

n-step Bootstrapping

Reinforcement Learning

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Recap



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Data Generation

— — —

2 steps:

1. Roll-in

2. Roll-out & compute supervision targets

Given s , a , how do we estimate $Q^\pi(s,a)$?

$$Q^\pi(s_t, a_t) = \mathbb{E}[\sum_{h=0}^{\infty} \gamma^h r_h | (s_0, a_0) = (s_t, a_t), a_{h+1} = \pi(s_h), s_{h+1} \sim p(\cdot | s_h, a_h)]$$

Monte-Carlo method: estimate this through sampling, execute until termination and then average many roll-outs to compute our estimate. **Note: True MC cannot be applied if infinite horizon, but we can adapt using the ‘trick’ shown in previous class**



Monte-Carlo Update

— — —

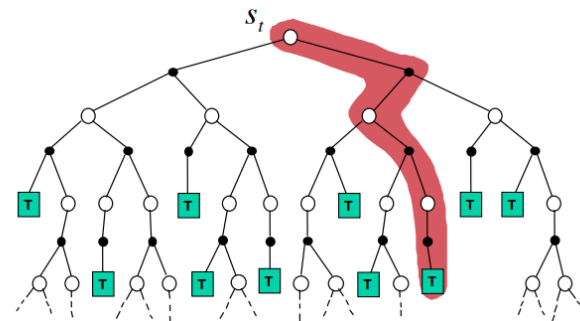
$$Q^\pi(s_t, a_t) = \mathbb{E}[\sum_{h=0}^{\infty} \gamma^h r_h | (s_0, a_0) = (s_t, a_t), a_{h+1} = \pi(s_h), s_{h+1} \sim p(\cdot | s_h, a_h)]$$

Monte-Carlo method: estimate this through sampling, execute until termination and then average many roll-outs to compute our estimate

Compute target: $y = G$

- G is the return
- The return is the sum of rewards

$$\sum_{h=0}^{\text{Termination}} \gamma^h r_h$$



MC Updates

Tabular:

$$Q(s,a) \leftarrow Q(s,a) + \alpha(G_i - Q(s,a))$$

we do this at every termination

Function Approximator:

$$\operatorname{argmin}_{Q \text{ in } \mathcal{Q}} \sum_{i=1}^N (Q(s_i, a_i) - G_i)^2$$

we store data and update in batch after a while or do online learning (at every datapoint - less stable)



MC Pros & Cons

— — —

Weaknesses:

- Needs some sort of termination
- Depends on many random actions, transitions, rewards
- Needs complete sequences of returns

Strengths:

- Unbiased
- Good convergence properties also with function approx
- Not very sensitive to initialization



Data Generation

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1. Roll-in

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Given s , a , how do we estimate $Q^\pi(s,a)$?

$$Q^\pi(s_t, a) = r_t + \gamma \mathbb{E}_{s' \sim p(\cdot | s, a)} [V^\pi(s')]$$

Monte-Carlo uses the actual return. In Temporal Difference we use an estimated return: our current V

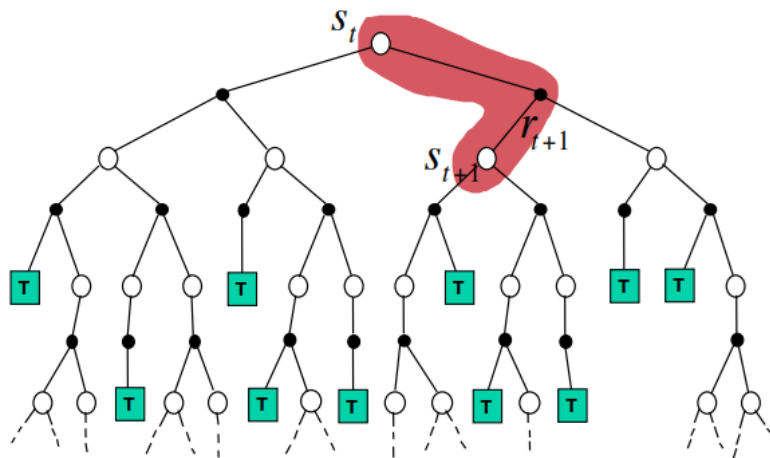


Temporal Difference Update

— — —

$$Q^\pi(s_t, a) = r_t + \gamma \mathbb{E}_{s' \sim p(\cdot | s, a)} [V^\pi(s')]$$

Temporal Difference method: estimate this through sampling, update our estimate towards the current reward and the current estimated return (*bootstrapping*) from incomplete episodes



Bootstrapping: an estimate of the next state value is used instead of the true next state value



TD Updates

Tabular:

$$Q(s,a) \leftarrow Q(s,a) + \alpha(r_i + \gamma Q(s', \cdot) - Q(s,a))$$

we do this at every timestep

Function Approximator:

$$\operatorname{argmin}_{Q \in \mathcal{Q}} \sum_{i=1}^N (Q(s_i, a_i) - r_i + \gamma Q(s', \cdot))^2$$

still we store data and update in batch after a while or do online learning (at every datapoint - less stable), but many more data-points than MC with same experience



TD Pros & Cons

Weaknesses:

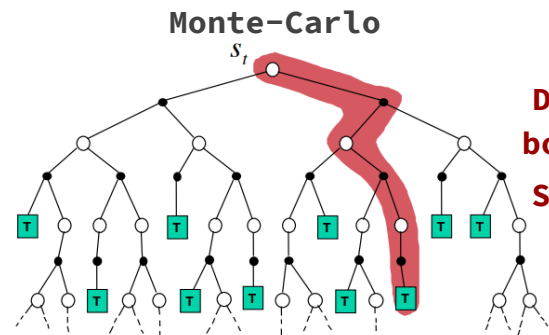
- Sensitive to initial value
- Biased estimate of Q^π

Strengths:

- Can learn at every step, from incomplete sequences and in continuing tasks easily
- Depends on just one action instead of a sequence like MC
- Converges but not always if function approx

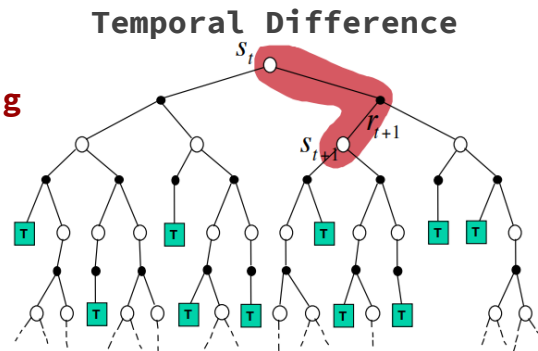
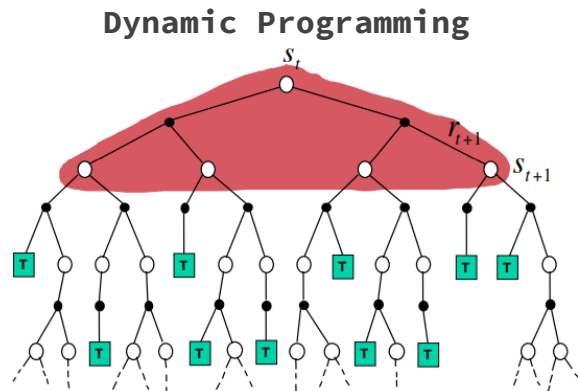


MC vs TD vs DP



Bootstrapping

Sampling



Bootstrapping

Compute expectation



ϵ -Greedy Exploration & Policy Improvement

— — —
Simplest idea: instead of only being greedy with respect to Q , try all actions with some probability

- probability $1-\epsilon$ choose the greedy action (do argmax)
 - probability ϵ choose a random action
- $$\pi(a|s) = \begin{cases} \epsilon/m + 1 - \epsilon & \text{if } a^* = \operatorname{argmax}_{a \in \mathcal{A}} Q(s, a) \\ \epsilon/m & \text{otherwise} \end{cases}$$

This handles the **exploration-exploitation trade-off**

For any ϵ -greedy policy π , the ϵ -greedy policy π' obtained by Q^π is an improvement, such that $V^{\pi'} \geq V^\pi$ holds

If we set $\epsilon = 1/k$, with k going to infinity

- we visit all state-action pairs infinitely many times
- the policy converges to a greedy policy

Greedy in the Limit with Infinite Exploration



ϵ -Greedy and MC

— — —

If we apply Greedy in the Limit with Infinite Exploration to MC we converge to the optimal Q^*

$$\epsilon \leftarrow 1/k$$

$$\pi \leftarrow \epsilon\text{-greedy}(Q)$$



ϵ -Greedy and TD

— — —

Remember $r_i + \gamma Q(s', \cdot)$?

How do we select \cdot ?

Sarsa: the target action is selected according to π (which can be ϵ -greedy with respect to Q)

Selects the target action according to the same policy we execute

ON-POLICY

Q-learning: the target action is greedy with respect to Q

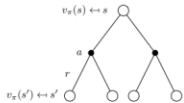

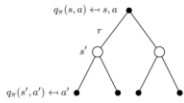
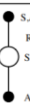
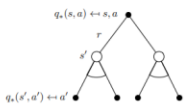
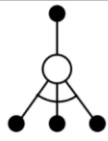
Selects the target action differently from the policy we execute (which must be ϵ -greedy, remember?)

OFF-POLICY



TD, Sarsa & Q-Learning vs DP

— — —

	Full Backup (DP)	Sample Backup (TD)	Full Backup (DP)	Sample Backup (TD)
Bellman Expectation Equation for $v_{\pi}(s)$	 <p>Iterative Policy Evaluation</p>	 <p>TD Learning</p>	Iterative Policy Evaluation $V(s) \leftarrow \mathbb{E}[R + \gamma V(S') \mid s]$	TD Learning $V(S) \stackrel{\alpha}{\leftarrow} R + \gamma V(S')$
Bellman Expectation Equation for $q_{\pi}(s, a)$	 <p>Q-Policy Iteration</p>	 <p>Sarsa</p>	Q-Policy Iteration $Q(s, a) \leftarrow \mathbb{E}[R + \gamma Q(S', A') \mid s, a]$	Sarsa $Q(S, A) \stackrel{\alpha}{\leftarrow} R + \gamma Q(S', A')$
Bellman Optimality Equation for $q_{*}(s, a)$	 <p>Q-Value Iteration</p>	 <p>Q-Learning</p>	Q-Value Iteration $Q(s, a) \leftarrow \mathbb{E}\left[R + \gamma \max_{a' \in \mathcal{A}} Q(S', a') \mid s, a\right]$	Q-Learning $Q(S, A) \stackrel{\alpha}{\leftarrow} R + \gamma \max_{a' \in \mathcal{A}} Q(S', a')$



End Recap



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A (statistical) Note on Bootstrapping

— — —

Is bootstrapping in RL the same as in statistics?



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Definition from statistics: *Bootstrapping is a method of inferring results for a population from results found on a collection of smaller random samples of that population, using replacement during the sampling process*

Replacement: every time an item is drawn from the pool, the same item remains a part of the sample pool



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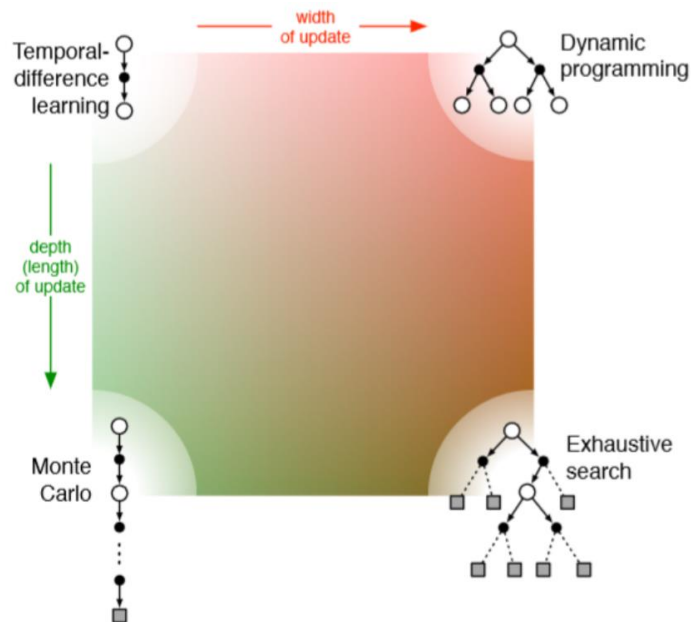
Replacement: every time an item is drawn from the pool, the same item remains a part of the sample pool

In RL we are basically doing the same: we infer results (Q) for all the states and actions, inferring them from results found on a collection of smaller random samples (the states that we actually have some information about). All states and actions are always in the ‘samplable’ pool.



MC vs TD vs DP

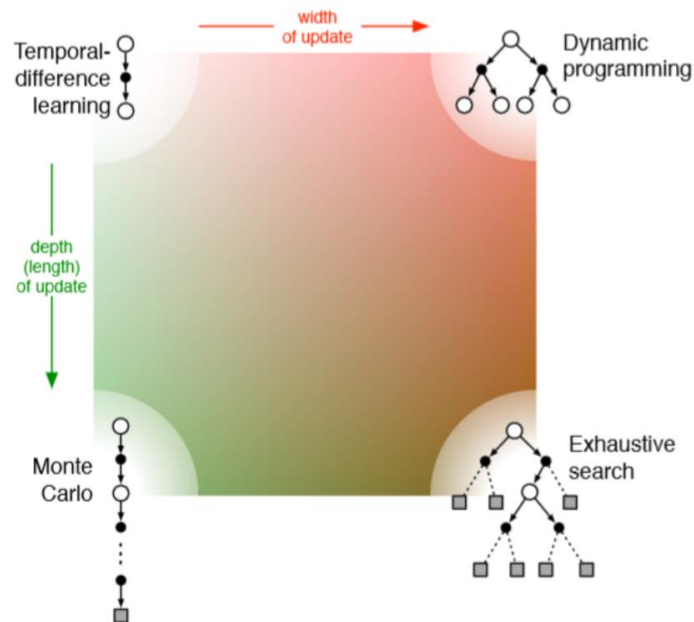
— — —



MC vs TD vs DP

— — —

- TD uses a single timestep
 - sometimes it's not enough to acquire any signal or significant state change
 - MC uses all timesteps
 - leads to high variance
- is there any intermediate?**



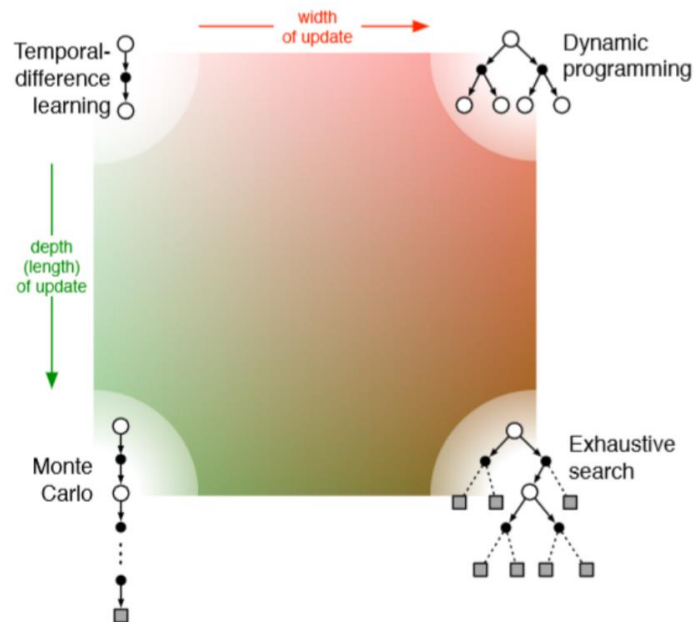
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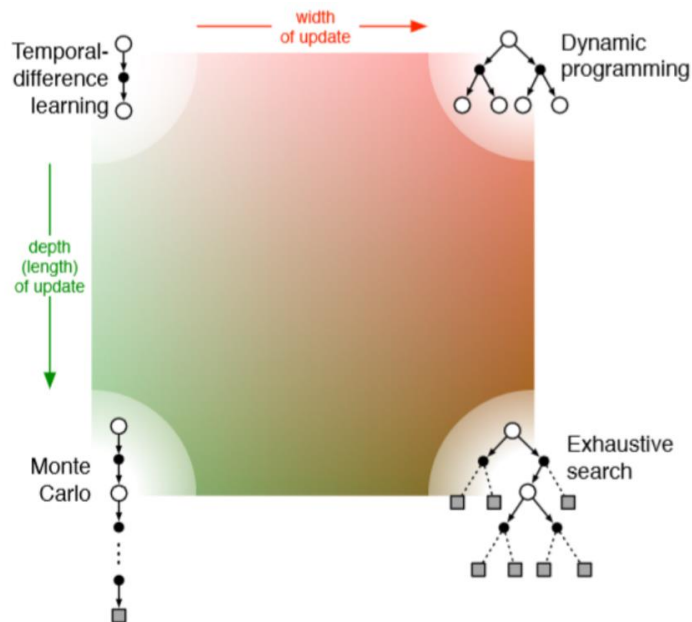
use n-step returns



n-step Returns

— — —

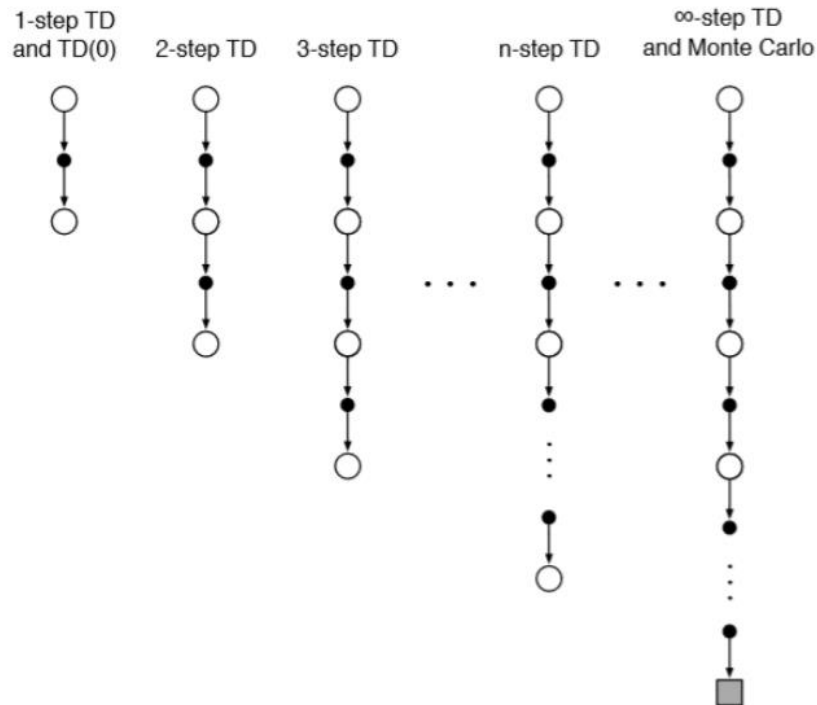
n-step returns are still make using of temporal difference, but use more than one reward



n-step Returns

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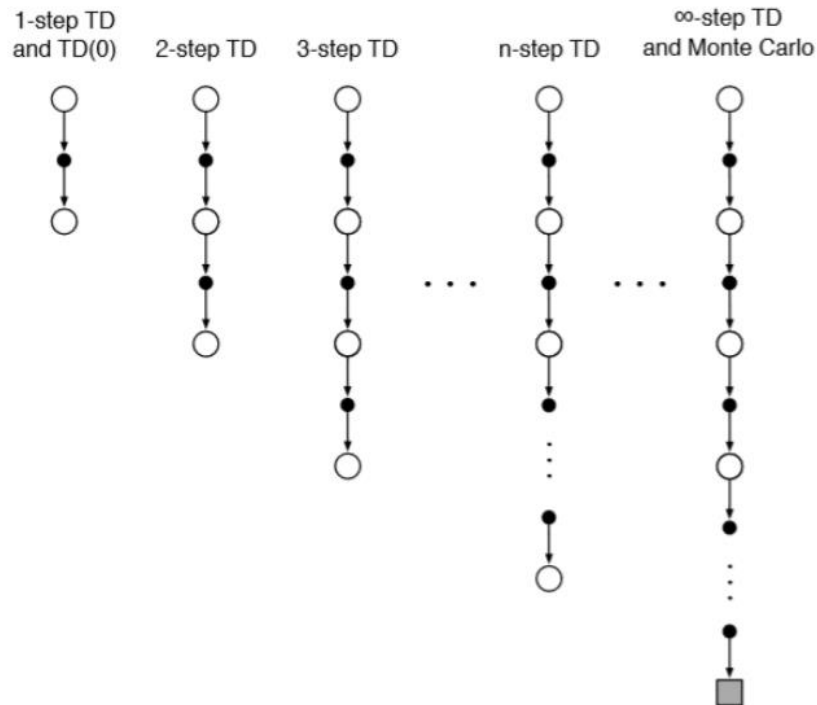
n-step returns are still made using of temporal difference, but use more than one reward

$$n = 1 \quad y = G_t^{(1)} = r_t + \gamma V(s_{t+1})$$

$$n = 2 \quad y = G_t^{(2)} = r_t + \gamma r_{t+1} + \gamma^2 V(s_{t+2})$$

...

$$n = \infty \quad y = G_t = y_{MC}$$



n-step Returns

n-step returns are still made using of temporal difference, but use more than one reward

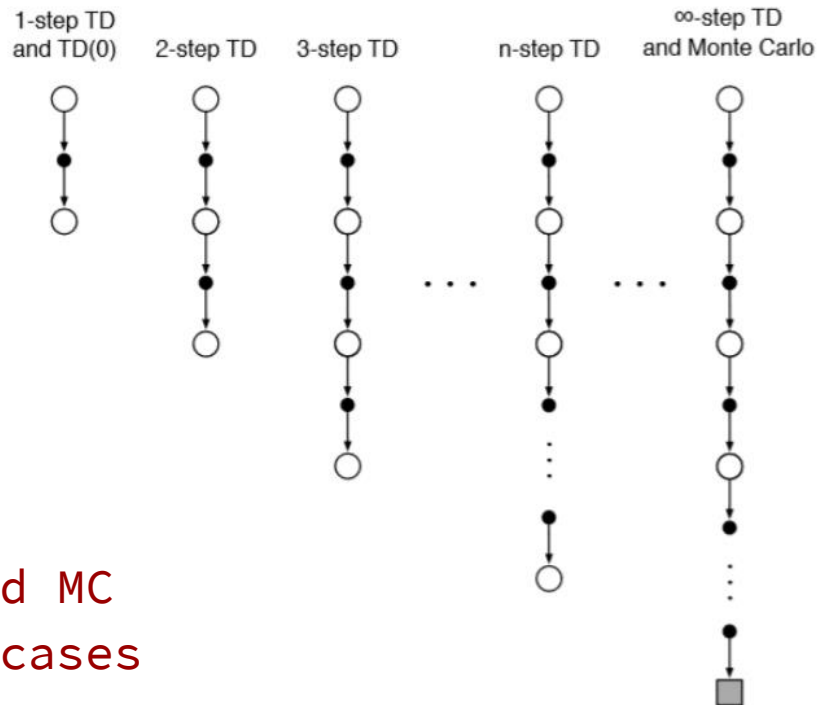
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1-step TD and MC
just extreme cases



n-step Returns

n-step returns are still made using of temporal difference, but use more than one reward

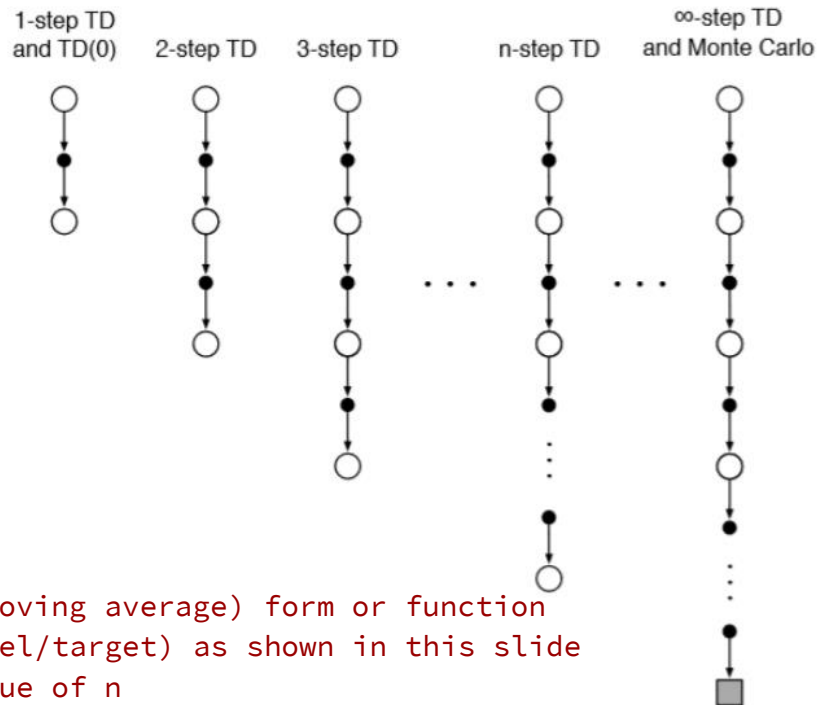
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$$n = \infty \quad y = G_t = y_{MC}$$

we still do our updates using the tabular (moving average) form or function approximation (l2-regression), with y (the label/target) as shown in this slide depending on the value of n



n-step TD in V

— — —

Input: a policy π

Algorithm parameters: step size $\alpha \in (0, 1]$, a positive integer n

Initialize $V(s)$ arbitrarily, for all $s \in \mathcal{S}$

All store and access operations (for S_t and R_t) can take their index mod $n + 1$

Loop for each episode:

 Initialize and store $S_0 \neq \text{terminal}$

$T \leftarrow \infty$

 Loop for $t = 0, 1, 2, \dots$:

 | If $t < T$, then:

 | Take an action according to $\pi(\cdot | S_t)$

 | Observe and store the next reward as R_{t+1} and the next state as S_{t+1}

 | If S_{t+1} is terminal, then $T \leftarrow t + 1$

 | $\tau \leftarrow t - n + 1$ (τ is the time whose state's estimate is being updated)

 | If $\tau \geq 0$:

 | $G \leftarrow \sum_{i=\tau+1}^{\min(\tau+n, T)} \gamma^{i-\tau-1} R_i$

 | If $\tau + n < T$, then: $G \leftarrow G + \gamma^n V(S_{\tau+n})$ ($G_{\tau:\tau+n}$)

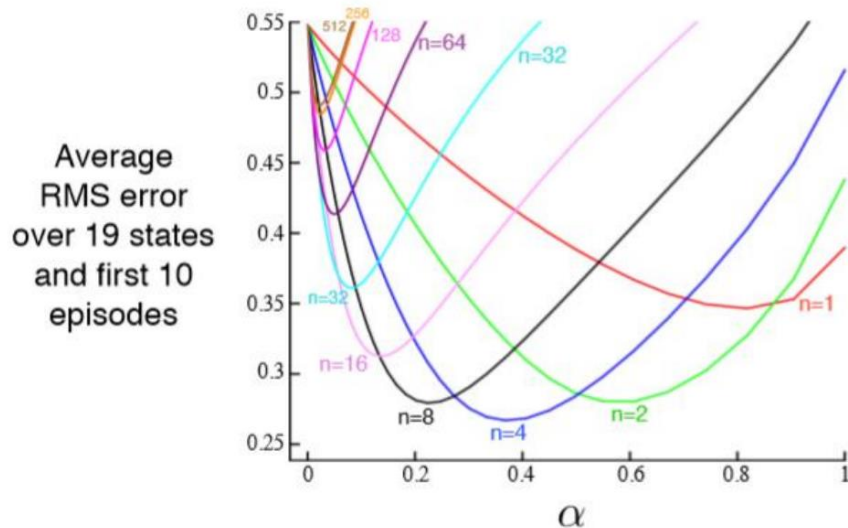
 | $V(S_\tau) \leftarrow V(S_\tau) + \alpha [G - V(S_\tau)]$

 Until $\tau = T - 1$



n-step TD in V

Extremes can potentially perform worse



n-step Sarsa

1-step Sarsa
aka Sarsa(0)



2-step Sarsa



3-step Sarsa



...

n-step Sarsa



Just compute the target using n-steps

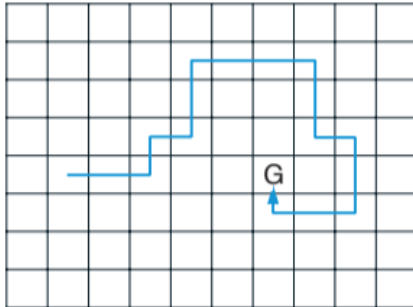
$$y = Q_{(n)}^{\pi} = r_t + \dots + \gamma^{n-1} r_{t+n-1} + \gamma^n Q^{\pi}(s_{t+n}, a \sim \pi(s_{t+n}))$$



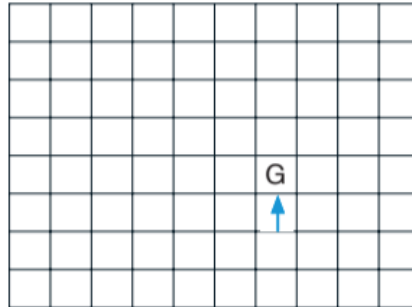
n-step Sarsa: Example

— — —

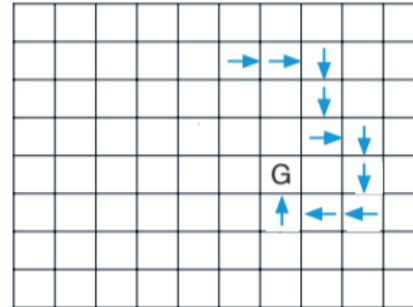
Path taken



Action values increased
by one-step Sarsa



Action values increased
by 10-step Sarsa



n-steps

— — —

But at this point, how do we pick n ? Why should we commit to a specific n ? Based on what?



Averaging n-step Returns

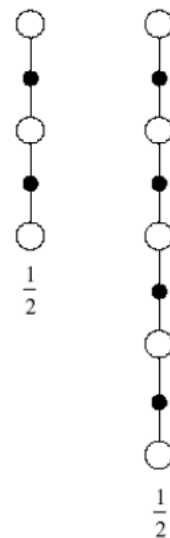
We can also solve this: average n-step returns over different lengths, thus combining information from different timesteps

$$n = 2 \quad G^{(2)}$$

$$n = 4 \quad G^{(4)}$$

$$y = 0.5G^{(2)} + 0.5G^{(4)}$$

One backup



λ -returns

— — —

Can we combine information from all timesteps?

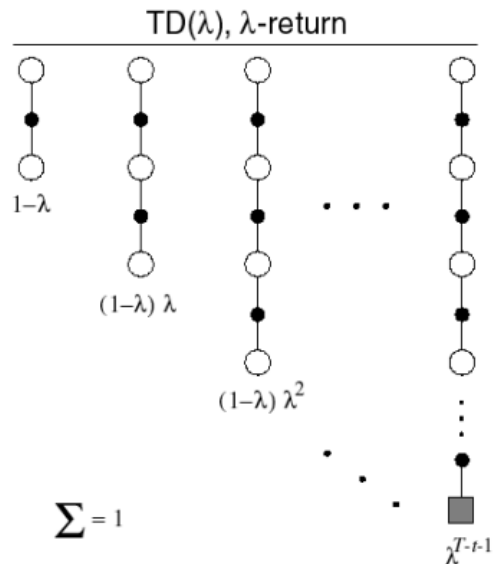


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Can we combine information from all timesteps?

Yes, λ -returns G_t^λ combine all n-step returns



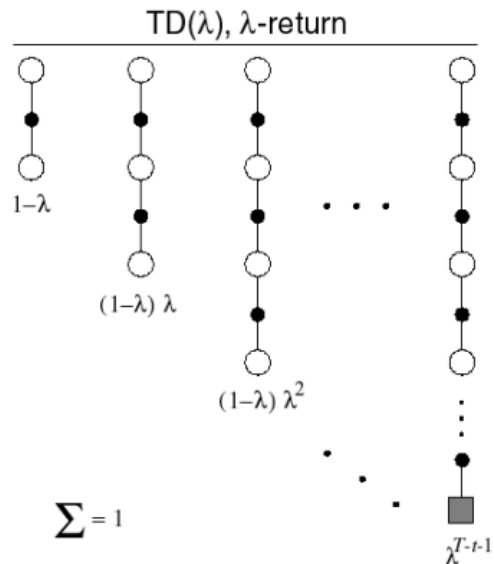
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- using a certain weight $(1-\lambda)\lambda^{n-1}$
- doing a weighted average

$$y = G_t^\lambda = (1-\lambda) \sum_{n=1}^{\infty} \lambda^{n-1} G_t^{(n)}$$



λ -returns & TD(λ)

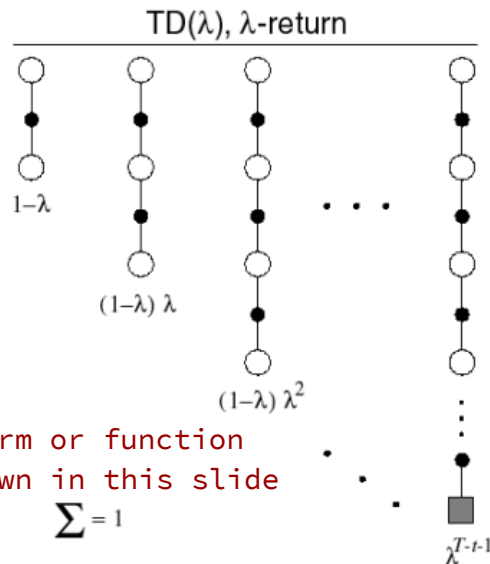
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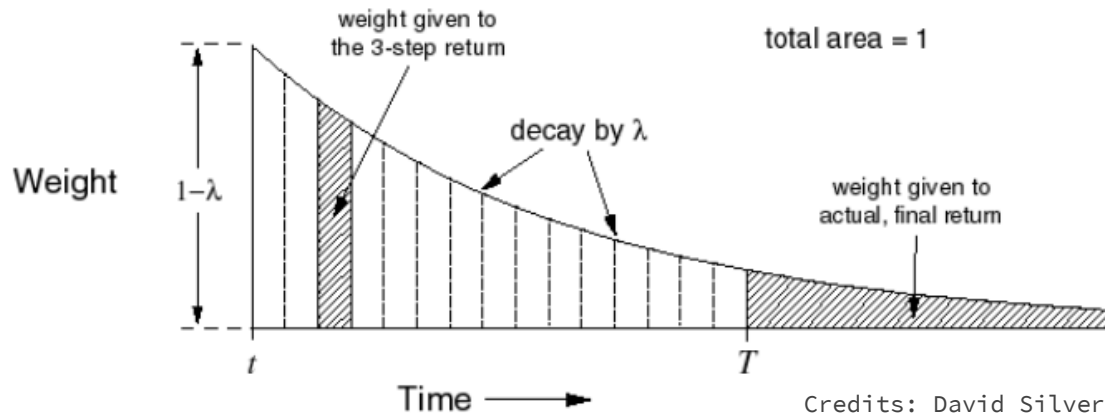
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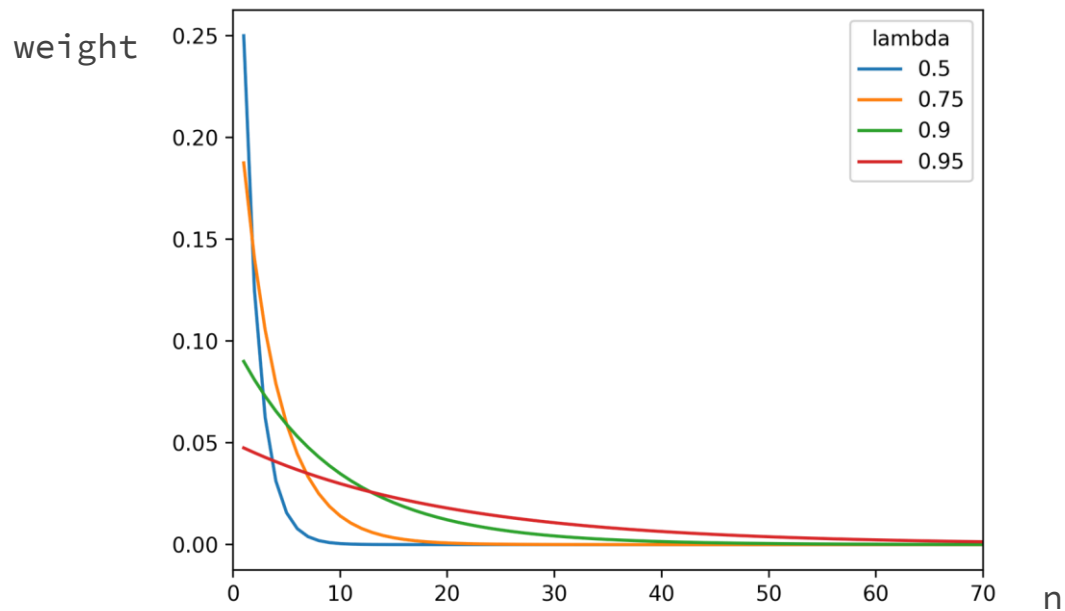
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TD(λ) Weights



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Forward-View TD(λ)

We can combine all n-steps using λ -returns G_t^λ but we are back at the problem of MC updates: we need to wait for termination



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Backward-View TD(λ)

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We can actually do better and still preserve the updates at every timestep by maintaining a virtually equivalent intuition under a different perspective: backward-view



Backward-View TD(λ)

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We will use **eligibility traces**



Eligibility Traces

— — —

Instead of waiting for *what is going to happen next*, we
will remember *what happened in the past*



Eligibility Traces

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We're specifically looking at a **credit assignment** problem



Credit Assignment

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We're specifically looking at a **credit assignment** problem

At the end of a football match a team either wins or loses. What contribution did each player provide to the win/loss?

This kind of analysis is called credit assignment, and we will assign credit to states (or states and actions)



Credit Assignment

Instead of waiting for *what is going to happen next*, we will remember *what happened in the past*

We're specifically looking at a **credit assignment** problem

Heuristics:

- **frequency:** most frequent states get credit
- **recency:** most recent states get credit



Eligibility Traces

Eligibility traces combine both credit assignment heuristics:

- keep an eligibility trace for all states s in S
- compute the eligibility trace as

$$e_0(s) = 0$$

$$e_t(s) = \gamma \lambda e_{t-1}(s) + \mathbf{I}(s_t=s)$$



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\mathbf{I} is the indicator function, which equals 1 if the condition inside is true, 0 otherwise



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recency



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frequency



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now use eligibility traces as scaling factor for TD error



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TD error (in V): $\delta_t = r_t + \gamma V^\pi(s_{t+1}) - V^\pi(s_t)$

- for **ALL** the states s in S update the value function estimate

$$V^\pi(s) \leftarrow V^\pi(s) + \alpha \delta_t e_t(s)$$



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We do our updates for all the states at each timestep: states that are not visited or haven't been visited in a while will have an eligibility value equal or close to zero, which means that our estimate for those states won't change much



Eligibility Traces

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- for **ALL** the states s in S update the value function estimate

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We propagate current error information (δ_t) into the states we visited in the past. This allows us to combine the n -step returns in an online fashion.



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This is still a TD method: still biased because of the bootstrapping. It should intuitively have less variance than MC because of the averaging of low-variance information, but this is not proved



Eligibility Traces and λ Values (0)

If $\lambda = 0$

$$e_0(s) = 0$$

$$e_t(s) = \mathbf{I}(s_t=s)$$

As a result we basically update only s_t as we do in standard TD(0)

$$V^\pi(s_t) \leftarrow V^\pi(s_t) + \alpha \delta_t$$



Eligibility Traces and λ Values (1)

If $\lambda = 1$ credit is maintained until the end of the episode

As a result, over the course of an episode, the total update to each state is the same as the total update for MC if the value function is updated just at the end of the episode (e.g., through a batch update)



Eligibility Traces and λ Values (1)

Consider a state s visited only once at time k :

- $e_t(s) = 0$ if $t < k$
- $e_t(s) = \gamma^{t-k}$ if $t \geq k$

The total updates that it cumulates are:

$$\sum_{t=0}^{T-1} \alpha \delta_t e_t(s) = \alpha \sum_{t=k}^{T-1} \gamma^{t-k} \delta_t = \alpha (G_k - V^{\pi}(s_t))$$



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$$\delta_k + \gamma \delta_{k+1} + \gamma^2 \delta_{k+2} + \dots + \gamma^{T-1-k} \delta_{T-1}$$



Eligibility Traces and λ Values (1)

— — —

$$\begin{aligned} & \delta_k + \gamma \delta_{k+1} + \gamma^2 \delta_{k+2} + \dots + \gamma^{T-1-k} \delta_{T-1} = \\ & \quad r_k + \gamma V^\pi(s_{k+1}) - V^\pi(s_k) + \\ & \quad \gamma r_{k+1} + \gamma^2 V^\pi(s_{k+2}) - \gamma V^\pi(s_{k+1}) + \\ & \quad \gamma^2 r_{k+2} + \gamma^3 V^\pi(s_{k+3}) - \gamma^2 V^\pi(s_{k+2}) + \\ & \quad \dots \\ & \quad \gamma^{T-1-k} r_{T-1} \end{aligned}$$



Eligibility Traces and λ Values (1)

— — —

$$\begin{aligned} & \delta_k + \gamma \delta_{k+1} + \gamma^2 \delta_{k+2} + \dots + \gamma^{T-1-k} \delta_{T-1} = \\ & \quad r_k + \cancel{\gamma V^\pi(s_{k+1}) - V^\pi(s_k)} + \\ & \quad \gamma r_{k+1} + \cancel{\gamma^2 V^\pi(s_{k+2}) - \gamma V^\pi(s_{k+1})} + \\ & \quad \gamma^2 r_{k+2} + \cancel{\gamma^3 V^\pi(s_{k+3}) - \gamma^2 V^\pi(s_{k+2})} + \\ & \quad \dots \\ & \quad \gamma^{T-1-k} r_{T-1} \end{aligned}$$



Eligibility Traces and λ Values (1)

$$\begin{aligned}
 &\delta_k + \gamma \delta_{k+1} + \gamma^2 \delta_{k+2} + \dots + \gamma^{T-1-k} \delta_{T-1} = \\
 &\quad r_k + \cancel{\gamma V^\pi(s_{k+1}) - V^\pi(s_k)} + \\
 &\quad \gamma r_{k+1} + \cancel{\gamma^2 V^\pi(s_{k+2}) - \gamma V^\pi(s_{k+1})} + \\
 &\quad \gamma^2 r_{k+2} + \cancel{\gamma^3 V^\pi(s_{k+3}) - \gamma^2 V^\pi(s_{k+2})} + \\
 &\quad \dots
 \end{aligned}$$

$$\gamma^{T-1-k} r_{T-1} =$$

$$r_k + \gamma r_{k+1} + \gamma^2 r_{k+2} + \gamma^{T-1-k} r_{T-1} - V^\pi(s_k) = G_t - V^\pi(s_k)$$



Eligibility Traces and λ Values (General)

Consider a state s visited only once at time k :

- $e_t(s) = 0$ if $t < k$
- $e_t(s) = (\gamma\lambda)^{t-k}$ if $t \geq k$

The total updates that it cumulates are:

$$\sum_{t=0}^{T-1} \alpha \delta_t e_t(s) = \alpha \sum_{t=k}^{T-1} (\gamma\lambda)^{t-k} \delta_t = \alpha (G_k^\lambda - V^\pi(s_t))$$

You can expand the definition of G_k^λ and prove it



Forward & Backward View Equivalence

— — —

Theorem: The sum of **offline** updates is identical for forward-view and backward-view

$$\sum_{t=0}^{T-1} \alpha \delta_t \mathbf{e}_t(s) = \sum_{t=0}^{T-1} \alpha (G_t^\lambda - V^\pi(s_t)) \mathbf{I}(s_t=s)$$



Forward & Backward View Equivalence

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- **offline:** apply update in batch at the end of the episode
- **online:** apply update at every timestep



Forward & Backward View Equivalence

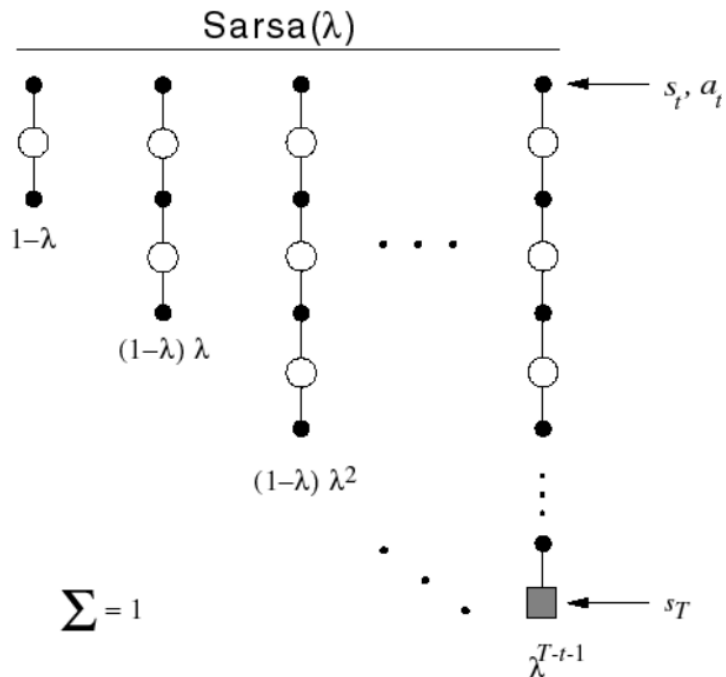
— — —

Offline updates	$\lambda = 0$	$\lambda \in (0, 1)$	$\lambda = 1$
Backward view	TD(0) 	TD(λ) 	TD(1)
Forward view	TD(0)	Forward TD(λ)	MC
Online updates	$\lambda = 0$	$\lambda \in (0, 1)$	$\lambda = 1$
Backward view	TD(0) 	TD(λ) ⧻	TD(1) ⧻
Forward view	TD(0)	Forward TD(λ)	MC

Credits: David Silver



Sarsa- λ : Forward View



Forward view:

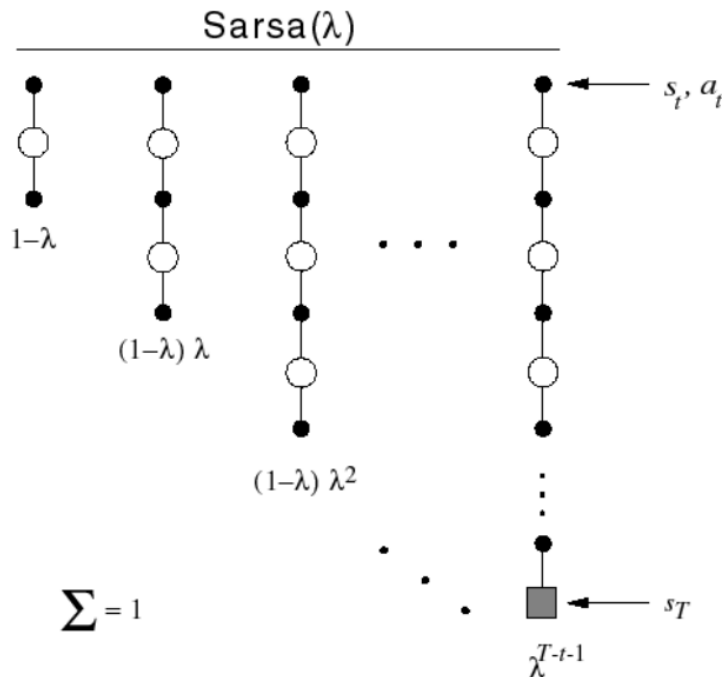
$$y = (1-\lambda) \sum_{n=1}^{\infty} \lambda^{n-1} Q_{(n)}^{\pi}$$

$$Q_{(n)}^{\pi} = r_t + \dots + \gamma^{n-1} r_{t+n-1} + \gamma^n Q^{\pi}(s_{t+n}, a \sim \pi(s_{t+n}))$$

$$Q(s, a) \leftarrow Q(s, a) + \alpha (y - Q(s, a))$$



Sarsa- λ : Backward View



Backward view:

$e_0(s,a) = 0$ and $e_t(s,a) = \gamma e_{t-1}(s,a) + \mathbf{I}(s_t=s, a_t=a)$
for all s,a

Update for all s,a every time:

$$\delta_t = r_t + \gamma Q^{\pi}(s_{t+1}, a \sim \pi(s_{t+1})) - Q^{\pi}(s_t, a_t)$$

$$Q(s,a) \leftarrow Q(s,a) + \alpha \delta_t e_t(s,a)$$



Sarsa- λ : Backward View

— — —

Initialize $Q(s, a)$ arbitrarily, for all $s \in \mathcal{S}, a \in \mathcal{A}(s)$

Repeat (for each episode):

$E(s, a) = 0$, for all $s \in \mathcal{S}, a \in \mathcal{A}(s)$

Initialize S, A

Repeat (for each step of episode):

Take action A , observe R, S'

Choose A' from S' using policy derived from Q (e.g., ϵ -greedy)

$\delta \leftarrow R + \gamma Q(S', A') - Q(S, A)$

$E(S, A) \leftarrow E(S, A) + 1$

For all $s \in \mathcal{S}, a \in \mathcal{A}(s)$:

$Q(s, a) \leftarrow Q(s, a) + \alpha \delta E(s, a)$

$E(s, a) \leftarrow \gamma \lambda E(s, a)$

$S \leftarrow S'; A \leftarrow A'$

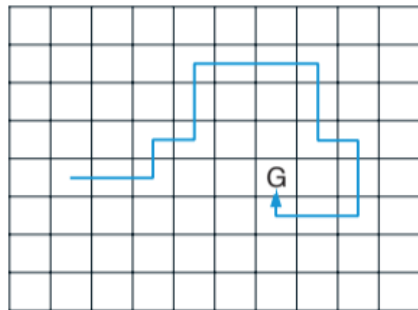
until S is terminal



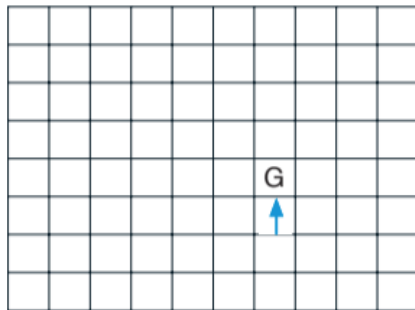
Sarsa- λ : Example

— — —

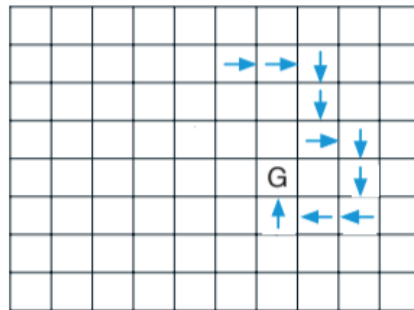
Path taken



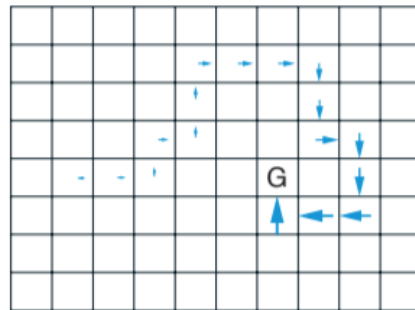
Action values increased
by one-step Sarsa



Action values increased
by 10-step Sarsa



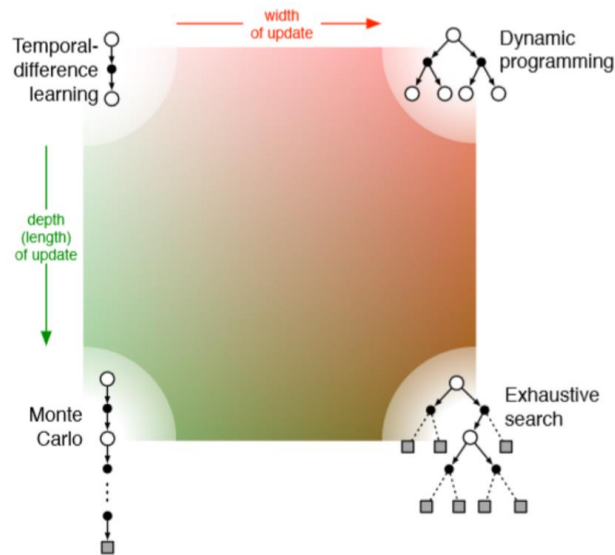
Action values increased
by Sarsa(λ) with $\lambda=0.9$



Going Wide vs Going Deep

So far we analyzed the depth of our updates, by considering the amount of sampling, which is:

- cheap computationally
- affected by sampling error
- easy to collect directly from the environment

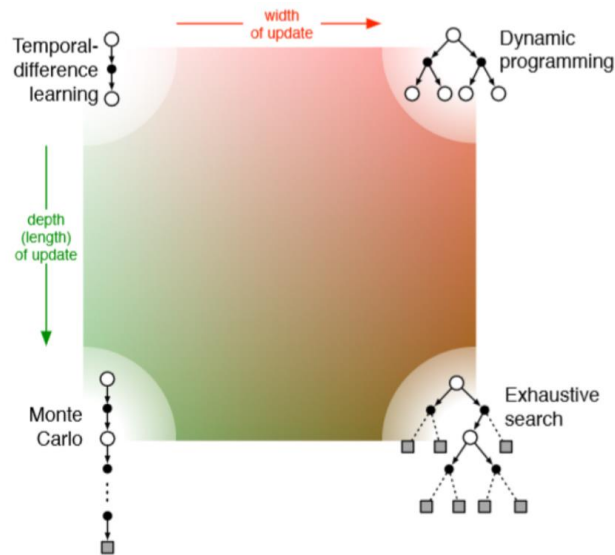


Going Wide vs Going Deep

So far we analyzed the depth of our updates, by considering the amount of sampling, which is:

- cheap computationally
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Can we also go wider with our updates?

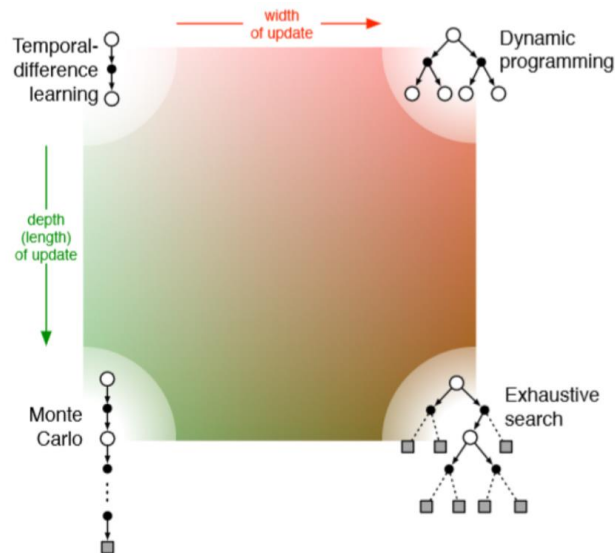


Going Wide vs Going Deep

So far we analyzed the depth of our updates, by considering the amount of sampling, which is:

- cheap computationally
- affected by sampling error
- easy to collect directly from the environment

Yes, we can use expected updates

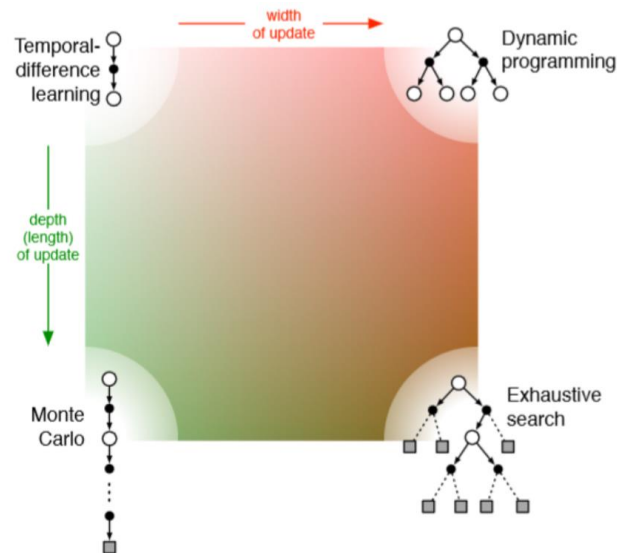


Going Wide vs Going Deep

— — —

Expected updates are

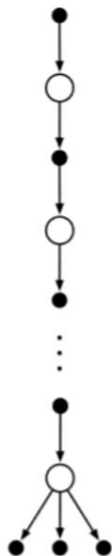
- computationally heavier
- exact (no sampling error)
- impossible to obtain without some distribution model



n-step Expected Sarsa

— — —

n-step
Expected Sarsa



Just compute the target using n-steps and an expectation over the policy at the end

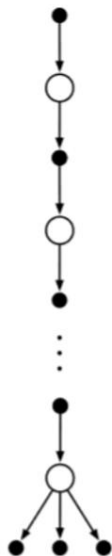
$$y = Q_{(n)}^{\pi} = r_t + \dots + \gamma^{n-1}r_{t+n-1} + \gamma^n \sum_a \pi(a|s_{t+n}) Q^{\pi}(s_{t+n}, a)$$



n-step Expected Sarsa

— — —

n-step
Expected Sarsa



Just compute the target using n-steps and an expectation over the policy at the end

$$y = Q_{(n)}^{\pi} = r_t + \dots + \gamma^{n-1}r_{t+n-1} + \gamma^n \sum_a \pi(a|s_{t+n}) Q^{\pi}(s_{t+n}, a)$$

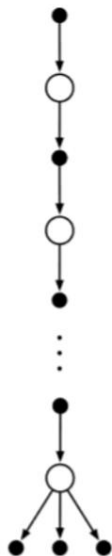
All sample transitions except the last one where we use a full distribution



n-step Expected Sarsa

— — —

n-step
Expected Sarsa



Just compute the target using n-steps and an expectation over the policy at the end

$$y = Q_{(n)}^{\pi} = r_t + \dots + \gamma^{n-1}r_{t+n-1} + \gamma^n \sum_a \pi(a|s_{t+n}) Q^{\pi}(s_{t+n}, a)$$

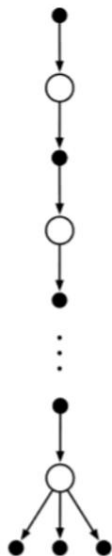
A tree-backup algorithm would have no sampling and all expectations



n-step Expected Sarsa

— — —

n-step
Expected Sarsa



Just compute the target using n-steps and an expectation over the policy at the end

$$y = Q_{(n)}^{\pi} = r_t + \dots + \gamma^{n-1}r_{t+n-1} + \gamma^n \sum_a \pi(a|s_{t+n}) Q^{\pi}(s_{t+n}, a)$$

Can we handle the degree of
sampling/expectation at each step?



$Q(\sigma)$

Use σ_t in $[0,1]$ to denote the degree of sampling at each timestep:

- 1 means full sampling
- 0 means full expectation
- can be a function of the state

At each timestep the TD error is

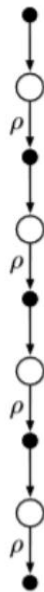
$$\delta_t = r_t + \gamma(\sigma_t Q^{\pi}(s_{t+1}, a \sim \pi(s_{t+1})) + (1-\sigma_t) \sum_a \pi(a|s_{t+1}) Q^{\pi}(s_{t+1}, a)) - Q^{\pi}(s_t, a_t)$$



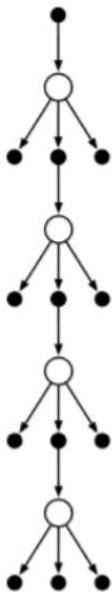
$Q(\sigma)$

— — —

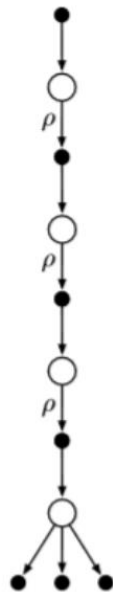
4-step
Sarsa



4-step
Tree backup



4-step
Expected Sarsa



4-step
 $Q(\sigma)$

