Machine Learning Theory 2024 Lecture 9

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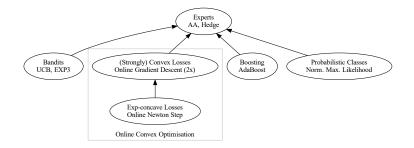
Bandit problems

- Adversarial bandit Setting
- EXP3 Algorithm and analysis
- Stochastic bandit Setting
- UCB Algorithm and analysis



Recap and Bandit Setting

Overview of Second Half of Course



Material: course notes on MLT website.

Recap: Setting

Protocol (Dot Loss Game)

• For
$$t = 1, 2, ...$$

- Learner chooses a distribution $w_t \in \Delta_K$ on K "experts".
- Adversary reveals loss vector ℓ_t ∈ [0, 1]^K.
 Learner's loss is the dot loss w^T_tℓ_t = ∑^K_{k=1} w^k_tℓ^k_t

Objective

Regret after *T* rounds:

$$R_T = \underbrace{\sum_{t=1}^{T} w_t^{\mathsf{T}} \ell_t}_{\text{Learner's loss}} - \underbrace{\min_{k} \sum_{t=1}^{T} \ell_t^k}_{\text{loss of best expert}}$$

A good learner has small regret, i.e. it approximately behaves as if it knows the best expert.

Recap: Method and Result

Definition (Hedge Algorithm)

The Hedge algorithm with learning rate η plays weights in round t:

$$w_t^k = \frac{e^{-\eta \sum_{s=1}^{t-1} \ell_s^k}}{\sum_{j=1}^{K} e^{-\eta \sum_{s=1}^{t-1} \ell_s^j}}.$$
 (Hedge)

or, equivalently, $w_1^k = rac{1}{K}$ and

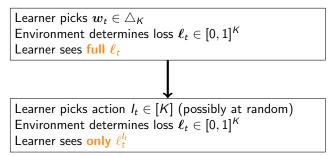
$$w_{t+1}^k = rac{w_t^k e^{-\eta \ell_t^k}}{\sum_{j=1}^K w_t^j e^{-\eta \ell_t^j}}$$
 (Hedge, incremental)

Theorem (Hedge Regret Bound)

The regret of Hedge with learning rate $\eta = \sqrt{rac{8 \ln K}{T}}$ is at most

$$R_T \leq \sqrt{T/2 \ln K}.$$

"Bandits": a (minor?) change of feedback



Radical upgrade: Learner actively controls which data are collected.

Applications

- Clinical trials (round=patient, action=treatment)
- Advertising (round=visitor, action=serving specific ad)
- Radio channel selection (wifi)

► ...

Main Questions

How difficult is it to learn from partial observations?

- How should learning algorithms be (re)designed?
 - Obtaining information requires executing sub-optimal actions
 - Exploration/Exploitation trade-off
- What is the effect of the environment model?
 - Adversarial
 - Stochastic

Different techniques, different complexity (regret rate)

Two Brilliant Ideas



Importance Weighted Loss Estimates

Optimism in Face of Uncertainty

Adversarial Bandits

Main Questions

How difficult is it to learn from partial observations?

The setup

Protocol (K-armed adversarial bandit)

- Adversary hides $\ell_t^k \in [0, 1]$ for all $t \leq T, k \leq K$.
- For t = 1, 2, ..., T
 - Learner picks arm I_t (typically by sampling $I_t \sim w_t$)
 - Learner observes and incurs loss $\ell_t^{l_t}$

Objective:

Expected regret w.r.t. best arm after T rounds:

$$\mathbb{E}[R_T] = \mathbb{E}_{I_1 \cdots I_T} \left[\sum_{t=1}^T \ell_t^{I_t} \right] - \min_k \sum_{t=1}^T \ell_t^k$$

Outline of this part

We will prove the following result:

Theorem (Main Adversarial Bandit Result)

There is an algorithm with regret

 $\mathbb{E}[R_T] \leq \sqrt{2TK \ln K}$

Ingredients:

- Importance weighted estimates
- Reduction to AA
- Tweaks to AA analysis

Importance Weighted Loss Estimates

- Opponent fixed ℓ_t .
- \blacktriangleright We draw $I_t \sim w_t$.
- We see $\ell_t^{I_t}$.

We only see one entry of ℓ_t . Can we still estimate the full ℓ_t ?

Definition (Loss Estimate)

The importance weighted loss estimate is $\hat{\ell}_t$ with entries $\hat{\ell}_t^k := \frac{\ell_t^{I_t}}{w_t^{I_t}} \mathbf{1}_{I_t=k}$.

Example

Say K = 4, $w_t = (0.1, 0.2, 0.3, 0.4)$, $\ell_t = (0.6, 0.7, 0.8, 0.9)$ and sampling from w_t gives $I_t = 3$. Then we see $\ell_t^{I_t} = \ell_t^3 = 0.8$ and form the estimate

$$\hat{\ell}_t = \begin{pmatrix} 0 \\ 0 \\ 0.8/0.3 = 2.66 \dots \\ 0 \end{pmatrix}$$

Importance Weighted Loss Estimates

Definition (Loss Estimate)

We pick $\hat{\ell}_t$ with $\hat{\ell}_t^k = \frac{\ell_t^{\prime_t}}{w_t^{l_t}} \mathbf{1}_{l_t=k}$.

Lemma (Unbiased Estimator)

 $\mathbb{E}_{I_t \sim w_t}[\hat{\ell}_t] = \ell_t.$

Proof.

For each k

$$\mathbb{E}_{I_t \sim w_t}[\hat{\ell}_t^k] = \sum_{I_t=1}^K w_t^{I_t} \frac{\ell_t^{I_t}}{w_t^{I_t}} \mathbf{1}_{I_t=k} = \sum_{I_t=1}^K \ell_t^{I_t} \mathbf{1}_{I_t=k} = \ell_t^k$$

Corollary

$$\mathbb{E}_{l_t \sim \boldsymbol{w}_t}[\boldsymbol{w}_t^\mathsf{T} \hat{\boldsymbol{\ell}}_t] = \boldsymbol{w}_t^\mathsf{T} \boldsymbol{\ell}_t = \mathbb{E}_{l_t \sim \boldsymbol{w}_t}[\boldsymbol{\ell}_t^{l_t}].$$

EXP3: AA + scaling + estimation

Slogan: EXP3 is AA applied to η -scaled importance weighted losses.

Definition (EXP3 Algorithm)

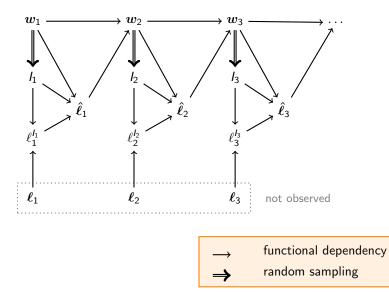
The *EXP3 algorithm* with *learning rate* $\eta > 0$ plays weights in round *t*:

$$w_t^k = \frac{e^{-\eta \sum_{s=1}^{t-1} \hat{\ell}_s^k}}{\sum_{j=1}^{K} e^{-\eta \sum_{s=1}^{t-1} \hat{\ell}_s^j}}.$$
 (EXP3)

or, equivalently, $w_1^k = \frac{1}{K}$ and

$$w_{t+1}^{k} = \frac{w_{t}^{k} e^{-\eta \hat{\ell}_{t}^{k}}}{\sum_{j=1}^{K} w_{t}^{j} e^{-\eta \hat{\ell}_{t}^{j}}}$$
(EXP3, incremental)

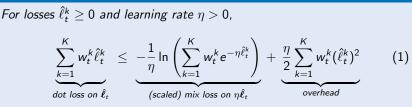
Dependency structure



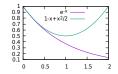
EXP3 Analysis: dot/mix loss

We would like to use the dot/mix loss relationship. For Hedge the losses ℓ_t are **bounded**, and we can use Hoeffding's Inequality. But for EXP3 the importance weighted loss estimates $\hat{\ell}_t$ are **not bounded** above. We need another relation.

Lemma



EXP3 Analysis: dot/mix loss



Proof.

For $x \ge 0$, we have $e^{-x} \le 1 - x + x^2/2$. Hence

$$\begin{aligned} -\ln\left(\sum_{k=1}^{K} w_{t}^{k} e^{-\eta \hat{\ell}_{t}^{k}}\right) &\geq -\ln\left(\sum_{k=1}^{K} w_{t}^{k} (1 - \eta \hat{\ell}_{t}^{k} + (\eta \hat{\ell}_{t}^{k})^{2}/2)\right) \\ &= -\ln\left(1 - \eta \sum_{k=1}^{K} w_{t}^{k} \hat{\ell}_{t}^{k} + \frac{\eta^{2}}{2} \sum_{k=1}^{K} w_{t}^{k} (\hat{\ell}_{t}^{k})^{2}\right) \\ &\geq \eta \sum_{k=1}^{K} w_{t}^{k} \hat{\ell}_{t}^{k} - \frac{\eta^{2}}{2} \sum_{k=1}^{K} w_{t}^{k} (\hat{\ell}_{t}^{k})^{2} \end{aligned}$$

Dividing by $\eta>0$ and moving the rightmost term over gives the lemma.

EXP3 Analysis: overhead term

Let's study that overhead term in expectation

Lemma

In round t, for the importance weighted loss estimator $\hat{\ell}_t$

$$\mathbb{E}_{I_t \sim w_t} \left[\sum_{k=1}^{K} w_t^k (\hat{\ell}_t^k)^2 \right] \leq K$$
(2)

Proof.

By definition of the importance weighted loss estimator

$$\mathbb{E}_{I_t \sim \boldsymbol{w}_t} \left[\sum_{k=1}^K w_t^k (\hat{\ell}_t^k)^2 \right] = \sum_{I_t=1}^K w_t^{I_t} \sum_{k=1}^K w_t^k \left(\frac{\ell_t^{I_t}}{w_t^{I_t}} \mathbf{1}_{I_t=k} \right)^2$$

Only the diagonal $I_t = k$ contributes, and the loss is bounded $\ell_t^{I_t} \in [0, 1]$, so

$$= \sum_{l_t=1}^{K} w_t^{l_t} w_t^{l_t} \frac{(\ell_t^{l_t})^2}{(w_t^{l_t})^2} = \sum_{l_t=1}^{K} (\ell_t^{l_t})^2 \leq K.$$

EXP3 Regret Bound

Theorem

The expected regret of EXP3 with learning rate $\eta > 0$ is

$$\mathbb{E}_{I_1 \cdots I_T} \left[\sum_{t=1}^T \ell_t^{I_t} \right] - \min_k \sum_{t=1}^T \ell_t^k \leq \frac{\ln K}{\eta} + \frac{TK\eta}{2}$$

Corollary

The expected regret of EXP3 with learning rate $\eta = \sqrt{\frac{2 \ln K}{TK}}$ is

$$\mathbb{E}_{I_1 \cdots I_T} \left[\sum_{t=1}^T \ell_t^{I_t} \right] - \min_k \sum_{t=1}^T \ell_t^k \leq \sqrt{2TK \ln K}$$

EXP3 Analysis

Proof.

Sum the mix/dot loss inequality (1) over rounds

$$\sum_{t=1}^{T} \sum_{k=1}^{K} w_t^k \hat{\ell}_t^k \leq \sum_{t=1}^{T} -\frac{1}{\eta} \ln \left(\sum_{k=1}^{K} w_t^k e^{-\eta \hat{\ell}_t^k} \right) + \sum_{t=1}^{T} \frac{\eta}{2} \sum_{k=1}^{K} w_t^k (\hat{\ell}_t^k)^2$$

Apply the AA regret bound (Lecture 8) to the middle sum

$$\sum_{t=1}^{T} \sum_{k=1}^{K} w_t^k \hat{\ell}_t^k \leq \min_k \sum_{t=1}^{T} \hat{\ell}_t^k + \frac{\ln K}{\eta} + \sum_{t=1}^{T} \frac{\eta}{2} \sum_{k=1}^{K} w_t^k (\hat{\ell}_t^k)^2$$

Take expectations, and pull the min out using Jensen's Inequality

$$\mathbb{E}_{I_1\cdots I_T}\left[\sum_{t=1}^T\sum_{k=1}^K w_t^k \hat{\ell}_t^k\right] \leq \min_k \mathbb{E}_{I_1\cdots I_T}\left[\sum_{t=1}^T \hat{\ell}_t^k\right] + \frac{\ln K}{\eta} + \mathbb{E}_{I_1\cdots I_T}\left[\sum_{t=1}^T \frac{\eta}{2}\sum_{k=1}^K w_t^k (\hat{\ell}_t^k)^2\right]$$

Use unbiasedness and our expected overhead bound (2) to conclude

$$\mathbb{E}_{I_1\cdots I_T}\left[\sum_{t=1}^T \ell_t^{I_t}\right] \leq \min_k \sum_{t=1}^T \ell_t^k + \frac{\ln K}{\eta} + T\frac{\eta}{2}K.$$

Conclusion of Adversarial Bandits part

An algorithm that can learn from **partial information** even with **adversarially determined losses**.

Observations:

- Efficient: run time is O(K) per round.
- Regret of EXP3 is $\sqrt{TK \ln K}$ compared to $\sqrt{T \ln K}$ for Hedge in full information setting.
- For \sqrt{KT} lower bound see bonus material.
- Exploration/exploitation. Unsampled arms get 0 estimated loss. So eventually they will get sampled.

Stochastic Bandits

Main Questions

How difficult is it to learn from **partial observations** if we assume the **environment is stochastic**?

Are we back in statistical learning?

Not quite:

- Yes: statistical model for environment
- ▶ No (Major): Learner actively controls which data are collected
- No (Minor): sequential evaluation

A completely different style of algorithm.

Setting

Protocol (*K*-armed stochastic bandit)

• Environment: distributions (ν_1, \ldots, ν_K) of arm rewards

- For t = 1, 2, ..., T
 - Learner picks arm I_t
 - Learner observes and receives reward $X_t \sim \nu_{I_t}$

Definition (Stochastic Bandit Notation)

The mean reward of arm k is $\mu^k = \mathbb{E}_{X \sim \nu_k}[X]$. The best arm is $i^* = \arg \max_k \mu^k$. The sub-optimality gap of arm i is $\Delta_i = \mu^{i^*} - \mu^i$.

Objective

Pseudo-regret after T rounds:

$$\bar{R}_{T} = T\mu^{i^{*}} - \underset{\substack{X_{1} \cdots X_{T} \\ l_{1} \cdots l_{T}}}{\mathbb{E}} \left\{ \sum_{t=1}^{T} \mu^{l_{t}} \right\}$$

Distributional Assumption and Its Consequences

We assume each arm's reward distribution ν_k is Gaussian $\mathcal{N}(\mu^k, 1)$.

Lemma (Chernoff Bound)

Let X_1, \ldots, X_t i.i.d. $\mathcal{N}(\mu, 1)$ with average $\hat{\mu}_t = \frac{1}{t} \sum_{i=1}^t X_i$. For any $\epsilon \geq 0$

$$\mathbb{P}\left\{\hat{\mu}_{t} \geq \mu + \epsilon\right\} \leq e^{-t\frac{\epsilon^{2}}{2}} \text{ and}$$

$$\mathbb{P}\left\{\hat{\mu}_{t} \leq \mu - \epsilon\right\} \leq e^{-t\frac{\epsilon^{2}}{2}}.$$

$$(3a)$$

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 (3a)

Equivalent confidence interval statements: for any $\delta \in (0, 1]$,

$$\mathbb{P}\left\{\mu \leq \hat{\mu}_t - \sqrt{\frac{2\ln\frac{1}{\delta}}{t}}\right\} \leq \delta \quad \text{and}$$

$$\mathbb{P}\left\{\mu \geq \hat{\mu}_t + \sqrt{\frac{2\ln\frac{1}{\delta}}{t}}\right\} \leq \delta.$$
(3b)

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Equivalent confidence interval statements: for any $\delta \in (0, 1]$,

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$$\mathbb{P}\left\{\mu \geq \hat{\mu}_t + \sqrt{\frac{2\ln\frac{1}{\delta}}{t}}\right\} \leq \delta.$$
(3b)

In fact, we may take **sub-Gaussian** rewards, *defined* to satisfy (3). This includes Gaussian, Bernoulli, non-parametric support $[\pm 1], \ldots$

Outline of this part

We will prove the following result:

Theorem (Main Stochastic Bandit Result)

There is an algorithm with pseudo-regret

$$ar{R}_T \leq C\left(\sum_{k
eq i^*}^{\kappa} rac{1}{\Delta_k}\right) \ln T + C'$$

Idea

For each arm, estimate its mean.

Empirical estimate of mean of arm *k* after *t* rounds:

$$\hat{\mu}_{t}^{k} = \frac{\sum_{s=1}^{t} X_{s} \mathbf{1}_{I_{s}=k}}{N_{t}^{k}} \quad \text{where} \quad N_{t}^{k} = \sum_{s=1}^{t} \mathbf{1}_{I_{s}=k}$$

Uncertainty quantification by means of a confidence interval

$$\mathsf{LCB}_{t}^{k} \coloneqq \hat{\mu}_{t}^{k} - \sqrt{\frac{2\alpha \ln(t+1)}{N_{t}^{k}}}$$
$$\mathsf{UCB}_{t}^{k} \coloneqq \hat{\mu}_{t}^{k} + \sqrt{\frac{2\alpha \ln(t+1)}{N_{t}^{k}}}$$

Claim: True mean $\mu^k \in [LCB_t^k, UCB_t^k]$ with near-certainty (probability ≈ 1).

Strategy: Sample the arm of highest UCB_t

UCB Algorithm

Definition (UCB Algorithm)

In round *t*, the UCB algorithm with parameter $\alpha > 2$ samples arm

$$I_t := \arg \max_k \ \mathsf{UCB}_{t-1}^k = \arg \max_k \ \hat{\mu}_{t-1}^k + \sqrt{\frac{2\alpha \ln(t)}{N_{t-1}^k}}$$

UCB sets I_t deterministically given the past $I_{< t}, X_{< t}$

Optimism in face of uncertainty:

Take the action of highest reward among any plausible bandit model.

Where we are heading

We will show

Theorem (UCB Regret Bound)

UCB with $\alpha > 2$ satisfies

$$\bar{R}_T = \sum_{k=1}^K \mathbb{E}[N_T^k] \Delta_k \leq \left(\sum_{k \neq i^*}^K \frac{1}{\Delta_i}\right) 8\alpha \ln T + \frac{\alpha}{\alpha - 2} \sum_{k=1}^K \Delta_k$$

Let $i^* = \arg \max_k \mu^k$ be the index of the arm of highest mean.

If in some round t the algorithm samples a suboptimal arm, $I_t = i \neq i^*$, one of three things must be the case

- ▶ We have not sampled arm *i* often; its confidence width is still large
- Arm *i* is overestimated (its LCB_{t-1}^{i} is too high).
- Arm i^* is underestimated (its UCB $_{t-1}^{i^*}$ is too low).

Lemma

If UCB samples suboptimal $I_t = i \neq i^*$ then (a) $UCB_{t-1}^{i^*} \leq \mu^{i^*}$ or (b) $LCB_{t-1}^i > \mu_i$ or (c) $N_{t-1}^i < \frac{8\alpha \ln t}{\Delta_i^2}$ where $\Delta_i = \mu^{i^*} - \mu^i$.

Proof.

Suppose not. Then

$$\begin{aligned} \mathsf{UCB}_{t-1}^{i^*} \stackrel{(a)}{\geq} \mu^{i^*} &= \mu^i + \Delta_i \stackrel{(c)}{\geq} \mu^i + 2\sqrt{\frac{2\alpha \ln t}{N_{t-1}^i}} \\ \stackrel{(b)}{\geq} \mathsf{LCB}_{t-1}^i + 2\sqrt{\frac{2\alpha \ln t}{N_{t-1}^i}} \stackrel{\text{def.}}{=} \mathsf{UCB}_{t-1}^i \end{aligned}$$

and this contradicts that UCB samples $I_t = i$.

NB: \mathbb{E} scopes the rewards $X_1 \cdots X_T$. UCB picks I_t deterministically.

The pseudo-regret can be rewritten as

$$\bar{R}_{T} = T\mu^{i^{*}} - \mathbb{E}\left[\sum_{t=1}^{T}\mu^{t}\right] = \sum_{k=1}^{K}\mathbb{E}[N_{T}^{k}]\Delta_{k}$$

It hence suffices to bound $\mathbb{E}[N_T^i]$ for suboptimal $i \neq i^*$.

We will show for each $k \neq i^*$

$$\mathbb{E}[N_T^k] \leq C \frac{8\alpha}{\Delta_k^2} \ln T + C'$$

Slogan: Sub-optimal arms are sampled logarithmically often

$$\begin{split} \mathbb{E}[N_{T}^{i}] &= \mathbb{E}\left[\sum_{t=1}^{T} \mathbb{1}_{I_{t}=i}\right] = \sum_{t=1}^{T} \mathbb{P}\left\{I_{t}=i\right\} \\ &= \sum_{t=1}^{T} \mathbb{P}\left\{I_{t}=i \text{ and } N_{t-1}^{i} < u\right\} + \sum_{t=1}^{T} \mathbb{P}\left\{I_{t}=i \text{ and } N_{t-1}^{i} \geq u\right\} \\ &\leq u + \sum_{t=u+1}^{T} \mathbb{P}\left\{I_{t}=i \text{ and } N_{t-1}^{i} \geq u\right\} \\ &\stackrel{\text{Lemma}}{\leq} u + \sum_{t=u+1}^{T} \mathbb{P}\left\{UCB_{t-1}^{i^{*}} \leq \mu^{i^{*}} \text{ or } LCB_{t-1}^{i} > \mu_{i}\right\} \\ &\stackrel{\text{Union bd.}}{\leq} u + \sum_{t=u+1}^{T} \mathbb{P}\left\{UCB_{t-1}^{i^{*}} \leq \mu^{i^{*}}\right\} + \sum_{t=u+1}^{T} \mathbb{P}\left\{LCB_{t-1}^{i} > \mu_{i}\right\} \end{split}$$

where $u = \lceil \frac{8\alpha \ln T}{\Delta_i^2} \rceil \le \frac{8\alpha \ln T}{\Delta_i^2} + 1.$

Confidence bounds are valid

We need to control two similar deviation events. For the first we will show

$$\sum_{t=u+1}^{T} \mathbb{P}\left\{\mathsf{UCB}_{t-1}^{i^*} \le \mu^{i^*}\right\} \le \sum_{t=u+1}^{T} \frac{1}{t^{\alpha-1}} \le \frac{1}{\alpha-2}.$$

Let $\tilde{\mu}_n^i$ be the average of the first n samples from arm i, so that $\hat{\mu}_{t-1}^i=\tilde{\mu}_{N_{t-1}^i}^i.$ Then

$$\begin{split} \mathbb{P}\left\{\mathsf{UCB}_{t-1}^{i^*} \leq \mu^{i^*}\right\} & \stackrel{\text{def}}{=} \mathbb{P}\left\{\hat{\mu}_{t-1}^{i^*} + \sqrt{\frac{2\alpha\ln(t)}{N_{t-1}^{i^*}}} \leq \mu^{i^*}\right\} \\ & = \mathbb{P}\left\{\hat{\mu}_{N_{t-1}^{i^*}}^{i^*} + \sqrt{\frac{2\alpha\ln(t)}{N_{t-1}^{i^*}}} \leq \mu^{i^*}\right\} \\ & \leq \mathbb{P}\left\{\exists s \in \{1, \dots, t\} : \hat{\mu}_s^{i^*} + \sqrt{\frac{2\alpha\ln(t)}{s}} \leq \mu^{i^*}\right\} \\ & \stackrel{\text{union bd}}{\leq} \sum_{s=1}^t \mathbb{P}\left\{\hat{\mu}_s^{i^*} + \sqrt{\frac{2\alpha\ln(t)}{s}} \leq \mu^{i^*}\right\} \\ & = \sum_{s=1}^t \mathbb{P}\left\{\mu^{i^*} - \hat{\mu}_s^{i^*} \geq \sqrt{\frac{2\alpha\ln(t)}{s}}\right\}^{\operatorname{Chernoft}} \sum_{s=1}^t e^{-s(\sqrt{\frac{2\alpha\ln(t)}{s}})^2/2} = \sum_{s=1}^t \frac{1}{t^\alpha} \end{split}$$

Overall result

We proved

Theorem (UCB Regret Bound)

UCB with $\alpha > 2$ satisfies

$$\bar{R}_T = \sum_{k=1}^K \mathbb{E}[N_T^k] \Delta_k \leq \left(\sum_{k \neq i^*}^K \frac{1}{\Delta_i}\right) 8\alpha \ln T + \left(1 + \frac{2}{\alpha - 2}\right) \sum_{k=1}^K \Delta_k$$

Conclusion of stochastic bandit part

An algorithm that can learn from partial information with stochastic losses.

Observations:

- Regret of UCB is In T whereas EXP3 is \sqrt{T} .
- Regret of UCB is **instance dependent** (through gaps Δ_i)
- Exploration/exploitation mechanism: confidence intervals + optimism
- Matching lower bounds exist (bonus material).