Artificial Intelligence

Reinforcement learning

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Multi-Armed Bandit



A row of N old-style slot machines

Basic definitions

N arms or bandits

Each arm a yields a random reward r with probability distribution $P(r \mid a)$

For simplicity, only Bernoullian rewards (i.e. either 0 or 1) will be considered here

Each time t in a sequence, the player (i.e. the agent) selects the arm $\pi(t)$ In other words, π is the *policy* adopted by the agent

Problem

Find a policy π that maximizes the <u>total reward</u> over time The policy will include random choices i.e. it will be *stochastic*

Multi-Armed Bandit: strategies

Informed (i.e. optimal) strategy

At all times, select the bandit with higher probability of reward:

$$\pi^*(t) = \operatorname{argmax}_a P_i(r = 1 \mid a)$$

Clearly, this strategy is optimal but requires knowing all distributions $P(r \mid a)$ With enough data (e.g. from other players), these distributions can be learnt

Random strategy

At all times, select a bandit a at random, with uniform probability

How does the Random strategy compare with the optimal, informed strategy?

Multi-Armed Bandit: basic definitions

Actions, Rewards

$$a \in \mathcal{A}$$
 in this case $a \in \{1, \dots, N\}$ $r \in \mathcal{R}$ in this case $r \in \{0, 1\}$

Probability distribution (unknown)

 $P(R \,|\, A)$ the probability of reward R for action A (i.e. two random variables)

Policy

 $\pi:\mathbb{N}^+ o\mathcal{A}$ at each time, defines which action will be taken, it may be <u>stochastic</u>

Q-value

The <u>expected</u> reward of action a

$$Q(a) := \mathbb{E}[R \, | \, A = a] = \sum_{r} r \, P(r \, | \, A = a)$$

Optimal Value

Maximum <u>expected</u> reward

$$V^* := Q(a^*) = \max_{a \in \mathcal{A}} Q(a)$$

Multi-Armed Bandit: evaluating strategies

Total Expected Regret

How far from optimality a policy is, considering the total reward over T trials For just <u>one</u> sequence of T trials, the *Total Regret with <u>expected</u> rewards* is

$$L(T) := TV^* - \sum_{t=1}^T Q(\pi(t))$$
 action taken at step t

In a more general definition, the *Total Expected Regret* is

$$\overline{L}(T):=TV^*-\sum_{a=1}^N\mathbb{E}[T_a(T)]Q(a)=\sum_{a=1}^N\mathbb{E}[T_a(T)]\Delta_a$$
 number of times action a is taken in T trials (i.e. a random variable)

where

$$\Delta_a := V^* - Q(a)$$

Multi-Armed Bandit: evaluating strategies

Total Expected Regret

$$\overline{L}(T) := TV^* - \sum_{a=1}^N \mathbb{E}[T_a(T)]Q(a) = \sum_{a=1}^N \mathbb{E}[T_a(T)]\Delta_a$$
 number of times action a is taken in T trials (i.e. a random variable)

where

$$\Delta_a := V^* - Q(a)$$

With the optimal policy π^* the total expected regret is 0.

Whereas, with the random policy the total expected regret grows linearly over time:

$$\overline{L}(T) = rac{T}{N} \sum_{a=1}^N \Delta_a$$
 ... since, with a random strategy $\mathbb{E}[T_a(T)] = rac{T}{N}$

Multi-Armed Bandit: Online learning

Adaptive policy: exploration vs. exploitation

exploration: make trials over the set of N arms to improve on estimates $\hat{Q}(a)$

exploitation: make use of the current best estimates $\hat{Q}(a)$

Greedy policy

Initialize all the estimates $\hat{Q}(a)$ at random Repeat:

- 1) select the bandit with the current best estimated reward $a = \operatorname{argmax}_a \hat{Q}(a)$
- 2) update the current estimate about a as

$$\hat{Q}(a) := \frac{\sum\limits_{t=1}^{T_a} r_{a,t}}{T_a} \quad \text{reward of arm a at trial t}$$
 Total number of times the arm \$a\$ has been played

Multi-Armed Bandit: Online learning

Adaptive policy: exploration vs. exploitation

exploration: make trials over the set of N arms to improve on estimates $\hat{Q}(a)$ **exploitation**: make use of the current best estimates $\hat{Q}(a)$

• ε -greedy policy $(0 < \varepsilon < 1)$

Initialize all the estimates $\,\hat{Q}(a)\,$ at random Repeat:

- 1) with probability (1ε) select the bandit $a = \operatorname{argmax}_a \hat{Q}(a)$ else (i.e. with probability ε) select one bandit at random
- 2) update the current estimate about a

$$\hat{Q}(a) := \frac{\sum\limits_{t=1}^{T_a} r_{a,t}}{T_a} \quad \text{reward of arm } a \text{ at trial } t$$
 total number of times the arm a has been played

Multi-Armed Bandit: Online learning

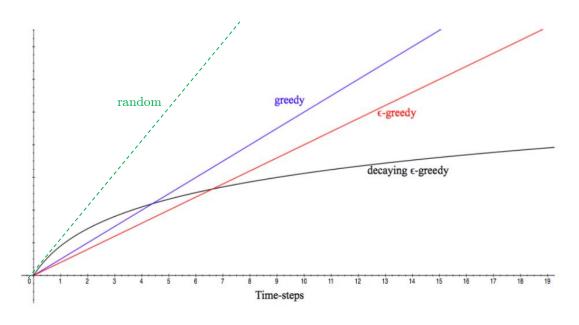
Adaptive policy: exploration vs. exploitation

exploration: make trials over the set of N arms to improve on estimates $\hat{Q}(a)$

exploitation: make use of the current best estimates $\hat{Q}(a)$

■ Experimental comparison of different strategies (*Total Expected Regret*)

After a certain period of time, the *greedy* strategy stops exploring and exploits its estimates whereas, the ε -greedy strategy keeps exploring and improving



Decaying
$$arepsilon$$
-greedy strategy: $arepsilon = rac{arepsilon_{initial}}{t}$

Multi-Armed Bandit: evaluating strategies

The two greedy strategies

They are *biased*: they depend on the initial random estimates

Optimistic variant: initially, set all $\hat{Q}(a) := 1$

The average total regret grows <u>linearly</u>, in the long run In fact:

- on the average, the *greedy* strategy will get stuck in a suboptimal choice
- the ε -greedy strategy will continue to choose an arm at random (with probability ε)

Can we do any better?

The decaying ε -greedy strategy does that... Is there a minimum, i.e. a lower bound?

Multi-Armed Bandit: Optimal online learning

■ Lower bound theorem [Lai & Robbins 1985]

Consider a generic, adaptive (i.e. learning) strategy for the multi-armed bandit problem with Bernoulli reward (i.e. $r \in \{0,1\}$)

$$\lim_{T \to \infty} \overline{L}(T) \ge \ln T \sum_{a \mid \Delta_a > 0} \frac{\Delta_a}{\text{kl}(Q(a), V^*)} \qquad \Delta_a := V^* - Q(a)$$

where

$$\mathrm{kl}(Q(a),V^*) := Q(a)\ln\frac{Q(a)}{V^*} + (1-Q(a))\ln\frac{(1-Q(a))}{(1-V^*)}$$
 the Kullback-Leibler divergence

In other words, we can achieve logarithmic growth for the total expected regret, but not better: on average, any adaptive strategy will choose suboptimal bandits a minimum number of times

$$\lim_{T \to \infty} \mathbb{E}[T_a(T)] \ge \frac{\ln T}{\mathrm{kl}(Q(a), V^*)}$$

Multi-Armed Bandit: UCB strategy

■ Upper confidence bound (UCB) strategy [Auer, Cesa-Bianchi and Fisher 2002]

Initialize all the estimates of the expected reward $\hat{Q}(a) := 0$ Play each arm once (to avoid zeroes in the formula below)

Repeat:

1) select the bandit $a = \operatorname{argmax}_k \left(\hat{Q}(a) + \sqrt{\frac{2 \ln T}{T_a}} \right)$

2) update the current estimate $\hat{Q}(a)$ as the *average* reward

Theorem

With the UCB strategy, $\lim_{T \to \infty} \mathbb{E}[T_a(T)] \leq \frac{8 \ln T}{\Delta_a^2} + c$ where it can be shown that $\frac{8}{\Delta_a^2} \geq \frac{1}{\mathrm{kl}(Q(a), V^*)}$ i.e. a (small) constant

(i.e. there is a reasonably small gap between the two bounds – near optimality)

total number of trials

the arm k has been played

Numerical example of the

confidence bound term

number of times

Multi-Armed Bandit: Thompson Sampling

■ Thompson Sampling strategy (also 'Bayesian Bandit') [Thompson, 1933]

Initialize all the expected reward $\hat{Q}(a) :\sim \operatorname{Beta}(x;1,1)$ i.e. assume this as a random variable

Repeat:

- 1) sample each of the N distributions to obtain an estimate $\,\hat{Q}(a)$
- 2) select the bandit $a = \operatorname{argmax}_a \hat{Q}(a)$
- 3) update the *posterior* distribution

$$\hat{Q}(a):\sim \mathrm{Beta}(x;R_a+1,\ T_a-R_a+1)$$
 total number of times the arm has been played total (Bernoulli) reward from this arm (i.e. number of wins)

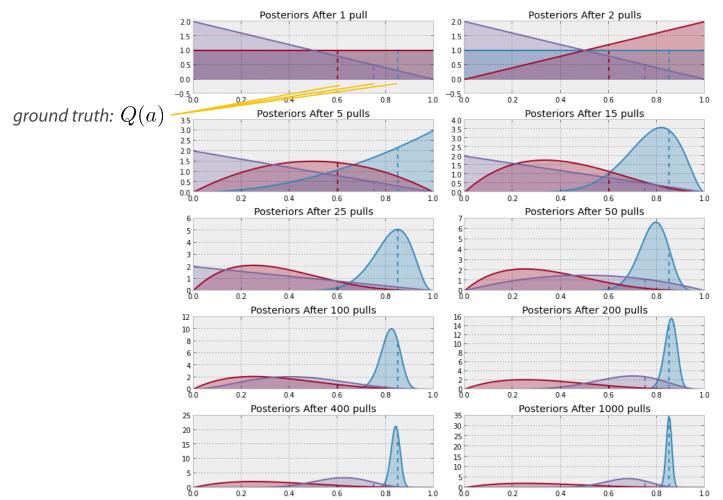
with this distribution

Theorem [Kaufmann et al., 2012]

The Thompson Sampling strategy has essentially the same theoretical bounds of the UCB strategy

Multi-Armed Bandit: Thompson Sampling

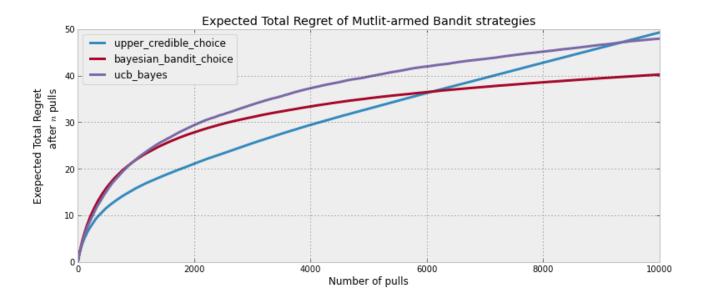
Thompson Sampling strategy (also 'Bayesian Bandit') [Thompson, 1933] Example run with 3 arms: trace of the posterior probabilities for each $\hat{Q}(a)$



Multi-Armed Bandit: Thompson Sampling

■ Thompson Sampling strategy (also 'Bayesian Bandit') [Thompson, 1933]

In practical experiments, this strategy shows better performances in the long run
[Chapelle & Li, 2011]



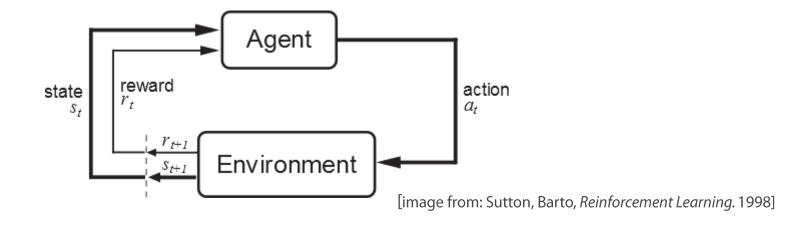
Actually, Thompson Sampling is a preferred strategy at Google Inc. (see https://support.google.com/analytics/answer/2846882?hl=en)

[image from: http://camdp.com/blogs/multi-armed-bandits]

Agent/Environment Interactions

With multi-armed bandits, the <u>context</u> never changes in the sense that the optimal choice does **not** depend on the current <u>state</u>

What if the actions of the agent change the state of its interaction with the environment?

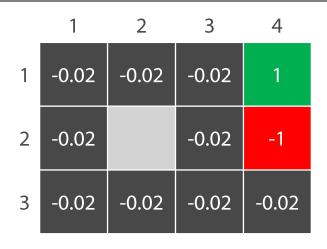


Examples:

- a_t could be a *move in a game*, whereby the agent changes the state of the game
- a_t could be a movement, whereby the agent changes its position in the environment

The agent could be wanting to learn an optimal strategy towards a given goal...

An example: gridworld



The <u>state</u> of the agent is the position on the grid: e.g. (1,1), (3,4), (2,3)

The effect of each move is somewhat stochastic, however: for example, a move ↑ has a slight probability of producing a different (and perhaps unwanted) effect

Entering each state yields the <u>reward</u> shown in each box above

There are two <u>absorbing states</u>: entering either the green or the red box means exiting the *gridworld* and completing the game

What is the best (i.e. maximally rewarding) movement policy?

the agent will end up here

but with probability 0.2

it might end up here

0.8

Markov Decision Process (MDP)



Formalization and abstraction of the gridworld example

Markov Decision Process: $\langle S, A, r, P, \gamma \rangle$

A set of *states*: $S = \{s_1, s_2, \dots\}$

A set of <u>actions</u>: $A = \{a_1, a_2, \dots\}$

A <u>reward function</u>: $r: \mathcal{S} \to \mathbb{R}$

A <u>transition probability distribution</u>: $P(S_{t+1} \mid S_t, A_t)$ (also called a <u>model</u>)

Markov property: the transition probability depends only on the previous state and action

$$P(S_{t+1} \mid S_t, A_t) = P(S_{t+1} \mid S_t, A_t, S_{t-1}, A_{t-1}, S_{t-2}, A_{t-2}, \dots)$$

A <u>discount factor</u>: $0 \le \gamma < 1$

Markov Decision Process (MDP): policies and values

The agent is supposed to adopt a *deterministic* <u>policy</u>: $\pi: \mathcal{S} \to \mathcal{A}$ In other words, the agent always chooses its *action* depending on the *state* alone

Given a policy π , the **state value function** is defined, for each state s as:

$$V^{\pi}(s) := \mathbb{E}[r(S_t) + \gamma r(S_{t+1}) + \gamma^2 r(S_{t+2}) + \dots \mid \pi, S_t = s]$$

Note the role of the discount factor: a value $\,\gamma < 1\,$ means that that future rewards could be weighted less (by the agent) than immediate ones

Note also that all states $\,S_t\,$ must be described by $\it random\ \it variables$: i.e. the policy is deterministic but the state transition is not

Note also that when the reward is *bounded*, i.e. $r(S) \leq r_{\text{max}}$

$$\sum_{t=0}^{\infty} \gamma^t \ r(S_t) \le r_{\max} \sum_{t=0}^{\infty} \gamma^t = r_{\max} \, rac{1}{1-\gamma}$$
 for $\gamma < 1$ this is the geometric series

Markov Decision Process (MDP): policies and values

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In the *gridworld* example:

- The set of states is finite
- The set of actions is finite
- For every policy, each entire story is <u>finite</u>
 Sooner or later the agent will fall into one of the absorbing states

Bellman equations

By working on the definition of value function:

$$V^{\pi}(s) := \mathbb{E}[r(S_t) + \gamma r(S_{t+1}) + \gamma^2 r(S_{t+2}) + \dots \mid \pi, S_t = s]$$

$$= \mathbb{E}[r(S_t) + \gamma (r(S_{t+1}) + \gamma r(S_{t+2}) + \dots) \mid \pi, S_t = s]$$

$$= r(s) + \gamma \mathbb{E}[r(S_{t+1}) + \gamma r(S_{t+2}) + \dots \mid \pi, S_t = s]$$

$$= r(s) + \gamma \sum_{s'} P(s' \mid s, \pi(s)) \cdot \mathbb{E}[r(S_{t+1}) + \gamma r(S_{t+2}) + \dots \mid \pi, S_{t+1} = s']$$

$$= r(s) + \gamma \sum_{S_{t+1}} P(S_{t+1} \mid s, \pi(s)) \cdot V^{\pi}(S_{t+1})$$

This means that in a Markov Decision Process:

$$V^{\pi}(s) = r(s) + \gamma \sum_{S_{t+1}} P(S_{t+1} \mid s, \pi(s)) \cdot V^{\pi}(S_{t+1})$$

This is true for any state, so there is one such equation for each of those If the set of states is <u>finite</u>, there are exactly |S| (linear) Bellman equations for |S| variables: in general, for any <u>deterministic</u> policy, V^{π} <u>can</u> be computed analytically

Optimal policy - Optimal value function

Basic definitions

$$\pi^*(s) := \underset{\pi}{\operatorname{argmax}} V^{\pi}(s), \ \forall s \in S$$
$$V^*(s) := \underset{\pi}{\operatorname{max}} V^{\pi}(s), \ \forall s \in S$$

Property: for every MDP, there exists such an optimal deterministic policy (possibly non-unique)

With Bellman Equations:

$$\max_{\pi} V^{\pi}(s) = r(s) + \gamma \max_{\pi} \left(\sum_{S_{t+1}} P(S_{t+1} \mid s, \pi(s)) \cdot V^{\pi}(S_{t+1}) \right)$$
$$V^{*}(s) = r(s) + \gamma \max_{\pi} \left(\sum_{S_{t+1}} P(S_{t+1} \mid s, \pi(s)) \cdot V^{*}(S_{t+1}) \right)$$
$$= r(s) + \gamma \max_{a} \left(\sum_{S_{t+1}} P(S_{t+1} \mid s, a) \cdot V^{*}(S_{t+1}) \right)$$

Therefore:

$$\pi^*(s) = \operatorname{argmax}_a \left(\sum_{S_{t+1}} P(S_{t+1} \mid s, a) V^*(S_{t+1}) \right)$$

Computing V^* directly from these equations is unfeasible, however There are in fact $|A|^{|S|}$ possible strategies

However, once V^* has been determined, π^* can be determined as well

Optimal value function: value iteration

Value iteration algorithm

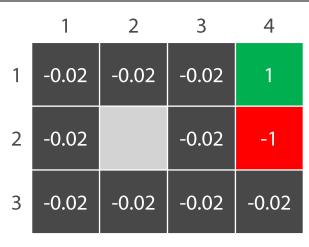
Initialize: $V(s) := r(s), \ \forall s \in S$ Repeat:

Note that there is no policy: all actions must be explored

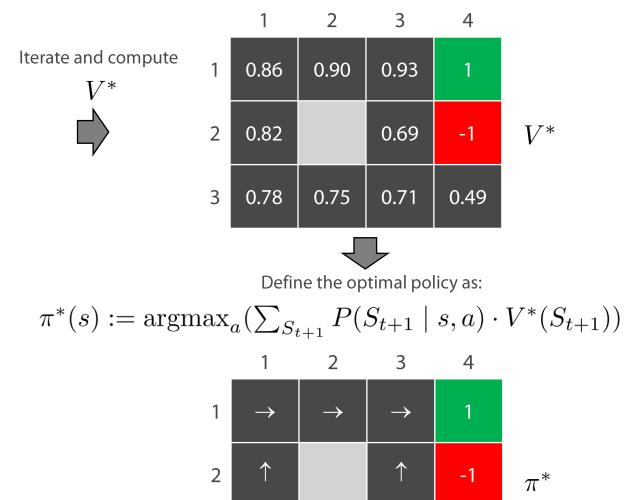
1) For every state, update:
$$V(s) := r(s) + \gamma \max_{a} \sum_{s'} P(s' \mid s, a) V(s')$$

Theorem: for every fair way (i.e. giving an equal chance) of visiting the states in S, this algorithm converges to V^{st}

Value iteration and optimal policy



Initialize states (e.g. using rewards as initial values)



 \leftarrow

3

Optimal policy: policy iteration

Policy iteration algorithm

Initialize $\pi(s), \forall s \in S$ at random *Repeat*:

This step is computationally expensive: either solve the equations or use value iteration (with fixed policy π)

- 1) For each state, compute: $V(s) := V^{\pi}(s)$
- 2) For each state, define: $\pi(s) := \operatorname{argmax}_a \sum_{s'} P(s' \mid s, a) V(s')$

Theorem: for every fair way (i.e. giving an equal chance) of visiting the states in S , this algorithm converges to π^*

As with the value iteration algorithm, this algorithm uses partial estimates to compute new estimates.

It is also greedy, in the sense that it exploits its current estimate $V^\pi(s)$

Policy iteration converges with very few number of iterations, but every iteration takes much longer time than that of value iteration

The tradeoff with value iteration is the <u>action space</u>: when action space is large and state space is small, policy iteration could be better

Offline vs. Online learning

Value iteration and policy iteration are offline algorithms

The \underline{model} , i.e. the Markov Decision Process is known What needs to be learn is the optimal policy π^*

In the algorithms, visiting states just means considering: there is no agent actually playing the game.

Different conditions: learning by doing ...

Suppose the <u>model</u> (i.e. the MDP) is NOT known, or perhaps known only in part Then the agent must learn by doing...

Action value function

An analogous of the value function $\,V^{\pi}$

Given a policy π , the **action value function** is defined, for each pair (s,a) as:

$$Q^{\pi}(s, a) := \sum_{S_{t+1}} P(S_{t+1} \mid s, a) \cdot V^{\pi}(S_{t+1})$$

$$= \sum_{S_{t+1}} P(S_{t+1} \mid s, a) \cdot \mathbb{E}[r(S_{t+1}) + \gamma r(S_{t+2}) + \dots \mid \pi, S_{t+1}]$$

$$= \sum_{S_{t+1}} P(S_{t+1} \mid s, a) \cdot [r(S_{t+1}) + \mathbb{E}[\gamma r(S_{t+2}) + \dots \mid \pi, S_{t+1}]]$$

$$= \sum_{S_{t+1}} P(S_{t+1} \mid s, a) \cdot [r(S_{t+1}) + \gamma Q^{\pi}(S_{t+1}, \pi(S_{t+1}))]$$

In other words, $Q^{\pi}(s,a)$ is the expected value of the reward in S_{t+1} by taking action a in state s and then following policy π from that point on

Following a similar line of reasoning, the *optimal* action value function is

$$Q^*(s, a) = \sum_{S_{t+1}} P(S_{t+1} \mid s, a) \cdot [r(S_{t+1}) + \gamma \max_{a'} Q^*(S_{t+1}, a')]$$

Q-Learning

• Q-learning algorithm (ε -greedy version)

Initialize $\hat{Q}(s,a)$ at random, put the agent is in a random state s Repeat:

- 1) Select the action $\argmax_a \hat{Q}(s,a)$ with probability $(1-\varepsilon)$ otherwise, select a at random
- 2) The agent is now in state s^\prime and has received the reward r
- 3) Update $\hat{Q}(s,a)$ by

$$\Delta \hat{Q}(s,a) = \alpha[r + \gamma \max_{a'} \hat{Q}(s',a') - \hat{Q}(s,a)]$$
 Exponential Moving Average (see later ...)

Note that step 1) is closely similar to a **multi-armed bandit**: in each state, the agent has to choose one among all actions in \mathcal{A} and this will produce a random reward...

Q-Learning

Q-learning algorithm

Theorem (Watkins, 1989): in the limit of that each action is played infinitely often and each state is visited infinitely often and $\alpha \to 0$ as experience progresses, then

$$\hat{Q}(s,a) \to Q^*(s,a)$$

with probability 1

The Q-learning algorithm bypasses the MDP entirely, in the sense that the optimal strategy is learnt without learning the model $P(S_{t+1} \mid S_t, A_t)$

An aside: moving averages

Following non-stationary phenomena

Average

Definition:
$$\overline{v}_T := \frac{1}{T} \sum_{k=1}^{T} v_k$$

Running implementation:

$$\overline{v}_T = \frac{1}{T}(v_T + \sum_{k=1}^{T-1} v_k) = \frac{1}{T}(v_T + (T-1)\overline{v}_{T-1})$$

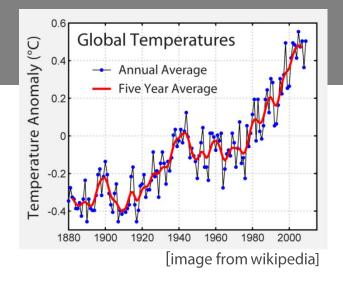
$$= \overline{v}_{T-1} + \frac{1}{T}(v_T - \overline{v}_{T-1}) = \frac{1}{T}v_T + (1 - \frac{1}{T})\overline{v}_{T-1}$$



$$\overline{v}_{T,n} := \frac{1}{n} \sum_{k=T-n}^{T} v_k$$

Exponential Moving Average (EMA)

$$\overline{v}_{T,lpha}:=lpha\,v_T+(1-lpha)\,\overline{v}_{T-1,lpha},\ \ lpha\in[0,1]$$
 "the weight of newer observations remains constant"

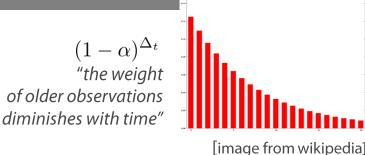


"the weight of newer observations diminishes with time"

An aside: moving averages

Exponential Moving Average (EMA)

$$\overline{v}_{T,\alpha} := \alpha v_T + (1-\alpha) \overline{v}_{T-1,\alpha}, \ \alpha \in [0,1]$$



Expanding:

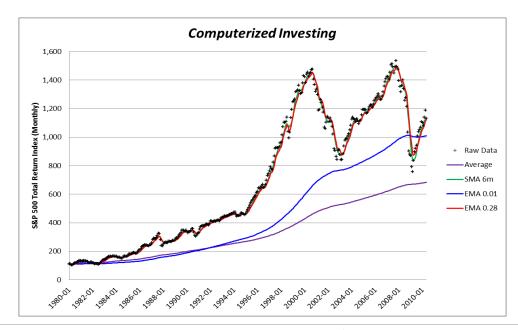
$$\overline{v}_{t,\alpha} = \alpha \, v_t + (1 - \alpha) \, \overline{v}_{t-1,\alpha}
= \alpha \, v_t + (1 - \alpha)(\alpha \, v_{t-1} + (1 - \alpha) \overline{v}_{t-2,\alpha})
= \alpha \, v_t + (1 - \alpha)(\alpha \, v_{t-1} + (1 - \alpha)(\alpha \, v_{t-2} + (1 - \alpha) \overline{v}_{t-3,\alpha}))
= \alpha \, (v_t + (1 - \alpha) \, v_{t-1} + (1 - \alpha)^2 \, v_{t-2}) + (1 - \alpha)^3 \, \overline{v}_{t-3,\alpha}$$

The weight of past contributions decays as

$$(1-\alpha)^{\Delta_t}$$

A SMA with n previous values is approximately equal to an EMA with

$$\alpha = \frac{2}{n+1}$$



Q-Learning revisited

• Q-learning algorithm (ε -greedy version)

Initialize $\hat{Q}(s,a)$ at random, put the agent is in a random state s Repeat:

- 1) Select the action $a=\mathrm{argmax}_a\hat{Q}(s,a)$ with probability $(1-\varepsilon)$ otherwise, select a at random
- 2) The agent is now in state s^\prime and has received the reward r
- 3) Update $\hat{Q}(s,a)$ by

$$\Delta \hat{Q}(s, a) = \alpha [r + \gamma \max_{a'} \hat{Q}(s', a') - \hat{Q}(s, a)]$$

By rewriting step 3)

$$\hat{Q}(s, a) = \hat{Q}(s, a) + \Delta \hat{Q}(s, a) = \hat{Q}(s, a) + \alpha [r + \gamma \max_{a'} \hat{Q}(s', a') - \hat{Q}(s, a)]$$

$$= \alpha [r + \gamma \max_{a'} \hat{Q}(s', a')] + (1 - \alpha) \hat{Q}(s, a)$$

Exponential Moving Average

compare with (see before):

$$Q^*(s, a) = \sum_{S_{t+1}} P(S_{t+1} \mid s, a) \cdot [r(S_{t+1}) + \gamma \max_{a'} Q^*(S_{t+1}, a')]$$

Expectation

SARSA

• SARSA algorithm (ε -greedy version)

Initialize $\hat{Q}(s,a)$ at random, put the agent is in a random state s Repeat:

- 1) Select the action $a=\mathrm{argmax}_a\hat{Q}(s,a)$ with probability $(1-\varepsilon)$ otherwise, select a at random
- 2) The agent is now in state s^\prime and has received the reward r
- 3) Select the action $a'=\mathrm{argmax}_a\hat{Q}(s',a)$ with probability $(1-\varepsilon)$ otherwise, select a' at random
- 4) Update $\hat{Q}(s,a)$ by

$$\Delta \hat{Q}(s,a) = \alpha [r + \gamma \hat{Q}(s',a') - \hat{Q}(s,a)]$$
 No more 'max' here

Q-learning is a an *off-policy* algorithm: each update involves $\max_{a'} \hat{Q}(s',a')$ (i.e. *exploration* is not taken into account) SARSA is a an *on-policy* algorithm: each update involves $\hat{Q}(s',a')$ (which involves the next policy action, *exploration* included)

SARSA vs Q-Learning

Cliff World

'S' is the start 'G' is the goal Each white box has $\,r=-1\,$ 'The Cliff' region has $\,r=-100\,$ and entails going back to 'S'

Experimental Results

SARSA finds a sub-optimal but safer path since its learning takes into account the ε risk of going off the cliff

Q-learning finds the optimal path but, occasionally, it falls off the cliff during learning due to the ε -greedy strategy

