Multi-Armed Bandits

Reading

- Sutton, Richard S., and Barto, Andrew G. Reinforcement learning: An introduction. MIT press, 2018.
  - http://www.incompleteideas.net/book/the-book-2nd.html
  - Chapter 2
- Slivkins, Aleksandrs. "Introduction to multi-armed bandits." Foundations and Trends® in Machine Learning 12.1-2 (2019)
  - https://arxiv.org/pdf/1904.07272
  - Chapter 1
- Agarwal, Alekh, et al. "Reinforcement learning: Theory and algorithms." *CS Dept., UW, WA, USA, Tech. Rep* 32 (2019): 96.
  - https://rltheorybook.github.io/rltheorybook_AJKS.pdf
  - Chapter 6 (will consider a modified version of their proof)

Overview

Rensselaer

- Multi-armed bandits have many applications
  - Dynamic advertising on websites
  - Dynamic pricing
  - Investment
  - etc.
- It's a sequential decision-making problem
  - Simpler than the general RL setting since there is no state
  - Pick one out of k actions at each step
- Agenda
  - formalize the standard multi-armed bandit setting
  - derive the popular confidence upper bound algorithm

Other Applications

- Suppose you are in a casino all by yourself
  - There are k slot machines, each with a different probability of success
  - At any given time, you can only be on one slot machine
  - You would like to learn which slot machine is the best
- Suppose you are a doctor
  - You are presented with a sick patient with a rare condition
  - There are a number of experimental treatments, but you don't know their probability of success
  - You would like to learn which treatment is the best

Multi-armed Bandits Formalization

- At each time, you can select 1 out of k actions
- Each action has an unknown expected reward
  - E.g., slot machine payout rate/treatment success rate
- Your goal is to learn the expected rewards over time
  - Then you select the action with highest expected reward
- Bonus points if you can minimize the number of attempts
  - At the beginning, you are in *exploration* phase
    - Trying different actions randomly and seeing the rewards
  - Eventually, you switch to the *exploitation* phase
    - When you have a good estimate of rewards, you pick actions to maximize the rewards
  - Balancing the 2 is one of the fundamental challenges in RL

Multi-armed Bandits Formalization, cont'd

Rensselaer

- The agent has K possible actions, i.e., $A = \{a_1, \dots, a_K\}$
- Each action a has an unknown reward function is
$$R_e(a) = \mathbb{E}[R_{t+1} | A_t = a]$$
  - where A_t is the random variable for the action at time step t
  - where R_{t+1} is the random variable for the reward at time step $t + 1$
    - By convention, the reward is received one step after the action is taken
- At each round t, you taken an action A_t and observe a reward R_{t+1}
- Goal: estimate $R_e(a)$ for all actions a and learn the best action
$$a^* = arg\max_a R_e(a)$$

Naïve Approach

- How do we estimate the expected reward of each action?
  - Hint: what probabilistic tools did we discuss?
- Try each action N number of times and collect the rewards
  - Calculate the average reward per action
  - As $N \to \infty$, the average will converge to the true expected reward (law of large numbers)
- What can we say about a specific finite N?
  - For any N, can construct a confidence interval around your current estimate
    - E.g., using a concentration bound like Hoeffding's inequality

Probability Aside: Hoeffding's Inequality

- Let $X_1, \dots, X_n$ be n independent random variables
  - Each bounded by $a_i \leq X_i \leq b_i$
- Let $S_n = X_1 + \cdots + X_n$
- Hoeffding's Theorem:

$$\mathbb{P}[S_n - \mathbb{E}[S_n] \geq t] \leq \exp\left\{-\frac{2t^2}{\sum_{i=1}^{n}(b_i - a_i)^2}\right\}$$

  - A type of concentration bound
  - Given a sample S_n, bound its deviation from the true mean
  - The larger t is, the higher the probability the mean is within t of the sample
  - The smaller the bounds $(b_i - a_i)$, the tighter the bound on S_n

Probability Aside: Hoeffding's Inequality, cont'd

Rensselaer

- Hoeffding's Theorem:

$$\mathbb{P}[S_n - \mathbb{E}[S_n] \geq t] \leq \exp\left\{-\frac{2t^2}{\sum_{i=1}^{n}(b_i - a_i)^2}\right\}$$

- Two-tailed version:

$$\mathbb{P}[|S_n - \mathbb{E}[S_n]| \geq t] \leq 2\exp\left\{-\frac{2t^2}{\sum_{i=1}^{n}(b_i - a_i)^2}\right\}$$

  - Essentially applying bound twice
    - Once for the case $\geq$ and once for the case $\leq$

Probability Aside: Hoeffding's Inequality, cont'd

- Suppose we know the reward varies by at most some $B > 0$
  - For simplicity, suppose $B = 1$
- The bound simplifies to:

$$\mathbb{P}[S_n - \mathbb{E}[S_n] \geq t] \leq \exp\left\{-\frac{2t^2}{n}\right\}$$

- Furthermore, suppose we are interested in bounding the mean

$$\mathbb{P}\left[\frac{1}{n}(S_n - \mathbb{E}[S_n]) \geq t\right] =$$

$$= \mathbb{P}[S_n - \mathbb{E}[S_n] \geq nt] \leq \exp\{-2t^2 n\}$$

Probability Aside: Hoeffding's Inequality, cont'd

Rensselaer

$$\mathbb{P}\left[\frac{1}{n}|S_n - \mathbb{E}[S_n]| \geq t\right] \leq 2\exp\{-2t^2 n\}$$

- How do we construct a 95%-confidence interval around $\frac{S_n}{n}$?
  - Solve for t such that

$$2\exp\{-2t^2 n\} = 0.05$$

i.e., $t = c\sqrt{\frac{1}{n}}$

  - where $c = \sqrt{-0.5 * \log(0.05/2)} = \sqrt{0.5 * \log(2/0.05)}$

- In general, for any confidence $1 - \delta$:

$$c = \sqrt{0.5 * \log(2/\delta)}$$

Probability Aside: Hoeffding's Inequality, cont'd

$$\mathbb{P}\left[\frac{1}{n}|S_n - \mathbb{E}[S_n]| \geq t\right] \leq 2\exp\{-2t^2 n\}$$

- How do we construct a $1-\delta$-confidence interval around $\frac{S_n}{n}$?
  - Set $t = c\sqrt{\frac{1}{n}}$
    - where $c = \sqrt{0.5 * \log(2/\delta)}$
- So finally:

$$\mathbb{P}\left[\frac{1}{n}|S_n - \mathbb{E}[S_n]| \geq c\sqrt{\frac{1}{n}}\right] \leq \delta$$

Probability Aside: Hoeffding's Inequality, cont'd

- So finally,

$$\mathbb{P}\left[\frac{1}{n}|S_n - \mathbb{E}[S_n]| \geq c\sqrt{\frac{1}{n}}\right] \leq \delta$$

- The $1-\delta$ confidence interval is thus

$$\left[\frac{S_n}{n} - c\sqrt{\frac{1}{n}}, \frac{S_n}{n} + c\sqrt{\frac{1}{n}}\right]$$

Naïve Approach, cont'd

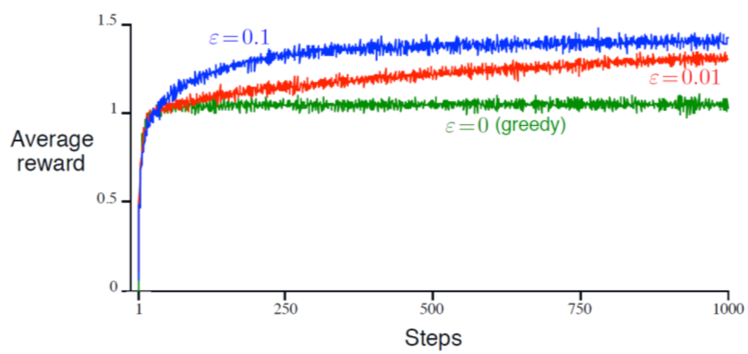
- The previous bound only works for a single action
  - Why?
  - Each action has a 95% probability of being within its confidence interval
  - What is the probability that all K actions are all within their confidence intervals?
    - Assuming actions are independent, then it is 0.95^K

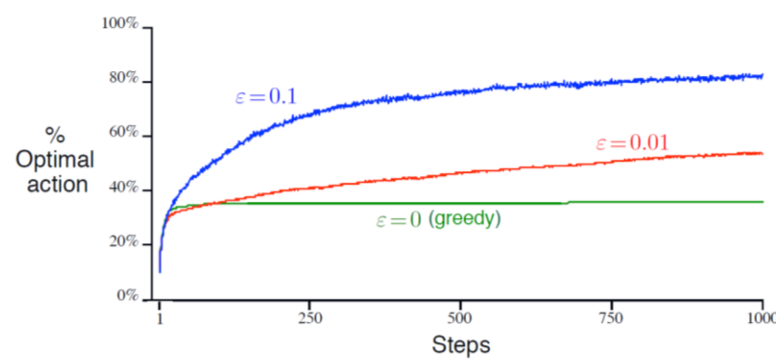
Multi-armed Bandits, the RL Approach

- In practice, we have to choose an action every time
  - Can't pre-collect N datapoints for each action
- So how do we choose that action?
  - Keep a running average of each action
  - At each step, choose the action with the highest average
- This is OK, but has a major limitation
  - Some actions may get very few points if they get a few bad samples
  - You are not guaranteed to find the best action in the limit
  - How do we fix this issue?

Multi-armed Bandits, the RL Approach

- ϵ-greedy action selection
- At each step, choose the action with the highest average
  - But with probability $1 - \epsilon$, for small $\epsilon > 0$
  - With probability ϵ, pick another action at random
    - $k - 1$ other actions, so other actions get $\frac{\epsilon}{k-1}$ probability each
- 10-armed example from the book
  - The $\epsilon = 0.1$ case converges fastest in this example
  - The $\epsilon = 0$ case eventually plateaus





Multi-armed Bandits, RL Approach Implementation

Rensselaer

- When computing the running average, we don't need to add up all past rewards every time
  - E.g., suppose average at time t is $q^t(a) = \frac{1}{t}\sum_{i=1}^{t} R_i$
  - When we receive R_{t+1}, what is the new average, in terms of $q^t(a)$?

$$
\begin{aligned}
q^{t+1}(a) &= \frac{R_1 + R_2 + \cdots + R_{t+1}}{t+1} \\
&= \frac{1}{t+1}(R_1 + \cdots + R_t) + \frac{1}{t+1} R_{t+1} \\
&= \frac{t}{t+1}\frac{(R_1 + \cdots + R_t)}{t} + \frac{1}{t+1} R_{t+1} \\
&= \frac{t}{t+1} q^t(a) + \frac{1}{t+1} R_{t+1} \\
&= q^t(a) + \frac{1}{t+1}\left(R_{t+1} - q^t(a)\right)
\end{aligned}
$$

Multi-armed Bandits, RL Approach Implementation, cont'd

Rensselaer

- When computing the running average, we don't need to add up all past rewards every time
  - E.g., suppose average at time t is $q^t(a) = \frac{1}{t}\sum_{i=1}^{t} R_i$
  - When we receive R_{t+1}, what is the new average, in terms of $q^t(a)$?

$$q^{t+1}(a) = q^t(a) + \frac{1}{t+1}\left(R_{t+1} - q^t(a)\right)$$

- Compute the difference between the new reward and the running average
  - This is a simple example of temporal difference learning (more later)

Successive Elimination Algorithm

- Can you design an algorithm that declares victory with high probability?
  - i.e., it keeps trying actions until it is 95%-confident that it has identified the best action
- For simplicity, suppose we have 2 actions
  - Suppose we keep running 95%-confidence intervals for each

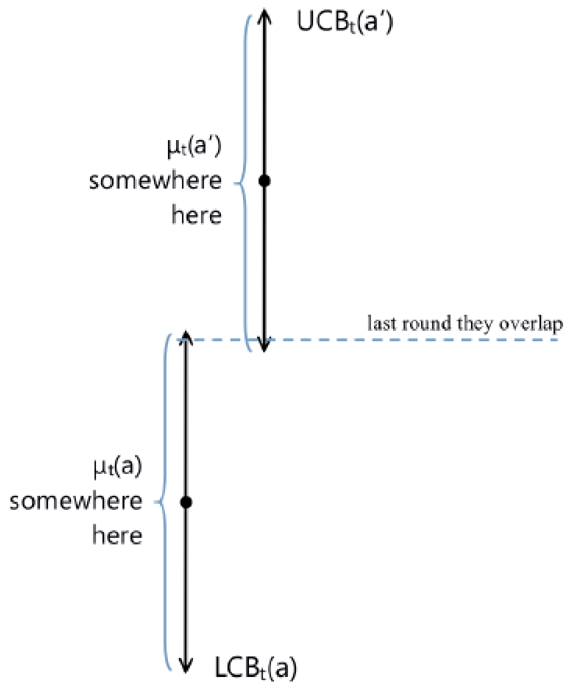
$$[LCB(a_1), UCB(a_1)], [LCB(a_2), UCB(a_2)]$$

- Can terminate algorithm when one interval is entirely larger than the other, e.g.,:

$$LCB(a_2) > UCB(a_1)$$

Successive Elimination Algorithm, cont'd

- What about more actions?
  - Successively eliminate actions whose upper bound is lower then the best action's lower bound



Successive Elimination Algorithm, cont'd

- Can't directly apply Hoeffding's inequality to calculate the confidence intervals
  - Why?
  - The rewards R_t are not necessarily independent!
  - Consider the following algorithm:
    - sample action a_1 two times and then only sample a_1 a 3rd time if $R_1 = R_2 = 0$
    - Clearly R_3 only exists when $R_1 = R_2 = 0$
  - How do we get around this issue?

Successive Elimination Algorithm, cont'd

- Suppose we are allowed to make a total of T actions
- Each action a gets a total of $0 < n(a) \leq T$ actions
  - Note that $n(a)$ is random and depends on the algorithm
  - Let $S_{n,a}$ be the sample average for the rewards received when taking action a
- The following bound holds for any algorithm

$$\mathbb{P}\left[\frac{1}{n(a)}\left|S_{n,a} - \mathbb{E}[S_{n,a}]\right| \geq \frac{\sqrt{2T\log(1/\delta)}}{n(a)}\right] \leq \delta$$

  - Proof requires theory of martingales
    - Shown at the end of this deck

Successive Elimination Algorithm, cont'd

- The following bound holds for any algorithm

$$\mathbb{P}\left[\frac{1}{n(a)}\left|S_{n,a} - \mathbb{E}[S_{n,a}]\right| \geq \frac{\sqrt{2T\log(1/\delta)}}{n(a)}\right] \leq \delta$$

- Very similar to the original Hoeffding bound
  - If we assume $T \approx n(a)$, we get

$$\mathbb{P}\left[\frac{1}{n(a)}\left|S_{n,a} - \mathbb{E}[S_{n,a}]\right| \geq \sqrt{\frac{2\log\left(\frac{1}{\delta}\right)}{n(a)}}\right] \leq \delta$$

  - Similar to original Hoeffding bound except $n(a)$ is random
- Ultimately the bounds are the same: T is fixed, so the choice of δ will determine the confidence interval size

Upper-Confidence-Bound Algorithm

Rensselaer

- We know that without exploration we are almost certainly going to converge to a suboptimal action
- On the other hand, too much exploration may take a long time to converge
  - So far, we've seen ϵ-greedy exploration, which indiscriminately selects the next action randomly
- Is there a way to perform targeted exploration?
- Pick the action with the highest UCB!
  - Why is this a good idea?
    - Either the highest-UCB action is already the best
    - or the highest-UCB action has a large confidence interval, which means it could benefit from more exploration
    - In both cases it makes sense to select that action

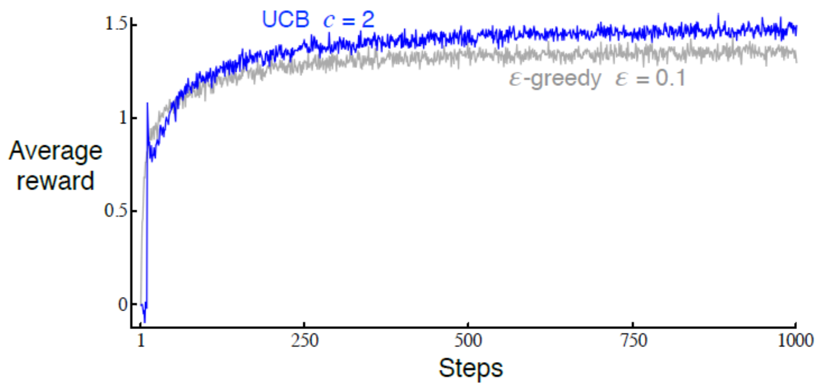
Upper-Confidence-Bound Algorithm, cont'd

Rensselaer

- Suppose we have a choice of K actions
- For $t \in [1, K]$:
  - Take each action once and observe the reward
- For $t > K$:
  - Calculate running reward averages $q^t(a_i)$ for each action a_i
  - Take action $a_t = a_{i^*}$, where $i^* = arg\max_i q^t(a_i) + \sqrt{\frac{c}{n(a_i)}}$
    - where $c = 2\log\left(\frac{1}{\delta}\right)$
      - Book uses a different c (no time to prove)
        - » Tighter confidence bounds can be derived specific to UCB
  - Observe corresponding reward r_t
    - Update$q^t(a_i)$ and increment $n(a_{i^*})$

Upper-Confidence-Bound Algorithm, cont'd

- UCB algorithm generally outperforms ϵ-greedy
- UCB is not widely used in the general RL setting, however
  - May introduce a lot of variance in a high-dimensional action space
    - If we have many actions, we will require a lot of data in order to try all actions enough times and get good confidence intervals



Conclusion

- Multi-armed bandits is a well-studied setting with a number of strong theoretical results
- It can be considered as a simplified RL setting where the environment has no state
- In this lecture, we considered the case where we made no assumptions about rewards
  - Except that they are bounded
- Next time, we'll look at Bayesian bandits where we assume a prior about the reward distribution

Proof of Confidence Bound

- Suppose we are allowed to make a total of T actions
- Each action a gets a total of $0 < n(a) \leq T$ actions
  - Note that $n(a)$ is random and depends on the algorithm
  - Let $S_{n,a}$ be the sample average for the rewards received when taking action a
- The following bound holds for any algorithm

$$\mathbb{P}\left[\frac{1}{n(a)}\left|S_{n,a} - \mathbb{E}[S_{n,a}]\right| \geq \frac{\sqrt{2T\log(1/\delta)}}{n(a)}\right] \leq \delta$$

- Sutton book uses a slightly different bound but

Probability Aside: Hoeffding-Azuma Inequality

- **Definition**: A sequence of random variables $X_0, \ldots, X_T$ is a martingale difference sequence if

$$\mathbb{E}[X_t] < \infty$$

$$\mathbb{E}[X_t | X_0, \ldots, X_{t-1}] = 0$$

- **Theorem [Hoeffding-Azuma Inequality]**: Let $X_0, \ldots, X_T$ be a martingale difference sequence and suppose $|X_t - X_{t-1}| \leq c_t$. Then, for all $\varepsilon > 0, T > 0$:

$$\mathbb{P}\left[\sum_{i=0}^{T} X_i \geq \epsilon\right] \leq \exp\left(\frac{-\epsilon^2}{2\sum_{i=1}^{T} c_i^2}\right)$$

Proof of Confidence Bound, cont'd

- Consider a fixed action a and fixed algorithm $\mathcal{A}$
  - Let $\hat{\mu}_a^t = \frac{S_{n_t,a}}{n_t(a)}$ be the running average at time step t
  - Let $\mu_a = \mathbb{E}[R_{t+1} | A_t = a]$ be the true expected reward for action a
  - Assume each action a is tried once initially, with random reward R_a
- Define the following random variables

$$X_0 = R_a - \mu_a, X_1 = \mathbf{1}\{A_1 = a\}(R_2 - \mu_a), \dots, X_T = \mathbf{1}\{A_T = a\}(R_{T+1} - \mu_a)$$

  - Each X_t is 0 when action a is not taken at time t and r_t otherwise (normalized to be 0-mean by subtracting μ_a)

Proof of Confidence Bound, cont'd

Rensselaer

- Define the following random variables
  $X_0 = R_a - \mu_a, X_1 = \mathbf{1}\{A_1 = a\}(R_2 - \mu_a), \dots, X_T = \mathbf{1}\{A_T = a\}(R_{T+1} - \mu_a)$
  - Each X_t is 0 when action a is not taken at time t and r_t otherwise (normalized to be 0-mean by subtracting μ_a)
- Notice that $\mathbb{E}[X_t | X_1, \dots, X_{t-1}] = 0$
  - Given all history, $\mathbf{1}\{A_1 = a\}$ is deterministic
    - Decided by the algorithm $\mathcal{A}$
  - Either $\mathbf{1}\{A_1 = a\} = 0$ (in which case expectation is 0)
  - Or $\mathbf{1}\{A_1 = a\} = 1$, in which case $\mathbb{E}[X_t | X_1, \dots, X_{t-1}] = \mathbb{E}[R_t - \mu_a] = 0$
- Thus, $X_1, \dots, X_T$ is a martingale difference sequence

Proof of Confidence Bound, cont'd

- Define the following random variables

$X_0 = R_a - \mu_a, X_1 = \mathbf{1}\{A_1 = a\}(R_2 - \mu_a), \dots, X_T = \mathbf{1}\{A_T = a\}(R_{T+1} - \mu_a)$

  - Each X_t is 0 when action a is not taken at time t and r_t otherwise (normalized to be 0-mean by subtracting μ_a)

- Also notice that $|X_t - X_{t-1}| \leq 1$ for all t
  - Recall $R_t \in [0,1]$, which means $\mu_a \in [0,1]$ and hence

$$R_t - \mu_a \in [0,1] \text{ and } X_t \in [0,1]$$

- By the Hoeffding-Azuma inequality, for any t

$$\mathbb{P}\left[\sum_{i=0}^{t} X_i \geq \epsilon\right] \leq \exp\left(\frac{-\epsilon^2}{2\sum_{i=1}^{t} 1^2}\right) \leq \exp\left(\frac{-\epsilon^2}{2t}\right)$$

Proof of Confidence Bound, cont'd

Rensselaer

- Define the following random variables

$$X_0 = R_a - \mu_a, X_1 = \mathbf{1}\{A_1 = a\}(R_2 - \mu_a), \dots, X_T = \mathbf{1}\{A_T = a\}(R_{T+1} - \mu_a)$$

- By the Hoeffding-Azuma inequality, for any fixed t

$$\mathbb{P}\left[\sum_{i=0}^{t} X_i \geq \epsilon\right] \leq \exp\left(\frac{-\epsilon^2}{2\sum_{i=0}^{t} 1^2}\right) \leq \exp\left(\frac{-\epsilon^2}{2t}\right)$$

- Notice that

$$\sum_{i=0}^{t} X_i = \sum_{i=0}^{t} \mathbf{1}\{A_i = a\}R_{i+1} - \sum_{i=0}^{t} \mathbf{1}\{A_i = a\}\mu_a$$
$$= S_{n_t,a} - n_t(a)\mu_a$$
$$= n_t(a)\hat{\mu}_a^t - n_t(a)\mu_a$$

Proof of Confidence Bound, cont'd

- Define the following random variables

$$X_0 = R_a - \mu_a, X_1 = \mathbf{1}\{A_1 = a\}(R_2 - \mu_a), \dots, X_T = \mathbf{1}\{A_T = a\}(R_{T+1} - \mu_a)$$

- By the Hoeffding-Azuma inequality, for any fixed t

$$\mathbb{P}\left[\sum_{i=0}^{t} X_i \geq \epsilon\right] \leq \exp\left(\frac{-\epsilon^2}{2\sum_{i=0}^{t} 1^2}\right) \leq \exp\left(\frac{-\epsilon^2}{2t}\right)$$

- Finally,

$$\left[\sum_{i=0}^{t} X_i \geq \epsilon\right] = \mathbb{P}[n_t(a)\hat{\mu}_a^t - n_t(a)\mu_a \geq \epsilon]$$

$$= \mathbb{P}\left[\hat{\mu}_a^t - \mu_a \geq \frac{\epsilon}{n_t(a)}\right] \leq \exp\left(\frac{-\epsilon^2}{2t}\right)$$

Proof of Confidence Bound, cont'd

$$\mathbb{P}\left[\hat{\mu}_a^t - \mu_a \geq \frac{\epsilon}{n_t(a)}\right] \leq \exp\left(\frac{-\epsilon^2}{2t}\right)$$

- Solving for $\delta = \exp\left(\frac{-\epsilon^2}{2t}\right)$, we get

$$\epsilon = \sqrt{-2t\log(\delta)} = \sqrt{2t\log(1/\delta)}$$

- Thus, for $1 - \delta$ confidence:

$$\mathbb{P}\left[\hat{\mu}_a^t - \mu_a \geq \frac{\sqrt{2t\log(1/\delta)}}{n_t(a)}\right] \leq \delta$$

  – Plugging in $T = t$, we get the final result