Exploration and exploitation

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Exploration vs. exploitation dilemma

Online decision-making involves a fundamental choice:

- Exploitation: Make the best decision given current information
- Exploration: Gather more information

Consequences

- The best long-term strategy may involve short-term sacrifices
- Only gather as much information as necessary to make the best overall decision

Four methods are presented

- optimistic initialization
- R-Max
- decaying ϵ-greedy
- UCB1

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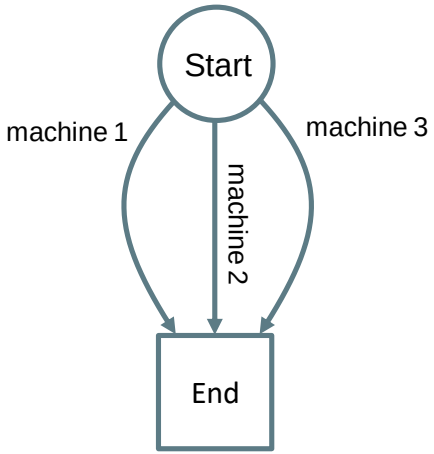
Example: Multi-armed bandits

- Three actions for a given state: Pull lever of slot machine 1/2/3 and get reward
- Special case: Probabilistic (non-deterministic) rewards R
- At time t, agent selects action a_t and gets reward R_t
- Goal: Maximize (average) reward R_t



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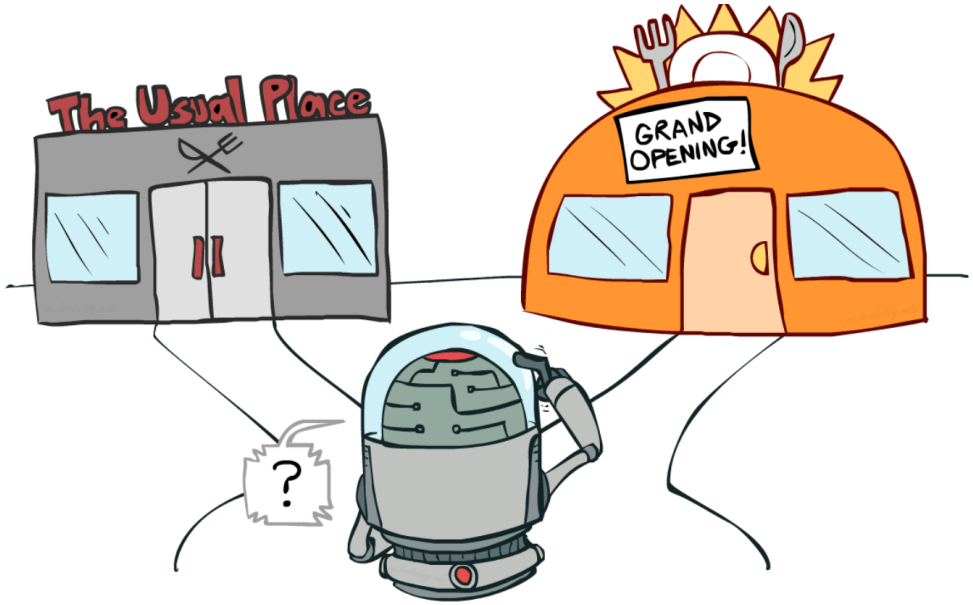
Related real life examples

- Should I stick to my current job or get a new one?
- How many prices should I compare before buying product X?
- Secretary problem



http://procaccia.info/courses/15381f16/slides/781_rl_rmax.pdf

Task: What other related examples come to your mind?

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Disclaimer: All methods described in this chapter are only thoroughly analyzed for multi-armed bandits and not for MDPs in general, although they also provide very good (but not optimal) results for MDPs with discrete actions

Difference between multi-armed bandit and general MPD

	Multi-armed bandit	MDP
episode length	1	usually > 1
reward	stochastic	usually deterministic
goal	max. (avg.) reward	max (avg.) discounted reward

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Regret

- Is based on the optimal V-value, defined as $V_* = \max_a Q_*(a)$
- Defines how much worse an action is compared to the optimal action at time step t

$$I_t = E[\, V_* - Q(A_t)\,]$$

Total regret

- Is the accumulated regret until timestep t

$$L_t = E\left[\sum_{\tau=1}^{t} V_* - Q(A_\tau)\right]$$

- Maximize return $\widehat{=}$ minimize total regret
- always executing the best action equals total regret of 0

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Counting regret

- the total regret depends on two factors
  - how bad an action is
    (**gap** $\Delta_a = V_* - Q(a)$ as difference of action a to optimal action)
  - how often the action is taken
    (count $N_t(a)$ as the number of selecting a until timestep t)
- the counting regret is a reformulation of the total regret as

$$L_t = E\left[\sum_{\tau=1}^{t} V_* - Q(A_\tau)\right]$$

← iterate over time steps τ

$$= \sum_{a \in \mathcal{A}} E[N_t(a)] \cdot \Delta_a$$

← iterate over actions a

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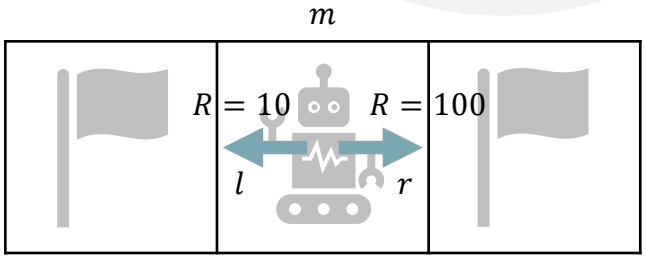

Example: Trivial robot maze

- Policy: Move right for two episodes, then move left for one episode.

$$V_*(m) = 100$$
$$Q(m, r) = 100 \quad \rightarrow \Delta_r = 0$$
$$Q(m, l) = 10 \quad \rightarrow \Delta_l = 90$$

- After n timesteps/episodes with counting regret

$$E[N_n(r)] = \frac{2}{3}n \quad \rightarrow \quad L_n = \frac{0 \cdot 2}{3}n + \frac{90 \cdot 1}{3}n = 30n$$
$$E[N_n(l)] = \frac{1}{3}n$$

- After n timesteps/episodes with total regret

$$L_n = E[\, 0 + 0 + 90 + 0 + 0 + 90 + \cdots \,] = 30n$$

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Total regret for different policies

- Optimal policy: Always pick the best action

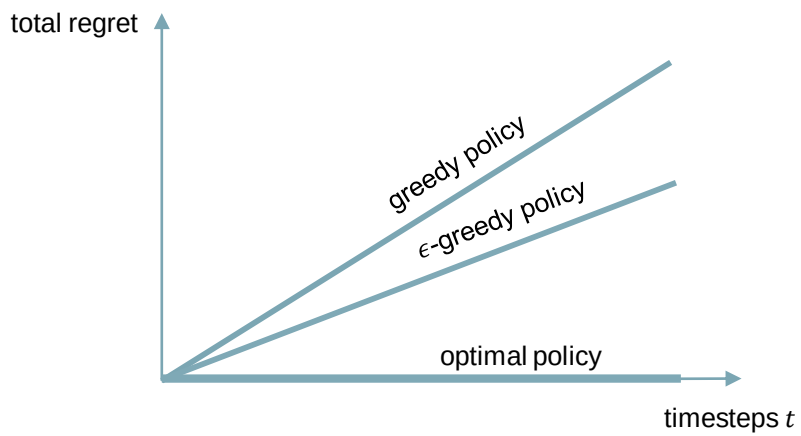
$$L_t = 0$$

- greedy policy: Sometimes (systematically) pick the wrong action

$$L_t = c \cdot t$$

- ϵ-greedy policy: With probability ϵ pick the wrong action

$$L_t = d \cdot t$$



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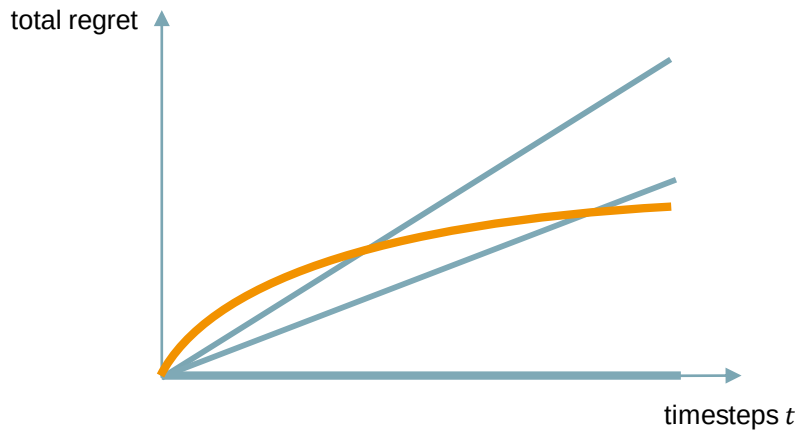
Other considerations

- If an algorithm explores forever, it will have a linear total regret
- If an algorithm explores never, it will have a linear total regret
- If an algorithm stops exploration too early, it will have a linear total regret

Are there exploration algorithms with sublinear total regret converging to an optimal policy?

→ yes



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Total regret lower bound

- defines how small the total regret can become
- depends on the reward distribution $\mathcal{R}^a$ when picking action a and the **Kullback-Leibler divergence KL** measuring the dissimilarity between two probability distributions
- Theorem (Lai and Robbins)

$$\lim_{t\to\infty} L_t \geq \log t \cdot \sum_{a|\Delta_a>0} \frac{\Delta_a}{KL(\mathcal{R}^a|\mathcal{R}^{a^*})}$$

the larger the gaps are, the worse it is on average if the wrong action is picked

most important: total regret increases logarithmically over t in the best case

sum over all actions with a gap > 0 (that are the suboptimal actions)

the smaller the KL divergence is, the more similar the reward distributions are and the more difficult it becomes to differentiate the reward distributions

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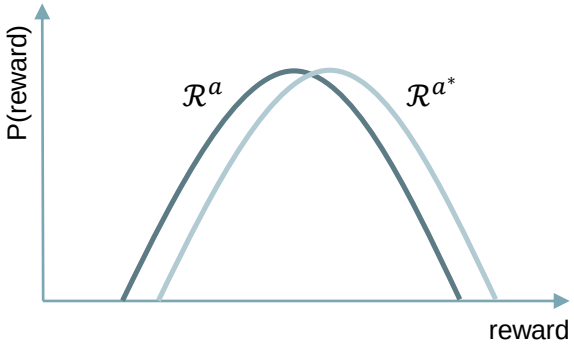
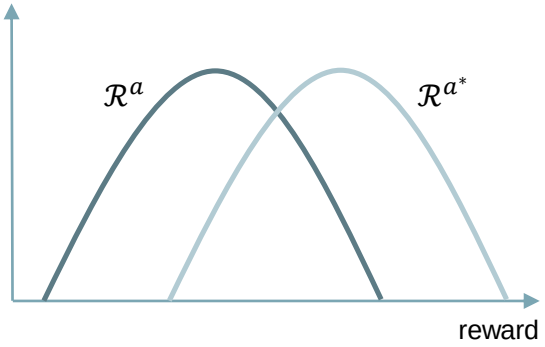
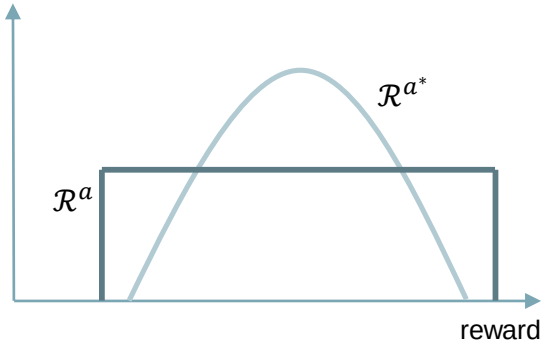
Example



small KL div



large KL div



large KL div

Task: Create different probability distributions and estimate the KL divergence

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Optimism in the face of uncertainty

- Is a heuristic/idea how to behave if one has to decide between multiple actions with unknown reward
- Colloquially: "If you have no idea about the outcome of an action, pick it. It might be the best"

https://medium.com/@uzair.ahmed2/optimism-a-path-to-success-4c7c4cc23fd7

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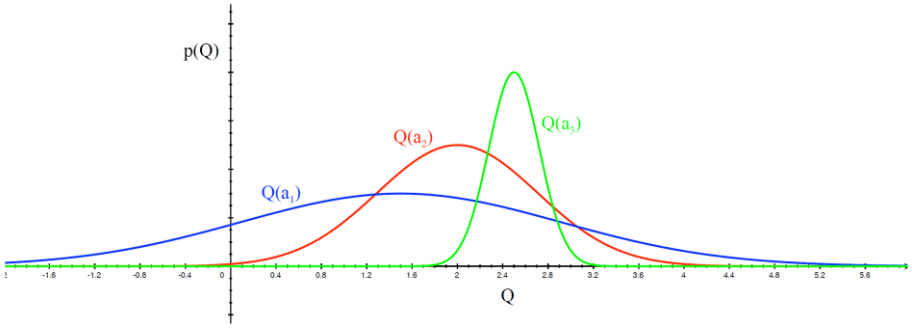
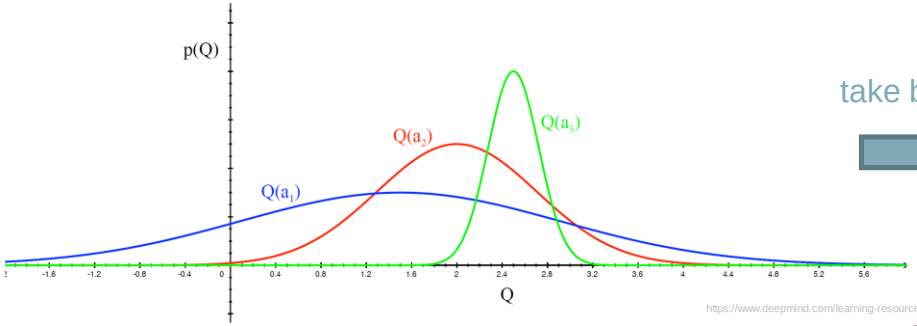
Example: Estimated reward distributions for three actions

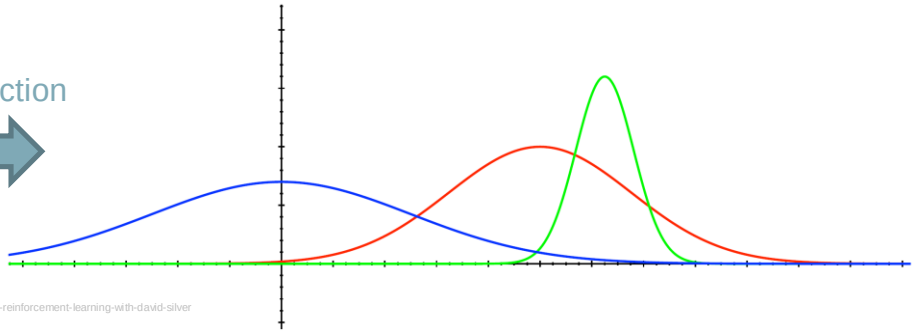
- A greedy policy would take the green action
- An optimistic policy would take the blue action



- After taking the blue action, one is more certain about the outcome of the blue action
  → might take another one next time



take blue action



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Optimistic initialization

- Initialize Q-function to a high value
- Then update it using MC evaluation / SARSA / Q-learning
  (SARSA / Q-learning may take long to converge if initial value is too large)
- Linear total regret when being combined with (ϵ-)greedy
  (no guarantee that optimal action will be taken after some time in every state)
- Standard for a lot of practical problems

Q-learning (off-policy TD control) for estimating $\pi \approx \pi_*$

Algorithm parameters: step size $\alpha \in (0, 1]$, small $\varepsilon > 0$
Initialize $Q(s, a)$, for all $s \in \mathcal{S}^+, a \in \mathcal{A}(s)$, arbitrarily except that $Q(terminal, \cdot) = 0$

Loop for each episode:
  Initialize S
  Loop for each step of episode:
    Choose A from S using policy derived from Q (e.g., ε-greedy)
    Take action A, observe R, S'
    $Q(S, A) \leftarrow Q(S, A) + \alpha\big[R + \gamma \max_a Q(S', a) - Q(S, A)\big]$
    $S \leftarrow S'$
  until S is terminal

Sutton, Barto: Reinforcement Learning

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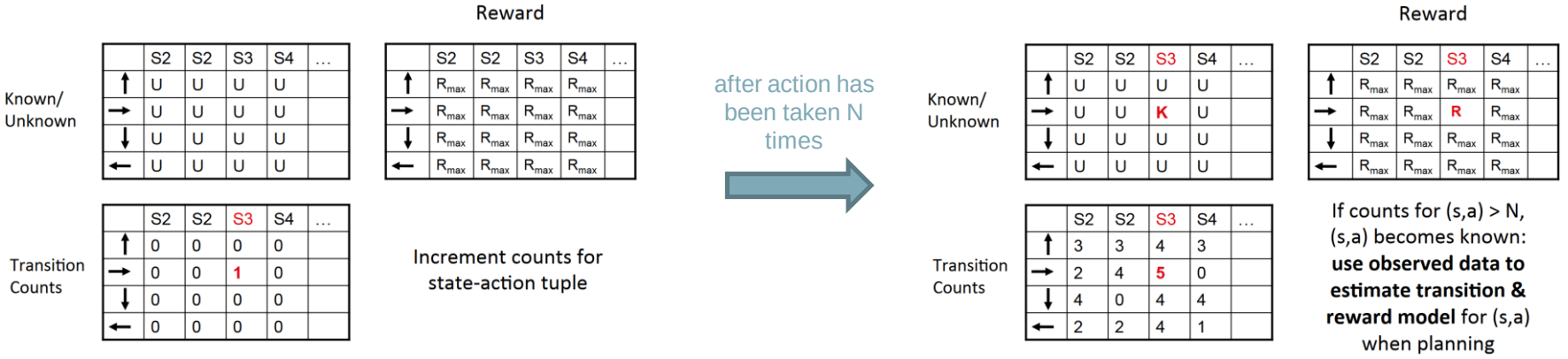
R-max

- Initialize rewards R to the maximum value R_{max}
- If the corresponding action has been taken N times, replace R_{max} with observed reward
- Linear total regret when being combined with (ϵ-)greedy
  (no guarantee that optimal action will be taken after some time in every state)

Example



http://procaccia.info/courses/15381f16/slides/781_rl_rmax.pdf

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Decaying ϵ-greedy exploration

- Decrease ϵ of ϵ-greedy exploration over time according to a special schedule
- Recap: ϵ-greedy exploration

$$\pi(a|s) = \begin{cases} 1 - \epsilon_t + \dfrac{\epsilon_t}{|\mathcal{A}(s)|} & \text{if } a \text{ maximizes } Q(s,a). \\ \dfrac{\epsilon_t}{|\mathcal{A}(s)|} & \text{for all other actions.} \end{cases}$$

- Decaying ϵ-greedy exploration: Update ϵ according to

$$\epsilon_t = \min\left(1, \frac{c}{d^2 t}\right)$$

c: tunable parameter > 0

t: time step

d: minimum gap $\min_a \Delta_a$

- Logarithmic asymptotic total regret but useless in practice, because gaps Δ_a are not known

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UCB1 (upper confidence bound)

- Estimate an upper confidence for each action value measuring the uncertainty of the true Q-function
- Depends on the number $N_t(a)$ than an action has been selected until time t
  - small $N_t(a)$ → estimated value is uncertain
  - large $N_t(a)$ → estimated value is certain
- UCB1 algorithm: Select action maximizing upper confidence bound as

$$a_t = \underset{a \in \mathcal{A}}{\operatorname{argmax}} \left(Q(a) + \sqrt{\frac{2 \log t}{N_t(a)}} \right)$$

- Logarithmic asymptotic total regret (but larger than lower bound), easy to implement
- Standard for a lot of practical problems

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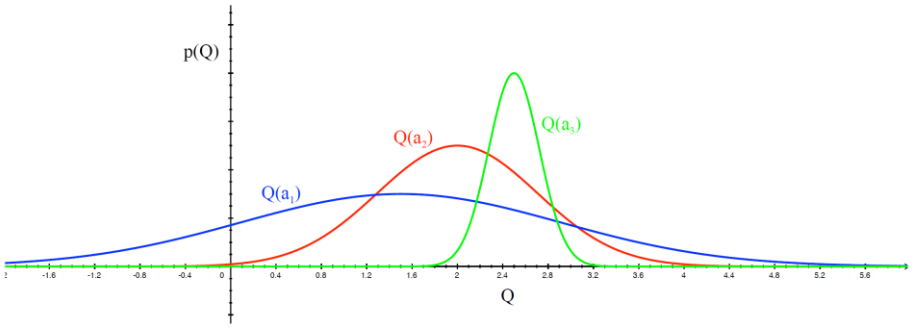
Thompson Sampling

- "randomly take action according to the probability you believe it is the optimal action" (Thompson 1933)
- Use internal (probabilistic) model to approximate the true Q-function
- At every time step
  - Sample from the approximated Q-function for every action
  - Select action with best sample outcome
  - Observe reward, update Q-function approximation
- Logarithmic asymptotic total regret (achieving lower bound)



https://www.deepmind.com/learning-resources/introduction-to-reinforcement-learning-with-david-silver

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Example: Thompson sampling

- 2 Bernoulli bandits (reward of 1 with prob. μ_i, otherwise 0)
- $\mu = [0.6, 0.4]$
- Rewards obtained so far shown on right side

- At time step $t = 14$
  - Approximate both bandits with e.g. beta-distribution
    Bandit 1: $\alpha = 4, \quad \beta = 2$
    Bandit 2: $\alpha = 3, \quad \beta = 4$
  - Sample from approximated Q-function for both bandits, e.g.
    Bandit 1: $Q_{sampled} = 0.68$
    Bandit 2: $Q_{sampled} = 0.56$
  - Select action with best sample outcome → Bandit 1
  - Observe reward of 1, update Q-function approximation
    Bandit 1: $\alpha = 5, \quad \beta = 2$
    Bandit 2: $\alpha = 3, \quad \beta = 4$

time	bandit	result
1	1	1
2	1	0
3	2	1
4	2	1
5	1	1
6	2	1
7	2	1
8	2	0
9	1	1
10	2	0
11	1	0
12	2	0
13	1	1

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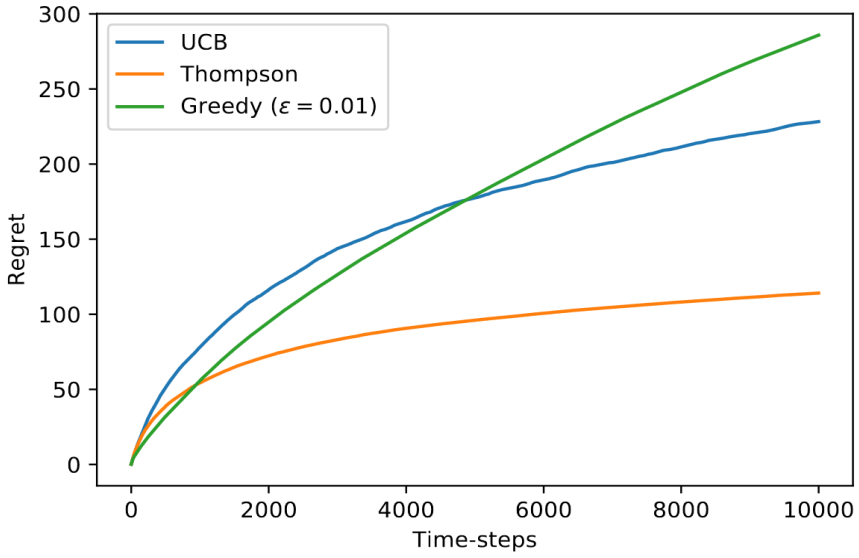
Example

- 5 Bernoulli bandits (give reward of 1 with probability μ_i, otherwise 0)
- $\mu = [0.6, 0.5, 0.4, 0.3, 0.2]$
- Shown is total regret over number of pulls



https://team.inria.fr/polaris/files/2019/05/Gast.pdf

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Example: Comparison of ϵ-greedy / UCB / Thompson

Example: Comparison of ϵ-greedy / UCB / Thompson

Example: Comparison of ϵ-greedy / UCB

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Comparison of all presented methods

Method	Pro	Con
Optimistic initialization	Simple, works well in practice	Linear total regret
R-max	Simple, works well in practice?	Linear total regret
ϵ-greedy	Simple, works well in practice	Linear total regret, param. ϵ
decaying ϵ-greedy	Near optimal	Unfeasible in practice
UCB1	Simple, works ok, near optimal	
Thompson sampling	Optimal	Complex for generic MDPs

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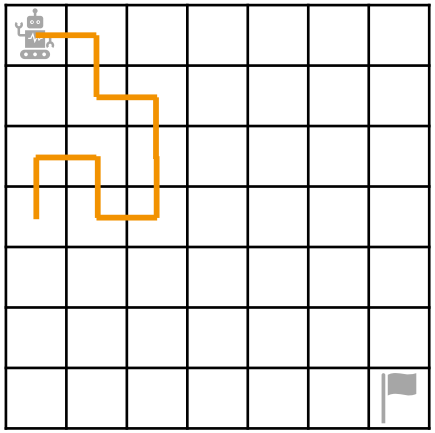
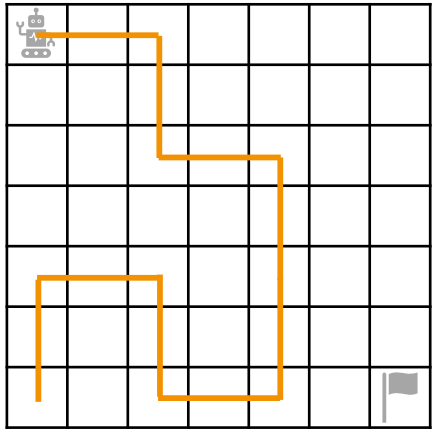
Other exploration techniques

Multi-step actions

- Execute the same action for n steps
- Well suited for continuous environments



1-step action



2-step action

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Count-based exploration

- Informal: Count how often you have been in each state and try to explore states that you haven't been to many times yet
- Use additive reward term of the form

$$R = \alpha R_{ext} + \beta R_{int}$$

  to favor exploration of new states (with weighting factors α, β)
- R_{ext} (extrinsic reward) is the original reward from the RL task (extrinsic reward)
- R_{int} (intrinsic reward) is a count-based exploration reward
  (high if state hasn't been visited often)
- Easy to implement for discrete states (need to store how often each state has been visited) but can be generalized also to continuous states

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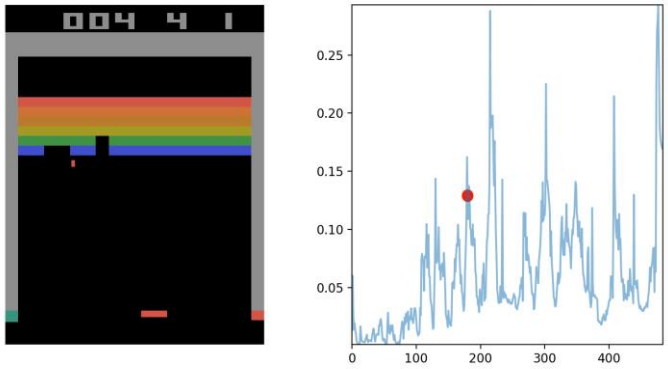
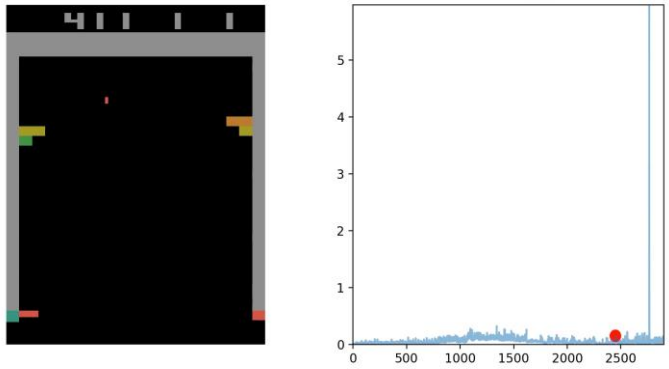
Prediction-based rewards

- Train a model to predict the outcome of the next action
- If the predicted outcome differs heavily from the true outcome (due to new states/rewards never seen before), assign a high intrinsic R_{int} reward to the corresponding action (similar to count-based exploration)

intrinsic reward at the beginning



intrinsic reward when passing the level for the first time



https://openai.com/blog/reinforcement-learning-with-prediction-based-rewards/

Note: Both prediction- and count-based rewards belong to the class of curiosity driven exploration

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Auxiliary tasks

- Fancy variant of reward shaping: Consider additional tasks (with corresponding rewards) that the agent has to solve along its way of solving the main task

Example

- Main task: Robot has to open a box, place an object into it and close the lid of the box afterwards again
- Auxiliary task 1: Box has been opened
- Auxiliary task 2: Object has been placed in the box
- Auxiliary task 3: Box has been closed

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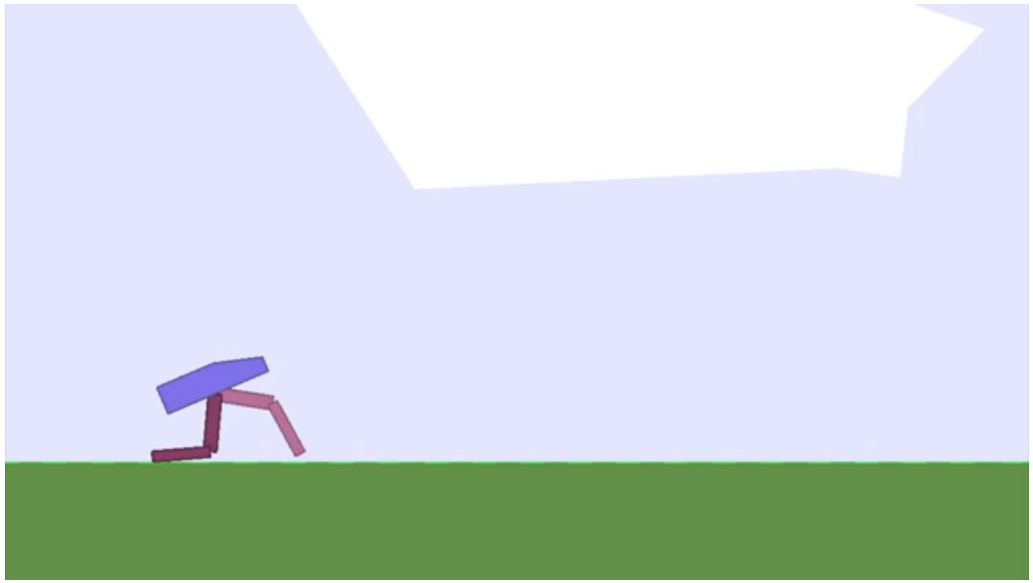
Curriculum learning

- Problem: Sometimes exploration does not help at all because the task is too difficult to be solved by an untrained agent
- Solution: Create a curriculum of environments, i.e. environments with increasing complexity until the previously unsolvable task can be solved



https://www.youtube.com/watch?v=D1WWhQY9N4g

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Brief summary

- Exploration vs. exploitation (sticking to known stuff vs. exploring something new) is a predominant problem in reinforcement learning
- There exist multiple methods with different implementation complexity favoring exploration
- A good overview of different methods is provided here

Kahoot!

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