Exploration: Contextual & Bayesian Bandits, Thompson Sampling

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Adapted from Wen Sun's slides

Recap

Exploration: the Big Pain of RL

We need to carefully and systematically explore (remember states we visited, and try to visit unexplored regions)

Exploration-Exploitation Trade-off: should we make the best decision given current information, or should we collect more information? In other words: should I sacrifice something now to get more in the future? (chicken-egg problem)

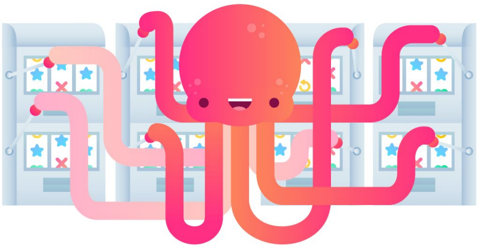
e.g., go to my favourite restaurant vs try a new one

Multi-Armed Bandit

Let's consider a simplified MDP to analyze exploration: **Multi-Armed Bandits**

- One single state
- K different arms (think of them as actions): $a_1, \ldots, a_k$
- Each arm has unknown reward distribution ν_i with mean $\mu_i = \mathbb{E}_{r\sim\nu_i}[r]$
- Every time we pull an arm we observe an i.i.d. reward

Multi-Armed Bandit: Interaction



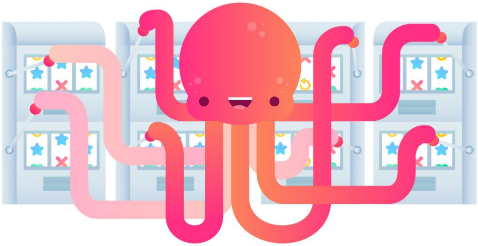
The interactive process that we deal with in MAB is the following:

For $t = 0, \ldots, T-1$:

1. Pull an arm I_t in $\{1, \ldots, K\}$ based on historical information
2. Observe i.i.d. reward $r_i \sim \nu_i$ of arm I_t (we do not observe rewards of untried arms)

But what are we trying to optimize exactly? **REGRET!**

Regret



We want to minimize our **opportunity loss**, which is expressed in the form of the regret

The regret is the **total expected reward if we pull the best arm for T rounds** VS the **total expected reward of the arms we pulled over T rounds**

$$\text{Regret}_T = \boxed{T\mu^\star} - \boxed{\sum_{t=0}^{T-1} \mu_{I_t}}$$

$$\mu^\star = \max_{i \in [K]} \mu_i$$

Greedy Algorithm

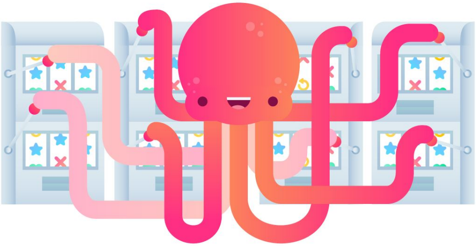
Algorithm:

- try each arm once
- commit to the one that has the highest observed reward

Problem: a (bad) arm with low μ_i may generate a high reward by chance, as we sample $r_i \sim \nu_i$ and it's i.i.d.

Consider two arms a_1, a_2: Reward dist for a_1: prob 60%: 1, else 0; for a_2: prob 40% 1, else 0. Now: a_1 is clearly better but with prob 16% we can observe (0, 1)

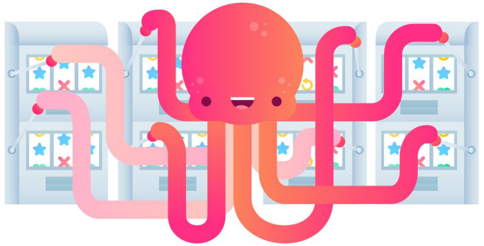
Explore & Commit Algorithm



1. Set $N = T/K$, where $T \gg K$ and K is the number of arms
2. For $k = 1, \ldots, K$: **(explore)**
   - pull arm k for N times
   - observe the set $\{r_i\}_{i=1}^{N} \sim \nu_i$
   - compute the empirical mean $\hat{\mu}_k = \sum_{i=1}^{N} r_i / N$
3. For $t = NK, \ldots, T$: **(commit)**
   - pull the best empirical arm

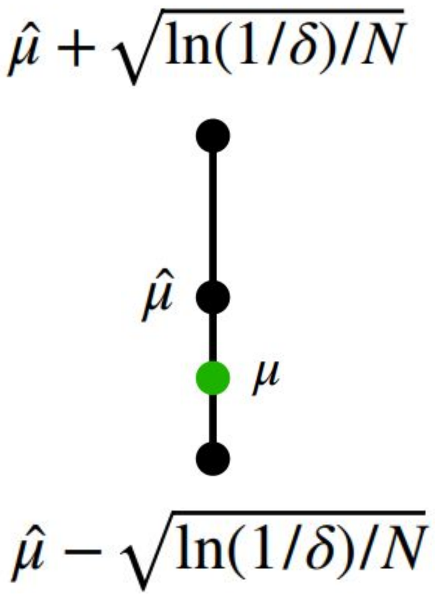
$$I_t = \arg\max_{i \in [K]} \hat{\mu}_i$$

Hoeffding Inequality



Do we have a confidence interval on our empirical mean? <u>During exploration, for each arm</u>, given a distribution with mean μ and N i.i.d. samples, we have with probability 1-δ:

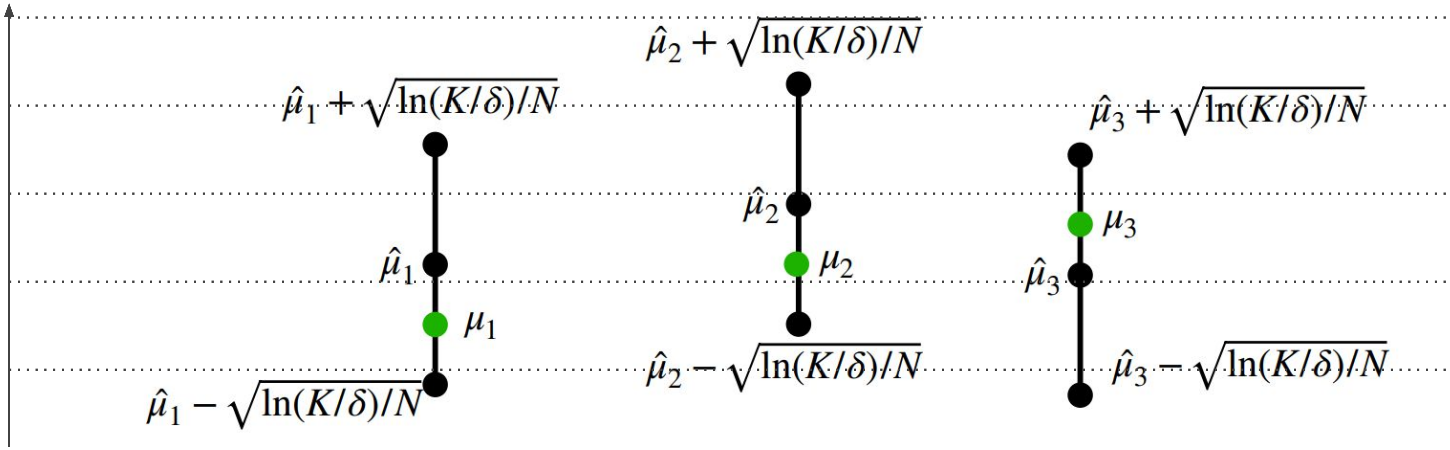
$$\left| \sum_{i=1}^{N} r_i/N - \mu_i \right| \leq O\left(\sqrt{\frac{\ln(1/\delta)}{N}}\right)$$

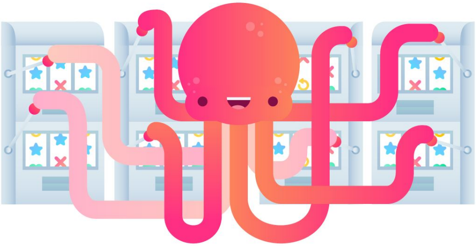


e.g., δ = 0.01, confidence bound holds with probability 99%

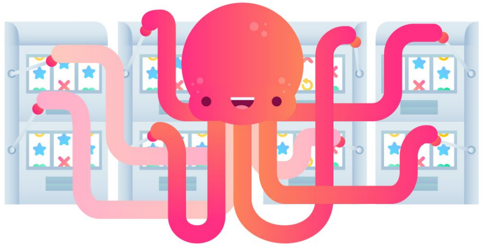
Hoeffding Inequality

Do we have a confidence interval on our empirical mean? During exploitation, for all arms, given a distribution with mean μ and N i.i.d. samples, we have with probability 1-δ:





Regret Calculation



- Empirical best arm:

$$\hat{I} = \arg\max_{i \in [K]} \hat{\mu}_i$$

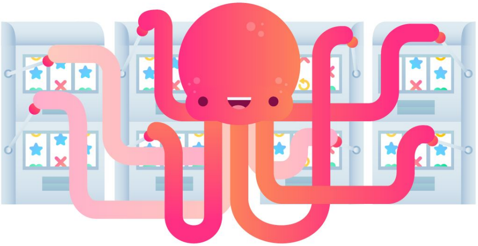
- Best arm:

$$I^\star = \arg\max_{i \in [K]} \mu_i$$

Total regret: $\mathrm{Regret}_T = \mathrm{Regret}_{explore} + \mathrm{Regret}_{exploit} \leq NK + 2T\sqrt{\frac{\ln(K/\delta)}{N}}$

To minimize our regret, we want to optimize N: take the gradient of the regret, set it to 0, solve for N

Regret Calculation



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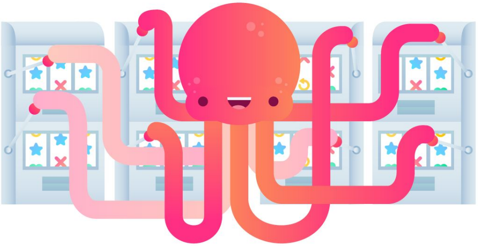
Total regret: $\text{Regret}_T = \text{Regret}_{explore} + \text{Regret}_{exploit} \leq NK + 2T\sqrt{\frac{\ln(K/\delta)}{N}}$

$$N = \left(\frac{T\sqrt{\ln(K/\delta)}}{2K}\right)^{2/3} \qquad \text{Regret}_T \leq O\left(T^{2/3}K^{1/3} \cdot \ln^{1/3}(K/\delta)\right)$$

Approaches 0 as T goes to infinite

Regret Decaying



The decaying rate of the regret using the explore & commit algorithm is kind of slow ($T^{2/3}$). Can we get something faster, like $O(\sqrt{T})$?

$O(\sqrt{T})$ is actually the minimum we can get as it is a lower bound (no algorithm ever will be faster than this)

Let's try to design a new algorithm

Statistics to Maintain & Confidence

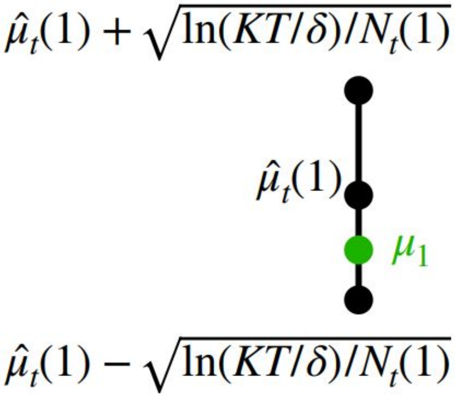
Let's write a list of generic statistics that we need to maintain in order to compute our confidence bounds and the regret

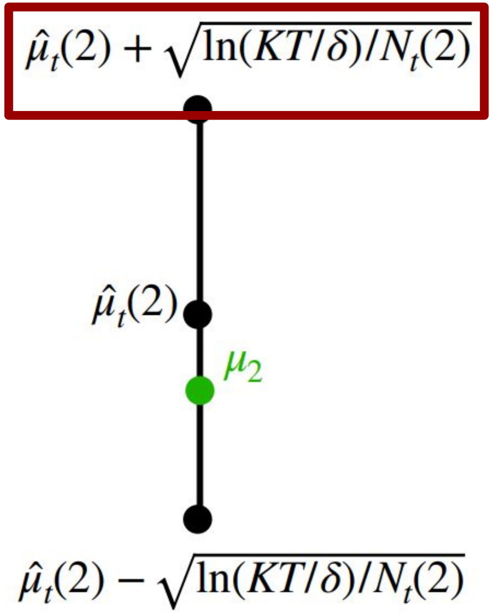
- # of times we have tried arm i $N_t(i) = \sum_{\tau=0}^{t-1} \mathbf{1}\{I_\tau = i\}$
- empirical mean so far $\hat{\mu}_t(i) = \sum_{\tau=0}^{t-1} \mathbf{1}\{I_\tau = i\} r_\tau / N_t(i)$

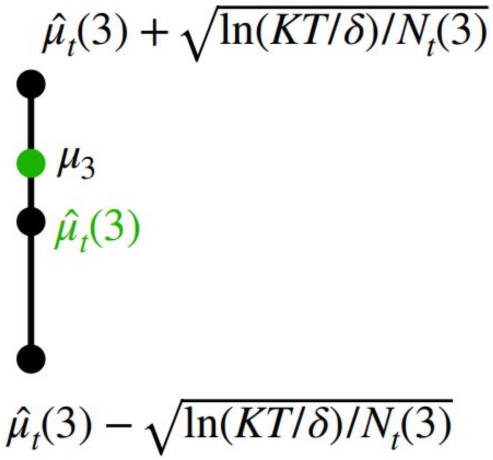
Confidence with probability 1-δ: $|\hat{\mu}_t(i) - \mu_i| \leq \sqrt{\dfrac{\ln(KT/\delta)}{N_t(i)}}$

Optimism in the Face of Uncertainty

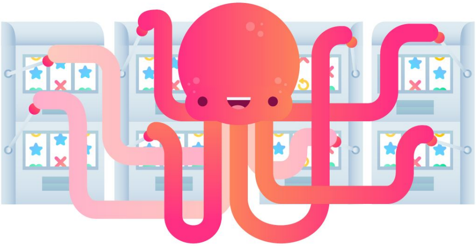
Let's pick the arm with the highest upper confidence bound (top of the confidence interval)







UCB Algorithm



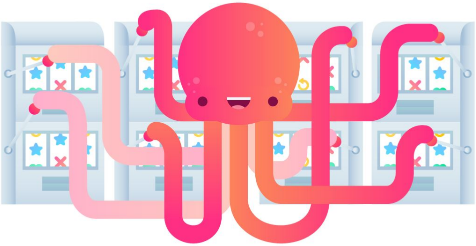
- For the first K iterations, pull each arm once
- For t = K, ..., T:
  - pick the action with the highest upper confidence bound

$$I_t = \arg\max_{i \in [K]} \left(\hat{\mu}_t(i) + \boxed{\sqrt{\frac{\ln(KT/\delta)}{N_t(i)}}} \right)$$

  - update statistics

Reward bonus is high if we did not try action many times: exploration

UCB Algorithm: Regret



$$\text{Regret-at-t} = \mu^\star - \mu_{I_t} \le \hat{\mu}_t(I_t) + \sqrt{\frac{\ln(TK/\delta)}{N_t(I_t)}} - \mu_{I_t} \le 2\sqrt{\frac{\ln(TK/\delta)}{N_t(I_t)}}$$

$$\text{Regret}_T = \sum_{t=0}^{T-1}\left(\mu^\star - \mu_{I_t}\right) \le \sum_{t=0}^{T-1} 2\sqrt{\frac{\ln(TK/\delta)}{N_t(I_t)}} \le 2\sqrt{\ln(TK/\delta)} \cdot \sum_{t=0}^{T-1}\sqrt{\frac{1}{N_t(I_t)}}$$

$$\sum_{t=0}^{T-1}\sqrt{\frac{1}{N_t(I_t)}} \le O\left(\sqrt{KT}\right) \longrightarrow$$ **With high probability** $\text{Regret}_T = \widetilde{O}\left(\sqrt{KT}\right)$

See also
https://wensun.github.io/CS4789_data/UCB_note_new.pdf

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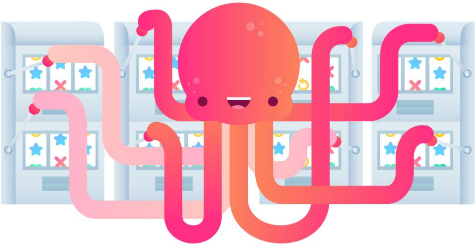
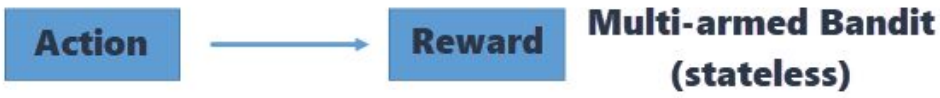
End Recap

From Multi-Armed to Contextual Bandits





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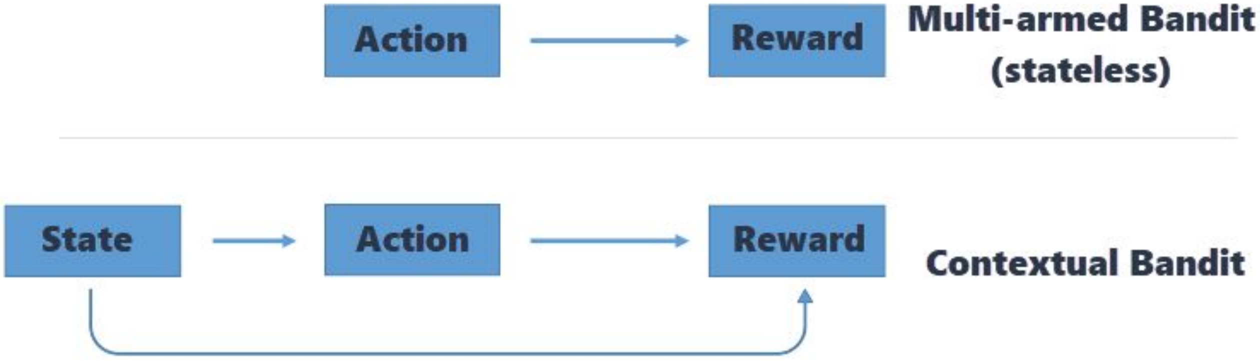
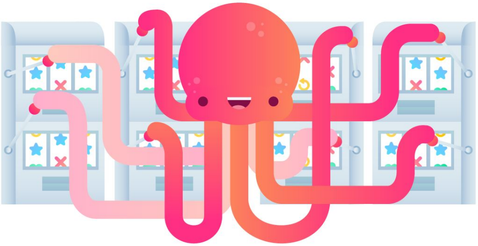


Contextual bandits add some context (state)

Contextual Bandits: Interaction

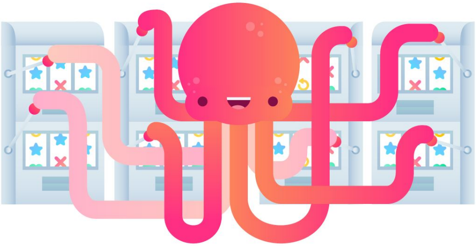


The interactive process that we deal with in CB is the following:

For t = 0, ..., T-1:

1. A new i.i.d. context x_t in X appears
2. Select an action a_t in A based on historical information and context
3. Observe reward $r(x_t,a_t)$ (which is context and arm dependent)

Contextual Bandits: Interaction



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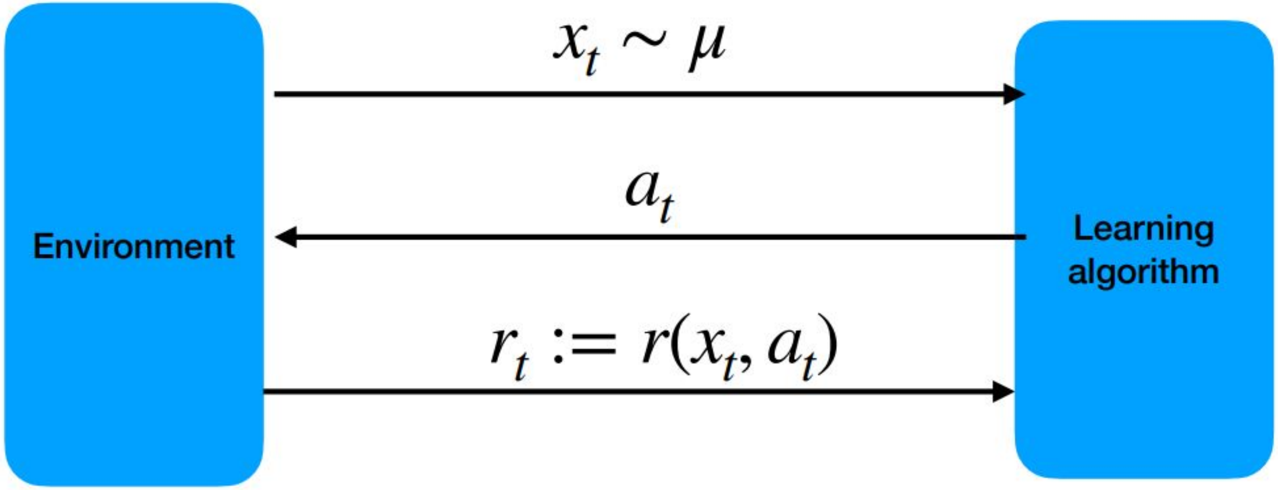
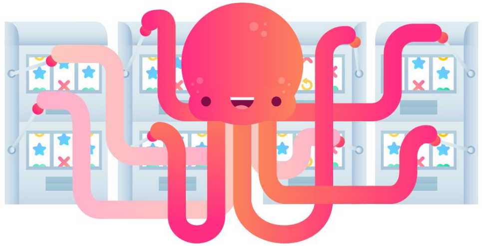
For simplicity we assume deterministic rewards, as the context is the challenge here

Contextual Bandits: Interaction



After we get reward, we start a new iteration: states do not depend on previous actions, they are just sampled in i.i.d. fashion

Contextual Bandits: Example



One domain of application of contextual bandits is recommendation systems:

- Context corresponds to user information (e.g., age, height, weight, job, etc.)
- Arms correspond to items to recommend (e.g., news, movies, etc.)
- Each arm has a click-through-rate (0/1 reward based on click) that we aim to maximize

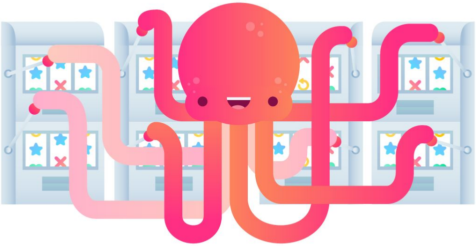
How do we decide which item to propose next, **in personalized way**?

Policy

A policy π:

- is a mapping from (all) states to actions;
- determines how agents select actions;
- can be deterministic ($a = \pi(s)$) or stochastic ($\pi(a|s)$ or $p(a|s)$ or $a \sim \pi(.|s)$)

Contextual Bandits: Regret



Optimal policy: $\pi^\star = \arg\max_{\pi \in \Pi} \mathbb{E}_{x \sim \mu} r(x, \pi(x))$

At every iteration $a_t = \pi_t(x_t)$ is selected and a reward $r(x_t, a_t)$ is received: the regret is the **total expected reward if we always use π^*** VS the **total expected reward if we use our learned sequence of policies**

$$\text{Regret}_T = \boxed{T\mathbb{E}_{x \sim \mu}[r(x, \pi^\star(x))]} - \boxed{\sum_{t=0}^{T-1} \mathbb{E}_{x \sim \mu}[r(x, \pi^t(x))]}$$

Note that policies are different at every iteration t

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Explore & Commit Algorithm

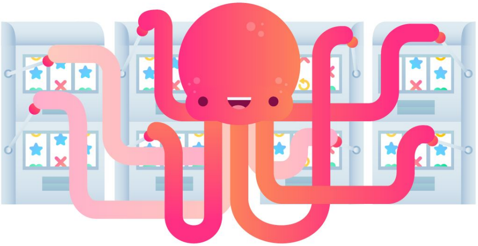
1. For t = 0, ..., N-1: **(explore)** for N iterations
    - observe state $x_t \sim \mu$
    - uniform-randomly sample $a_t \sim \mathrm{Unif}(A)$ choose uniformely random an action from the set of actions A
    - observe reward $r_t = r(x_t, a_t)$
    - build, for x_t, an unbiased estimate of $\mathbb{E}_{a_t \sim p} \hat{\mathbf{r}}[a] = r(x_t, a), \forall a$
2. Compute policy

$$\hat{\pi} = \arg\max_{\pi \in \Pi} \sum_{i=0}^{N-1} \hat{\mathbf{r}}_i[\pi(x_i)]$$

based on the gathered data, create the policy

3. For t = N, ..., T-1: **(commit)** exploit the learned policy
    - observe state $x_t \sim \mu$
    - play arm $a_t = \hat{\pi}(x_t)$

Explore & Commit Algorithm



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2. Compute policy

$$\hat{\pi} = \arg\max_{\pi \in \Pi} \sum_{i=0}^{N-1} \hat{\mathbf{r}}_i[\pi(x_i)]$$

If we know $p(a_t)$, given we sample from p

3. For t = N, ..., T-1: **(commit)**
   - observe state $x_t \sim \mu$
   - play arm $a_t = \hat{\pi}(x_t)$

$$\hat{\mathbf{r}}[a] = \frac{r(x_t, a)\mathbf{1}[a = a_t]}{p(a_t)} \qquad \begin{bmatrix} 0 \\ 0 \\ \cdots \\ r_t/p(a_t) \\ 0, \\ \cdots \\ 0 \end{bmatrix}$$

So if you know the probability of drawing a_t
you use it, otherwise you assume Unif so p(a_t) = 1 / |A|

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Explore & Commit Algorithm

1. For t = 0, ..., N-1: **(explore)**
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2. Compute policy

$$\hat{\pi} = \arg\max_{\pi \in \Pi} \sum_{i=0}^{N-1} \hat{\mathbf{r}}_i[\pi(x_i)]$$

Given we are sampling from $\mathrm{Unif}(A)$

$$\hat{\mathbf{r}}_t[a] = \begin{cases} 0 & a \neq a_t \\ \dfrac{r_t}{1/|\mathcal{A}|} & a = a_t \end{cases}$$

p(a_t) = 1 / |A|

3. For t = N, ..., T-1: **(commit)**
   - observe state $x_t \sim \mu$
   - play arm $a_t = \hat{\pi}(x_t)$

This table is the policy

Sampling from Unif(A). Also the state x_i is chosen randomly

π	action
x_1	a_1
x_2	a_1

these action column is populated at the end of the exercise with the argmax

$t=0$	$t=1$	$t=2$
x_1	x_2	x_1
a_1	a_1	a_2
$r_0 = 1$	$r_1 = 0.5$	$r_2 = 0$
$\hat{r}_0 = \begin{bmatrix} 1 \\ 0.5 \\ 0 \end{bmatrix}$	$\hat{r}_1 = \begin{bmatrix} 0.5 \\ 0.5 \\ 0 \end{bmatrix}$	$\hat{r}_2 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$

$$0.5 = \frac{r}{\frac{1}{|A|}}$$

these are the sum of the reward over time that are associated to x1

x_1

$$\begin{bmatrix} 2 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 2 \\ 0 \end{bmatrix} \leftarrow a_1$$

we choose the argmax

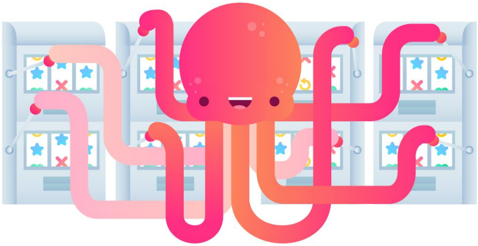
x_2

$$\begin{bmatrix} 1 \\ 0 \end{bmatrix} \leftarrow a_1$$

the index of argmax indicate the index of the action.

In this way we can make the policy

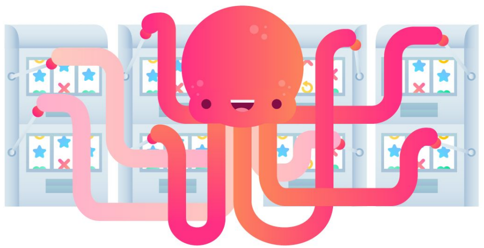
Explore & Commit Algorithm: Regret



$$\text{Regret}_T = T\mathbb{E}_{x\sim\mu}[r(x,\pi^\star(x))] - \sum_{t=0}^{T-1}\mathbb{E}_{x\sim\mu}[r(x,\pi^t(x))] = O\left(T^{2/3}K^{1/3}\cdot\ln(|\Pi|)^{1/3}\right)$$

Regret also depends on the size of the space/class of policies that we are considering

ε-Greedy



Instead of setting a threshold for exploring and then committing, we can try to interleave exploration and exploitation

1. For t = 0, ..., T: **(interleave exploration & exploitation)**
   - observe state $x_t \sim \mu$
   - $a_t \sim p_t = \boxed{(1-\varepsilon)\delta(\pi^t(x_t))} + \boxed{\varepsilon \mathrm{Unif}(A)}$
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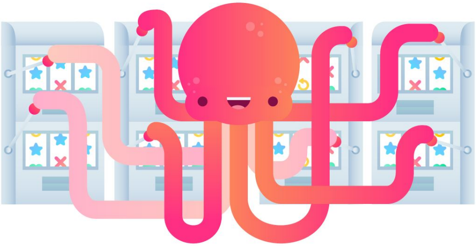
2. Update policy

$$\pi^{t+1} = \arg\max_{\pi \in \Pi} \sum_{i=0}^{t} \hat{\mathbf{r}}_i[\pi(x_i)]$$

ε = 0 -> exploit

ε = 1 -> uniformly explore

ε-Greedy



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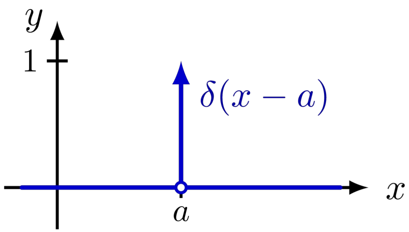
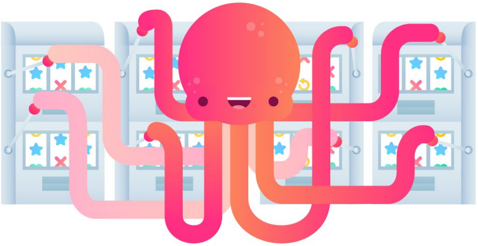
Dirac delta function



ε-Greedy



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Step 3: Gradually decay ε

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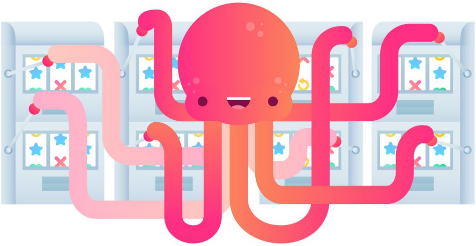
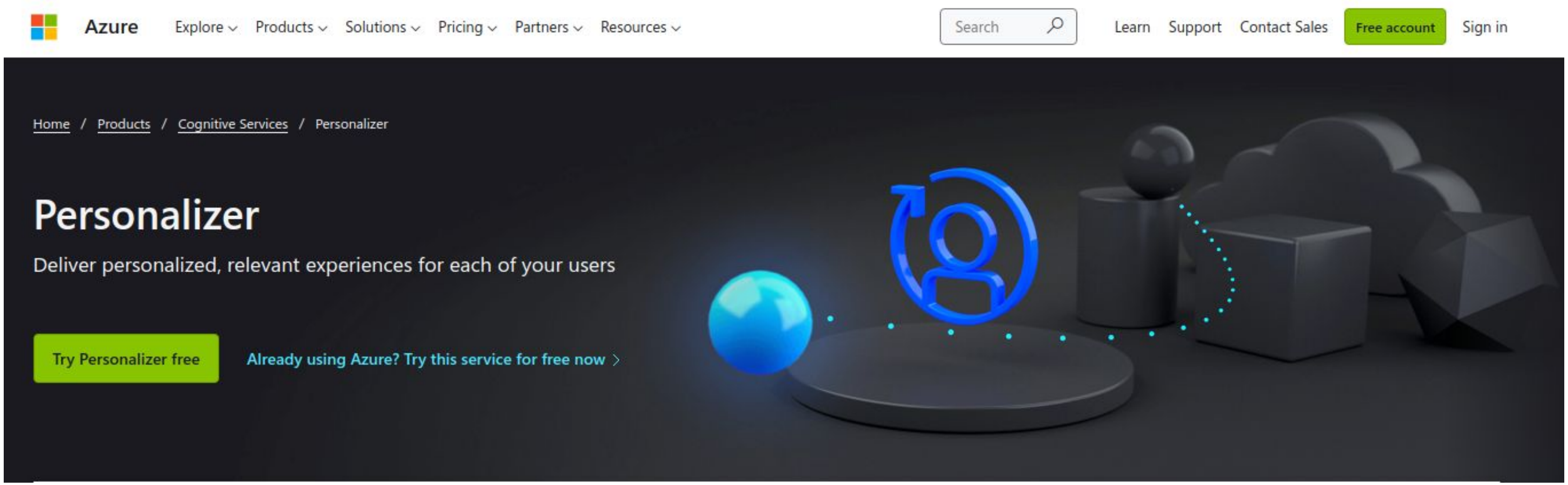
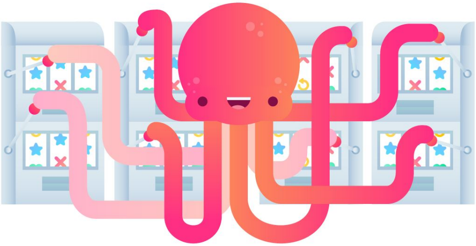
Real World Example



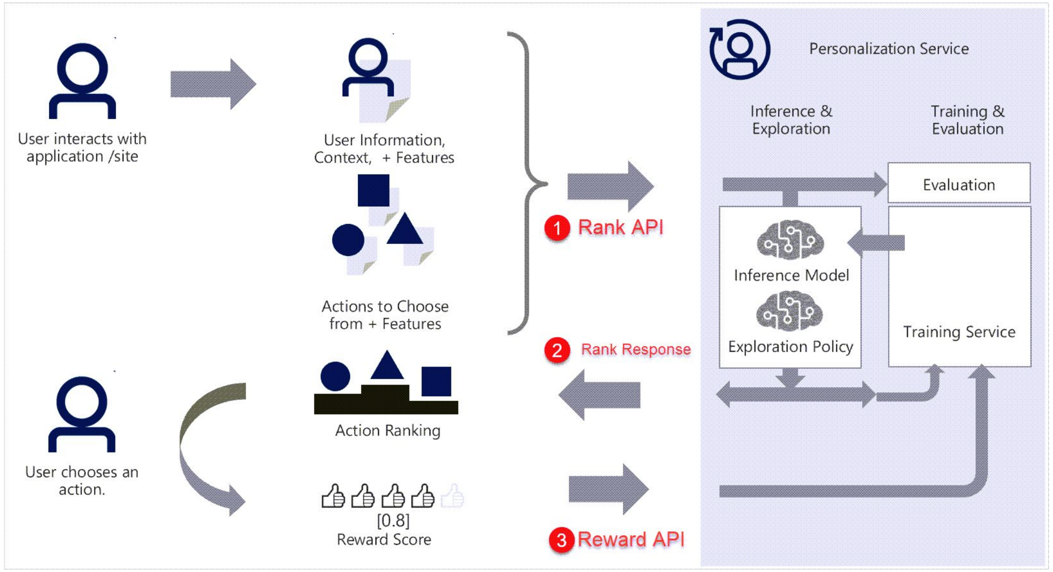
Algorithms for CB are actually used here: https://azure.microsoft.com/en-us/products/cognitive-services/personalizer/



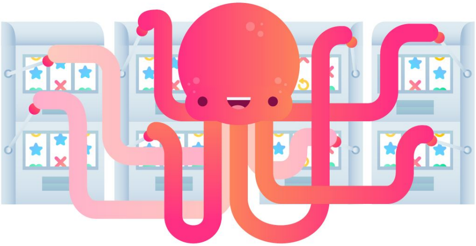
Real World Example



See https://learn.microsoft.com/en-us/azure/cognitive-services/personalizer/how-personalizer-works



Bayes Theorem Recall



This is the prior: i.e. what you believed before you saw the evidence.

This is the likelihood of seeing that evidence if your hypothesis is correct.

This is the posterior

$$p(H \mid D) = \frac{p(H)\,p(D \mid H)}{p(D)}$$

This is the normalizing constant:
i.e. The likelihood of that evidence under any circumstances.

Bayesian Bandits

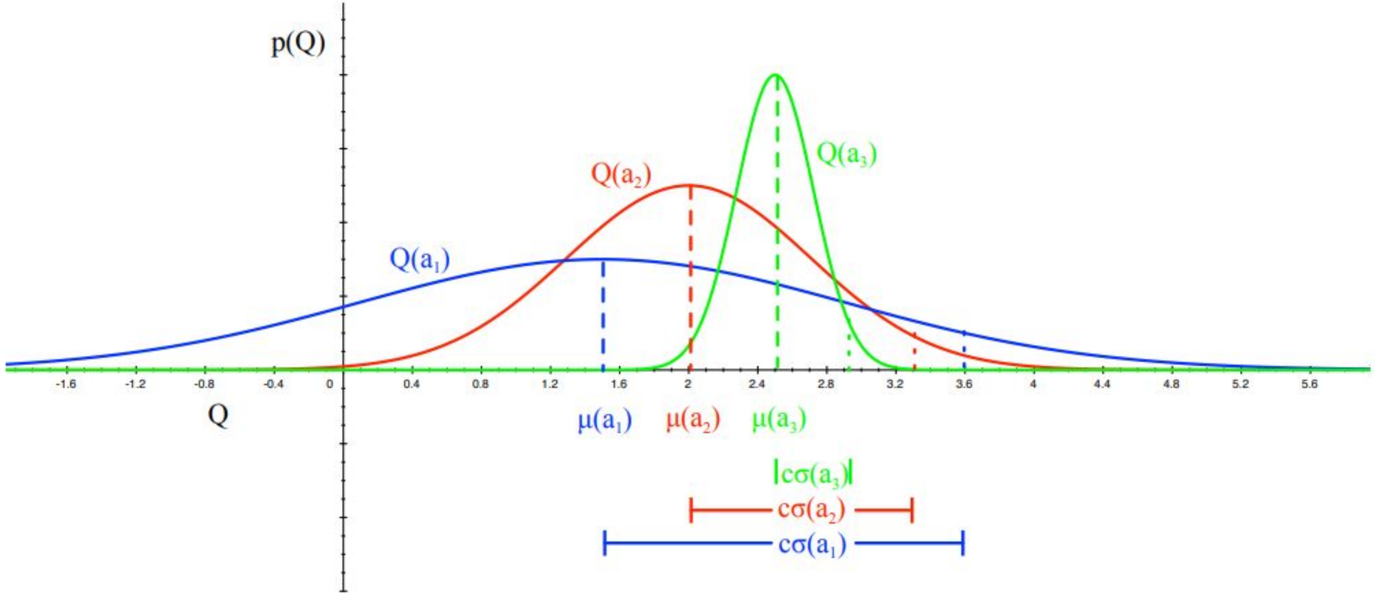
So far we have made no assumptions about the reward distribution ν_i, we only derived bounds on rewards

In Bayesian Bandits, however:

- We exploit *prior* knowledge of rewards
- Update a *posterior distribution* of rewards based on historical information
- Use posterior to guide exploration using:
  - upper confidence bounds (Bayesian UCB)
  - probability matching (Thompson Sampling)

Gaussian Bayesian Bandits Example

Assume ν_i is a Gaussian $N(\mu(i),\ \sigma^2(i))$



Gaussian Bayesian Bandits Example

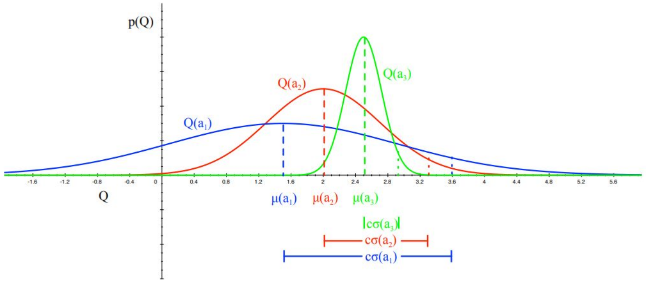
- Prior is often $N(0, 1)$
- Posterior update, given history h_t, is done as follows:

$$p(\mu_t(i),\sigma^2_t(i)\,|\,h_t) \propto p(\mu_i,\sigma^2_i)\prod_{t|k=i}\boxed{N(r_t\,|\,\mu_{t-1}(k),\ \sigma^2_{t-1}(k))}$$

Product over all timesteps *t* that select action *i* with the corresponding Gaussian parameters for that timestep

or more simply

$$p(\mu_t(i),\sigma^2_t(i)\,|\,r_t) \propto p(\mu(i),\sigma^2(i))N(r_t\,|\,\mu_{t-1}(i),\ \sigma^2_{t-1}(i))$$



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Gaussian Bayesian Bandits: UCB

Now we are modelling a distribution, so we already have confidence

What is confidence for Gaussians?

Gaussian Bayesian Bandits: UCB

Now we are modelling a distribution, so we already have confidence

What is confidence for Gaussians? **standard deviation**

Let’s do UCB by selecting the action with highest standard deviation

$$a_t = \text{argmax}_{i \text{ in } K}\, \mu_t(i) + c\sigma_t(i)/\sqrt{N_t(i)}$$

Gaussian Bayesian Bandits: Thompson Sampling

Thompson sampling is a way to do distribution matching: select action according to the probability that that action is optimal

- Optimistic in the face of uncertainty as uncertain actions have higher probability of satisfying maximization
- Uses sampling to avoid actual probability matching complications

Gaussian Bayesian Bandits: Thompson Sampling

For t = 0, ..., T:

1. for each arm i = 1, ..., K:
    - sample $\hat{\mathbf{r}}_i$ independently from $N(\mu_{t-1}(i), \sigma^2_{t-1}(i))$
2. pull arm

$$I_t = \arg\max_{i \in [K]} \hat{\mathbf{r}}_i$$

3. observe reward r_t
4. update posterior distribution $p(\mu_t(i), \sigma^2_t(i) | r_t)$

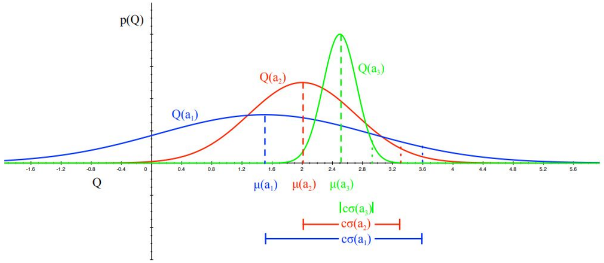
Gaussian Bayesian Bandits: Thompson Sampling

For t = 0, ..., T:

This is an estimation of the reward, in more generic MDPs this can be replaced with the Q function: we estimate a distribution of Q

1. for each arm i = 1, ..., K:
   - sample $\boxed{\hat{\mathbf{r}}_i}$ independently from $N(\mu_{t-1}(i),\ \sigma^2_{t-1}(i))$
2. pull arm

$$I_t = \arg\max_{i \in [K]} \hat{\mathbf{r}}_i$$



3. observe reward r_t
4. update posterior distribution $p(\mu_t(i), \sigma^2_t(i) \mid r_t)$

This can be done with different distributions as well