

# **Approximate Policy Iteration and Variants**

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# Review 1: $Q^*/V^*$

$V^*(s)$  := maximum expected total reward starting from state  $s$

$Q^*(s, a)$  := maximum expected total reward starting from state  $s$  and taking action  $a$  **for one step**, and then following the optimal strategy

**Value Iteration to approximate  $Q^*/V^*$  :** (for finding the optimal policy)

For  $i = 1, 2, \dots$

$$Q_i(s, a) \leftarrow R(s, a) + \gamma \sum_{s'} P(s'|s, a) V_{i-1}(s') \quad \text{for all } (s, a)$$

$$V_i(s) = \max_a Q_i(s, a) \quad \text{for all } s$$

## Review 2: $Q^\pi / V^\pi$

Fix a policy  $\pi$

$V^\pi(s) :=$  expected total reward starting from state  $s$  and **following policy  $\pi$**

$Q^\pi(s, a) :=$  expected total reward starting from state  $s$  and taking action  $a$  for one step, and then **following policy  $\pi$**

$\mathcal{R} \rightarrow Q^\pi$

(\*) **Approximate  $Q^\pi / V^\pi$  :** (for evaluating a given policy)

For  $i = 1, 2, \dots$

$$Q_i(s, a) \leftarrow R(s, a) + \gamma \sum_{s'} P(s'|s, a) V_{i-1}(s') \quad \text{for all } (s, a)$$

$$V_i(s) = \sum_a \pi(a|s) Q_i(s, a) \quad \text{for all } s$$

# Policy Iteration

Another way (other than value iteration) to find the optimal policy in an MDP

# Policy Iteration

$$\text{VI } \underbrace{Q_i(s,a)} \leftarrow R(s,a) + \gamma \sum_{s'} p(s'|s,a) \max_{a'} Q_{i-1}(s',a')$$

## Policy Iteration

For  $i = 1, 2, \dots$

$$\forall s, \quad \pi_i(s) \leftarrow \operatorname{argmax}_a Q^{\pi_{i-1}}(s, a)$$

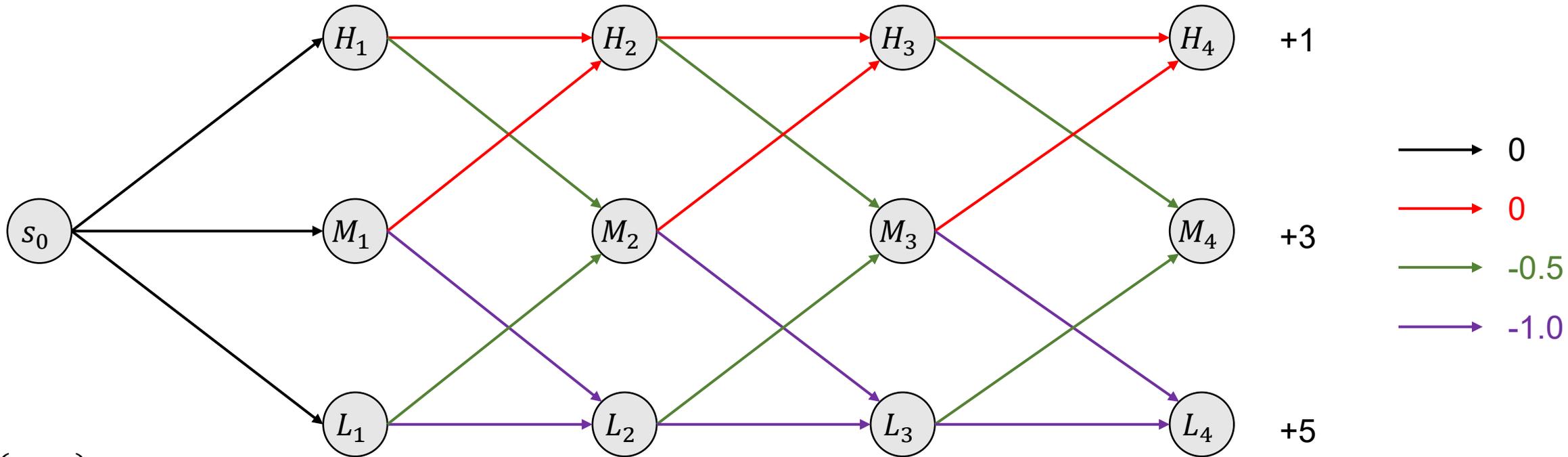
Call the (\*) algo to calculate  $Q^{\pi_i}$

In VI, there might not exist a policy  $\pi$ , such that  $Q_i = Q^\pi$

**Theorem (monotonic improvement).** Policy Iteration ensures

$$\forall s, a, \quad \underline{Q^{\pi_i}(s, a) \geq Q^{\pi_{i-1}}(s, a)}$$

When converged (i.e.,  $\pi_i = \pi_{i-1}$ ), we have  $\pi_i = \pi^*$ .



$$Q^\pi(s_0, \nearrow) =$$

$$Q^\pi(s_0, \rightarrow) =$$

$$Q^\pi(s_0, \searrow) =$$

$$Q^\pi(H_1, R) =$$

$$Q^\pi(H_2, R) =$$

$$Q^\pi(H_3, R) =$$

$$Q^\pi(H_1, G) =$$

$$Q^\pi(H_2, G) =$$

$$Q^\pi(H_3, G) =$$

$$Q^\pi(M_1, R) =$$

$$Q^\pi(M_2, R) =$$

$$Q^\pi(M_3, R) =$$

$$Q^\pi(M_1, P) =$$

$$Q^\pi(M_2, P) =$$

$$Q^\pi(M_3, P) =$$

$$Q^\pi(L_1, G) =$$

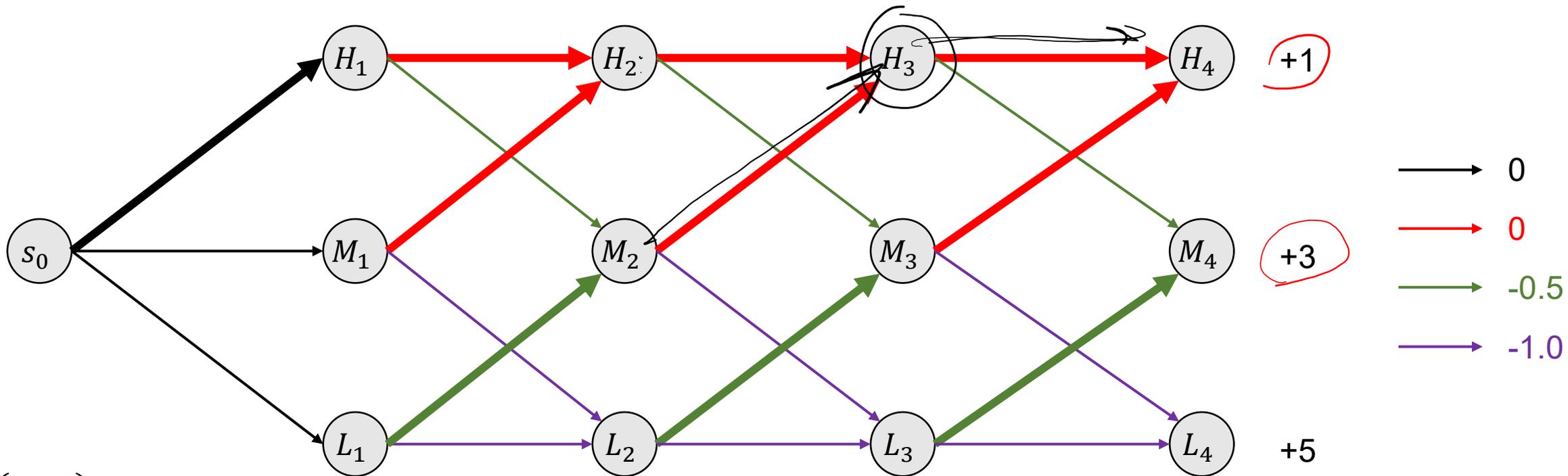
$$Q^\pi(L_2, G) =$$

$$Q^\pi(L_3, G) =$$

$$Q^\pi(L_1, P) =$$

$$Q^\pi(L_2, P) =$$

$$Q^\pi(L_3, P) =$$



$$Q^\pi(s_0, \nearrow) =$$

$$Q^\pi(s_0, \rightarrow) =$$

$$Q^\pi(s_0, \searrow) =$$

$$Q^\pi(H_1, R) =$$

$$Q^\pi(H_2, R) =$$

$$Q^\pi(H_3, R) = 0 + 1 = 1$$

$$Q^\pi(H_1, G) =$$

$$Q^\pi(H_2, G) = -0.5 + 1$$

$$Q^\pi(H_3, G) = -0.5 + 3 = 2.5$$

$$Q^\pi(M_1, R) =$$

$$Q^\pi(M_2, R) = 0 + 1$$

$$Q^\pi(M_3, R) =$$

$$Q^\pi(M_1, P) =$$

$$Q^\pi(M_2, P) =$$

$$Q^\pi(M_3, P) = 4$$

$$Q^\pi(L_1, G) =$$

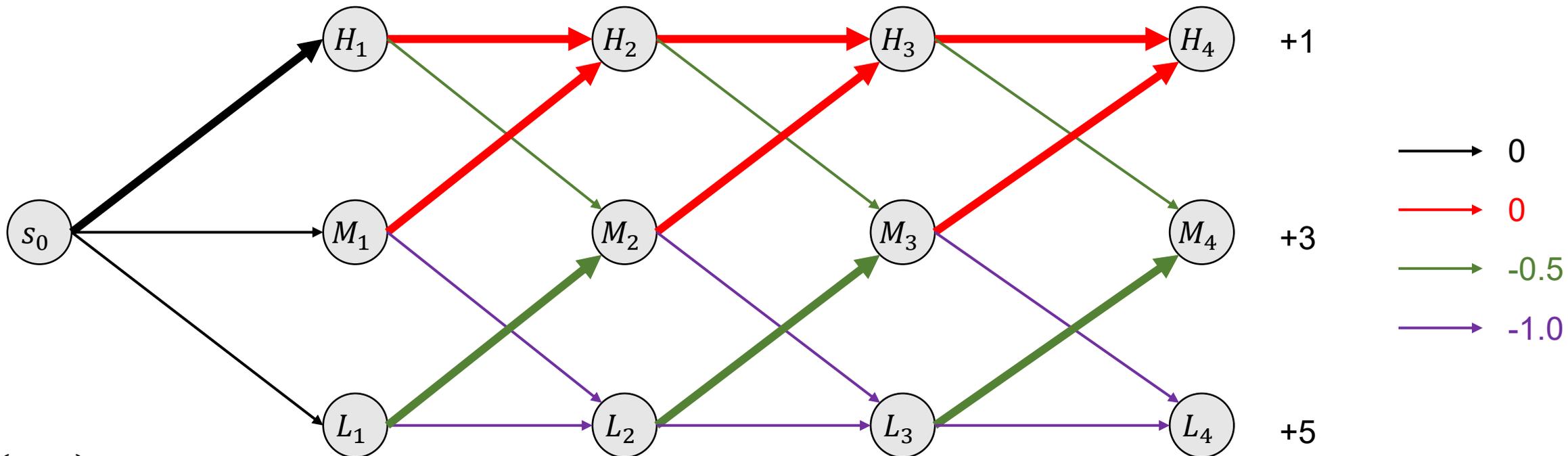
$$Q^\pi(L_2, G) =$$

$$Q^\pi(L_3, G) =$$

$$Q^\pi(L_1, P) =$$

$$Q^\pi(L_2, P) =$$

$$Q^\pi(L_3, P) =$$



$$Q^\pi(s_0, \nearrow) = 1$$

$$Q^\pi(s_0, \rightarrow) = 1$$

$$Q^\pi(s_0, \searrow) = 0.5$$

$$Q^\pi(H_1, R) = 1$$

$$Q^\pi(H_2, R) = 1$$

$$Q^\pi(H_3, R) = 1$$

$$Q^\pi(H_1, G) = 0.5$$

$$Q^\pi(H_2, G) = 0.5$$

$$Q^\pi(H_3, G) = 2.5$$

$$Q^\pi(M_1, R) = 1$$

$$Q^\pi(M_2, R) = 1$$

$$Q^\pi(M_3, R) = 1$$

$$Q^\pi(M_1, P) = -0.5$$

$$Q^\pi(M_2, P) = 1.5$$

$$Q^\pi(M_3, P) = 4$$

$$Q^\pi(L_1, G) = 0.5$$

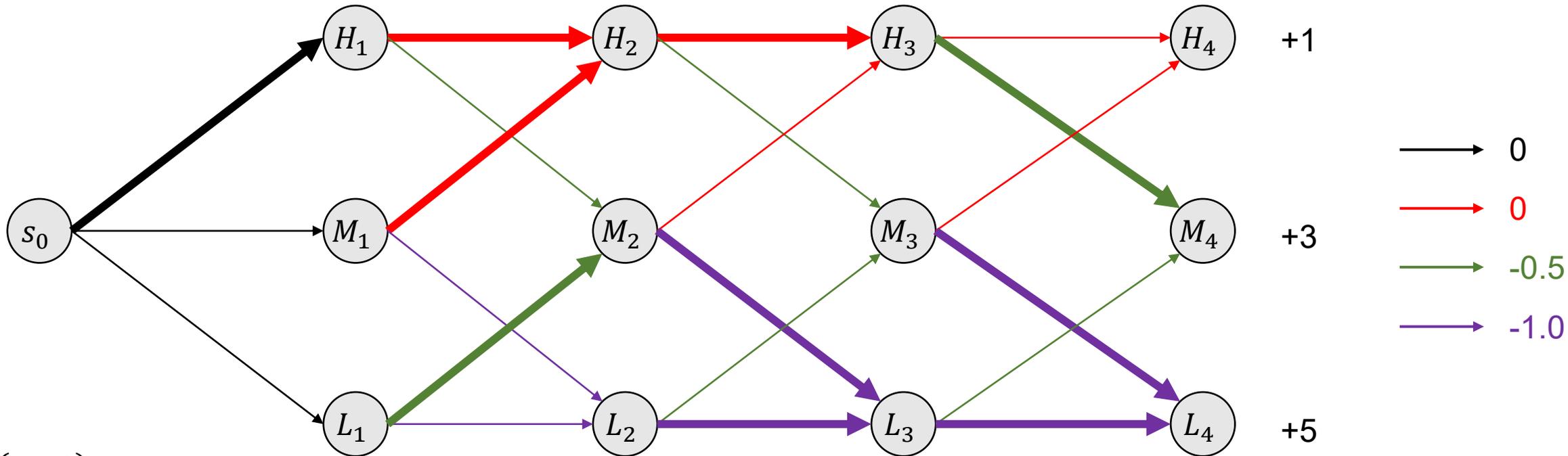
$$Q^\pi(L_2, G) = 0.5$$

$$Q^\pi(L_3, G) = 2.5$$

$$Q^\pi(L_1, P) = -0.5$$

$$Q^\pi(L_2, P) = 1.5$$

$$Q^\pi(L_3, P) = 4$$



$$Q^\pi(s_0, \nearrow) =$$

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$$Q^\pi(H_1, R) =$$

$$Q^\pi(H_2, R) =$$

$$Q^\pi(H_3, R) =$$

$$Q^\pi(H_1, G) =$$

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$$Q^\pi(M_1, P) =$$

$$Q^\pi(M_2, P) =$$

$$Q^\pi(M_3, P) =$$

$$Q^\pi(L_1, G) =$$

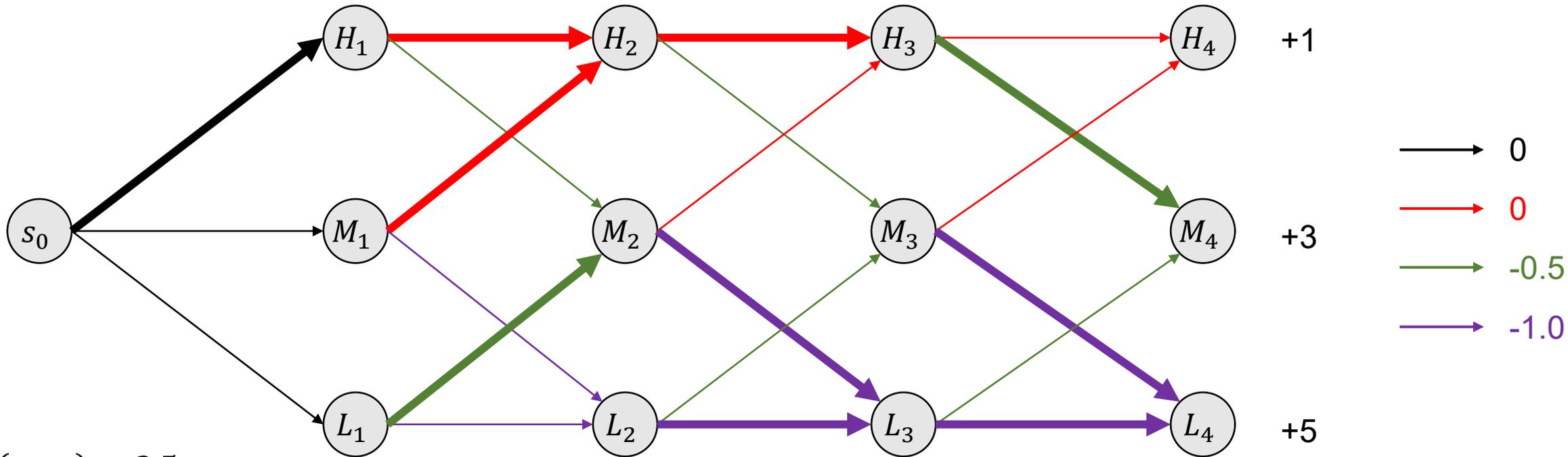
$$Q^\pi(L_2, G) =$$

$$Q^\pi(L_3, G) =$$

$$Q^\pi(L_1, P) =$$

$$Q^\pi(L_2, P) =$$

$$Q^\pi(L_3, P) =$$



$$Q^\pi(s_0, \nearrow) = 2.5$$

$$Q^\pi(s_0, \rightarrow) = 2.5$$

$$Q^\pi(s_0, \searrow) = 2.5$$

$$Q^\pi(H_1, R) = 2.5$$

$$Q^\pi(H_2, R) = 2.5$$

$$Q^\pi(H_3, R) = 1$$

$$Q^\pi(H_1, G) = 2.5$$

$$Q^\pi(H_2, G) = 3.5$$

$$Q^\pi(H_3, G) = 2.5$$

$$Q^\pi(M_1, R) = 2.5$$

$$Q^\pi(M_2, R) = 2.5$$

$$Q^\pi(M_3, R) = 1$$

$$Q^\pi(M_1, P) = 2$$

$$Q^\pi(M_2, P) = 3$$

$$Q^\pi(M_3, P) = 4$$

$$Q^\pi(L_1, G) = 2.5$$

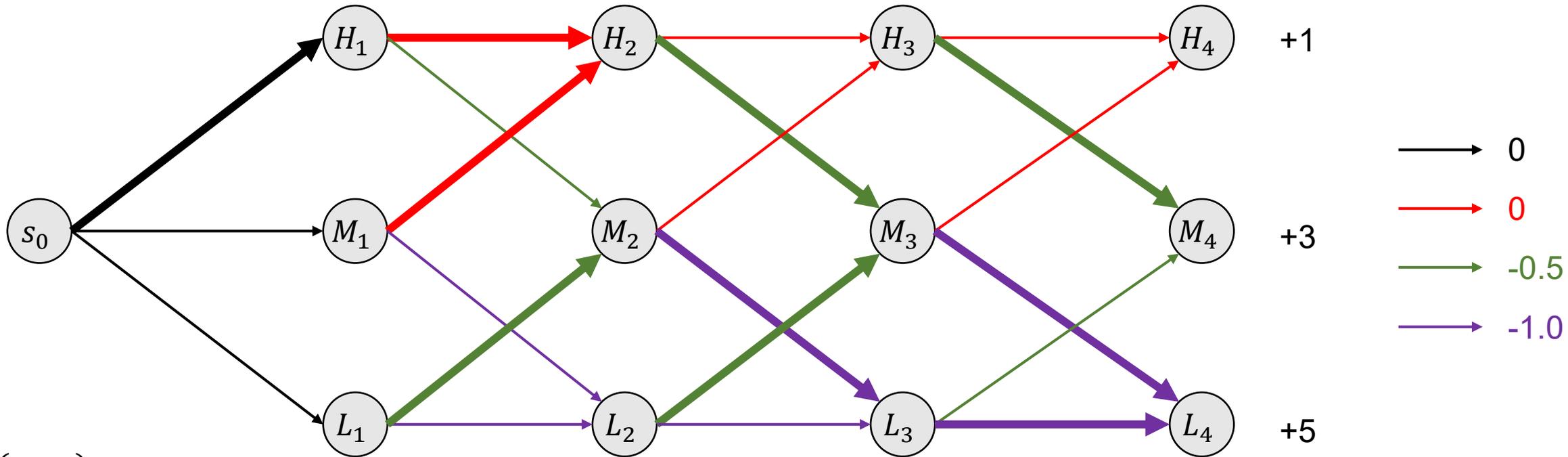
$$Q^\pi(L_2, G) = 3.5$$

$$Q^\pi(L_3, G) = 2.5$$

$$Q^\pi(L_1, P) = 2$$

$$Q^\pi(L_2, P) = 3$$

$$Q^\pi(L_3, P) = 4$$



$$Q^\pi(s_0, \nearrow) =$$

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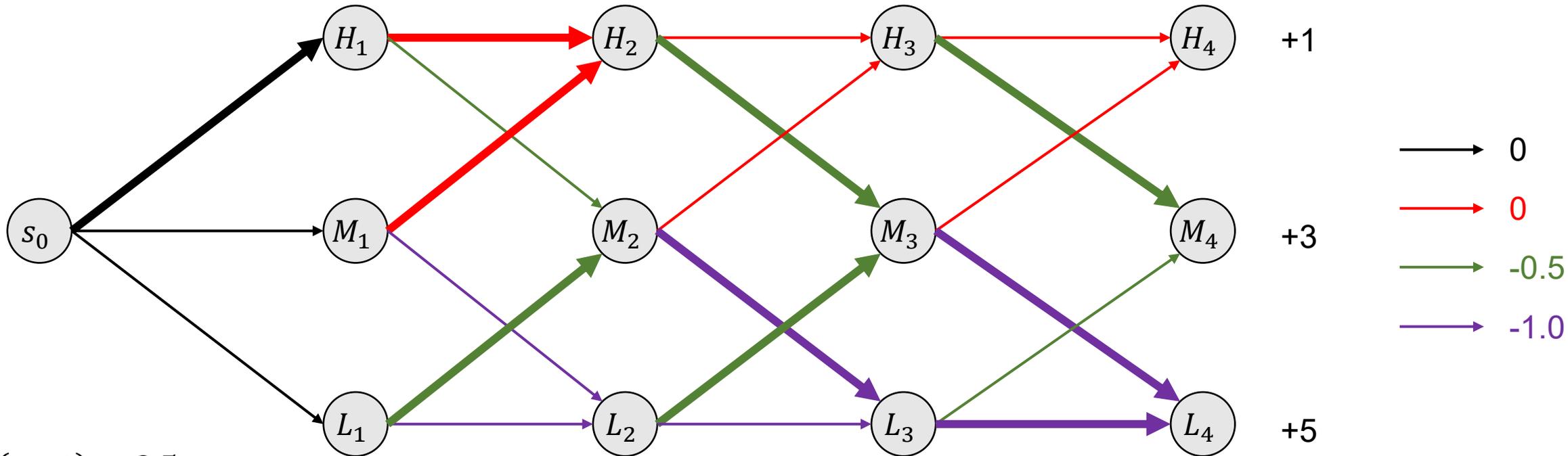
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$$Q^\pi(s_0, \nearrow) = 3.5$$

$$Q^\pi(s_0, \rightarrow) = 3.5$$

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$$Q^\pi(H_1, R) = 3.5$$

$$Q^\pi(H_2, R) = 2.5$$

$$Q^\pi(H_3, R) = 1$$

$$Q^\pi(H_1, G) = 2.5$$

$$Q^\pi(H_2, G) = 3.5$$

$$Q^\pi(H_3, G) = 2.5$$

$$Q^\pi(M_1, R) = 3.5$$

$$Q^\pi(M_2, R) = 2.5$$

$$Q^\pi(M_3, R) = 1$$

$$Q^\pi(M_1, P) = 2.5$$

$$Q^\pi(M_2, P) = 3$$

$$Q^\pi(M_3, P) = 4$$

$$Q^\pi(L_1, G) = 2.5$$

$$Q^\pi(L_2, G) = 3.5$$

$$Q^\pi(L_3, G) = 2.5$$

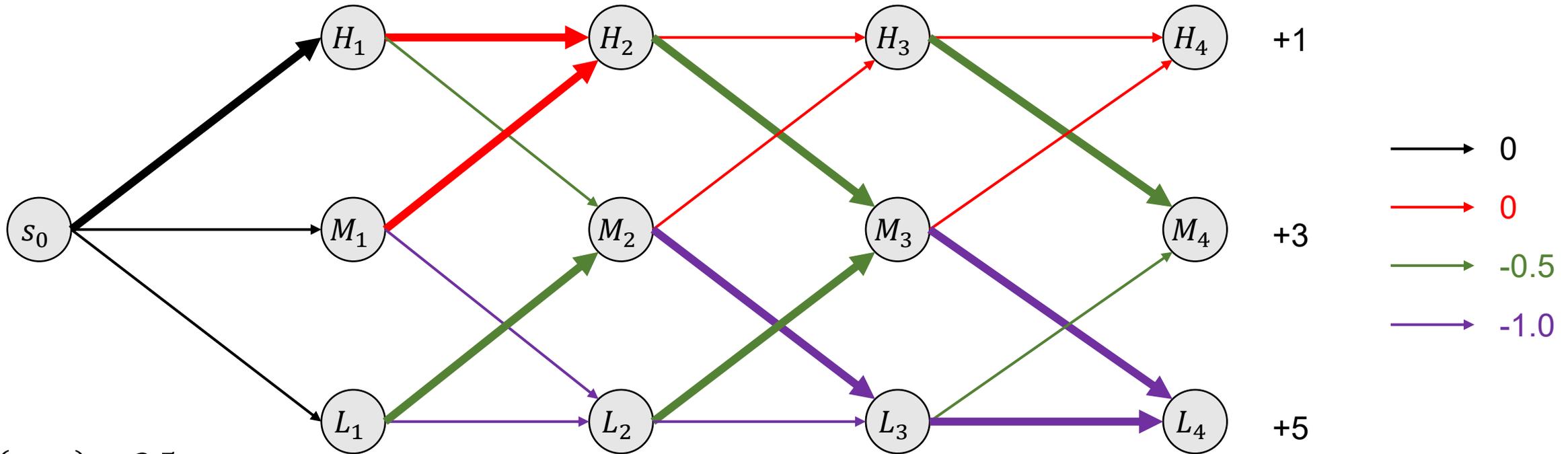
$$Q^\pi(L_1, P) = 2.5$$

$$Q^\pi(L_2, P) = 3$$

$$Q^\pi(L_3, P) = 4$$

$$\underline{\pi_{i(s)}} = \underset{\text{argmax}}{\text{argmax}} Q^{\pi_{i-1}}(s, a)$$

$$\underline{\pi_i = \pi_{i-1}}$$



$$Q^\pi(s_0, \nearrow) = 3.5$$

$$Q^\pi(s_0, \rightarrow) = 3.5$$

$$Q^\pi(s_0, \searrow) = 2.5$$

$$Q^\pi(H_1, R) = 3.5$$

$$Q^\pi(H_2, R) = 2.5$$

$$Q^\pi(H_3, R) = 1$$

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$$Q^\pi(H_2, G) = 3.5$$

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$$Q^\pi(L_2, G) = 3.5$$

$$Q^\pi(L_3, G) = 2.5$$

$$Q^\pi(L_1, P) = 2.5$$

$$Q^\pi(L_2, P) = 3$$

$$Q^\pi(L_3, P) = 4$$

$\pi_{i+1} = \pi_i \Rightarrow$  converged

# **Policy Evaluation with Samples**

# Policy Iteration

For  $k = 1, 2, \dots$

Calculate  $Q^{\pi_k}(s, a) \quad \forall s, a$

Policy Evaluation

$\pi_{k+1}(s) = \operatorname{argmax}_a Q^{\pi_k}(s, a) \quad \forall s$

Policy Improvement

# Policy Iteration with Samples

For  $k = 1, 2, \dots$

For  $i = 1, 2, \dots, N$ :

Choose action  $a_i \sim \pi_{\theta_k}(\cdot | s_i)$

Receive reward  $r_i \sim R(s_i, a_i)$  and  $s'_i \sim P(\cdot | s_i, a_i)$

$s_{i+1} = s'_i$  if episode continues,  $s_{i+1} \sim \rho$  if episode ends

$(s_i, a_i, r_i, s'_i)$

Data collection

Evaluate  $Z_k(s, a) \approx Q^{\pi_{\theta_k}}(s, a)$  for  $s = s_1, \dots, s_N$  and all  $a$

or  $Z_k(s, a) \approx Q^{\pi_{\theta_k}}(s, a) - b_k(s)$  for  $s = s_1, \dots, s_N$  and all  $a$

Policy Evaluation

Update  $\theta_{k+1}$  from  $\theta_k$  using the estimators  $\{Z_k(s_i, a)\}_{i=1}^N$

Using any technique we introduced for policy-based contextual bandits

Policy Improvement

# Monte Carlo Estimators

# Policy Evaluation with Monte Carlo Estimator

Recall

$$Q^{\pi}(s_i, a_i) = \mathbb{E}[r_i + \gamma r_{i+1} + \gamma^2 r_{i+2} + \gamma^3 r_{i+3} + \dots + \gamma^\tau r_{i+\tau}] \text{ following } \pi$$

*(Handwritten red annotations:  $r_i + \gamma r_{i+1} + \gamma^2 r_{i+2} + \gamma^3 r_{i+3} + \dots + \gamma^\tau r_{i+\tau}$  is circled in red.  $Q^{\pi}(s_i, a_i)$  is also circled in red. An arrow points from the text 'End of episode' to the  $\tau$  in the exponent of the last term.)*

(Expected sum of reward starting from  $(s_i, a_i)$  and following  $s_{i+1}$ ) End of episode

A natural estimator  $Z_k(s_i, a)$  with  $\mathbb{E}[Z_k(s_i, a)] = Q^{\pi_{\theta_k}}(s_i, a)$ :

$$Z_k(s_i, a) = \frac{r_i + \gamma r_{i+1} + \gamma^2 r_{i+2} + \dots + \gamma^\tau r_{i+\tau} - b(s_i)}{\pi_{\theta_k}(a|s_i)} \mathbb{I}\{a_i = a\}$$

*(Handwritten red annotations: The numerator  $r_i + \gamma r_{i+1} + \gamma^2 r_{i+2} + \dots + \gamma^\tau r_{i+\tau}$  is circled in red.  $Q^{\pi_{\theta_k}}(s_i, a)$  is written in red above the equation.)*

Contextual bandit special case:  $Z_k(x_i, a) = \hat{r}(x_i, a) = \frac{r_i - b(x_i)}{\pi_{\theta_k}(a|x_i)} \mathbb{I}\{a_i = a\}$  (see e.g. Page 34 [here](#))

# Policy Iteration with Samples (w/ Monte Carlo Estimator)

For  $k = 1, 2, \dots$

For  $i = 1, 2, \dots, N$ :

Choose action  $a_i \sim \pi_{\theta_k}(\cdot | s_i)$

Receive reward  $r_i \sim R(s_i, a_i)$  and  $s'_i \sim P(\cdot | s_i, a_i)$

$s_{i+1} = s'_i$  if episode continues,  $s_{i+1} \sim \rho$  if episode ends

Define for  $i = 1, 2, \dots, N$  and for all  $a$ :

$$Z_k(s_i, a) = \frac{r_i + \gamma r_{i+1} + \gamma^2 r_{i+2} + \dots + \gamma^\tau r_{i+\tau} - b_k(s_i)}{\pi_{\theta_k}(a | s_i)} \mathbb{I}\{a_i = a\}$$

$$\theta_{k+1} = \operatorname{argmax}_{\theta} \left\{ \frac{1}{N} \sum_{i=1}^N \left( \sum_a \pi_{\theta}(a | s_i) \underline{Z_k(s_i, a)} - \frac{1}{\eta} \operatorname{KL}(\pi_{\theta}(\cdot | s_i), \pi_{\theta_k}(\cdot | s_i)) \right) \right\}$$

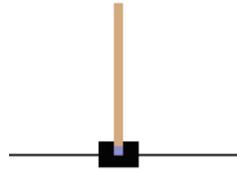
$$\stackrel{\circlearrowleft}{=} \operatorname{argmax}_{\theta} \left\{ \frac{1}{N} \sum_{i=1}^N \left( \frac{\pi_{\theta}(a_i | s_i)}{\pi_{\theta_k}(a_i | s_i)} (r_i + \gamma r_{i+1} + \dots + \gamma^\tau r_{i+\tau} - b_k(s_i)) - \frac{1}{\eta} \operatorname{KL}(\pi_{\theta}(\cdot | s_i), \pi_{\theta_k}(\cdot | s_i)) \right) \right\}$$

Data collection

Policy Evaluation

Policy Improvement

# A Caveat



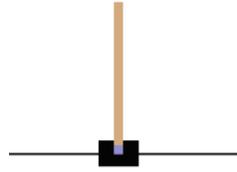
The **episode end** may go beyond the **end of the data collection phase**



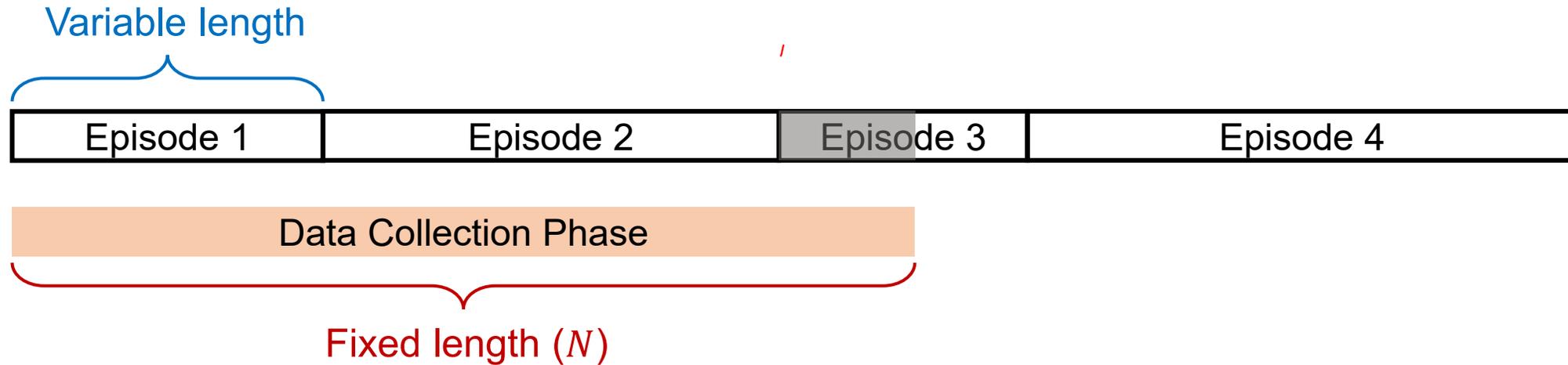
Therefore, for part of the data (the gray segment above), we're unable to create correct Monte Carlo estimator

$$\underline{Z}_k(s_i, a) = \frac{\overset{Q^{ZOR}(s_i, a_i)}{r_i + \gamma r_{i+1} + \gamma^2 r_{i+2} + \dots + \gamma^\tau r_{i+\tau}} - b_k(s_i)}{\pi_{\theta_k}(a|s_i)} \mathbb{I}\{a_i = a\}$$

# A Caveat



The **episode end** may go beyond the **end of the data collection phase**



Solutions:

- Use variable length data collection phase that always include complete episodes
- Drop the incomplete-episode samples (the gray part)
- Use alternative estimators we will discuss next

For  $k=1, 2, \dots$



For  $i=1, 2, \dots, N$ :

Choose  $a_i \sim \pi_{\theta_k}(\cdot | s_i)$

Receive  $r_i \sim \mathcal{R}(s_i, a_i)$ ,  $s_{i+1} \sim P(\cdot | s_i, a_i)$

$s_{i+1} = s_i'$  if the episode continues, and  $s_{i+1} \sim p$  if the episode terminates

// This procedure gives us  $(s_1, a_1, r_1, s_2, a_2, r_2, \dots, s_N, a_N, r_N)$

Define

$$Z_k(s_i, a) = \frac{\sum_{j=i}^N \gamma^{j-i} r_j}{\pi_{\theta_k}(a | s_i)} \mathbb{1}\{a_i = a\}$$

create estimator  $Z_k(s_i)$   
for  $Q^{\pi_{\theta_k}}(s, a)$

$$\hat{r}_k(x_i, a) = \frac{r_i - \text{baseline}}{\pi_{\theta_k}(a | x_i)} \mathbb{1}\{a_i = a\} \quad (\text{conditional bandits})$$

$$\theta_{k+1} = \operatorname{argmax}_{\theta} \left\{ \sum_{i=1}^N \pi_{\theta}(a | s_i) \underline{Z}_k(s_i, a) - \frac{1}{2} \text{KL}(\pi_{\theta}(\cdot | s_i), \pi_{\theta_k}(\cdot | s_i)) \right\}$$

# **Temporal Difference Estimators**

# Recall: Policy Iteration with Samples

For  $k = 1, 2, \dots$

For  $i = 1, 2, \dots, N$ :

Choose action  $a_i \sim \pi_{\theta_k}(\cdot | s_i)$

Receive reward  $r_i \sim R(s_i, a_i)$  and  $s'_i \sim P(\cdot | s_i, a_i)$

$s_{i+1} = s'_i$  if episode continues,  $s_{i+1} \sim \rho$  if episode ends

Evaluate  $Z_k(s, a) \approx Q^{\pi_{\theta_k}}(s, a)$  for  $s = s_1, \dots, s_N$  and all  $a$

or  $Z_k(s, a) \approx Q^{\pi_{\theta_k}}(s, a) - b_k(s)$  for  $s = s_1, \dots, s_N$  and all  $a$

Update  $\theta_{k+1}$  from  $\theta_k$  using the estimators  $\{Z_k(s_i, a)\}_{i=1}^N$

Using any technique we introduced for policy-based contextual bandits

Data collection

$\sum_{k(s, a)}$

$\delta_i \sim b(x_i)$

$\pi(a | s_i)$

Policy Evaluation

Policy Improvement

# More General Ways to Create $Q^{\pi_{\theta_k}}(s, a)$ Estimators

Our goal is to create an estimator  $Z_k(s_i, a)$  with  $\mathbb{E}[Z_k(s_i, a)] = Q^{\pi_{\theta_k}}(s_i, a)$

Previously we set

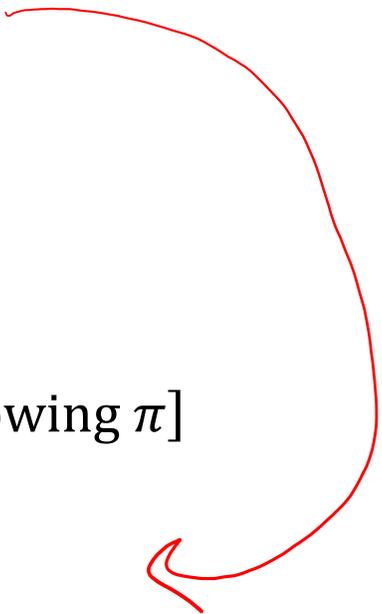
$$Z_k(s_i, a) = \frac{r_i + \gamma r_{i+1} + \gamma^2 r_{i+2} + \dots + \gamma^\tau r_{i+\tau} - b_k(s_i)}{\pi_{\theta_k}(a|s_i)} \mathbb{I}\{a_i = a\}$$

*just samples from the environment*

In general, the following is a valid estimator:

$$Z_k(s_i, a) = \frac{\text{Any estimation of } Q^{\pi_{\theta_k}}(s_i, a_i) - b_k(s_i)}{\pi_{\theta_k}(a|s_i)} \mathbb{I}\{a_i = a\}$$

# Using Another Neural Network to Approximate $V^\pi$

$$\begin{aligned}
 Q^\pi(s_i, a_i) &= \mathbb{E}[R(s_i, a_i) + \gamma R(s_{i+1}, a_{i+1}) + \dots + \gamma^\tau R(s_{i+\tau}, a_{i+\tau}) \mid \text{following } \pi] \\
 &= \mathbb{E}[R(s_i, a_i) + \gamma V^\pi(s_{i+1}) \mid \text{following } \pi] \\
 &= \mathbb{E}[R(s_i, a_i) + \gamma R(s_{i+1}, a_{i+1}) + \gamma^2 V^\pi(s_{i+2}) \mid \text{following } \pi] \\
 &= \mathbb{E}[R(s_i, a_i) + \gamma R(s_{i+1}, a_{i+1}) + \gamma^2 R(s_{i+2}, a_{i+2}) + \gamma^3 V^\pi(s_{i+3}) \mid \text{following } \pi] \\
 &\quad \vdots \\
 &= \mathbb{E}[R(s_i, a_i) + \gamma R(s_{i+1}, a_{i+1}) + \dots + \gamma^\tau R(s_{i+\tau}, a_{i+\tau})]
 \end{aligned}$$


For example, the following is an estimator for  $Q^{\pi_{\theta_k}}(s_i, a)$ :

$$Z_k(s_i, a) = \frac{r_i + \underbrace{\gamma \hat{V}(s_{i+1})}_{\approx \gamma(r_{i+1} + \gamma r_{i+2} + \gamma^2 r_{i+3} + \dots)} - b_k(s_i)}{\pi_{\theta_k}(a|s_i)} \mathbb{I}\{a_i = a\} \quad \text{where } \hat{V} \approx V^{\pi_{\theta_k}}$$

# Using Another Neural Network to Approximate $V^\pi$

How to estimate  $V^\pi$ ?

With true reward and transition:

Repeat:

$$V_{k+1}(s) \leftarrow \sum_a \pi(a|s) \left( R(s, a) + \gamma \sum_{s'} P(s'|s, a) V_k(s') \right) \quad \text{for all } s$$

With samples  $(s_1, a_1, r_1, s_2, a_2, r_2, \dots)$  collected from  $\pi$  and neural network  $V_\phi(s)$ :

Repeat:

$$\phi_{k+1} \leftarrow \underset{\phi}{\operatorname{argmin}} \frac{1}{N} \sum_{i=1}^N \left( V_\phi(s_i) - r_i - \gamma V_{\phi_k}(s_{i+1}) \right)^2$$

# Policy Iteration with Samples (w/ TD Estimator)

For  $k = 1, 2, \dots$

For  $i = 1, 2, \dots, N$ :

Choose action  $a_i \sim \pi_{\theta_k}(\cdot | s_i)$

Receive reward  $r_i \sim R(s_i, a_i)$  and  $s'_i \sim P(\cdot | s_i, a_i)$

$s_{i+1} = s'_i$  if episode continues,  $s_{i+1} \sim \rho$  if episode ends

Define for  $i = 1, 2, \dots, N$  and for all  $a$ :

$$Z_k(s_i, a) = \frac{r_i + \gamma V_{\phi_k}(s_{i+1}) - b_k(s_i)}{\pi_{\theta_k}(a | s_i)} \mathbb{I}\{a_i = a\}$$

$$\theta_{k+1} = \operatorname{argmax}_{\theta} \left\{ \frac{1}{N} \sum_{i=1}^N \left( \sum_a \pi_{\theta}(a | s_i) Z_k(s_i, a) - \frac{1}{\eta} \operatorname{KL}(\pi_{\theta}(\cdot | s_i), \pi_{\theta_k}(\cdot | s_i)) \right) \right\}$$

Perform several times:  $\phi \leftarrow \phi - \alpha \nabla_{\phi} \frac{1}{N} \sum_{i=1}^N \left( V_{\phi}(s_i) - r_i - \gamma V_{\phi_k}(s_{i+1}) \right)^2$

Data collection

Policy Evaluation

Policy Improvement

+  $V_{\phi}$  update

# Policy Iteration with Samples (w/ TD Estimator)

For  $k = 1, 2, \dots$

For  $i = 1, 2, \dots, N$ :

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$s_{i+1} = s'_i$  if episode continues,  $s_{i+1} \sim \rho$  if episode ends

Define for  $i = 1, 2, \dots, N$  and for all  $a$ :

$$Z_k(s_i, a) = \frac{r_i + \gamma r_{i+1} + \gamma^2 V_{\phi_k}(s_{i+2}) + b(s_i)}{\pi_{\theta_k}(a | s_i)} \mathbb{I}\{a_i = a\}$$

$$\theta_{k+1} = \operatorname{argmax}_{\theta} \left\{ \frac{1}{N} \sum_{i=1}^N \left( \sum_a \pi_{\theta}(a | s_i) Z_k(s_i, a) - \frac{1}{\eta} \operatorname{KL}(\pi_{\theta}(\cdot | s_i), \pi_{\theta_k}(\cdot | s_i)) \right) \right\}$$

Perform several times:  $\phi \leftarrow \phi - \alpha \nabla_{\phi} \frac{1}{N} \sum_{i=1}^N \left( V_{\phi}(s_i) - r_i - \gamma V_{\phi_k}(s_{i+1}) \right)^2$

Data collection

Policy Evaluation

Policy Improvement

+  $V_{\phi}$  update

$$\underbrace{Z_k(s_i, a)}_{\text{MC}} = \frac{r_i + \gamma r_{i+1} + \gamma^2 r_{i+2} + \dots + \gamma^T r_{i+T} - b(s_i)}{\pi_{\theta_k}(a|s_i)} \mathbb{I}(a_i = a) \quad \text{MC}$$

high variance  
unbiased

$$= \frac{r_i + \gamma V_{\phi_k}(s_{i+1}) - b(s_i)}{\pi_{\theta}(a|s_i)} \mathbb{I}(a_i = a) \quad \text{TD}$$

lower variance  
more biased

$$\Rightarrow \frac{r_i + \gamma r_{i+1} + \gamma^2 r_{i+2} + \dots + \gamma^m r_{i+m} + \gamma^{m+1} V_{\phi_k}(s_{i+m+1})}{\pi_{\theta}(a|s_i)} \quad (\text{general})$$

If  $T < m$

$$\frac{r_i + \gamma r_{i+1} + \dots + \gamma^T r_{i+T}}{\pi_{\theta}(a|s_i)}$$

# A Family of $Z_k$ Estimators

$$Z_k(s_i, a) = \frac{r_i + \gamma r_{i+1} + \dots + \gamma^{\tau-i} r_\tau - b_k(s_i)}{\pi_{\theta_k}(a|s_i)} \mathbb{I}\{a_i = a\} \quad \text{Monte Carlo (MC) Estimator}$$

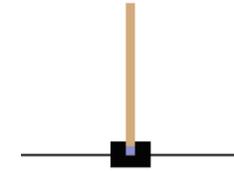
$$Z_k(s_i, a) = \frac{r_i + \gamma V_\phi(s'_{i+1}) - b_k(s_i)}{\pi_{\theta_k}(a|s_i)} \mathbb{I}\{a_i = a\} \quad \text{Temporal Difference (TD) Estimator}$$

$$Z_k(s_i, a) = \frac{r_i + \gamma r_{i+1} + \gamma^2 r_{i+2} + \dots + \gamma^m r_{i+m} + V_\phi(s'_{i+m+1}) - b_k(s_i)}{\pi_{\theta_k}(a|s_i)} \mathbb{I}\{a_i = a\}$$

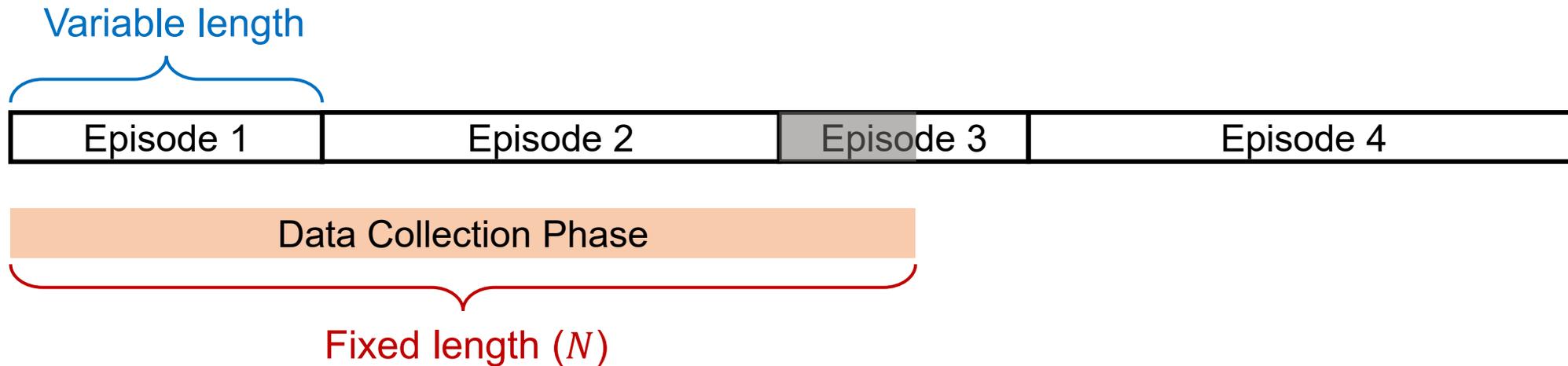
Multi-step TD Estimator

(If the episode ends before  $m$  steps, this falls back to the MC estimator)

# Recall: A Caveat of MC Estimator



The **episode end** may go beyond the **end of the data collection phase**



Issue: we may not construct  $r_i + \gamma r_{i+1} + \gamma^2 r_{i+2} + \dots + \gamma^{\tau_i} r_{i+\tau_i}$  for all  $i$

**Solution:** use  $r_i + \gamma r_{i+1} + \gamma^2 r_{i+2} + \dots + \gamma^{N-i} r_N + \gamma^{N-i+1} V_\phi(s'_N)$  if  $i$  is in an incomplete episode

# Recall: A Caveat of MC Estimator

E.g.,  $N = 16$ . Episodes end at steps 5, 11, 19

For  $i = 1, \dots, 5$ :

$$Z_k(s_i, a) = \frac{r_i + \gamma r_{i+1} + \dots + \gamma^{5-i} r_5 - b_k(s_i)}{\pi_{\theta_k}(a|s_i)} \mathbb{I}\{a_i = a\}$$

For  $i = 6, \dots, 11$ :

$$Z_k(s_i, a) = \frac{r_i + \gamma r_{i+1} + \dots + \gamma^{11-i} r_{11} - b_k(s_i)}{\pi_{\theta_k}(a|s_i)} \mathbb{I}\{a_i = a\}$$

For  $i = 12, \dots, 16$ :

$$Z_k(s_i, a) = \frac{r_i + \gamma r_{i+1} + \dots + \gamma^{16-i} r_{16} + \gamma^{17-i} V_{\phi}(s'_{16}) - b_k(s_i)}{\pi_{\theta_k}(a|s_i)} \mathbb{I}\{a_i = a\}$$

# How to Calculate $Z_k$ Efficiently for MC Estimator

Assume we have collected  $(s_1, a_1, r_1, s'_1), (s_2, a_2, r_2, s'_2), \dots, (s_N, a_N, r_N, s'_N)$ , where  $s_{i+1} = s'_i$  if  $s'_i$  is not a terminal state, and  $s_{i+1}$  is redrawn from initial state otherwise.

How to calculate

$$r_i + \gamma r_{i+1} + \gamma^2 r_{i+2} + \dots + \gamma^{\tau_i} r_{i+\tau_i}$$

$$r_i + \gamma r_{i+1} + \gamma^2 r_{i+2} + \dots + \gamma^{N-i} r_N + \gamma^{N-i+1} V_\phi(s'_N)$$

efficiently for all  $i = 1, \dots, N$  ?

Naïve implementation requires  $O(N \times \text{episode\_length})$  time

# How to Calculate $Z_k$ Efficiently for MC Estimator

For an incomplete episode

For a complete episode that ends at  $\tau$

# How to Calculate $Z_k$ Efficiently for MC Estimator

$$G_{N+1} = V_\phi(s'_N)$$

For  $i = N, N - 1, \dots, 1$ :

If  $s'_i$  is a terminal state:

$$G_i = r_i$$

Else:

$$G_i = r_i + \gamma G_{i+1}$$

For  $i = 1, \dots, N$ :

$$\text{Define } Z_k(s_i, a) = \frac{G_i - b_k(s_i)}{\pi_{\theta_k}(a|s_i)} \mathbb{I}\{a_i = a\}$$

Remark: For TD estimator,  $G_i$  is simply calculated as  $r_i + \gamma V_\phi(s'_i)$

For general ( $m$ -step) estimator, we can also design efficient algorithm (omitted)

# Policy Iteration with Samples

For  $k = 1, 2, \dots$

For  $i = 1, 2, \dots, N$ :

Choose action  $a_i \sim \pi_{\theta_k}(\cdot | s_i)$

Receive reward  $r_i \sim R(s_i, a_i)$  and  $s'_i \sim P(\cdot | s_i, a_i)$

$s_{i+1} = s'_i$  if episode continues,  $s_{i+1} \sim \rho$  if episode ends

Define for  $i = 1, 2, \dots, N$  and for all  $a$ :

$$Z_k(s_i, a) = \frac{\mathbf{G}_i - b_k(s_i)}{\pi_{\theta_k}(a | s_i)} \mathbb{I}\{a_i = a\} \quad \text{with } b_k(s_i) = V_{\phi}(s_i)$$

$$\theta_{k+1} = \operatorname{argmax}_{\theta} \left\{ \frac{1}{N} \sum_{i=1}^N \left( \sum_a \pi_{\theta}(a | s_i) Z_k(s_i, a) - \frac{1}{\eta} \operatorname{KL}(\pi_{\theta}(\cdot | s_i), \pi_{\theta_k}(\cdot | s_i)) \right) \right\}$$

Perform several times:  $\phi \leftarrow \phi - \alpha \nabla_{\phi} \frac{1}{N} \sum_{i=1}^N \left( V_{\phi}(s_i) - r_i - \gamma V_{\phi_k}(s_{i+1}) \right)^2$

Data collection

Policy Evaluation

Policy Improvement

+  $V_{\phi}$  update

# Generalized Policy Iteration

$N = \infty \Rightarrow$  Policy Iteration

$N = 1 \Rightarrow$  Value Iteration for policy optimization

For  $i = 1, 2, \dots$

$$\pi_i(s) = \operatorname{argmax}_a Q_i(s, a) \quad \leftarrow \text{Policy update}$$

$$Q \leftarrow Q_i$$

Repeat for  $N$  times:

$$Q(s, a) \leftarrow R(s, a) + \gamma \sum_{s', a'} P(s' | s, a) \pi_i(a' | s') Q(s', a') \quad \leftarrow \text{Value update}$$

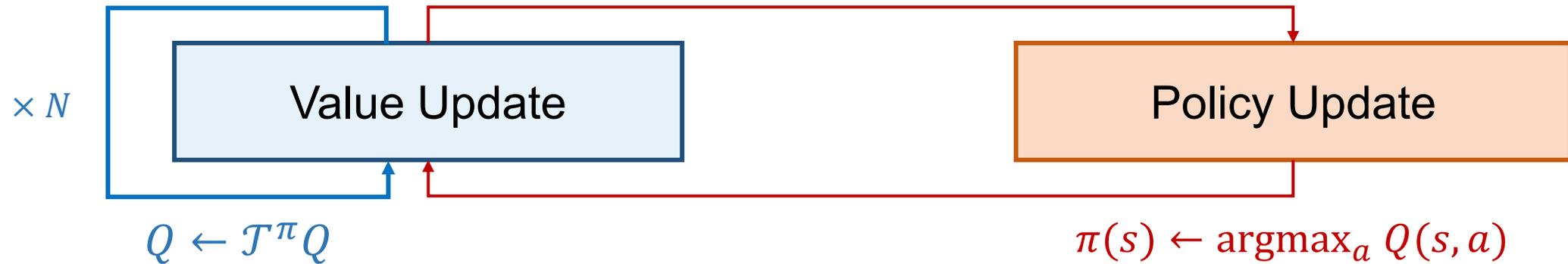
$$Q_{i+1} \leftarrow Q$$

**Notice:** in value iteration, there may not exist a policy  $\pi$  such that  $Q_i = Q^\pi$

In contrast, in policy iteration we have  $Q_i = Q^{\pi_{i-1}}$

VI can be viewed as PI **with incomplete policy evaluation**

# Generalized Policy Iteration



$$Q \leftarrow \mathcal{T}^\pi Q \text{ means } Q(s, a) \leftarrow R(s, a) + \gamma \sum_{s', a'} P(s' | s, a) \pi(a' | s') Q(s', a') \quad \text{for all } s, a$$

- Provide a unified view for algorithms approximating optimal policy with known  $P, R$
- Provide a unified view for “value-based” and “policy-based” algorithms
- Compared with bandits:
  - The  $R$  is replaced by  $Q$  (could be  $Q^\pi$  or  $Q^*$ ) to capture the long-term goal of the learner

# Summary for Policy-Based RL Algorithms

- We introduce Policy Iteration, an algorithm that iterates between **policy evaluation** and **policy improvement**, assuming access to true transition and reward
- We introduce the PPO algorithm for MDPs
  - Almost the same as its special case in contextual bandits, except that we replace  $\hat{r}_k(x, a)$  (an estimator for  $r(x, a)$ ) by  $Z_k(s, a)$  (an estimator for  $Q^{\pi_{\theta_k}}(s, a)$ )
  - There are a family of estimators you may choose from, depending on how much the algorithm relies on  $V_\phi$  or real reward collected from environments
  - $V_\phi$  also serves the baseline
- We introduce Generalized Policy Iteration as a way to unify Policy Iteration and Value Iteration