n-step Bootstrapping

Reinforcement Learning

Roberto Capobianco



Recap



Data Generation

- 2 steps:
- 1. Roll-in
- 2. Roll-out & compute supervision targets

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

$$Q^{\pi}(s_{+},a_{+}) = \mathbb{E}\left[\sum_{h=0}^{\infty} \gamma^{h} r_{h} | (s_{h},a_{h}) = (s_{+},a_{+}), a_{h+1} = \pi(s_{h}), s_{h+1} = \pi(s_{h}),$$

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

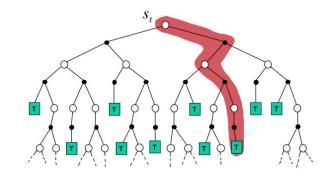
Monte-Carlo Update

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





Credits: David Silver

MC Updates

Tabular:

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

we do this at every termination

Function Approximator:

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

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

- 2 steps:
- 1. Roll-in
- 2. Roll-out & compute supervision targets

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

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

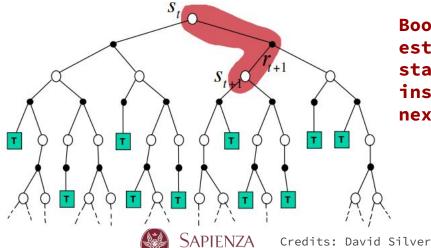
Monte-Carlo uses the actual return. In Temporal Difference we use an estimated return: our current V



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:

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

we do this at every timestep

Function Approximator:

$$\operatorname{argmin}_{0 \text{ in } 0} \sum_{i=1}^{N} (Q(s_i, a_i) - r_i + \gamma Q(s', .))^2$$

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

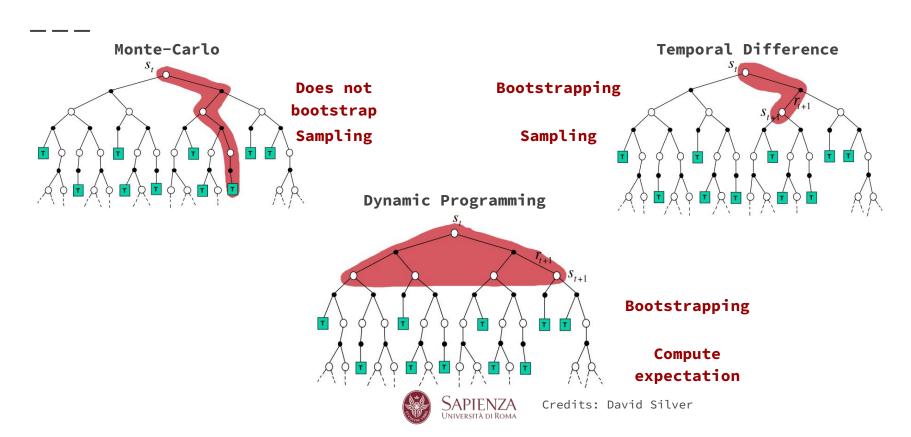
Weaknesses:

- Sensitive to initial value
- ullet Biased estimate of ${\bf Q}^\pi$

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
- Convergences but not always if function approx





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) $\pi(a|s) = \begin{cases} \epsilon/m + 1 - \epsilon & \text{if } a^* = \arg\max_{a \in \mathcal{A}} Q(s,a) \\ \epsilon/m & \text{otherwise} \end{cases}$

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 \mathbf{Q}^{\star}

$$\epsilon \leftarrow 1/k$$
 $\pi \leftarrow \epsilon$ -greedy(Q)



ϵ -Greedy and TD

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

How do we select •?

Sarsa: the target action is selected according to π (which can be eps-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 eps-greedy, remember?)

OFF-POLICY



TD, Sarsa & Q-Learning vs DP

1		
	Full Backup (DP)	Sample Backup (TD)
Bellman Expectation	$v_{\tau}(s) \leftarrow s$ $v_{\tau}(s') \leftarrow s'$	•
Equation for $v_{\pi}(s)$	Iterative Policy Evaluation	TD Learning
Bellman Expectation	$q_{\pi}(s, a) \leftrightarrow s, a$ r s' $q_{\pi}(s', a') \leftrightarrow a'$	S.A R S'
Equation for $q_{\pi}(s, a)$	Q-Policy Iteration	Sarsa
Bellman Optimality Equation for $q_*(s, a)$	$q_*(s,a) \leftrightarrow s,a$ $q_*(s',a') \leftrightarrow a'$ Q-Value Iteration	Q-Learning

Full Backup (DP)	Sample Backup (TD)
Iterative Policy Evaluation	TD Learning
$V(s) \leftarrow \mathbb{E}\left[R + \gamma V(S') \mid s\right]$	$V(S) \stackrel{\alpha}{\leftarrow} R + \gamma V(S')$
Q-Policy Iteration	Sarsa
$Q(s, a) \leftarrow \mathbb{E}\left[R + \gamma Q(S', A') \mid s, a\right]$	$Q(S,A) \stackrel{\alpha}{\leftarrow} R + \gamma Q(S',A')$
Q-Value Iteration	Q-Learning
$Q(s, a) \leftarrow \mathbb{E}\left[R + \gamma \max_{a' \in \mathcal{A}} Q(S', a') \mid s, a\right]$	$Q(S,A) \stackrel{\alpha}{\leftarrow} R + \gamma \max_{a' \in \mathcal{A}} Q(S',a')$

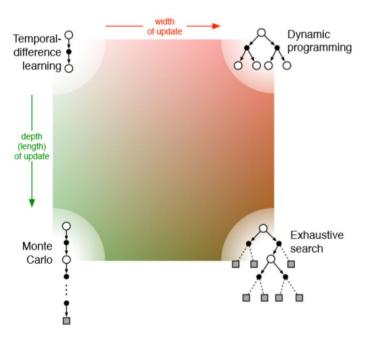


Credits: David Silver

End Recap

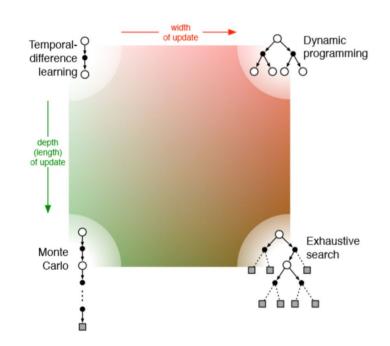


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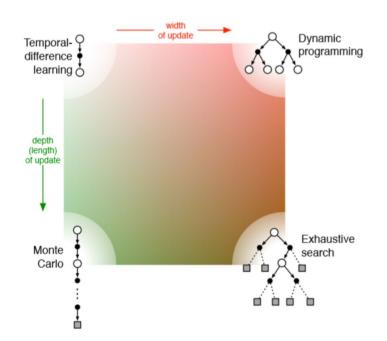
- TD uses a single timestep sometimes it's not enough to acquire any signal or significant state change
- MC uses all timesteps
 leads to high varianceis there any intermediate?





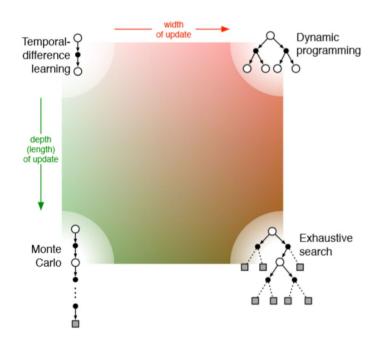
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- MC uses all timesteps

is there any intermediate?
 use n-step returns



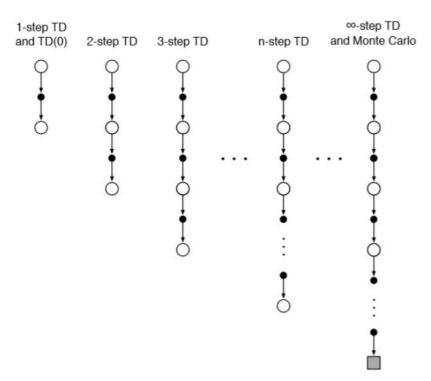


n-step returns are still make using of temporal difference, but use more than one reward





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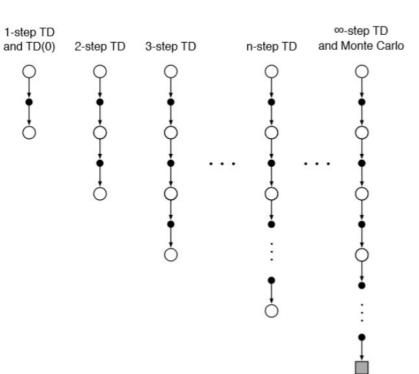


n-step returns are still make using of temporal difference, but use more than one reward

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

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





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

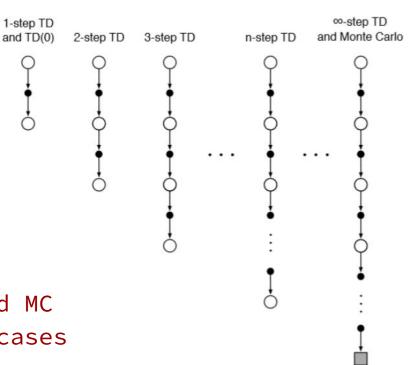
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1-step TD and MC just extreme cases



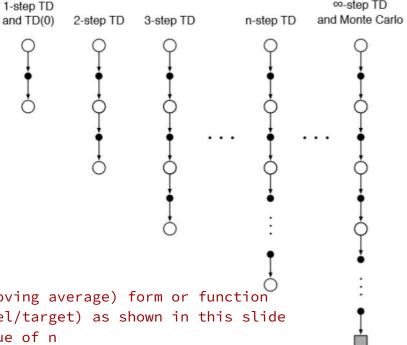


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. . .

y = G = ywe still do oul oul oul of 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



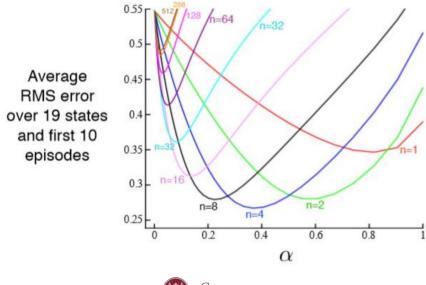
n-step TD in V

```
Input: a policy \pi
Algorithm parameters: step size \alpha \in (0,1], a positive integer n
Initialize V(s) arbitrarily, for all s \in 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, ...:
       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 (\tau is the time whose state's estimate is being updated)
      If \tau > 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})
V(S_{\tau}) \leftarrow V(S_{\tau}) + \alpha [G - V(S_{\tau})]
                                                                                                       (G_{\tau:\tau+n})
   Until \tau = T - 1
```



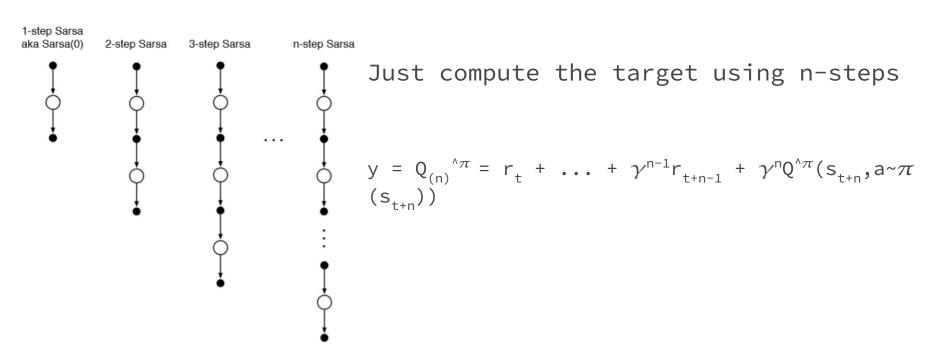
n-step TD in V

Extremes can potentially perform worse



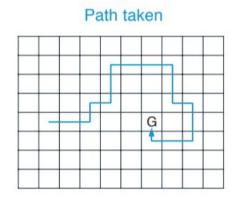


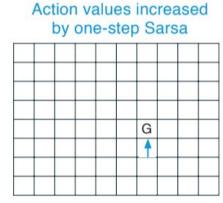
n-step Sarsa

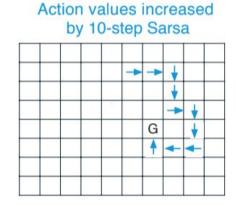




n-step Sarsa: Example









n-steps

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



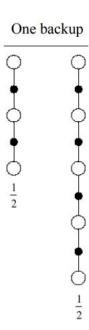
Averaging n-step Returns

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

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

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

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





λ -returns

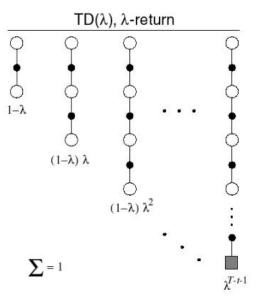
Can we combine information from all timesteps?



λ-returns

Can we combine information from all timesteps?

Yes, λ -returns $\mathsf{G}_{\scriptscriptstyle\mathsf{t}}^{\;\lambda}$ combine all n-step returns





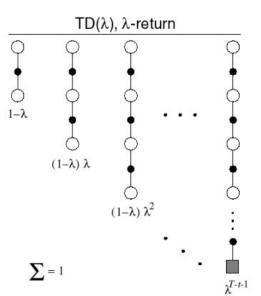
λ-returns

Can we combine information from all timesteps?

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

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

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





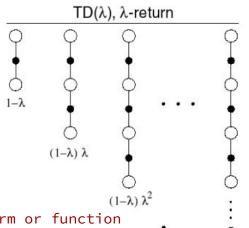
λ -returns & TD(λ)

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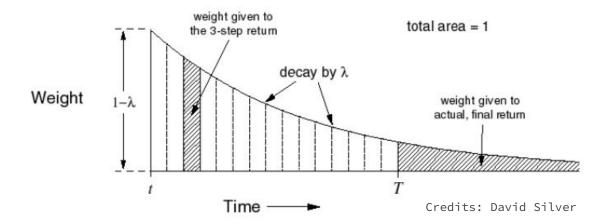


we still do our updates using the tabular (moving average) form or function approximation (l2-regression), with y (the label/target) as shown in this slide depending on the value of n $\sum = 1$



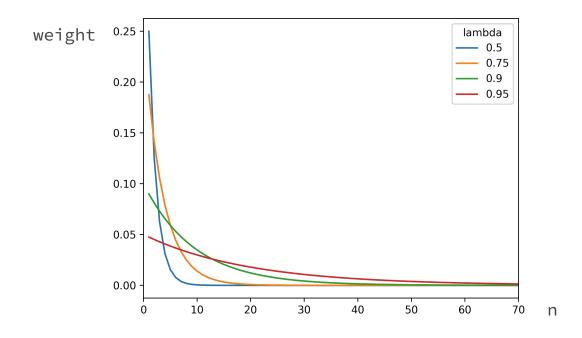
$TD(\lambda)$ Weights

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$TD(\lambda)$ Weights





Forward-View $TD(\lambda)$

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 $TD(\lambda)$

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 $TD(\lambda)$

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

We will use eligibility traces



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



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We're specifically looking at a credit assignment problem



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

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 combine both credit assignment heuristics:

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

$$e_0(s) = 0$$

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



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I is the indicator function, which equals 1 if the condition inside is true, 0 otherwise



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

• for ALL the states s in S update the value function estimate

$$V^{\wedge \pi}(s) \leftarrow V^{\wedge \pi}(s) + \alpha \delta_{+} e_{+}(s)$$



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

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

$$V^{\wedge \pi}(s) \leftarrow V^{\wedge \pi}(s) + \alpha \delta_{+} e_{+}(s)$$

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 equals or close to zero, which means that our estimate for those states won't change much



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

$$\mathbf{e_{_{0}}(s)} = \mathbf{0}$$

$$\mathbf{e_{_{t}}(s)} = \gamma\lambda\mathbf{e_{_{t-1}}(s)} + \mathbf{I}(\mathbf{s_{_{t}}} = \mathbf{s})$$
 TD error (in V):
$$\delta_{_{t}} = \mathbf{r_{_{t}}} + \gamma\mathbf{V^{^{^{^{^{}}}}}(s_{_{t+1}})} - \mathbf{V^{^{^{^{^{}}}}}(s_{_{t}})}$$

• for ALL the states s in S update the value function estimate

$$V^{\wedge \pi}(s) \leftarrow V^{\wedge \pi}(s) + \alpha \delta_{+} e_{+}(s)$$

We propagate current error information $(\delta_{\rm t})$ into the states we visited in the past. This allows us to combine the n-step returns in an online fashion.



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

$$e_{0}(s) = 0$$

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TD error (in V):
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• for ALL the states s in S update the value function estimate

$$V^{\wedge \pi}(s) \leftarrow V^{\wedge \pi}(s) + \alpha \delta_{+} e_{+}(s)$$

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



If
$$\lambda = 0$$

$$e_0(s) = 0$$

 $e_t(s) = I(s_t=s)$

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

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



If λ = 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)



Consider a state s visited only once at time k:

- $e_{+}(s) = 0 \text{ if } t < k$
- $e_t(s) = \gamma^{t-k} \text{ if } t \ge k$

The total updates that it cumulates are:

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



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



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

$$r_{k} + \gamma V^{\wedge \pi}(s_{k+1}) - V^{\wedge \pi}(s_{k}) +$$

$$\gamma r_{k+1} + \gamma^{2} V^{\wedge \pi}(s_{k+2}) - \gamma V^{\wedge \pi}(s_{k+1}) +$$

$$\gamma^{2} r_{k+2} + \gamma^{3} V^{\wedge \pi}(s_{k+3}) - \gamma^{2} V^{\wedge \pi}(s_{k+2}) +$$

$$\dots$$



 $\gamma^{\mathsf{T-1-k}}\mathsf{r}_{\mathsf{T-1}}$

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

$$r_{k} + \gamma V^{n} (s_{k+1}) - V^{n} (s_{k}) +$$

$$\gamma r_{k+1} + \gamma^{2} V^{n} (s_{k+2}) - \gamma V^{n} (s_{k+1}) +$$

$$\gamma^{2} r_{k+2} + \gamma^{3} V^{n} (s_{k+3}) - \gamma^{2} V^{n} (s_{k+2}) +$$

$$\cdots$$

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



$$\begin{split} \delta_{k} + \gamma \delta_{k+1} + \gamma^{2} \delta_{k+2} + \dots + \gamma^{T-1-k} \delta_{T-1} &= \\ r_{k} + \gamma V^{\wedge \pi}(s_{k+1}) - V^{\wedge \pi}(s_{k}) &+ \\ \gamma r_{k+1} + \gamma^{2} V^{\wedge \pi}(s_{k+2}) - \gamma V^{\wedge \pi}(s_{k+1}) &+ \\ \gamma^{2} r_{k+2} + \gamma^{3} V^{\wedge \pi}(s_{k+3}) - \gamma^{2} V^{\wedge \pi}(s_{k+2}) &+ \\ \dots & \\ \gamma^{T-1-k} r_{T-1} &= \\ r_{k} + \gamma r_{k+1} + \gamma^{2} r_{k+2} + \gamma^{T-1-k} r_{T-1} - V^{\wedge \pi}(s_{k}) &= G_{t} - V^{\wedge \pi}(s_{k}) \end{split}$$



Consider a state s visited only once at time k:

- $e_{+}(s) = 0 \text{ if } t < k$
- $e_{t}(s) = (\gamma \lambda)^{t-k} \text{ if } t \ge k$

The total updates that it cumulates are:

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

You can expand the definition of $G_{k}^{\ \lambda}$ and prove it



Forward & Backward View Equivalence

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

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



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

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



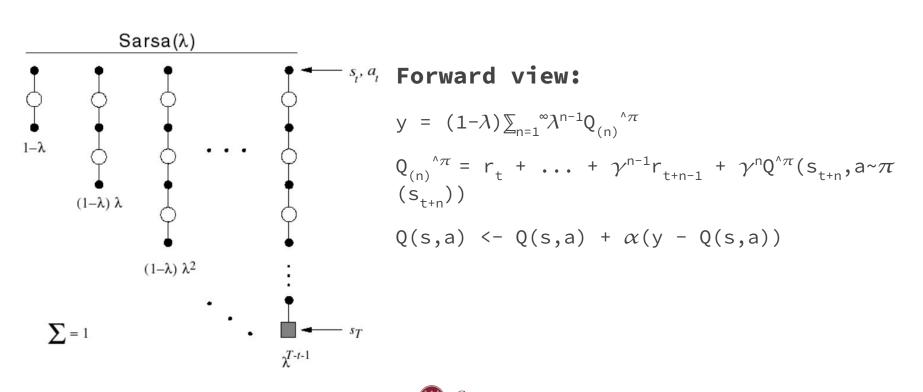
Forward & Backward View Equivalence

Offline updates	$\lambda = 0$	$\lambda \in (0,1)$	$\lambda = 1$
Backward view	TD(0)	$TD(\lambda)$	TD(1)
	II		II
Forward view	TD(0)	Forward $TD(\lambda)$	MC
Online updates	$\lambda = 0$	$\lambda \in (0,1)$	$\lambda = 1$
Backward view	TD(0)	$TD(\lambda)$	TD(1)
	11	*	#
Forward view	TD(0)	Forward TD(λ)	MC

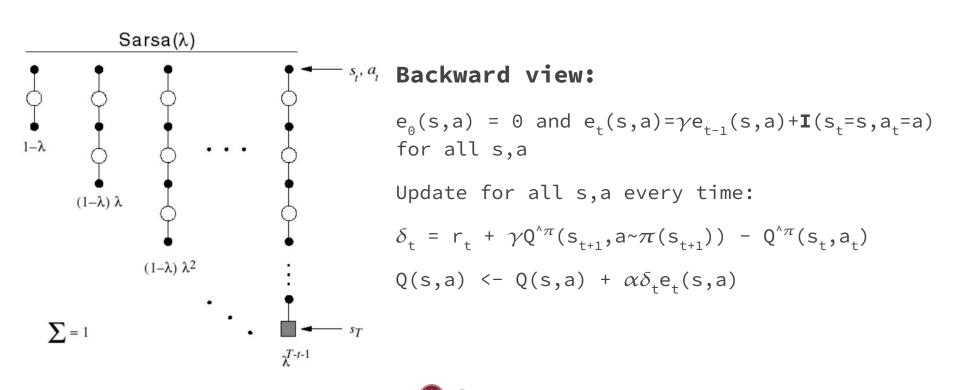
Credits: David Silver



Sarsa-*λ*: **Forward View**



Sarsa-\(\lambda\): Backward View

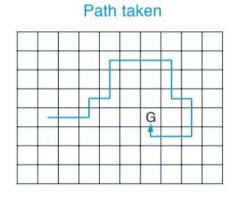


Sarsa-λ: Backward View

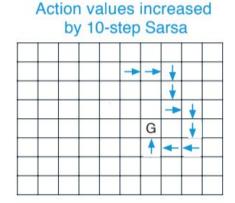
```
Initialize Q(s, a) arbitrarily, for all s \in S, a \in A(s)
Repeat (for each episode):
   E(s, a) = 0, for all s \in S, a \in A(s)
   Initialize S, A
   Repeat (for each step of episode):
       Take action A, observe R, S'
       Choose A' from S' using policy derived from Q (e.g., \varepsilon-greedy)
       \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
```

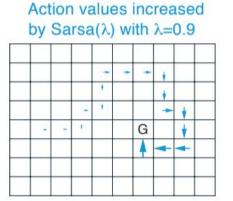


Sarsa-*\lambda*: Example





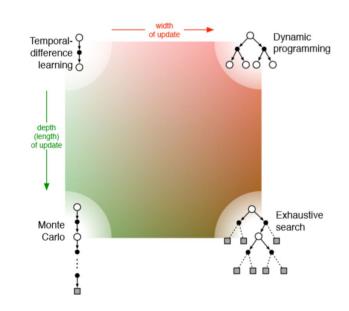






So far we analyzed the depth of our updates, by considering the amount of sampling, which is:

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

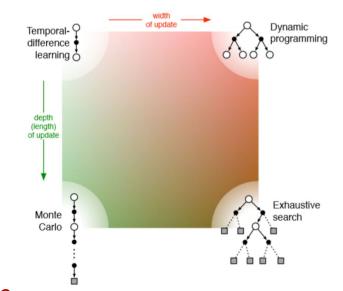




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Can we also go wider with our updates?

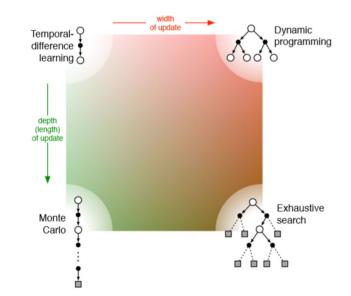




So far we analyzed the depth of our updates, by considering the amount of sampling, which is:

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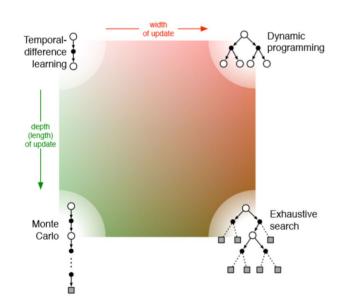
Yes, we can use expected updates





Expected updates are

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







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

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



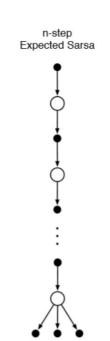


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All sample transitions except the last one where we use a full distribution





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

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

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





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

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

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

$$\delta_{t} = r_{t} + \gamma(\boldsymbol{\sigma}_{t}Q^{^{^{\prime}\pi}}(s_{t+1}, a \sim \pi(s_{t+1})) + (1 - \boldsymbol{\sigma}_{t}) \sum_{a} \pi(a|s_{t+1}) Q^{^{^{\prime}\pi}}(s_{t+1}, a)) - Q^{^{^{\prime}\pi}}(s_{t}, a_{t})$$



$Q(\sigma)$

