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Lecture ~~9~~: Exploration and Exploitation

Slides from David Silver

How to plan when you know how your actions affect your environment?

MDP lectures

How to learn from data about how your environment works?

Machine Learning lectures

How to trade off collecting data vs. accomplishing goals?

Today (also VPI lecture)

Putting it all together:

RL lectures next week

Exploration vs. Exploitation Dilemma

- Online decision-making involves a fundamental choice:
  - Exploitation: Make the best decision given current information
  - Exploration: Gather more information
- The best long-term strategy may involve short-term sacrifices
- Gather enough information to make the best overall decisions

Examples

- Restaurant Selection

  Exploitation Go to your favourite restaurant
  Exploration Try a new restaurant

- Online Banner Advertisements

  Exploitation Show the most successful advert
  Exploration Show a different advert

- Oil Drilling

  Exploitation Drill at the best known location
  Exploration Drill at a new location

- Game Playing

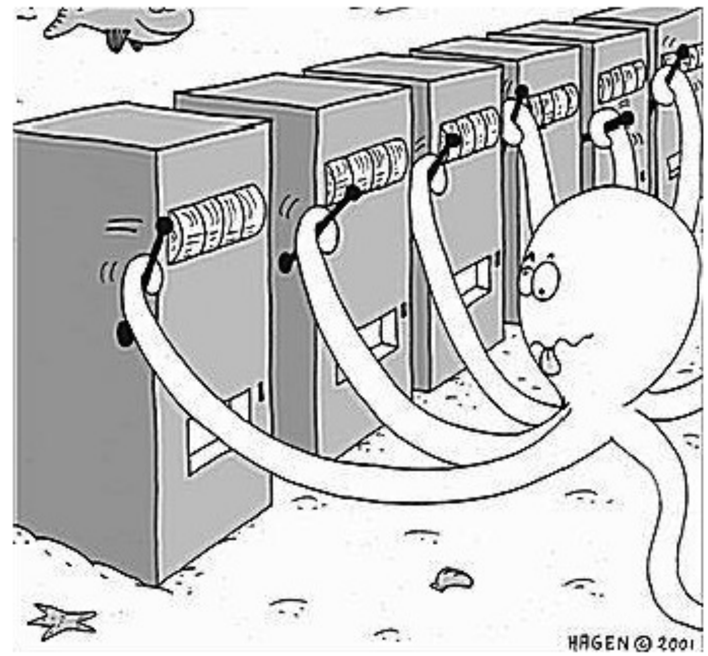
  Exploitation Play the move you believe is best
  Exploration Play an experimental move

Principles

- Naive Exploration
    - Add noise to greedy policy (e.g. ϵ-greedy)
- Optimistic Initialisation
    - Assume the best until proven otherwise
- Optimism in the Face of Uncertainty
    - Prefer actions with uncertain values
- Probability Matching
    - Select actions according to probability they are best

The Multi-Armed Bandit

- A multi-armed bandit is a tuple $\langle \mathcal{A}, \mathcal{R} \rangle$
- $\mathcal{A}$ is a known set of m actions (or "arms")
- $\mathcal{R}^a(r) = \mathbb{P}[r|a]$ is an unknown probability distribution over rewards
- At each step t the agent selects an action $a_t \in \mathcal{A}$
- The environment generates a reward $r_t \sim \mathcal{R}^{a_t}$
- The goal is to maximise cumulative reward $\sum_{\tau=1}^{t} r_\tau$



Regret

- The *action-value* is the mean reward for action a,

$$Q(a) = \mathbb{E}\left[r|a\right]$$

- The *optimal value* V^* is

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

- The *regret* is the opportunity loss for one step

$$l_t = \mathbb{E}\left[V^* - Q(a_t)\right]$$

Algorithm for selecting a_t may have randomness

- The *total regret* is the total opportunity loss

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

- Maximise cumulative reward $\equiv$ minimise total regret

Counting Regret

Algorithm for selecting a_t may have randomness

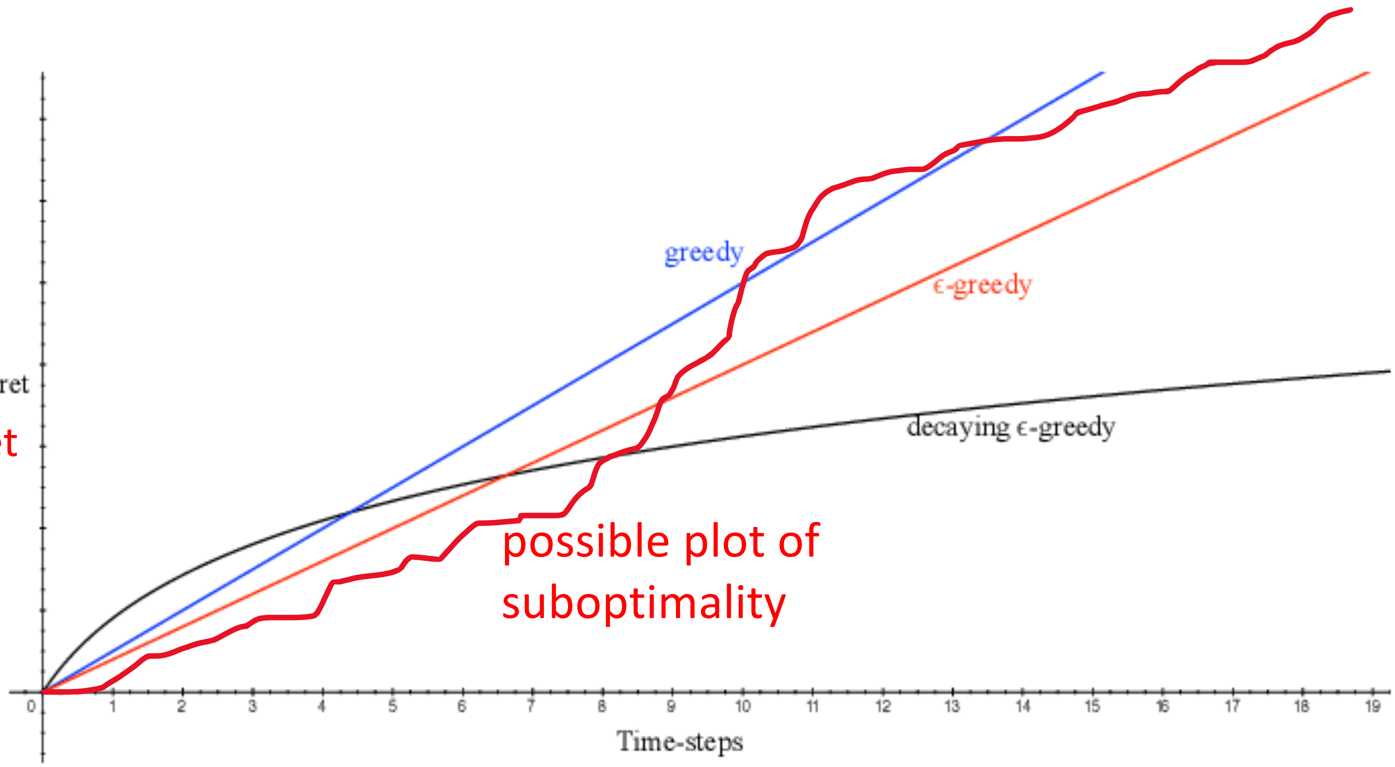
- The *count* $N_t(a)$ is expected number of selections for action a
- The *gap* Δ_a is the difference in value between action a and optimal action a^*, $\Delta_a = V^* - Q(a)$
- Regret is a function of gaps and the counts

$$
\begin{aligned}
L_t &= \mathbb{E}\left[\sum_{\tau=1}^{t} V^* - Q(a_\tau)\right] \\
&= \sum_{a \in \mathcal{A}} \mathbb{E}\left[N_t(a)\right] \left(V^* - Q(a)\right) \\
&= \sum_{a \in \mathcal{A}} \mathbb{E}\left[N_t(a)\right] \Delta_a
\end{aligned}
$$

- A good algorithm ensures small counts for large gaps
- Problem: gaps are not known!

Linear or Sublinear Regret

Remember regret is *expectation* of suboptimality



- If an algorithm forever explores it will have linear total regret
- If an algorithm never explores it will have linear total regret
- Is it possible to achieve sublinear total regret?

Greedy Algorithm

```
action_counts = [0 for a in range(n_actions)]
total_reward_per_action = [0 for a in range(n_actions)]

for t in range(inf):
        Qhat_a = [total_reward_per_action[a] / action_counts[a] for a in range(n_actions)]
        a_t = argmax(Qhat_a)
        r_t = take_action_and_get_random_reward(a_t)
        action_counts[a_t] += 1
        total_reward_per_action[a_t] += r_t
```

Greedy Algorithm

- We consider algorithms that estimate $\hat{Q}_t(a) \approx Q(a)$
- Estimate the value of each action by Monte-Carlo evaluation

$$\hat{Q}_t(a) = \frac{1}{N_t(a)} \sum_{t=1}^{T} r_t \mathbf{1}(a_t = a)$$

- The *greedy* algorithm selects action with highest value

$$a_t^* = \underset{a \in \mathcal{A}}{\operatorname{argmax}}\, \hat{Q}_t(a)$$

- Greedy can lock onto a suboptimal action forever
- $\Rightarrow$ Greedy has linear total regret

Regret

- The *action-value* is the mean reward for action a,

$$Q(a) = \mathbb{E}[r|a]$$

- The *optimal value* V^* is

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

- The *regret* is the opportunity loss for one step

$$l_t = \mathbb{E}[V^* - Q(a_t)]$$

- The *total regret* is the total opportunity loss

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

- The *gap* Δ_a is the difference in value between action a and optimal action a^*, $\Delta_a = V^* - Q(a)$

Actual rewards don't affect what we call regret.

Regret is only a function of the actions and the *expected* payout of those actions.

ϵ-Greedy Algorithm

- The ϵ-*greedy* algorithm continues to explore forever
  - With probability $1 - \epsilon$ select $a = \underset{a \in \mathcal{A}}{\operatorname{argmax}} \hat{Q}(a)$
  - With probability ϵ select a random action
- Constant ϵ causes a positive lower bound on regret :(

$$l_t \geq \frac{\epsilon}{\mathcal{A}} \sum_{a \in \mathcal{A}} \Delta_a$$

- $\Rightarrow$ ϵ-greedy has linear total regret

ϵ-Greedy Algorithm

```
action_counts = [0 for a in range(n_actions)]
total_reward_per_action = [0 for a in range(n_actions)]

for t in range(inf):
        Qhat_a = [total_reward_per_action[a] / action_counts[a] for a in range(n_actions)]
        a_t = argmax(Qhat_a)
        if random_uniform_between_0_and_1() < epsilon:
                a_t = random_action(n_actions)
        r_t = take_action_and_get_random_reward(a_t)
        action_counts[a_t] += 1
        total_reward_per_action[a_t] += r_t
```

Optimistic Initialisation

- Simple and practical idea: initialise $Q(a)$ to high value
- Update action value by incremental Monte-Carlo evaluation
- Starting with $N(a) > 0$

$$\hat{Q}_t(a_t) = \hat{Q}_{t-1} + \frac{1}{N_t(a_t)}(r_t - \hat{Q}_{t-1})$$

- Encourages systematic exploration early on
- But can still lock onto suboptimal action
- $\Rightarrow$ greedy + optimistic initialisation has linear total regret
- $\Rightarrow$ ϵ-greedy + optimistic initialisation has linear total regret

Optimistic Initialisation

```
action_counts = [5 for a in range(n_actions)]
total_reward_per_action = [10 for a in range(n_actions)]

for t in range(inf):
        Qhat_a = [total_reward_per_action[a] / action_counts [a] for a in range(n_actions)]
        a_t = argmax(Qhat_a)
        if random_uniform_between_0_and_1() < epsilon:
                a_t = random_action(n_actions)
        r_t = take_action_and_get_random_reward(a_t)
        action_counts[a_t] += 1
        total_reward_per_action[a_t] += r_t
```

Decaying ϵ_t-Greedy Algorithm

- Pick a decay schedule for $\epsilon_1, \epsilon_2, ...$
- Consider the following schedule

$$c > 0$$
$$d = \min_{a|\Delta_a>0} \Delta_i$$
$$\epsilon_t = \min \left\{ 1, \frac{c|\mathcal{A}|}{d^2 t} \right\}$$

- Decaying ϵ_t-greedy has *logarithmic* asymptotic total regret!
- Unfortunately, schedule requires advance knowledge of gaps
- Goal: find an algorithm with sublinear regret for any multi-armed bandit (without knowledge of $\mathcal{R}$)

Decaying ϵ_t-Greedy Algorithm

```
action_counts = [0 for a in range(n_actions)]
total_reward_per_action = [0 for a in range(n_actions)]

for t in range(inf):
        Qhat_a = [total_reward_per_action[a] / action_counts[a] for a in range(n_actions)]
        a_t = argmax(Qhat_a)
        epsilon_t = min{1, starting_epsilon / (t+1)}
        if random_uniform_between_0_and_1() < epsilon_t:
                a_t = random_action(n_actions)
        r_t = take_action_and_get_random_reward(a_t)
        action_counts[a_t] += 1
        total_reward_per_action[a_t] += r_t
```

Lower Bound

- The performance of any algorithm is determined by similarity between optimal arm and other arms
- Hard problems have similar-looking arms with different means
- This is described formally by the gap Δ_a and the similarity in distributions $KL(\mathcal{R}^a || \mathcal{R}^{a^*})$

Theorem (Lai and Robbins)

Asymptotic total regret is at least logarithmic in number of steps

expected reward of best action - expected reward of a

For large enough *t*:

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

a measure of how different the reward distributions are

Regret

- The *action-value* is the mean reward for action a,

$$Q(a) = \mathbb{E}[r|a]$$

- The *optimal value* V^* is

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

- The *regret* is the opportunity loss for one step

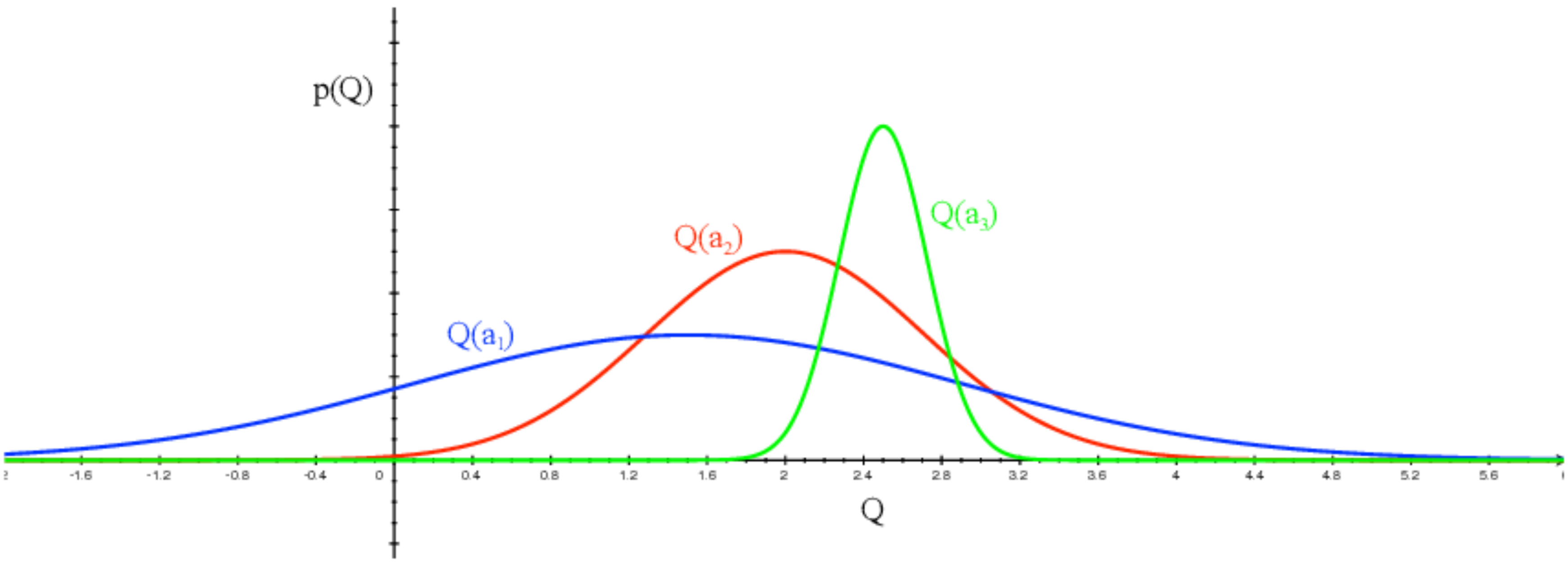
$$l_t = \mathbb{E}[V^* - Q(a_t)]$$

- The *total regret* is the total opportunity loss

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

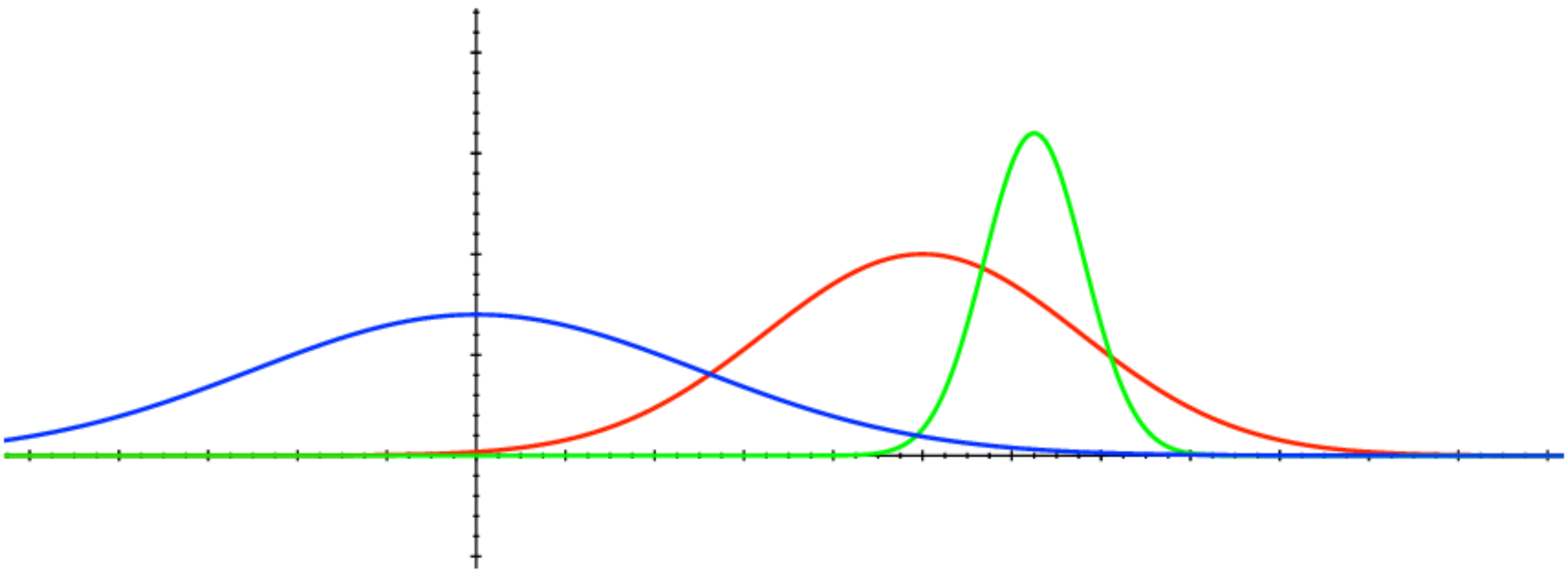
- The *gap* Δ_a is the difference in value between action a and optimal action a^*, $\Delta_a = V^* - Q(a)$

Optimism in the Face of Uncertainty



- Which action should we pick?
- The more uncertain we are about an action-value
- The more important it is to explore that action
- It could turn out to be the best action

Optimism in the Face of Uncertainty (2)



- After picking blue action
- We are less uncertain about the value
- And more likely to pick another action
- Until we home in on best action

Upper Confidence Bounds

- Estimate an upper confidence $\hat{U}_t(a)$ for each action value
- Such that $Q(a) \leq \hat{Q}_t(a) + \hat{U}_t(a)$ with high probability
- This depends on the number of times $N(a)$ has been selected
  - Small $N_t(a) \Rightarrow$ large $\hat{U}_t(a)$ (estimated value is uncertain)
  - Large $N_t(a) \Rightarrow$ small $\hat{U}_t(a)$ (estimated value is accurate)
- Select action maximising Upper Confidence Bound (UCB)

$$a_t = \operatorname*{argmax}_{a \in \mathcal{A}} \hat{Q}_t(a) + \hat{U}_t(a)$$

Hoeffding's Inequality

Theorem (Hoeffding's Inequality)

Let $X_1, ..., X_t$ be i.i.d. random variables in [0,1], and let $\overline{X}_t = \frac{1}{\tau} \sum_{\tau=1}^{t} X_\tau$ be the sample mean. Then

$$\mathbb{P}\left[\mathbb{E}\left[X\right] > \overline{X}_t + u\right] \leq e^{-2tu^2}$$

- We will apply Hoeffding's Inequality to rewards of the bandit
- conditioned on selecting action a

$$\mathbb{P}\left[Q(a) > \hat{Q}_t(a) + U_t(a)\right] \leq e^{-2N_t(a)U_t(a)^2}$$

Calculating Upper Confidence Bounds

- Pick a probability p that true value exceeds UCB
- Now solve for $U_t(a)$

$$e^{-2N_t(a)U_t(a)^2} = p$$

$$U_t(a) = \sqrt{\frac{-\log p}{2N_t(a)}}$$

- Reduce p as we observe more rewards, e.g. $p = t^{-4}$
- Ensures we select optimal action as $t \to \infty$

$$U_t(a) = \sqrt{\frac{2\log t}{N_t(a)}}$$

UCB1

- This leads to the UCB1 algorithm

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

Theorem

The UCB algorithm achieves logarithmic asymptotic total regret

For large enough *t*: $$L_t \leq 8 \log t \sum_{a|\Delta_a>0} \Delta_a$$

UCB1

```
action_counts = [0 for a in range(n_actions)]
total_reward_per_action = [0 for a in range(n_actions)]

for t in range(inf):
        Qhat_a = [total_reward_per_action[a] / action_counts[a] for a in range(n_actions)]
        Qoptimist_a = [Qhat_a[a] + sqrt(2 log t / action_counts[a]) for a in range(n_actions)]
        a_t = argmax(Qoptimist_a)
        r_t = take_action_and_get_random_reward(a_t)
        action_counts[a_t] += 1
        total_reward_per_action[a_t] += r_t
```

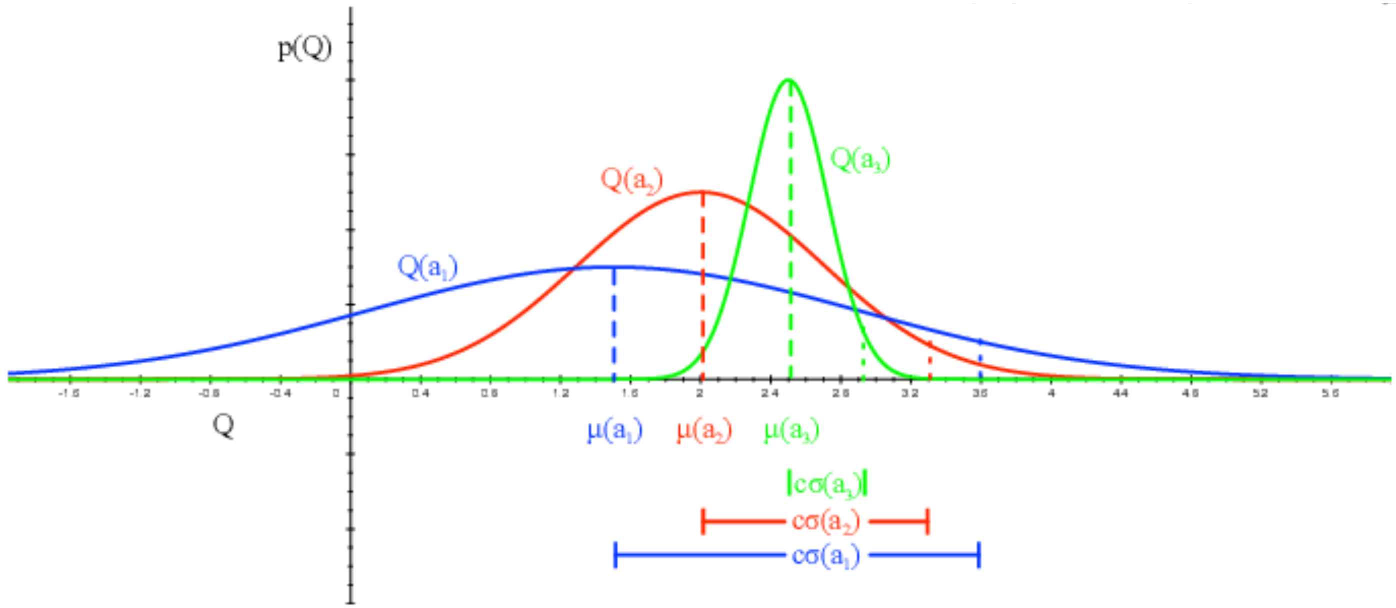
Why optimism?

- If you're optimistic when you don't know…
  - you check it out and learn the truth
- If you're pessimistic when you don't know…
  - you never check it out and never learn the truth
- Definition of *admissible* for a heuristic?
- If there's one environment with lots of dangers and another environment with no major dangers…
  - Which environment would you rather be optimistic in? Which environment would you rather be pessimistic in?

Bayesian Bandits

- So far we have made no assumptions about the reward distribution $\mathcal{R}$
  - Except bounds on rewards
- Bayesian bandits exploit prior knowledge of rewards, $p[\mathcal{R}]$
- They compute posterior distribution of rewards $p[\mathcal{R} \mid h_t]$
  - where $h_t = a_1, r_1, ..., a_{t-1}, r_{t-1}$ is the history
- Use posterior to guide exploration
  - Upper confidence bounds (Bayesian UCB)
  - Probability matching (Thompson sampling)
- Better performance if prior knowledge is accurate

Bayesian UCB Example: Independent Gaussians



- Maintain Gaussian probability distributions over the expected reward for each action
- Choose the action that maximizes mean + c * standard deviation

Probability Matching

- Probability matching selects action a according to probability that a is the optimal action

$$\pi(a \mid h_t) = \mathbb{P}\left[Q(a) > Q(a'), \forall a' \neq a \mid h_t\right]$$

- Probability matching is optimistic in the face of uncertainty
  - Uncertain actions have higher probability of being max
- Can be difficult to compute analytically from posterior

Thompson Sampling

- Thompson sampling implements probability matching

$$\begin{aligned} \pi(a \mid h_t) &= \mathbb{P}\left[Q(a) > Q(a'), \forall a' \neq a \mid h_t\right] \\ &= \mathbb{E}_{\mathcal{R}|h_t}\left[\mathbf{1}(a = \operatorname*{argmax}_{a \in \mathcal{A}} Q(a))\right] \end{aligned}$$

- Use Bayes law to compute posterior distribution $p\left[\mathcal{R} \mid h_t\right]$
- Sample a reward distribution $\mathcal{R}$ from posterior
- Compute action-value function $Q(a) = \mathbb{E}\left[\mathcal{R}_a\right]$
- Select action maximising value on sample, $a_t = \operatorname*{argmax}_{a \in \mathcal{A}} Q(a)$
- Thompson sampling achieves Lai and Robbins lower bound!

Value of Information

- Exploration is useful because it gains information
- Can we quantify the value of information?
  - How much reward a decision-maker would be prepared to pay in order to have that information, prior to making a decision
  - Long-term reward after getting information - immediate reward
- Information gain is higher in uncertain situations
- Therefore it makes sense to explore uncertain situations more
- If we know value of information, we can trade-off exploration and exploitation *optimally*

Contextual Bandits

- A contextual bandit is a tuple $\langle \mathcal{A}, \mathcal{S}, \mathcal{R} \rangle$
- $\mathcal{A}$ is a known set of actions (or "arms")
- $\mathcal{S} = \mathbb{P}[s]$ is an unknown distribution over states (or "contexts")
- $\mathcal{R}_s^a(r) = \mathbb{P}[r|s, a]$ is an unknown probability distribution over rewards
- At each step t
  - Environment generates state $s_t \sim \mathcal{S}$
  - Agent selects action $a_t \in \mathcal{A}$
  - Environment generates reward $r_t \sim \mathcal{R}_{s_t}^{a_t}$
- Goal is to maximise cumulative reward $\sum_{\tau=1}^{t} r_\tau$

Linear Regression

How many of each kind of movie has the user watched?					Properties of recommended movie					
Oscar winner	Will Farrell vibes	Action	Slow pace	Docu-mentary	Num Oscar noms	Year made	Will Farrell vibes	Slow pace	Act-ion	Reward
0	0	2	0	0	2	2020	0	1	0	0
1	0	0	0	3	0	2017	0	0	0	0
1	0	0	1	0	5	1999	0	1	0	0
0	0	0	0	0	0	2008	1	0	0	1
0	1	0	0	0	0	2012	1	0	1	1
0	0	2	0	0	0	2024	0	0	1	-1

$\phi(s_T, a_T)$

Reward: 0 for not clicking; 1 for watching; -1 for watching part and quitting

Linear Regression

- Action-value function is expected reward for state s and action a

$$Q(s,a) = \mathbb{E}\left[r | s, a\right]$$

- Estimate value function with a linear function approximator

$$Q_\theta(s,a) = \phi(s,a)^\top \theta \approx Q(s,a)$$

- Estimate parameters by least squares regression

$$A_t = \sum_{\tau=1}^{t} \phi(s_\tau, a_\tau)\phi(s_\tau, a_\tau)^\top$$

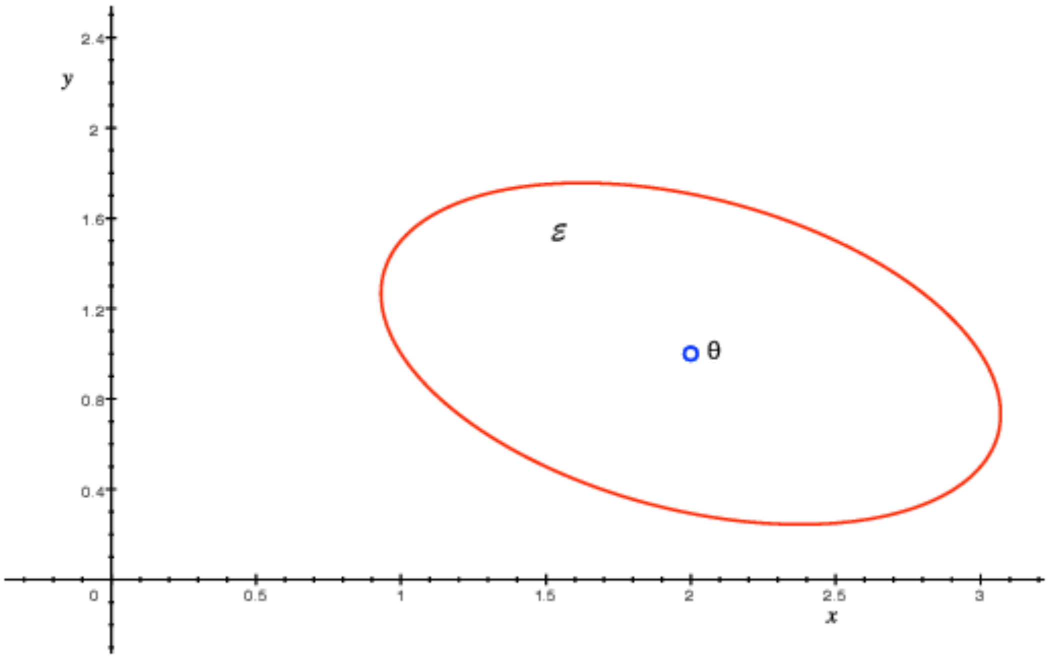
$$b_t = \sum_{\tau=1}^{t} \phi(s_\tau, a_\tau) r_\tau$$

$$\theta_t = A_t^{-1} b_t$$

Linear Upper Confidence Bounds

- Least squares regression estimates the mean action-value $Q_\theta(s, a)$
- But it can also estimate the variance of the action-value $\sigma^2_\theta(s, a)$ *sklearn.linear_model.BayesianRidge.predict() returns both*
- i.e. the uncertainty due to parameter estimation error
- Add on a bonus for uncertainty, $U_\theta(s, a) = c\sigma$
- i.e. define UCB to be c standard deviations above the mean

Geometric Interpretation



- Define confidence ellipsoid $\mathcal{E}_t$ around parameters θ_t
- Such that $\mathcal{E}_t$ includes true parameters θ^* with high probability
- Use this ellipsoid to estimate the uncertainty of action values
- Pick parameters within ellipsoid that maximise action value

$$\underset{\theta \in \mathcal{E}}{\operatorname{argmax}} \; Q_\theta(s, a)$$

Exploration/Exploitation Principles to MDPs

The same principles for exploration/exploitation apply to MDPs

Reinforcement Learning: Unknown MDPs

- We've seen how to compute the optimal policy in a known MDP
- We've just discussed a bandit setting with one state (no transitions)
  - But the reward function is unknown
- What if we are in an MDP, but we don't know the transition function *or* the reward function?

Greedy (And Slow) RL Algorithm

- Finite state space, finite action space
- For simplicity, say reward only depends on new state

```
transition_counts = array of zeros of size S x A x S
state_counts = array of zeros of size S
rewards_by_state = array of zeros of size S
s = get_initial_state()
while True:
        transition_matrix = estimate_T(transition_counts)
        reward_function = estimate_R(state_counts, rewards_by_state)
        policy = solve_mdp(transition_matrix, reward_function)        # expensive!
        a = policy[s]
        s’, r = get_next_state_and_reward(s, a)
        transition_counts[s][a][s’] += 1
        state_counts[s’] += 1
        rewards_by_state[s’] += r
```

Optimistic Initialisation: Model-Based RL

- Construct an optimistic model of the MDP
- Initialise transitions to go to heaven
  - (i.e. transition to terminal state with r_{max} reward)
- Solve optimistic MDP by favourite planning algorithm
  - policy iteration
  - value iteration
  - tree search
  - ...
- Encourages systematic exploration of states and actions
- e.g. RMax algorithm (Brafman and Tennenholtz)

(Slightly modified) Rmax Algorithm

```
transition_counts = array of zeros of size (S+1) x A x (S+1)
state_counts = array of zeros of size S+1
rewards_by_state = array of zeros of size S+1
rewards_by_state[-1] = rmax                    # maximum possible reward (“heaven state”)
state_counts[-1] = 1
for s in range(S+1):
        for a in range(A):
                transition_counts[s][a][-1] += 1    # pretend we’ve seen transition to heaven
s = get_initial_state()
while True:
        transition_matrix = estimate_T(transition_counts)        # real Rmax waits to update
                                                                   until count is high enough
        reward_function = estimate_R(state_counts, rewards_by_state)
        policy = solve_mdp(transition_matrix, reward_function)
        a = policy[s]
        s’, r = get_next_state_and_reward(s, a)
        transition_counts[s][a][s’] += 1
        state_counts[s’] += 1
        rewards_by_state[s’] += r
```