

Adaptive Methods for *Lecture* Data-based Decision Making 8

IN-STK 5000 / 9000

Autumn 2022

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UNIVERSITY OF OSLO

dScience – Centre for Computational and Data Science



← News and events ← dScience events

Norwegian version of this page

Data Science Day @ UiO 2022

dScience would like to welcome the Data Science community to the fifth annual Data Science Day.

dScience events

News

Time and place: Oct. 19, 2022 5:00 PM-10:00 PM, The Science Library and Sophus Lie's auditorium Add to calendar

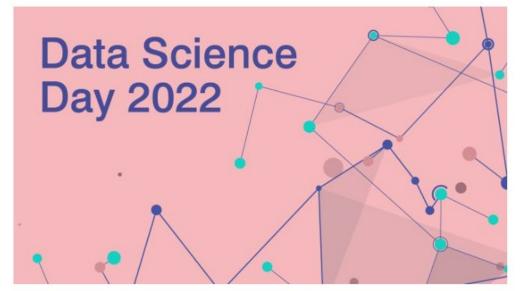


Illustration: Colourbox / AstroMaria

What we talk about today: Online Machine Learning



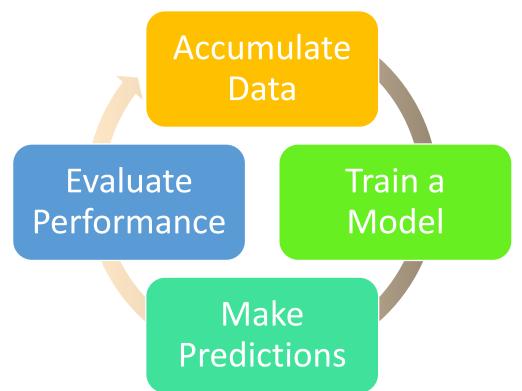
Online Learning

Vs.

Sources: Wikipedia, River tutorial, ...

Recommendations: Awesome online machine learning (github)

Sequentially update ML model as more data becomes available!



Offline Learning

Learn from one *batch* of data (use complete dataset in one go).

- → Problem:
 - Data might not fit in memory
 - Data only available over time

Data Streams

Reactive Data Streams:

- Receive unfiltered live data.
 E.g., clicks on website, heart rate measures, ...
- No influence over observations!



Proactive Data Streams:

- Control over the data stream.
 (Timing, order, etc. of observations)
 E.g., read data from file in specific order.
- Turn reactive streams into proactive: Save database and process offline.
- → <u>Challenge</u>:

Model trained offline (on proactive data) should perform correctly on reactive data.

Online Learning - Advantages

- Handles streams or updates of data → Adaptive to changes!
- Applications:
 - Recommender systems,
 - Anomaly detection,
 - Finance market, ...
- Learn from one data point at a time:
 - No need to train a new model from scratch
 - No need to store all historic data
- Can be applied for cases where one-shot learning is not feasible due to abundance of data (out-of-core learning)

Online Learning - Challenges

- Monitoring for changes and continued retraining
 - → How often necessary?
- Reduced performance compared to offline learning on complete data (if the distribution is static).
- Evaluation: Cross-validation Data must be in realistic order.

Concept Drifts

Data X (and labels y) is drawn from a probability distr. P

• Supervised learning: Learn function f(x) = y that predicts labels

Concept drift \approx Distribution P changes over time

- Virtual concept drift: P(X) changes, while f remains unchanged.
- Real concept drift: P(X, y) changes, i.e., f changes!
 - Abrupt change: Concept changes abruptly at given time.
 - Gradual change: Gradual concept change over time steps.
- Example: Energy consumption over year, traffic over week, ...
- Unsupervised learning: Learn clusters, patterns, latent features, ...
 → only virtual concept drifts are relevant

Drift Detector

- Offline learning performs badly under concept drifts
- Online learning updates model based on new data and can adapt to new concepts
- → Trigger model updates when concept drifts occur!

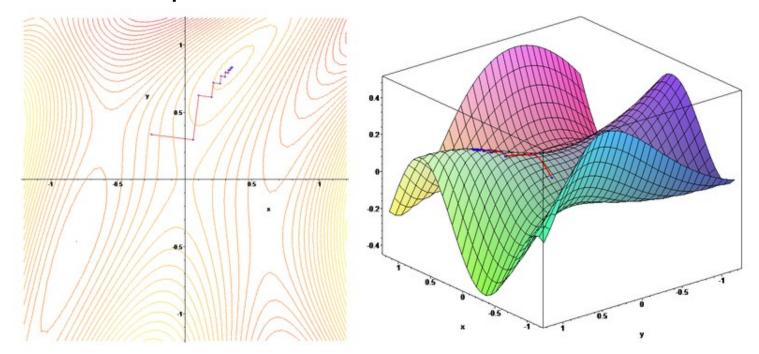
Drift-aware methods:

- Employ change detection mechanism ≈ drift detector
- Monitor model performance based on some metric
 Trigger model update when performance worsens



Online Regression via Stochastic Gradient Descent

- Gradient Descent: Find a local minimum of a function F.
 - \rightarrow Start from a random point, then repeatedly "take a step" in the direction of the steepest descent = $-\nabla F$



See Wikipedia on Gradient Descent

Online Regression via Stochastic Gradient Descent

- Gradient Descent: Find a local minimum of a function F.
 - \rightarrow Start from a random point, then repeatedly "take a step" in the direction of the steepest descent = $-\nabla F$
- GD for Regression: Min. prediction error F(x, w) (e.g. MAE, MSE)
 - for regression function with parameters w
 - over complete data set x!
 - Update: $w_{n+1} = w_n \gamma \nabla F(x, w_n), n \ge 0.$
- Stochastic GD: Update parameters w sequentially for each data point individually $x_1, x_2, ...$:

$$w_{n+1} = w_n - \gamma \nabla F(x_n, w_n), n \geq 0.$$

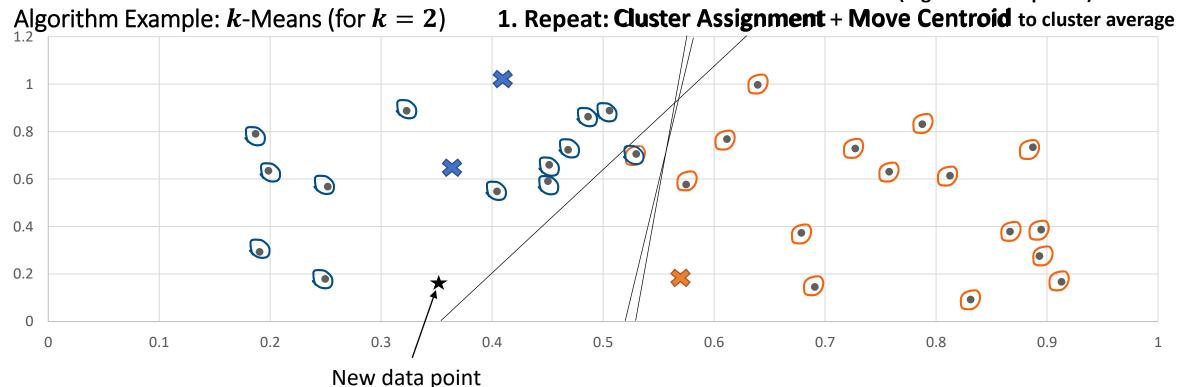
→ Can be updated as new data becomes available!

Online Clustering with k-Means

New data point (x, y):

- Allocate new point to a cluster (by nearest cluster center).
- Shift cluster center according to new point.

0. Insert k random cluster centroids (e.g. on k data points)



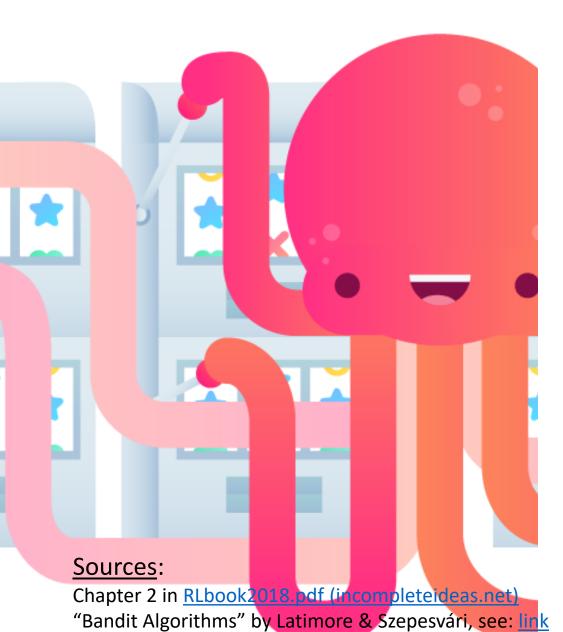
River

online-ml/river: C Online machine learning in Python (github.com)

- Python Library for Online Machine Learning
- Merger between scikit-multiflow and creme
- Includes:
 - Algorithms (for classification, regression, clustering, bandits)
 - data-transformation methods,
 - drift detectors,
 - datasets,
 - performance metrics







INSTK5100 in 2022: Course material

Another Online Problem:

Multi-armed Bandits

- Online problem:
 At every step choose an action
- Feedback:
 (numeric) reward for action
 → Proactive Data Stream

Multi-armed Bandits: Setting



 $\overline{R_t \sim P_{A_t}}$

 A_t

agent

environment

15

• The Bandits:



Actions: At any time step choose one arm to pull.

• Loop: Select action A_t , observe feedback

(reward) R_t from unknown distribution P_{A_t} .

Goal: Maximise rewards over time.

A. George

The Exploration Exploitation Trade-off

<u>Exploration</u>: Try out new actions that might turn out to be beneficial (but might not).

• Exploitation: Play actions that have been played in the past and turned out to be good.

→ Only exploring or only exploiting is suboptimal (prevents us from achieving high rewards)

→ We need to find an appropriate tradeoff between exploring and exploiting!





Which arm should I pull next?
Should I try a new one?

Note: Exploration-Exploitation
Dilemma is not an issue for un/supervised learning problems



k-Bandits Problem: Example

- Trying out Restaurants/Bars in Oslo:
- Not every visit (to the same place) is equally good/bad
- Want to sequentially choose a place to go:
 - Select promising places!
 - → Need to learn which places are good!











k-Bandits Problem: Example

- Medical treatments:
- Suppose there are several treatments available
- The treatments have unknown success rates
- Want to sequentially prescribe treatments to patients:
 - Give promising treatments to patients!
 - → Need to learn which treatment is most effective!



Estimating Action Values

At time t:
Action $A_t \in [k]$ Reward $R_t \sim P_{A_t}$ Selection prob. $P_{strategy}(a,t)$ Est. val. $Q^t(a)$ Real val. $q^*(a) = \mathbb{E}[R_t|A_t = a]$

• The value of an action is its expected reward:

$$\mathbf{q}^*(\mathbf{a}) = \mathbb{E}[R_t | A_t = a] = \int_{r \in R} r \, \mathrm{d}P_a(r).$$

- \rightarrow Reward distribution is unknown, thus the values of actions are also unknown!
- <u>Idea</u>: Estimate the values of actions based on prior feedback!

The **estimated value of an action** at time t: $Q^t(a)$ \rightarrow We want $Q^t(a)$ to be close to $q^*(a)$.

• Sample-average:

$$\overline{Q^{t}(a)} = \frac{\sum rewards \ when \ a \ was \ played}{\# \ a \ was \ played \ in \ prior \ rounds} = \frac{\sum_{i=1}^{t-1} R_{i} \cdot \mathbb{I}_{A_{i}=a}}{\sum_{i=1}^{t-1} \mathbb{I}_{A_{i}=a}} \qquad \text{if } \sum_{i=1}^{t-1} \mathbb{I}_{A_{i}=a} \neq 0$$

 $Q^{t}(a) = 0$ (or any other constant) otherwise

Expected Total Reward

At time t:
Action $A_t \in [k]$ Reward $R_t \sim P_{A_t}$

Selection prob. $P_{strategy}(a, t)$

Est. val. $Q^{t}(a)$

Real val. $q^*(a) = \mathbb{E}[R_t|A_t = a]$

- Let $P_{strategy}(a, t)$ denote the probability of pulling arm a in round t according to a fixed strategy.
- The **expected total reward** achieved by the strategy over *T* rounds is:

$$\mathbb{E}[\sum_{t=0...T-1} R_t] = \sum_{t=0...T-1} \sum_{a \in [k]} P_{strategy}(a,t) \cdot \mathbb{E}[R_t | A_t = a] = \sum_{t=0...T-1} \sum_{a \in [k]} P_{strategy}(a,t) \cdot q^*(a)$$

Quality Measure: Regret

Action $A_t \in [k]$ Reward $R_t \sim P_{A_t}$ Selection prob. $P_{strategy}(a, t)$

Est. val. $Q^{t}(a)$

At time *t*:

Real val. $q^*(a) = \mathbb{E}[R_t | A_t = a]$

Best val. q^{max} , best arm a^*

• The **expected total reward** achieved by the strategy over *T* rounds is:

$$\mathbb{E}\left[\sum_{t=0\dots T-1} R_t\right] = \sum_{t=0\dots T-1} \sum_{a\in[k]} P_{strategy}(a,t) \cdot q^*(a)$$

- Intuition: Find a strategy that is as close as possible to always pulling the "best" arm a^* with value q^{max}
- The **regret** of a strategy is

$$\operatorname{regret}_{\mathbf{T}}(\operatorname{strategy}) = \mathbf{T} \cdot q^{max} - \mathbb{E}[\sum_{t=0\dots T-1} R_t]$$
$$= \dots = \sum_{a \in [k]} [q^{max} - q^*(a)] \cdot \mathbb{E}[\# \ a \ is \ pulled]$$

- The regret is always ≥ 0 .
- The regret of a strategy that selects only best action (actions with maximal value) is 0.
- Ideally, we play a strategy that gives us a regret that is sub-linear in T.
- There is a known lower bound on the regret: $O(\sqrt{T \cdot k})$

The Exploration Exploitation Trade-off

<u>Exploration</u>: Try out new actions that might turn out to be beneficial (but might not).

<u>Exploitation</u>: Play actions that have been played in the past and turned out to be good.

→ Only exploring or only exploiting is suboptimal (prevents us from achieving high rewards)

→ We need to find an appropriate tradeoff between exploring and exploiting!

Exploration: Trying out (possibly random) actions.

 \rightarrow Helps us getting better estimates of the action values $Q^t(a)$ and to identify

the best action for future turns.

<u>Exploitation</u>: Playing a greedy action, i.e.,

one with currently highest estimated value $argmax_{a \in \lceil k \rceil} Q^t(a)$ (always exists!).

→ Gives us highest expected immediate reward w.r.t to our current estimates.

Let's take a Quiz...

... go to Mentimeter!

Let's take a break...

Back on in 5 min!

Multi-armed Bandits: Setting



 $\overline{R_t \sim P_{A_t}}$

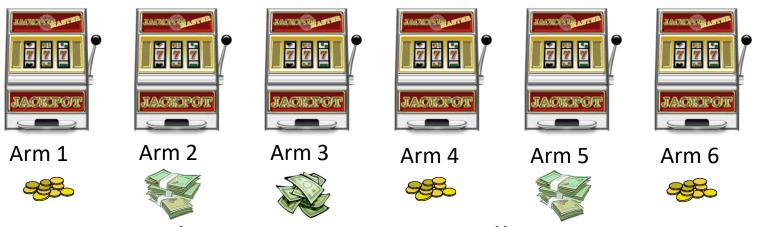
 A_t

agent

environment

26

• The Bandits:



Actions: At any time step choose one arm to pull.

• Loop: Select action A_t , observe feedback

(reward) R_t from unknown distribution P_{A_t} .

Goal: Maximise rewards over time (e.g. min. prediction error).

A Simple Strategy: Explore-Then-Commit (ETC)

Simulating 3 arms with m=2

For $t < m \cdot k$:

- Choose action $A_{t \bmod k}$
- Observe reward R_t

For $t \ge m \cdot k$:

• Compute $Q^{m \cdot k - 1}(a) = \frac{\sum_{i=0}^{m \cdot k - 1} R_i \cdot \mathbb{I}_{A_i = a}}{m}$

• Select arm $A_t \in argmax_{a \in [k]} Q^{k \cdot m - 1}(a)$



Round	Arm 1 $R_t \mid N^{t+1} \mid Q^{t+1}$	Arm 2 $R_t \mid N^{t+1} \mid Q^{t+1}$	Arm 3 $R_t \mid N^{t+1} \mid Q^{t+1}$
0	0_ 1		
1		0 1	
2			1 1
3	1 2 1/2		
4		1 2 1/2	
5			0 2 1/2
6			
7		???	
8			
9			
10			

A Simple Strategy: Explore-Then-Commit (ETC)

Simulating 3 arms with m=3

For $t < m \cdot k$:

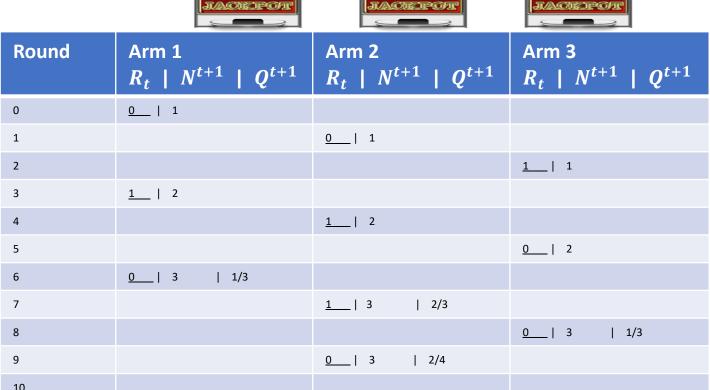
- Choose action $A_{t \bmod k}$
- Observe reward R_t

For
$$t \ge m \cdot k$$
:

Compute

$$Q^{m \cdot k - 1}(a) = \frac{\sum_{i=0}^{m \cdot k - 1} R_i \cdot \mathbb{I}_{A_i = a}}{m}$$

• Select arm $A_t \in argmax_{a \in [k]} Q^{k \cdot m - 1}(a)$



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Explore-Then-Commit (ETC): Regret

• The regret of ETC after T rounds is

At time t:
Action $A_t \in [k]$ Reward $R_t \sim P_{A_t}$ Selection prob. $P_{strategy}(a,t)$ Est. val. $Q^t(a)$ Real val. $q^*(a) = \mathbb{E}[R_t|A_t = a]$ Best val. q^{max} , best arm a^*

$$regret_T(ETC)$$

$$\leq \sum_{a \in [k]} [q^{max} - q^*(a)] \cdot m + \sum_{a \in [k]} [q^{max} - q^*(a)] \cdot (T - m \cdot k) \cdot \exp\left(-\frac{m(q^{max} - q^*(a))^2}{4}\right)$$

- Problem dependent regret bound:
 - Depends on the specific instance (because it includes the terms $q^{max} q^*(a)$).
- Exploration-Exploitation:
 - If *m* is large, i.e., we explore a lot, then the first term gets large.
 - If m is small, i.e., we concentrate on exploitation, then the second term gets large.
- Linear in T: We can't get lower average regret by increasing the number of rounds (after $T > m \cdot k$).

€-Greedy Action Selection

- Exploit:
 - Most of the time.
- <u>Explore</u>:

Instead of a fixed explore phase, just sometimes (randomly) choose to explore.

 \rightarrow Exploration chance: $\epsilon \in [0,1]$

At time t: Action $A_t \in [k]$ Reward $R_t \sim P_{A_t}$ Selection prob. $P_{strategy}(a,t)$ Est. val. $Q^t(a)$ Real val. $q^*(a) = \mathbb{E}[R_t|A_t = a]$ Best val. q^{max} , best arm a^*

€-Greedy Action Selection

- Let $\epsilon \in [0,1]$.
- Initialise $Q^0(a) = const.$ for all $a \in [k]$.
- Initialise $N^0(a) = 0$ for all $a \in [k]$, number times each arm was pulled.
- For $t = 0 \dots T 1$:
 - With probability (1ϵ) : $A_t = argmax_{a \in [k]}Q^t(a)$ # select a greedy action
 - With probability ϵ : $A_t \sim U([k])$ # sample uniformly rand. from $\{1, ..., k\}$
 - Receive reward R_t
 - $N^{t+1}(A_t) += 1$ and $N^{t+1}(a) = N^t(a)$ for all other actions a.

•
$$Q^{t+1}(a) = \begin{cases} Q^{t}(a) + \frac{1}{N^{t+1}(a)} [R_t - Q^t(a)] & \text{if } a = A_t \\ Q^t(a) & \text{otherwise} \end{cases}$$

At time t:
Action $A_t \in [k]$ Reward $R_t \sim P_{A_t}$ Selection prob. $P_{strategy}(a,t)$ Est. val. $Q^t(a)$ #pulls $N^t(a)$ Real val. $q^*(a) = \mathbb{E}[R_t|A_t = a]$ Best val. q^{max} , best arm a^*





€-Greedy Action Selection

- Let $\epsilon \in [0,1]$.
- Initialise $Q^0(a) = const.$ for all $a \in [k]$.
- Initialise $N^0(a) = 0$ for all $a \in [k]$, number times each arm was pulled.
- For $t = 0 \dots T 1$:
 - With probability (1ϵ) : $A_t = argmax_{a \in [k]}Q^t(a)$ # select a greedy action
 - With probability ϵ : $A_t \sim U([k])$

sample uniformly rand. from $\{1, ..., k\}$

At time *t*:

Action $A_t \in [k]$

Reward $R_t \sim P_{A_t}$

Est. val. $Q^{t}(a)$

#pulls $N^t(a)$

Selection prob. $P_{strategy}(a, t)$

Real val. $q^*(a) = \mathbb{E}[R_t|A_t = a]$

Best val. q^{max} , best arm a^*

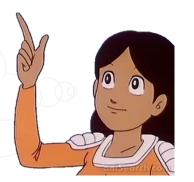
- Receive reward R_t
- $N^{t+1}(A_t) += 1$ and $N^{t+1}(a) = N^t(a)$ for all other actions a.

$$Q^{t+1}(a) = \frac{\left[Q^t(a) + \frac{1}{1-1} \left[R_t - \Omega^t(a)\right]\right]}{\left[Q^t(a) + \frac{1}{1-1} \left[R_t - \Omega^t(a)\right]\right]}$$

$$if \alpha = A_{-}$$

If $T \to \infty$ can we guarantee $Q^t(a) \to q^*(a)$ for all actions a?

Yes: Because for $T \to \infty$ we will select every arm infinitely often.

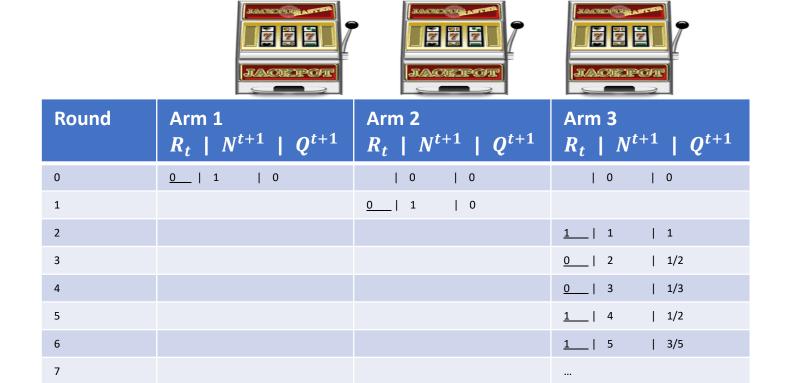


Simulating 3 arms with $\epsilon = 0$ \rightarrow only greedy actions

Initialise

- $Q^0(a) = 0$ for all $a \in [3]$
- $N^0(a) = 0$ for all $a \in [3]$

- Choose greedy action A_t
- Observe reward R_t
- $N^{t+1}(A_t) += 1$
- $Q^{t+1}(A_t) = Q^t(A_t) + \frac{1}{N^{t+1}(A_t)} [R_t Q^t(A_t)]$

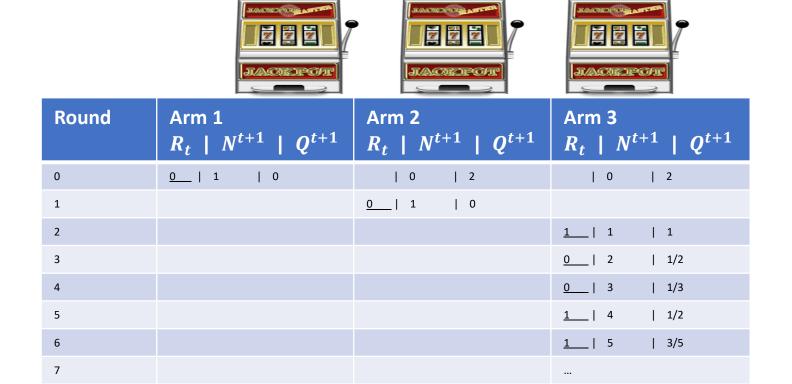


Simulating 3 arms with $\epsilon = 0$ only greedy actions

Initialise

- $Q^0(a) = 2$ for all $a \in [3]$
- $N^0(a) = 0$ for all $a \in [3]$

- Choose greedy action A_t
- Observe reward R_t
- $N^{t+1}(A_t) += 1$
- $Q^{t+1}(A_t) = Q^t(A_t) + \frac{1}{N^{t+1}(A_t)} [R_t Q^t(A_t)]$



Simulating 3 arms with $\epsilon = 0$ \rightarrow only greedy actions

Initialise

- $Q^0(a) = -1$ for all $a \in [3]$
- $N^0(a) = 0$ for all $a \in [3]$

- Choose greedy action A_t
- Observe reward R_t
- $N^{t+1}(A_t) += 1$
- $Q^{t+1}(A_t) = Q^t(A_t) + \frac{1}{N^{t+1}(A_t)} [R_t Q^t(A_t)]$



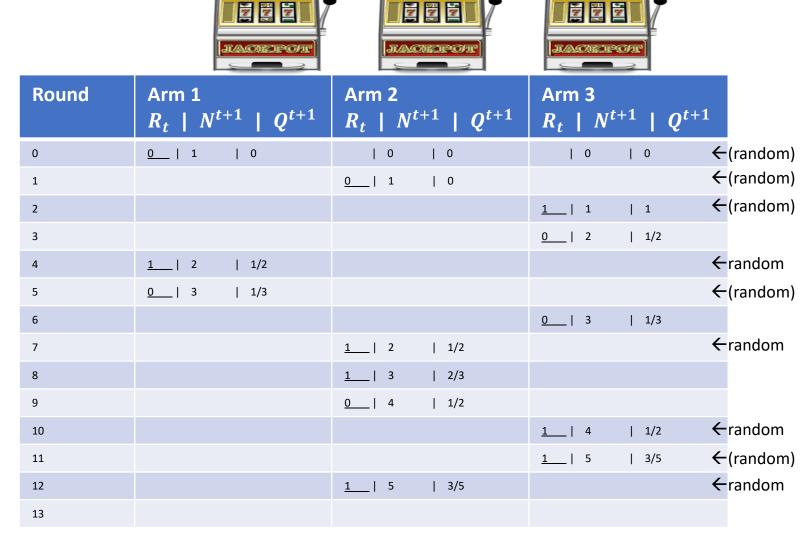
Round	Arm 1 $R_t \mid N^{t+1} \mid Q^{t+1}$	Arm 2 $R_t \mid N^{t+1} \mid Q^{t+1}$	Arm 3 $R_t \mid N^{t+1} \mid Q^{t+1}$
0	0 1 0	0 -1	0 -1
1	1 2 1/2		
2	0 3 1/3		
3	0 4 1/4		
4	<u>0</u> 5 1/5		
5	0 6 1/6		
6	0 7 1/7		
7			

Simulating 3 arms with $\epsilon = 0.5$ random actions ~half the time

Initialise

- $Q^0(a) = 0$ for all $a \in [3]$
- $N^0(a) = 0$ for all $a \in [3]$

- Choose action A_t (greedy/rand.)
- Observe reward R_t
- $N^{t+1}(A_t) += 1$
- $Q^{t+1}(A_t) = {1 \over Q^t(A_t) + {1 \over N^{t+1}(A_t)}} [R_t Q^t(A_t)]$



€-Greedy Action Selection: Summary

- Exploration rate can be tuned by varying the parameter $\epsilon \in [0,1]$.
- ϵ -Greedy has linear regret: regret_T $(\epsilon Greedy) \in O(T)$.
- Advantages:
 - Easy to implement!
 - Vary the exploration parameter over time $\epsilon_t \in [0,1]$ such that, e.g., exploration rate decreases.

Issues:

• When ϵ -Greedy selects a non-greedy action, it does not differentiate between any of the actions (just picks uniformly at random)

Non-Stationary Rewards



• Reward of arm A_t follows unknown distribution $P(r_t|A_t=a)=P_{\theta_a}(r)$.

Example:

- Bernoulli distribution: P_{θ_a} , such that $r = \begin{cases} 1 \ with \ prob. & \theta_a \\ 0 \ with \ prob. \ 1 \theta_a \end{cases}$.
- Normal distribution: P_{θ_a} , with mean $\theta_{a,\mu}$ and standard deviation $\theta_{a,\sigma}$.

- Now: Let us consider non-stationary rewards i.e., a Concept Drift!
 - → The distribution of the rewards can change over time.
 - → We want to give more recent rewards more weight than rewards from long ago timesteps...

€-Greedy Action Selection with weighted averages

- Let $\epsilon \in [0,1]$.
- Initialise $Q^0(a) = const.$ for all $a \in [k]$.
- Initialise $N^0(a) = 0$ for all $a \in [k]$, number times each arm was pulled.
- For $t = 0 \dots T 1$:
 - With probability (1ϵ) : $A_t = argmax_{a \in [k]}Q^t(a)$ # select a greedy action
 - With probability ϵ : $A_t \sim \mathrm{U}([\mathrm{k}])$ # sample uniformly rand. from $\{1,\ldots,k\}$
 - Receive reward R_t
 - $N^{t+1}(A_t) += 1$ and $N^{t+1}(a) = N^t(a)$ for all other actions a.

•
$$Q^{t+1}(a) = \begin{cases} Q^t(a) + \alpha^t(a)[R_t - Q^t(a)] & \text{if } a = A_t \\ Q^t(a) & \text{otherwise} \end{cases}$$

Weighted Averages

• Constant step size $\alpha \in (0,1]$:

$$Q^{t+1}(a) = Q^{t}(a) + \alpha \cdot [R_{t} - Q^{t}(a)] = \dots$$

= $(1-\alpha)^{N^{t+1}(a)} Q^{0}(a) + \sum_{i=1}^{t} \alpha (1-\alpha)^{N^{t+1}(a)-N^{i+1}(a)} R_{i} \mathbb{I}_{A_{i}=a}$

• Non-Constant step size $\alpha^t(a) \in (0,1] : \rightarrow$ time and action dependent! $Q^{t+1}(a) = Q^t(a) + \alpha^t(a) \cdot [R_t - Q^t(a)]$

If reward functions were stationary:

For which step size functions $\alpha^t(a)$ can we guarantee $Q^t(a) \rightarrow q^*(a)$ for $t \rightarrow \infty$?

Weighted Averages: Convergence for stationary reward distributions

• Condition for convergence of ϵ -Greedy with **stationary** rewards and $\epsilon > 0$:

```
(Or any other strategy that pulls all arms infinitely many times as T \to \infty)
```

We can guarantee $Q^t(a) \to q^*(a)$ for $t \to \infty$ if for all $a \in [k]$

- 1. $\sum_{t=1}^{\infty} \alpha_t(a) = \infty$ and
- 2. $\sum_{t=1}^{\infty} (\alpha_t(a))^2 < \infty$
- Constant step size $\alpha \in (0,1]$: Condition 2. is not satisfied!
 - → No convergence to true action-values.
 - → But: still good for non-stationary rewards.

• Non-Constant step size $\alpha^t(a) \in (0,1]$: Example: $\alpha^t(a) = 1/N^{t+1}(a)$ [sample-average method]

→ Guaranteed convergence to true action-values by condition 1. and 2.

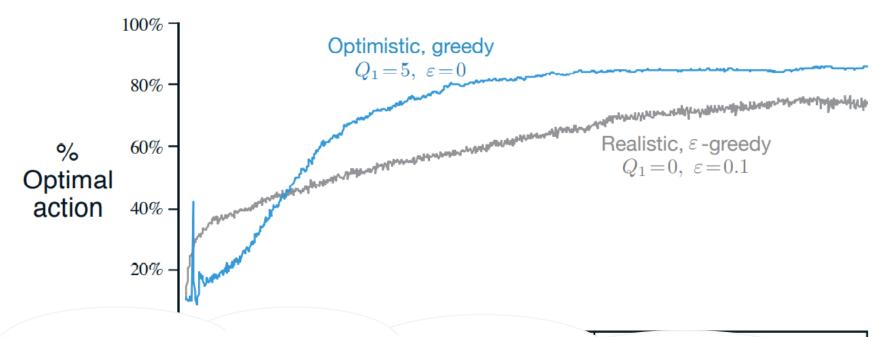
Optimistic Initial Values

- Let $\epsilon \in [0,1]$.
- Initialise $Q^0(a) = const.$ for all $a \in [k]$.
- Initialise $N^0(a) = 0$ for all $a \in [k]$ the number of times each arm has been pulled.
- For t = 0 ... T
 - With probabilit
 - With probabilit
 - Receive reward R
 - $N^{t+1}(A_t) += 1$
- $Q^{t+1}(a) = \begin{cases} Q^t \\ Q^t \end{cases}$

- Initial values create "bias"
 - → for sample average: disappears after all arms have been selected once
 - \rightarrow for const. α bias persists but decreases over time
- Can incorporate prior knowledge on the arms
- Can be used to incentivize exploration in the beginning → setting optimistic values

andom from $\{1, \dots, k\}$

Optimistic Initial Values (see Chapter 2.6 in [Link])



Optimistic initial values:

- exploration is only encouraged in a few initial rounds
- only useful in stationary distribution
- if reward distributions change, new exploration might be necessary



1000

Upper-Confidence-Bound Action Selection

- Idea: Select actions that are "uncertain", but "promising".
- <u>Principle</u>: Optimism in the face of uncertainty!
 - → Find upper confidence bounds on the value estimates and choose the arm with the best bound:

$$A_t = \arg\max_{a} Q^t(a) + c \sqrt{\frac{\ln(t)}{N_t(a)}}.$$

- → Upper confidence bounds get tighter provided more data.
- → Intuitively, we will not select a suboptimal arm too often.
- Can be implemented such that the regret is: $\operatorname{regret}_{\mathbf{T}}(UCB) \in \mathcal{O}(\sqrt{k \cdot T \cdot \log(T)} + \sum_{a \in [k]} q^{max} q^*(a))$. \rightarrow close to optimal!

... more on that next time!

Let's continue the Quiz...

... go to Mentimeter!