langle v(a_1), v(a_2) \rangle + 2\gamma \right) \cdot \langle v(a_2), v(a^*) \rangle,$$

$$Q_h^\pi(\bar{a}_1, a^*) = \langle v(a_1), v(a^*) \rangle + 2\gamma$$

## Verifying the Assumptions: Realizability and the Large Gap

**Lemma:** For all  $(s, a)$ , we have  $Q_h^*(s, a) = \langle \phi(s, a), v(a^*) \rangle$  and the “gap” is  $\geq \gamma/4$ .

**Proof:** throughout  $a_2 \neq a^*$

- First, let's verify  $Q^\pi(s, a) = \langle \phi(s, a), v(a^*) \rangle$  is the value of the policy  $\pi(\bar{a}) = a^*$ .  
By induction, we can show:

$$Q_h^\pi(\bar{a}_1, a_2) = \left( \langle v(a_1), v(a_2) \rangle + 2\gamma \right) \cdot \langle v(a_2), v(a^*) \rangle,$$

$$Q_h^\pi(\bar{a}_1, a^*) = \langle v(a_1), v(a^*) \rangle + 2\gamma$$

- **Proving optimality:** for  $a_2 \neq a^*, a_1$

$$Q_h^\pi(\bar{a}_1, a_2) \leq 3\gamma^2, \quad Q_h^\pi(\bar{a}_1, a^*) = \langle v(a_1), v(a^*) \rangle + 2\gamma \geq \gamma > 3\gamma^2$$

$\implies \pi$  is optimal

## Verifying the Assumptions: Realizability and the Large Gap

**Lemma:** For all  $(s, a)$ , we have  $Q_h^*(s, a) = \langle \phi(s, a), v(a^*) \rangle$  and the “gap” is  $\geq \gamma/4$ .

**Proof:** throughout  $a_2 \neq a^*$

- First, let's verify  $Q^\pi(s, a) = \langle \phi(s, a), v(a^*) \rangle$  is the value of the policy  $\pi(\bar{a}) = a^*$ .  
By induction, we can show:

$$Q_h^\pi(\bar{a}_1, a_2) = \left( \langle v(a_1), v(a_2) \rangle + 2\gamma \right) \cdot \langle v(a_2), v(a^*) \rangle,$$

$$Q_h^\pi(\bar{a}_1, a^*) = \langle v(a_1), v(a^*) \rangle + 2\gamma$$

- **Proving optimality:** for  $a_2 \neq a^*, a_1$

$$Q_h^\pi(\bar{a}_1, a_2) \leq 3\gamma^2, \quad Q_h^\pi(\bar{a}_1, a^*) = \langle v(a_1), v(a^*) \rangle + 2\gamma \geq \gamma > 3\gamma^2$$

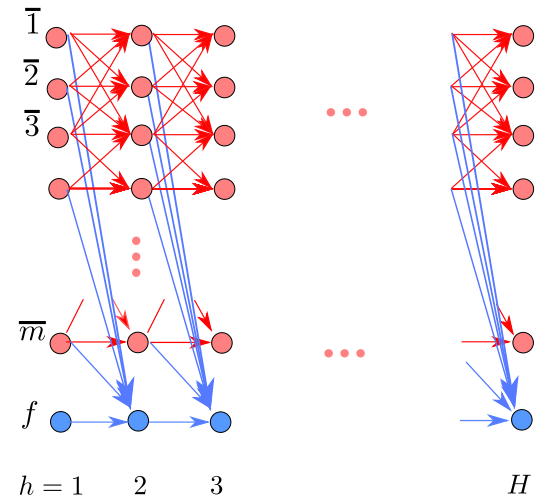
$\implies \pi$  is optimal

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

$$V_h^*(\bar{a}_1) - Q_h^*(\bar{a}_1, a_2) = Q_h^\pi(\bar{a}_1, a^*) - Q_h^\pi(\bar{a}_1, a_2) > \gamma - 3\gamma^2 \geq \frac{1}{4}\gamma.$$

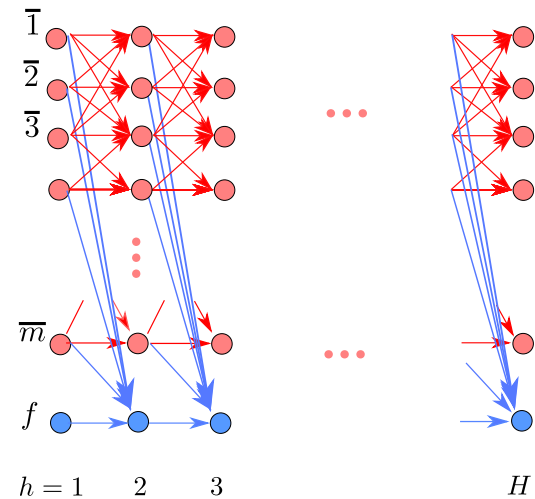
$$\gamma = \frac{1}{4}$$

# The information theoretic proof:



# The information theoretic proof:

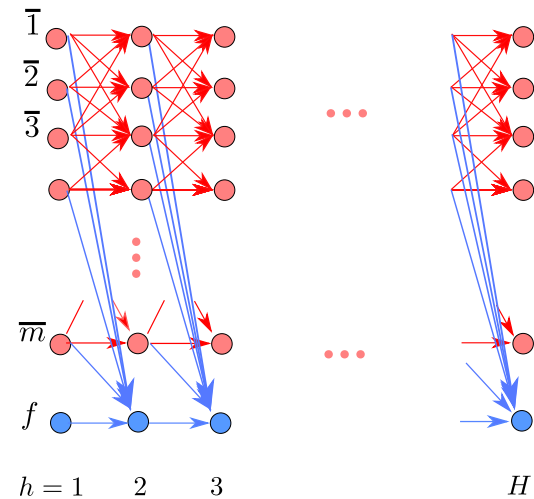
Proof: When is info revealed about  $\mathcal{M}_{a^*}$ , indexed by  $a^*$ ?



## The information theoretic proof:

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

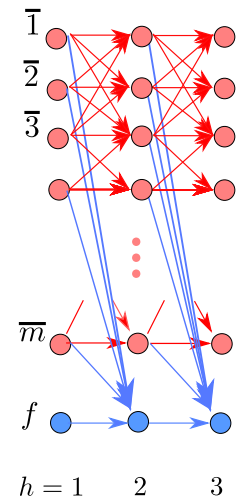
- Features:** The construction of  $\phi$  does not depend on  $a^*$ .



## The information theoretic proof:

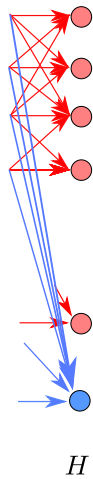
**Proof:** When is info revealed about  $\mathcal{M}_{a^*}$ , indexed by  $a^*$ ?

- **Features:** The construction of  $\phi$  does not depend on  $a^*$ .
- **Transitions:** if we take  $a^*$ , only then does the dynamics leak info about  $a^*$  (but there  $O(2^d)$  actions)



...

...



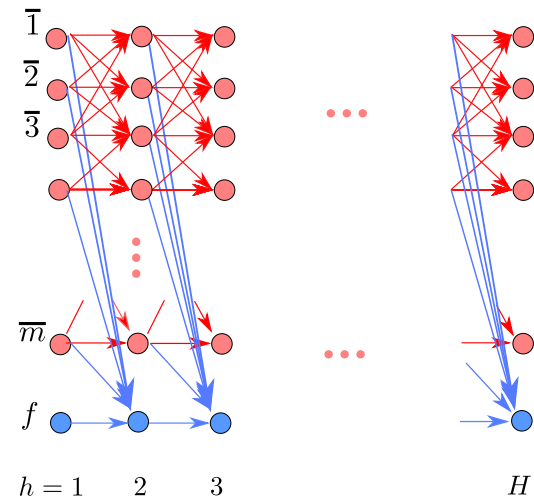
$H$



## The information theoretic proof:

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

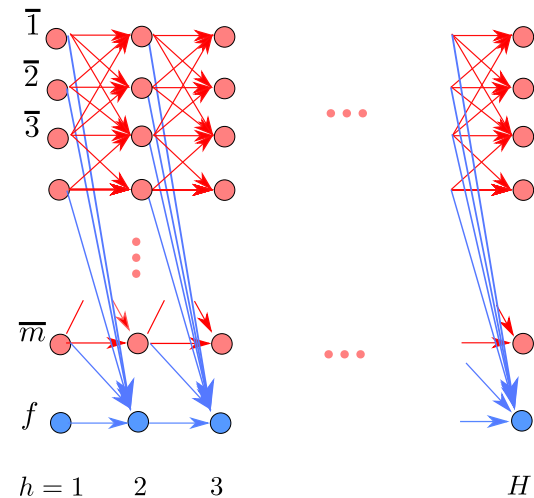
- **Features:** The construction of  $\phi$  does not depend on  $a^*$ .
- **Transitions:** if we take  $a^*$ , only then does the dynamics leak info about  $a^*$  (but there  $O(2^d)$  actions)
- **Rewards:** two cases which leak info about  $a^*$ 
  - (1) if we take  $a^*$  at any  $h$ , then reward leaks info about  $a^*$  (but there  $m = O(2^d)$  actions)
  - (2) also, if we terminate at  $s_H \neq f$ , then the reward  $r_H$  leaks info about on  $a^*$
- But there is always at least 1/4 chance of moving to  $f$
- So need at least  $O((4/3)^H)$  trajectories to hit  $s_H \neq f$



## The information theoretic proof:

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

- **Features:** The construction of  $\phi$  does not depend on  $a^*$ .
  - **Transitions:** if we take  $a^*$ , only then does the dynamics leak info about  $a^*$  (but there  $O(2^d)$  actions)
  - **Rewards:** two cases which leak info about  $a^*$ 
    - (1) if we take  $a^*$  at any  $h$ , then reward leaks info about  $a^*$  (but there  $m = O(2^d)$  actions)
    - (2) also, if we terminate at  $s_H \neq f$ , then the reward  $r_H$  leaks info about on  $a^*$
- But there is always at least 1/4 chance of moving to  $f$
  - So need at least  $O((4/3)^H)$  trajectories to hit  $s_H \neq f$
- $\implies$  need  $\Omega(\min(2^d, 2^H))$  samples to discover  $\mathcal{M}_{a^*}$ .

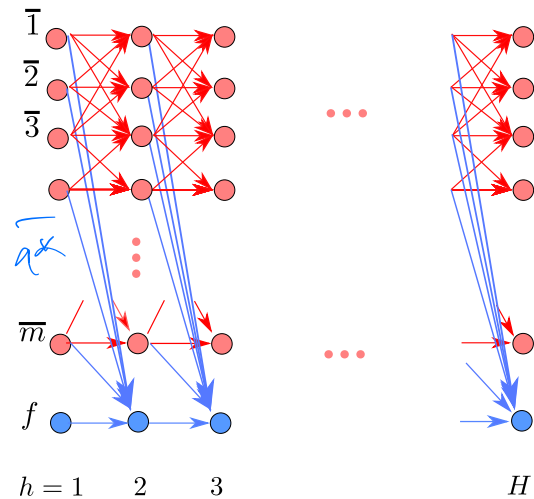


## The information theoretic proof:

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

- **Features:** The construction of  $\phi$  does not depend on  $a^*$ .
  - **Transitions:** if we take  $a^*$ , only then does the dynamics leak info about  $a^*$  (but there  $O(2^d)$  actions)
  - **Rewards:** two cases which leak info about  $a^*$ 
    - (1) if we take  $a^*$  at any  $h$ , then reward leaks info about  $a^*$  (but there  $m = O(2^d)$  actions)
    - (2) also, if we terminate at  $s_H \neq f$ , then the reward  $r_H$  leaks info about on  $a^*$
- But there is always at least 1/4 chance of moving to  $f$
  - So need at least  $O((4/3)^H)$  trajectories to hit  $s_H \neq f$
- $\implies$  need  $\Omega(\min(2^d, 2^H))$  samples to discover  $\mathcal{M}_{a^*}$ .

**Caveats:** Haven't handled the state  $\bar{a}^*$  carefully.



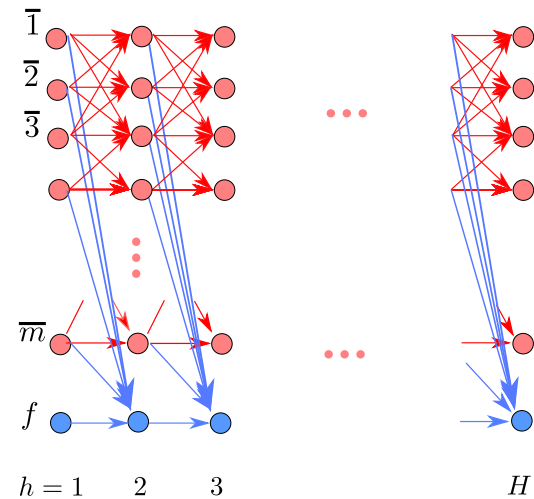
## The information theoretic proof:

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

- **Features:** The construction of  $\phi$  does not depend on  $a^*$ .
  - **Transitions:** if we take  $a^*$ , only then does the dynamics leak info about  $a^*$  (but there  $O(2^d)$  actions)
  - **Rewards:** two cases which leak info about  $a^*$ 
    - (1) if we take  $a^*$  at any  $h$ , then reward leaks info about  $a^*$  (but there  $m = O(2^d)$  actions)
    - (2) also, if we terminate at  $s_H \neq f$ , then the reward  $r_H$  leaks info about on  $a^*$
- But there is always at least 1/4 chance of moving to  $f$
  - So need at least  $O((4/3)^H)$  trajectories to hit  $s_H \neq f$
- $\implies$  need  $\Omega(\min(2^d, 2^H))$  samples to discover  $\mathcal{M}_{a^*}$ .

**Caveats:** Haven't handled the state  $\bar{a}^*$  carefully.

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



# Part-3: Discussion

RL is different from SL.

+ we have seen negative results.

How do we obtain positive results?

How should we approach generalization in RL?

## How should we approach generalization in RL?

- We have seen that:

## How should we approach generalization in RL?

- We have seen that:
  - agnostic learning is not possible in RL  
(unless we pay an exponential in  $H$  dependence)



## How should we approach generalization in RL?

- We have seen that:
  - agnostic learning is not possible in RL  
(unless we pay an exponential in  $H$  dependence)
  - simple linear realizability assumptions are also not sufficient

## How should we approach generalization in RL?

- We have seen that:
  - agnostic learning is not possible in RL  
(unless we pay an exponential in  $H$  dependence)
  - simple linear realizability assumptions are also not sufficient
- What next?

## How should we approach generalization in RL?

- We have seen that:
  - agnostic learning is not possible in RL  
(unless we pay an exponential in  $H$  dependence)
  - simple linear realizability assumptions are also not sufficient
- What next?
  - **Structural Assumptions:** Need even stronger assumptions. We start this study (**today**) with the stronger linear Bellman completeness. More examples of this in “Part 2”.

## How should we approach generalization in RL?

- We have seen that:
  - agnostic learning is not possible in RL  
(unless we pay an exponential in  $H$  dependence)
  - simple linear realizability assumptions are also not sufficient
- What next?
  - **Structural Assumptions:** Need even stronger assumptions. We start this study (**today**) with the stronger linear Bellman completeness. More examples of this in “Part 2”.
  - **Distribution Dependent Results:** We will see examples of this approach when we consider approximate dynamic programming. And more refined bounds when we consider policy gradient methods.

## How should we approach generalization in RL?

- We have seen that:
  - agnostic learning is not possible in RL  
(unless we pay an exponential in  $H$  dependence)
  - simple linear realizability assumptions are also not sufficient
- What next?
  - **Structural Assumptions:** Need even stronger assumptions. We start this study (**today**) with the stronger linear Bellman completeness. More examples of this in “Part 2”.
  - **Distribution Dependent Results:** We will see examples of this approach when we consider approximate dynamic programming. And more refined bounds when we consider policy gradient methods.
  - **Imitation learning and behavior cloning:** models where the agent has input from, effectively, a teacher.