## Simons Tutorial: Online Learning and Bandits Part I

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## Positioning this Tutorial

- Building up tools in support of RL
- Exploring surrounding viewpoints, problems and methods
- Soaking up "Culture"


## Working Definitions

Context: interactive decision making in unknown environment Aim: Design systems to amass reward in many environments.

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Main distinction: model of environment

- Reinforcement Learning action affects future state
- Bandits action affects observation
- Full Inf. Online Learning action affects reward


## On the Menu

Two parts:
(1) Full Information Online Learning
(2) Bandits (w. Alan Malek)

## Full Information Online Learning

1. Two Basic Problems

Online Convex Optimisation; Online Gradient Descent
The Experts Problem; Exponential Weights
2. Two Peeks Beyond the Basics

Follow the Regularised Leader and Mirror Descent
Online Quadratic Optimisation; Online Newton Step
3. Applications

Classical Optimisation
Stochastic Optimisation
Saddle Points in Two-player Zero-Sum Games
4. Conclusion and Extensions

Two Basic Problems

## Setup

- Focus on losses (negative rewards)
- Model Environment as Adversary
- Online Convex Optimisation (OCO) abstraction.


## OCO Problem

## Protocol: Online Convex Optimisation

Given: game length $T$, convex action space $\mathcal{U} \subseteq \mathbb{R}^{d}$
For $t=1,2, \ldots, T$,

- The learner picks action $w_{t} \in \mathcal{U}$
- The adversary picks convex loss $f_{t}: \mathcal{U} \rightarrow \mathbb{R}$
- The learner observes $f_{t} \triangleleft$ full information
- The learner incurs loss $f_{t}\left(w_{t}\right)$


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The goal: control the regret (w.r.t. the best point after $T$ rounds)

$$
\mathcal{R}_{T}=\sum_{t=1}^{T} f_{t}\left(\boldsymbol{w}_{t}\right)-\min _{u \in \mathcal{U}} \sum_{t=1}^{T} f_{t}(u)
$$

using a computationally efficient algorithm for learner.

## Design Principle

Learner needs to "chase" the best point $\arg \min _{\boldsymbol{u} \in \mathcal{U}} \sum_{t=1}^{T} f_{t}\left(\boldsymbol{w}_{t}\right)$. But doing so naively overfits.

Idea: add regularisation. Two manifestations:

- Penalise excentricity "FTRL style"
- Update iterates, but only slowly "MD style"

Will see examples of both. For our purposes, these are roughly equivalent

## Online Gradient Descent (OGD) Algorithm

Let $\mathcal{U}$ be a convex set containing 0 . Fix a learning rate $\eta>0$.

## Algorithm: Online Gradient Descent (OGD)

OGD with learning rate $\eta>0$ plays

$$
\boldsymbol{w}_{1}=\mathbf{0} \quad \text { and } \quad \boldsymbol{w}_{t+1}=\Pi_{\mathcal{U}}\left(\boldsymbol{w}_{t}-\eta \nabla f_{t}\left(\boldsymbol{w}_{t}\right)\right)
$$

where $\Pi_{\mathcal{U}}(\boldsymbol{w})=\arg \min _{\boldsymbol{u} \in \mathcal{U}}\|\boldsymbol{u}-\boldsymbol{w}\|$ is the projection onto $\mathcal{U}$.


Figure 1: OGD update

## Online Gradient Descent Result

## Algorithm: OGD

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## Assumption: Boundedness

Bounded domain $\max _{\boldsymbol{u} \in \mathcal{U}}\|\boldsymbol{u}\| \leq D$ and gradients $\left\|\nabla f_{t}\left(\boldsymbol{w}_{t}\right)\right\| \leq G$.

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## Theorem (OGD regret bd, Zinkevich 2003)

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Tuning $\eta=\frac{D}{G \sqrt{T}}$ results in $\mathcal{R}_{T} \leq D G \sqrt{T}$.
Sublinear regret: learning overhead per round $\rightarrow 0$.

## Proof of OGD regret bound

Using convexity, we may analyse the tangent upper bound

$$
f_{t}\left(\boldsymbol{w}_{t}\right)-f_{t}(\boldsymbol{u}) \leq\left\langle\boldsymbol{w}_{t}-\boldsymbol{u}, \nabla f_{t}\left(w_{t}\right)\right\rangle
$$

Moreover,

$$
\begin{aligned}
\left\|\boldsymbol{w}_{t+1}-\boldsymbol{u}\right\|^{2} & =\left\|\Pi_{\mathcal{U}}\left(\boldsymbol{w}_{t}-\eta \nabla f_{t}\left(\boldsymbol{w}_{t}\right)\right)-\boldsymbol{u}\right\|^{2} \\
& \leq\left\|\boldsymbol{w}_{t}-\eta \nabla f_{t}\left(\boldsymbol{w}_{t}\right)-\boldsymbol{u}\right\|^{2} \\
& =\left\|\boldsymbol{w}_{t}-\boldsymbol{u}\right\|^{2}-2 \eta\left\langle\boldsymbol{w}_{t}-\boldsymbol{u}, \nabla f_{t}\left(\boldsymbol{w}_{t}\right)\right\rangle+\eta^{2}\left\|\nabla f_{t}\left(\boldsymbol{w}_{t}\right)\right\|^{2}
\end{aligned}
$$

Hence

$$
\left\langle\boldsymbol{w}_{t}-\boldsymbol{u}, \nabla f_{t}\left(\boldsymbol{w}_{t}\right)\right\rangle \leq \frac{\left\|\boldsymbol{w}_{t}-\boldsymbol{u}\right\|^{2}-\left\|\boldsymbol{w}_{t+1}-\boldsymbol{u}\right\|^{2}}{2 \eta}+\frac{\eta}{2}\left\|\nabla f_{t}\left(\boldsymbol{w}_{t}\right)\right\|^{2}
$$

## Proof of OGD regret bound (ctd)

Summing over $T$ rounds, we find

$$
\begin{aligned}
\mathcal{R}_{T}^{u} & \leq \sum_{t=1}^{T}\left\langle\boldsymbol{w}_{t}-\boldsymbol{u}, \nabla f_{t}\left(\boldsymbol{w}_{t}\right)\right\rangle \\
& \leq \underbrace{\sum_{t=1}^{T} \frac{\left\|\boldsymbol{w}_{t}-\boldsymbol{u}\right\|^{2}-\left\|\boldsymbol{w}_{t+1}-\boldsymbol{u}\right\|^{2}}{2 \eta}+\frac{\eta}{2} \sum_{t=1}^{T}\left\|\nabla f_{t}\left(\boldsymbol{w}_{t}\right)\right\|^{2}}_{\text {telescopes }} \\
& \leq \frac{\|\boldsymbol{u}\|^{2}-\left\|\boldsymbol{w}_{T+1}-\boldsymbol{u}\right\|^{2}}{2 \eta}+\frac{\eta}{2} \sum_{t=1}^{T}\left\|\nabla f_{t}\left(\boldsymbol{w}_{t}\right)\right\|^{2} \\
& \leq \frac{D^{2}}{2 \eta}+\frac{\eta}{2} T G^{2}
\end{aligned}
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## Theorem

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## Proof (by probabilistic argument).

Consider interval $\mathcal{U}=[-1,1]$ and linear losses $f_{t}(u)=x_{t} \cdot u$ with i.i.d. Rademacher coefficients $x_{t} \in\{ \pm 1\}$. Any algorithm has expected loss zero. The expected loss of the best action ( $\pm 1$ ) is $-\mathbb{E}\left[\left|\sum_{t=1}^{T} x_{t}\right|\right]=-\Omega(\sqrt{T})$. Then as the expected regret is $\mathbb{E}\left[\mathcal{R}_{T}\right]=\Omega(\sqrt{T})$, there is a deterministic witness.

Here, the regret arises from overfitting of the best point.

## OGD Discussion

- Adversarial result, super strong!
- Proof reveals it is really about linear losses.
- Matching lower bounds

Successful in practise:

- Practically all deep learning uses versions of online gradient descent (e.g. TensorFlow has AdaGrad [Duchi et al., 2011]) even though objective not convex.


## From Learning Parameters to Picking Actions

We now turn to the second elementary online learning task.

- Decision Theoretic Online Learning
- Experts setting (also: Hedge setting)
- Prediction with Expert Advice


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## Protocol: Prediction With Expert Advice

Given: game length $T$, number $K$ of experts
For $t=1,2, \ldots, T$,

- Learner chooses a distribution $w_{t} \in \triangle_{K}$ on $K$ "experts".
- Adversary reveals loss vector $\ell_{t} \in[0,1]^{K}$.
- Learner's loss is the dot loss $\boldsymbol{w}_{t}^{\top} \ell_{t}=\sum_{k=1}^{K} w_{t}^{k} \ell_{t}^{k}$


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using a computationally efficient algorithm for learner.

## Let's apply what we know

Observations:

- Dot loss $\boldsymbol{u} \mapsto \boldsymbol{u}^{\top} \ell_{t}$ is linear (hence convex).
- Gradient $\ell_{t} \in[0,1]^{K}$ bounded by $\left\|\ell_{t}\right\| \leq \sqrt{K}$.
- Probability simplex $\triangle_{K}$ is contained in unit ball.

So: Instance of Online Convex Optimisation.
OGD with $D=1$ and $G=\sqrt{K}$ gives $\mathcal{R}_{T} \leq \sqrt{K T}$.

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Q: Optimal?
Maybe not. There are no points with loss difference $\sqrt{K}$ in the simplex...

## Exponential Weigths / Hedge Algorithm

## Algorithm: Exponential Weights (EW)

EW with learning rate $\eta>0$ plays weights in round $t$ :

$$
\begin{equation*}
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}}} . \tag{EW}
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or, equivalently, $w_{1}^{k}=\frac{1}{K}$ and

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w_{t+1}^{k}=\frac{w_{t}^{k} e^{-\eta \ell_{t}^{k}}}{\sum_{j=1}^{K} w_{t}^{j} e^{-\eta \ell_{t}^{j}}}
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Theorem (EW regret bd, Freund and Schapire 1997)
The regret of EW is bounded by $\mathcal{R}_{T} \leq \frac{\ln K}{\eta}+T \frac{\eta}{8}$.

## Corollary

Tuning $\eta=\sqrt{\frac{8 \ln K}{T}}$ yields $\mathcal{R}_{T} \leq \sqrt{T / 2 \ln K}$.

## EW Analysis

Applying Hoeffding's Lemma to the loss of each round gives

$$
\sum_{t=1}^{T} \boldsymbol{w}_{t}^{\top} \ell_{t} \leq \sum_{t=1}^{T}(\underbrace{\frac{-1}{\eta} \ln \left(\sum_{k=1}^{K} w_{t}^{k} e^{-\eta \ell_{t}^{k}}\right)}_{\text {"mix loss" }}+\underbrace{\eta / 8}_{\text {overhead }})
$$

Crucial observation is that cumulative mix loss telescopes

$$
\begin{aligned}
\sum_{t=1}^{T} \frac{-1}{\eta} \ln \left(\sum_{k=1}^{K} w_{t}^{K} e^{-\eta \ell_{t}^{k}}\right) & =\sum_{t=1}^{T} \frac{-1}{\eta} \ln \left(\sum_{k=1}^{K} \frac{e^{-\eta \sum_{s=1}^{t-1} \ell_{s}^{k}}}{\sum_{j=1}^{K} e^{-\eta \sum_{s=1}^{t-1} \ell_{s}^{j}}} e^{-\eta \ell_{t}^{k}}\right) \\
& =\sum_{t=1}^{T} \frac{-1}{\eta} \ln \left(\frac{\sum_{k=1}^{K} e^{-\eta \sum_{s=1}^{t} \ell_{s}^{k}}}{\sum_{j=1}^{K} e^{-\eta \sum_{s=1}^{t-1} \ell_{s}^{\prime}}}\right) \\
& \stackrel{\text { telescopes }}{=} \frac{-1}{\eta} \ln \left(\sum_{k=1}^{K} e^{-\eta \sum_{t=1}^{T} e_{t}^{k}}\right)+\frac{\ln K}{\eta} \\
& \leq \min _{k \in[K]} \sum_{t=1}^{T} l_{t}^{K}+\frac{\ln K}{\eta} .
\end{aligned}
$$

## Summary so far

Balancing act: "model complexity" vs "overfitting"

Theorem (OGD)

$$
\mathcal{R}_{T} \leq \frac{D^{2}}{2 \eta}+\frac{\eta}{2} G^{2} T
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Theorem (EW)
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Generates many follow-up questions:

- What if horizon $T$ is not fixed? Anytime guarantees?
- What if gradient bound $G$ is not known a priori?
- Can we have the actual gradient norms?
- What if model complexity $(D)$ is not known? Not uniformly bounded? See Orabona and Cutkosky ICML'20 tutorial.


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Two Peeks Beyond the Basics

## FTRL/MD "sneak peek"

Q: What if my domain does not look like either ball or simplex?

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## Algorithm: Follow the Regularised Leader (FTRL)

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\boldsymbol{w}_{t+1}=\underset{\boldsymbol{u} \in \mathcal{U}}{\arg \min } \sum_{s=1}^{t}\left\langle\boldsymbol{u}, \nabla f_{s}\left(w_{s}\right)\right\rangle+\frac{1}{\eta} R(\boldsymbol{u})
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## Algorithm: Mirror Descent (MD)

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Examples:

## Regularizer $R$

OGD sq. Euclidean norm EW Shannon entropy

Bregman Divergence $B$
sq. Euclidean distance
Kullback-Leibler divergence

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Bregman Divergence $B$
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Kullback-Leibler divergence

Other entropies: Burg, Tsallis, Von Neumann, ... Connections to continuous exponential weights [van der Hoeven et al., 2018].

## FTRL/MD "sneak peak" performance

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$$

## Theorem (AdaFTRL, Orabona and Pál 2015)

Fix a norm $\|\cdot\|$ with associated dual norm $\|\cdot\|_{\star}$. Let $R: \mathcal{U} \rightarrow\left[0, D^{2}\right]$ be strongly convex w.r.t. $\|\cdot\|$. AdaFTRL ensures

$$
\mathcal{R}_{T} \leq 2 D \sqrt{\sum_{t=1}^{T}\left\|\nabla f_{t}\left(w_{t}\right)\right\|_{\star}^{2}}+2 \cdot \text { loss range }
$$

## Quadratic Losses

So far we used convexity to "linearise"

$$
f_{t}(\boldsymbol{u}) \geq f_{t}\left(\boldsymbol{w}_{t}\right)+\left\langle\boldsymbol{u}-\boldsymbol{w}_{t}, \nabla f_{t}\left(\boldsymbol{w}_{t}\right)\right\rangle,
$$

and our methods essentially operated on linear losses. But what if we know there is curvature?

- How to represent/quantify curvature?
- How to efficiently manipulate curvature?
- How much can we reduce the regret?


## Curvature assumptions

## Assumption: Quadratic loss lower bound

There is a matrix $M_{t} \succeq \mathbf{0}$ such that

$$
f_{t}(\boldsymbol{u}) \geq \underbrace{f_{t}\left(\boldsymbol{w}_{t}\right)+\left\langle\boldsymbol{u}-\boldsymbol{w}_{t}, \nabla f_{t}\left(\boldsymbol{w}_{t}\right)\right\rangle+\frac{1}{2}\left(\boldsymbol{u}-\boldsymbol{w}_{t}\right)^{\top} \boldsymbol{M}_{t}\left(\boldsymbol{u}-\boldsymbol{w}_{t}\right)}_{=: q_{t}(\boldsymbol{u})}
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for each $\boldsymbol{u} \in \mathcal{U}$.

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$$

for each $\boldsymbol{u} \in \mathcal{U}$.
Two main classes of instances

- squared Euclidean distance: $f_{t}(u)=\frac{1}{2}\left\|u-x_{t}\right\|^{2}$ satisfies the assumption with $\boldsymbol{M}_{t}=\boldsymbol{I}$. More generally, strongly convex functions have $M_{t} \propto I$.
- linear regression: $f_{t}(\boldsymbol{u})=\left(y_{t}-\left\langle\boldsymbol{u}, \boldsymbol{x}_{t}\right\rangle\right)^{2}$ satisfies the assumption with $M_{t}=x_{t} x_{t}^{\top}$. More generally, exp-concave functions have $\boldsymbol{M}_{t} \propto \nabla_{t} f_{t}\left(\boldsymbol{w}_{t}\right) \nabla_{t} f_{t}\left(\boldsymbol{w}_{t}\right)^{\top}$.


## ONS Algorithm

## Algorithm: Online Newton Step (FTRL variant)

$$
\boldsymbol{w}_{t+1}=\underset{\boldsymbol{u} \in \mathcal{U}}{\arg \min } \sum_{s=1}^{t} q_{s}(\boldsymbol{u})+\frac{1}{2}\|\boldsymbol{u}\|^{2}
$$

Computing the iterate $w_{t+1}$ amounts to minimising a convex quadratic. Often (depending on $\mathcal{U}$ ) closed-form solution or 1d line search.

- For $M_{t} \propto I$, takes $O(d)$ per round.
- For rank-one $M_{t}$, can do update in $O\left(d^{2}\right)$ per round.
- In both cases, need to take care of projection onto $\mathcal{U}$.


## ONS Performance

## Algorithm: Online Newton Step (FTRL version)

$$
\boldsymbol{w}_{t+1}=\underset{\boldsymbol{u} \in \mathcal{U}}{\arg \min } \sum_{s=1}^{t} q_{s}(\boldsymbol{u})+\frac{1}{2}\|\boldsymbol{u}\|^{2}
$$

## Theorem (ONS strcvx bd, Hazan et al. 2006)

For the strongly convex case $M_{t} \propto I$, ONS guarantees

$$
\mathcal{R}_{T}=O(\ln T)
$$

Algorithm reduces to OGD with specific decreasing step-size $\eta_{t}$

## Theorem (ONS expccv bd, Hazan et al. 2006)

For the exp-concave case $M_{t} \propto g_{t} g_{t}^{\top}$, ONS guarantees

$$
\mathcal{R}_{T}=O(d \ln T)
$$

## ONS Discussion

- Convex quadratics closed under taking sums. Run-time independent of $T$.
- Curvature gives huge reduction in regret: $\sqrt{T}$ to $\ln T$.
- Matrix sketching techniques allow trading off run-time $O\left(d^{2}\right)$ vs $O(d)$ with regret $O(\ln T)$ vs $O(\sqrt{T})$ [Luo et al., 2016].

Applications

## Application 1: Offline Optimisation

## Problem

Given gradient access to a convex $f$, find a near-optimal point.

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Given gradient access to a convex $f$, find a near-optimal point.
Idea: run OGD on $f_{t}=f$ for $T$ rounds. Regret bound gives

$$
\sum_{t=1}^{T} f\left(\boldsymbol{w}_{t}\right)-T \min _{\boldsymbol{u} \in \mathcal{U}} f(\boldsymbol{u}) \leq G D \sqrt{T}
$$

We may divide by $T$ and apply convexity to find

$$
f\left(\frac{1}{T} \sum_{t=1}^{T} w_{t}\right)-\min _{u \in \mathcal{U}} f(u) \leq \frac{G D}{\sqrt{T}}
$$

Find $\epsilon$-suboptimal point (iterate average) after $T=\frac{G^{2} D^{2}}{\epsilon^{2}}$ rounds.

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Find $\epsilon$-suboptimal point (iterate average) after $T=\frac{G^{2} D^{2}}{\epsilon^{2}}$ rounds.

Why would we optimise this way? For example, what if $f_{t} \rightarrow f$.

## Application 2: Online to Batch

## Assumption: stochastic setting

Suppose training set $f_{1}, \ldots, f_{T}$ and test point $f$ drawn i.i.d. from unknown $\mathbb{P}$.

## Problem

Learn a point $\hat{w}_{T}$ from the training set that generalises to $\mathbb{P}$, i.e. behaves like $\boldsymbol{u}^{*}=\arg \min _{\boldsymbol{u} \in \mathcal{U}} \mathbb{E}_{f}[f(\boldsymbol{u})]$

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i.e. behaves like $\boldsymbol{u}^{*}=\arg \min _{\boldsymbol{u} \in \mathcal{U}} \mathbb{E}_{f}[f(\boldsymbol{u})]$

Idea: use online learning algorithm on training set $f_{1}, \ldots, f_{T}$, to get iterates $w_{1}, \ldots, w_{T}$. Output the average iterate estimator

$$
\hat{\boldsymbol{w}}_{T}=\frac{1}{T} \sum_{t=1}^{T} \boldsymbol{w}_{t}
$$

## Theorem

An online regret bound $R_{T} \leq B(T)$ implies

$$
\mathbb{E}_{i i d} f_{1}, \ldots, f_{T}, f\left[f\left(\hat{w}_{T}\right)-f\left(u^{*}\right)\right] \leq \frac{B(T)}{T}
$$

## Application 3: Computing Saddle Points

Assumption: convex-concave
Fix an objective function

$$
g(x, y)
$$

convex in $x$, concave in $y$.

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The game value is

$$
V^{*}=\min _{x} \max _{y} g(x, y)=\max _{y} \min _{x} g(x, y)
$$

An $\epsilon$-saddle point $(\bar{x}, \bar{y})$ satisfies

$$
V^{*}-\epsilon \leq \min _{x} g(x, \bar{y}) \leq V^{*} \leq \max _{y} g(\bar{x}, y) \leq V^{*}+\epsilon
$$

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Find an $\epsilon$-saddle point

## Application 3: Computing Saddle Points

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An $\epsilon$-saddle point ( $\bar{x}, \bar{y}$ ) satisfies

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$$

## Problem

Find an $\epsilon$-saddle point

Idea: play regret minimisation algorithms for $x$ and $y$.

## Application 3: Saddle Point Algorithm

## Algorithm: approximate saddle point solver

## For $t=1,2, \ldots, T$

- Players play $x_{t}$ and $y_{t}$.
- Players see loss functions $x \mapsto+g\left(x, y_{t}\right)$ and $y \mapsto-g\left(x_{t}, y\right)$.

Output average iterate pair $\bar{x}_{T}=\frac{1}{T} \sum_{t=1}^{T} x_{t}$ and $\bar{y}_{T}=\frac{1}{T} \sum_{t=1}^{T} y_{t}$
Assume the players have regret (bounds) $\mathcal{R}_{T}^{\chi}$ and $\mathcal{R}_{T}^{y}$, i.e.

$$
\begin{aligned}
& \sum_{t=1}^{T}+g\left(x_{t}, y_{t}\right)-\min _{x} \sum_{t=1}^{T}+g\left(x, y_{t}\right) \leq \mathcal{R}_{T}^{x} \\
& \sum_{t=1}^{T}-g\left(x_{t}, y_{t}\right)-\min _{y} \sum_{t=1}^{T}-g\left(x_{t}, y\right) \leq \mathcal{R}_{T}^{y}
\end{aligned}
$$

## Theorem (self-play, Freund and Schapire 1999)

$\bar{x}_{T}$ and $\bar{y}_{T}$ form an $\frac{\mathcal{R}_{T}^{x}+\mathcal{R}_{T}^{y}}{T}$-saddle point.

## Application 3: Saddle Point Analysis

$$
\begin{aligned}
V^{*} & =\min _{x} \max _{y} g(x, y) \\
& \leq \max _{y} g\left(\bar{x}_{T}, y\right) \\
& \leq \max _{y} \frac{1}{T} \sum_{t=1}^{T} g\left(x_{t}, y\right) \\
& \leq \frac{1}{T} \sum_{t=1}^{T} g\left(x_{t}, y_{t}\right)+\frac{\mathcal{R}_{T}^{y}}{T} \\
& \leq \min _{x} \frac{1}{T} \sum_{t=1}^{T} g\left(x, y_{t}\right)+\frac{\mathcal{R}_{T}^{x}+\mathcal{R}_{T}^{y}}{T} \\
& \leq \min _{x} g\left(x, \bar{y}_{T}\right)+\frac{\mathcal{R}_{T}^{x}+\mathcal{R}_{T}^{y}}{T} \\
& \leq \min _{x} \max _{y} g(x, y)+\frac{\mathcal{R}_{T}^{x}+\mathcal{R}_{T}^{y}}{T} \\
& =V^{*}+\frac{\mathcal{R}_{T}^{x}+\mathcal{R}_{T}^{y}}{T}
\end{aligned}
$$

## Conclusion and Extensions

## Conclusion

- Online Learning a powerful and versatile tool
- Environment-as-black-box. Adversarial.
- Foundation for optimisation, statistical learning, games, ...


## Conclusion

- Online Learning a powerful and versatile tool
- Environment-as-black-box. Adversarial.
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Some (of many) cool things we left out:

- First-order (small loss) and second-order (small variance) bounds
- Adaptivity to friendly stochastic environments (best of both worlds, interpolation)
- Optimism (predicting the upcoming gradient)
- Non-stationarity (tracking, adaptive/dynamic regret, path length)
- Beyond convexity (star-convex, geometrically convex, ...)
- Supervised Learning and (stochastic) complexities (VC, Littlestone, Rademacher, ...)


## Thanks!

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## Simons Tutorial: Online Learning and Bandits Part II

Wouter Koolen and Alan Malek
August 31st, 2020

## What is a Bandit?

## The Basic Bandit Game

## Protocol: Finite-Arm Bandits

Given: game length $T$, number of arms $K$
For $t=1,2, \ldots, T$,

- The learner picks action $I_{t} \in\{1, \ldots, K\}$
- The adversary simultaneously picks rewards

$$
r_{t} \in\{1, \ldots, K\} \rightarrow[0,1]
$$

- The learner observes and receives $r_{t}\left(I_{t}\right)$
- The learner does not observe $r_{t}(i)$ for $i \neq I_{t}$

The goal: control the regret (a random variable)

$$
\mathcal{R}_{T}=\underbrace{\max _{i} \sum_{t=1}^{T} r_{t}(i)}_{\text {Best action in hindsight }}-\sum_{t=1}^{T} r_{t}\left(I_{t}\right)
$$

## Bandits are Super Simple MDP

- $S=\{$ the_state $\}, P($ the_state $\mid$ the_state,$a)=1$
- Why should we care about this in RL?
- Creates a tension between
- Exploration (learning about the loss of actions)
- Exploitation (playing actions that will have low regret)
- Exploration/Exploitation is absent in full-information but very present in reinforcement learning
- Model is simple enough to allow for comprehensive theory
- Easily incorporates adversarial data
- Useful algorithm design principles


## The Regret

$$
\mathcal{R}_{T}=\underbrace{\max _{i} \sum_{t=1}^{T} r_{t}(i)}_{\text {Best action in hindsight }}-\sum_{t=1}^{T} r_{t}\left(I_{t}\right)
$$

- $\mathcal{R}_{T}$ is a random variable we do not observe
- Different objectives, from easiest to hardest
- Pseudo-regret $\overline{\mathcal{R}_{T}}=\max _{i} \mathbb{E}\left[\sum_{t=1}^{T} r_{t}(i)\right]-\mathbb{E}\left[\sum_{t=1}^{T} r_{t}\left(I_{t}\right)\right]$
- Expected regret $\mathbb{E}\left[\mathcal{R}_{T}\right]=\mathbb{E}[\underbrace{\max _{i} \sum_{t=1}^{T} r_{t}(i)}_{\text {can depend on } I_{t}}-\sum_{t=1}^{T} r_{t}\left(I_{t}\right)]$
- High probability bounds on the realized regret


## The Regret

$$
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- Expected regret $\mathbb{E}\left[\mathcal{R}_{T}\right]=\mathbb{E}[\underbrace{\max _{i} \sum_{t=1}^{T} r_{t}(i)}_{\text {can depend on } I_{t}}-\sum_{t=1}^{T} r_{t}\left(I_{t}\right)]$
- High probability bounds on the realized regret
- We always have $\overline{\mathcal{R}_{T}} \leq \mathbb{E}\left[\mathcal{R}_{T}\right]$
- If the adversary is reactive, then the distribution of $r_{t}$ can be a function of $I_{1}, \ldots, I_{t-1}$
- Otherwise, the adversary is oblivious and $\overline{\mathcal{R}_{T}}=\mathbb{E}\left[\mathcal{R}_{T}\right]$


## Our Focus

- Introduce most popular bandit problems
- Adversarial Bandits
- Stochastic Bandits
- Pure Exploration Bandits
- Contextual Bandits (time permitting)
- Concentrate on useful algorithm design principles
- Exponential weights (still useful)
- Optimism in the face of Uncertainty
- Probability matching (i.e. Thompson sampling)
- Action-Elimination


## Other Settings that Have Been Considered

- Data models for $r_{t}$
- chosen by an adversary
- sampled i.i.d.
- stochastic with adversarial perturbations...
- Action spaces
- Finite number of arms
- A vector space ( $r_{t}$ are functions)
- Combinatorial (e.g. subsets, paths on a graph)
- Objectives
- Pseudo-regret (the expectation over the learner's randomness)
- Realized regret (with high probability)
- Best-arm identification a.k.a. pure exploration
- Side information
- Linear rewards
- Competing with a policy class


## Adversarial Bandits

## Adversarial Protocol

## Protocol: Finite-Arm Adversarial Bandits

Given: game length $T$, number of arms $K$
For $t=1,2, \ldots, T$,

- The learner picks action $I_{t} \in\{1, \ldots, K\}$
- The adversary simultaneously picks losses $\ell_{t} \in[0,1]^{K}$
- The learner observes and receives $\ell_{t}\left(I_{t}\right)$
- The results are easier to state using losses instead of rewards
- Randomization of $I_{t}$ is essential
- We are familiar with adversarial data from the first half
- The simple idea of estimating $\ell_{t}$ from $\ell_{t}\left(I_{t}\right)$ and then applying a full-information algorithm works very well


## Algorithm Design Principle: Exponential Weights

## Algorithm: Exp3 [Auer et al., 2002b]

Given: number of arms $K$, learning rate $\eta>0$, length $T$ Initialize $p_{1}(i)=1 / K, \hat{L}_{0}(i)=0$ for all $i \in[K]$

For $t=1,2, \ldots, T$ :

- Sample $I_{t} \sim p_{t}$ and observe $\ell_{t}\left(I_{t}\right)$
- Estimate $\hat{\ell}_{t}(i)=\frac{\ell_{t}\left(l_{t}\right)}{p_{t}\left(l_{t}\right)} \mathbb{1}_{\left\{I_{t}=i\right\}}$ and $\hat{L}_{t}=\hat{\ell}_{t}+\hat{L}_{t-1}$
- Calculate $W_{t}=\sum_{j} e^{-\eta \hat{L}_{t}(j)}$ and $p_{t+1}(i)=\frac{1}{W_{t}} e^{-\eta \hat{L}_{t}(i)}$


## Algorithm Design Principle: Exponential Weights

## Algorithm: Exp3 [Auer et al., 2002b]

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For $t=1,2, \ldots, T$ :

- Sample $I_{t} \sim p_{t}$ and observe $\ell_{t}\left(I_{t}\right)$
- Estimate $\hat{\ell}_{t}(i)=\frac{\ell_{t}\left(I_{t}\right)}{p_{t}\left(I_{t}\right)} \mathbb{1}_{\left\{I_{t}=i\right\}}$ and $\hat{L}_{t}=\hat{\ell}_{t}+\hat{L}_{t-1}$
- Calculate $W_{t}=\sum_{j} e^{-\eta \hat{L}_{t}(j)}$ and $p_{t+1}(i)=\frac{1}{W_{t}} e^{-\eta \hat{L}_{t}(i)}$
- Exp3 $=$ Exponential Weights for Exploration and Exploitation
- $\hat{\ell}_{t}$ is the importance-weighted estimator of $\ell_{t}$
- $\hat{\ell}_{t}$ is unbiased:

$$
\mathbb{E}_{l_{t} \sim p_{t}}\left[\hat{\ell}_{t}(i)\right]=\mathbb{E}\left[\frac{\ell_{t}\left(I_{t}\right)}{p_{t}\left(I_{t}\right)} \mathbb{1}_{\left\{I_{t}=i\right\}}\right]=\sum_{j} p_{t}(j) \frac{\ell_{t}(j)}{p_{t}(j)} \mathbb{1}_{\{j=i\}}=\ell_{t}(i) .
$$

- Exp3 runs exponential weights on $\hat{\ell}_{t}$


## Exp3: Abridged Analysis

- Using the same $\frac{W_{t}}{W_{t-1}}$ telescoping procedure as in the full information case with $i^{*}$ arbitrary but fixed,

$$
\sum_{t=1}^{T} \sum_{j} p_{t}(j) \mathbb{E}\left[\hat{\ell}_{t}(j)-\hat{L}_{T}\left(i^{*}\right)\right] \leq \frac{\log (K)}{\eta}+\frac{\eta}{2} \sum_{t=1}^{T} \mathbb{E}\left[\sum_{j} p_{t}(j) \hat{\ell}_{t}(j)^{2}\right] .
$$

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\sum_{t=1}^{T} \sum_{j} p_{t}(j) \mathbb{E}\left[\hat{\ell}_{t}(j)-\hat{L}_{T}\left(i^{*}\right)\right] \leq \frac{\log (K)}{\eta}+\frac{\eta}{2} \sum_{t=1}^{T} \mathbb{E}\left[\sum_{j} p_{t}(j) \hat{\ell}_{t}(j)^{2}\right]
$$

- Because $\hat{\ell}_{t}$ is unbiased,

$$
\sum_{t=1}^{T} \sum_{j} p_{t}(j) \mathbb{E}\left[\hat{\ell}_{t}(j)-\hat{L}_{T}\left(i^{*}\right)\right]=\sum_{t=1}^{T} \sum_{j} p_{t}(j) \ell_{t}(j)-L_{T}\left(i^{*}\right) \geq \overline{\mathcal{R}}_{T} .
$$

## Exp3: Abridged Analysis

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$$
\sum_{t=1}^{T} \sum_{j} p_{t}(j) \mathbb{E}\left[\hat{\ell}_{t}(j)-\hat{L}_{T}\left(i^{*}\right)\right] \leq \frac{\log (K)}{\eta}+\frac{\eta}{2} \sum_{t=1}^{T} \mathbb{E}\left[\sum_{j} p_{t}(j) \hat{\ell}_{t}(j)^{2}\right] .
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- Because $\hat{\ell}_{t}$ is unbiased,

$$
\sum_{t=1}^{T} \sum_{j} p_{t}(j) \mathbb{E}\left[\hat{\ell}_{t}(j)-\hat{L}_{T}\left(i^{*}\right)\right]=\sum_{t=1}^{T} \sum_{j} p_{t}(j) \ell_{t}(j)-L_{T}\left(i^{*}\right) \geq \overline{\mathcal{R}}_{T} .
$$

- Bounding the variance term turns out to be easy:
$\mathbb{E}\left[\sum_{j} p_{t}(j) \frac{\ell_{t}\left(I_{t}\right)^{2}}{p_{t}\left(I_{t}\right)^{2}} \mathbb{1}_{\left\{I_{t}=i\right\}}\right] \leq \mathbb{E}\left[\sum_{j} p_{t}(j) \frac{\mathbb{1}_{\left\{I_{t}=i\right\}}}{p_{t}\left(I_{t}\right)^{2}}\right]=\mathbb{E}\left[\frac{1}{p_{t}\left(I_{t}\right)}\right]=K$.


## Exp3: Analysis

So, plugging this in, we find

$$
\sum_{t=1}^{T} \mathbb{E}\left[\ell\left(I_{t}\right)\right]-L_{T}\left(i^{*}\right) \leq \frac{\log (K)}{\eta}+\frac{\eta}{2} T K .
$$

## Theorem (Exp3 upper bound [Auer et al., 2002b])

With $\eta=\sqrt{\frac{2 \log (T)}{T K}}$, Exp3 has $\overline{\mathcal{R}}_{T} \leq \sqrt{2 T K \log (K)}$.
Only get pseudo-Regret bounds because the $i^{*}$ in the proof was fixed, not a function of $I_{1}, \ldots, I_{T}$

## Lower Bounds

Theorem (Adversarial Bandits lower bound [Auer et al., 2002b])
Any adversarial bandit algorithm must have

$$
\overline{\mathcal{R}}_{T}=\Omega(\sqrt{T K})
$$

- Exp3 upper bound: $\overline{\mathcal{R}}_{T} \leq \sqrt{2 T K \log (K)}$
- First matching upper bound achieved by INF [Audibert and Bubeck, 2009] (which is Mirror Descent)


## Upgrades

- High Probability bounds: requires a lower-variance estimate of $\hat{\ell}_{t}$ or an algorithm that keeps $p_{t}(i)$ away from zero
- Exp3.P [Auer et al., 2002b] uses $\hat{\ell}_{t}(i)=\frac{1_{\left\{l_{t}=i\right\}} \ell_{t}\left(l_{t}\right)-\beta}{p_{t}\left(I_{t}\right)}$
- Exp3-IX [Neu, 2015] uses $\hat{\ell}_{t}(i)=\frac{\left.1_{\left\{l_{t}=i=1\right.}\right\}_{t}\left(l_{t}\right)}{p_{t}\left(l_{t}\right)+\gamma}$
- Experts with bandits; each arm is an expert that recommends actions: you compete with the best expert (Exp4 algorithm) [Auer et al., 2002b]
- Competing with strategies that can switch [Auer, 2002]
- Feedback determined by a graph [Mannor and Shamir, 2011]
- Partial Monitoring [Bartók et al., 2014]
- Combinatorial action spaces...


## Stochastic Bandits

## Protocol

## Protocol: Stochastic Bandits

Given: game length $T$, number of arms $K$, reward distributions $\nu_{1}, \ldots, \nu_{K}$

For $t=1,2, \ldots, T$,

- The learner picks action $I_{t} \in\{1, \ldots, K\}$
- The learner observes and receives reward $X_{t} \sim \nu_{l_{t}}$


## Protocol

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For $t=1,2, \ldots, T$,

- The learner picks action $I_{t} \in\{1, \ldots, K\}$
- The learner observes and receives reward $X_{t} \sim \nu_{l_{t}}$
- Stochastic bandits is an old problem [Thompson, 1933]
- We will use the following notation
- Reward of arm $i$ is sampled from $\nu_{i}$ with $\mu_{i}:=\mathbb{E}_{X \sim \nu_{i}}[X]$
- $i^{*}=\arg \max _{i} \mu_{i}$ is the best arm
- Gaps $\Delta_{i}:=\mu_{i^{*}}-\mu_{i} \geq 0$,
- Number of pulls $N_{i, t}:=\sum_{s=1}^{t} \mathbb{1}_{\left\{l_{s}=i\right\}}$
- Empirical mean $\hat{\mu}_{i, t}:=\frac{\left.\sum_{s=1}^{t} x_{s 1} 1_{\{l s}=i\right\}}{N_{i, t}}$


## Protocol

## Protocol: Stochastic Bandits

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For $t=1,2, \ldots, T$,

- The learner picks action $I_{t} \in\{1, \ldots, K\}$
- The learner observes and receives reward $X_{t} \sim \nu_{l_{t}}$
- We still want to minimize the expected regret, which has the useful decomposition

$$
\mathbb{E}\left[\mathcal{R}_{T}\right]=T \mu_{i^{*}}-\sum_{t=1}^{T} \mathbb{E}\left[X_{t}\right]=\sum_{i} \Delta_{i} \mathbb{E}\left[N_{i, T}\right]
$$

## Protocol

## Protocol: Stochastic Bandits

Given: game length $T$, number of arms $K$, reward distributions $\nu_{1}, \ldots, \nu_{K}$

For $t=1,2, \ldots, T$,

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$$

Assumption: 1-sub-Gaussian reward distributions
For all stochastic bandit problems, we will assume that all arms are 1-sub-Gaussian, i.e. $\mathbb{E}_{X \sim \mu}\left[e^{\lambda(X-\mu)^{2}-\lambda^{2} / 2}\right] \leq 1$. For $X_{1}, \ldots, X_{t}$, This implies the Hoeffding bound

$$
P\left(\frac{1}{t} \sum_{s=1}^{t} X_{s}-\mu_{i} \geq \epsilon\right) \leq e^{-\frac{e^{2} t}{2}} .
$$

## Warm-up: Explore-Then-Commit

## Algorithm: Explore-Then-Commit

Given: Game length $T$, exploration parameter $M$
For $t=1,2, \ldots, M K$ :

- Choose $i_{t}=(t \bmod K)$, see $X_{t} \sim \nu_{i_{t}}$

Compute empirical means $\hat{\mu}_{i, m k}$
For $t=M K+1, M K+2, \ldots, T$ :

- Pull arm $i=\arg \max _{i} \hat{\mu}_{i, m K}$
- The first strategy you might try
- A proof idea that we will return to: bound regret by first bounding $\mathbb{E}\left[N_{i, T}\right]$.
- In this simple algorithm,

$$
\mathbb{E}\left[N_{i, T}\right]=M+(T-M K) P\left(i=\underset{j}{\arg \max } \hat{\mu}_{j, M K}\right)
$$

## Explore-Then-Commit Upper Bound

Using the sub-Gaussian concentration bound,

$$
\begin{aligned}
P\left(i=\underset{j}{\arg \max } \hat{\mu}_{j, M K}\right) & \leq P\left(\hat{\mu}_{i, M K} \geq \hat{\mu}_{i^{*}, M K}\right) \\
& =P\left(\left(\hat{\mu}_{i, M K}-\mu_{i}\right) \geq\left(\hat{\mu}_{i^{*}, M K}-\mu_{i^{*}}\right)+\Delta_{i}\right) \\
& \leq e^{-\frac{M \Delta_{i}^{2}}{4}} \text { (the difference is } \sqrt{2 / M} \text {-sub-Gaussian) }
\end{aligned}
$$

## Explore-Then-Commit Upper Bound

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& \leq e^{-\frac{M \Delta_{i}^{i}}{4}} \text { (the difference is } \sqrt{2 / M} \text {-sub-Gaussian) }
\end{aligned}
$$

## Theorem (Explore-Then-Commit upper bound)

$$
\mathbb{E}\left[\mathcal{R}_{T}\right]=\sum_{i} \Delta_{i} \mathbb{E}\left[N_{i, T}\right] \leq \sum_{i=1}^{K} \Delta_{i}\left(M+(T-M K) e^{-\frac{M \Delta_{i}^{2}}{4}}\right)
$$

- For the two arm case, if we know $\Delta$, then $m=\frac{4}{\Delta_{1}^{2}} \log \frac{T \Delta_{1}^{2}}{4}$, results in $\mathbb{E}\left[\mathcal{R}_{T}\right] \leq \sum_{i=1}^{K} \frac{4}{\Delta_{1}} \log \frac{T \Delta_{1}^{2}}{4}+T \frac{4}{T \Delta_{1}^{2}}=O\left(\frac{K \log (T)}{\Delta_{1}}\right)$
- But we don't know $\Delta$...can we be adaptive?


## Algorithm Design Principle: OFU

- OFU: Optimism in the Face of Uncertainty
- We establish some confidence set for the problem instance (e.g. means) to within some confidence set
- We then assume the most favorable instance in the confidence set and act greedily


## Algorithm Design Principle: OFU

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- We then assume the most favorable instance in the confidence set and act greedily


## Algorithm: UCB1 [Auer et al., 2002a]

Given: Game length $T$
Initialize: play every arm once
For $t=K+1,2, \ldots, T$ :

- Compute upper confidence bounds $B_{i, t-1}=\sqrt{\frac{6 \log (t)}{N_{i, t-1}}}$
- Choose $I_{t}=\arg \max _{i} \hat{\mu}_{i, t-1}+B_{i, t-1}$, observe $X_{t} \sim \nu_{l_{t}}$
- Update $N_{i, t}=N_{i, t-1}+\mathbb{1}_{\left\{I_{t}=i\right\}}$ and $\hat{\mu}_{i, t}=\frac{\sum_{s=1}^{t} 1_{\left\{I_{s}=i\right\}} X_{s}}{N_{i, t}}$


## UCB Illustration

Round 1


## UCB Illustration

Round 2


## UCB Illustration

Round 3


## UCB: Intuition

- Naturally balances exploration and exploitation: an arm has a high UCB if
- It has a high $\hat{\mu}_{i, t}$, or
- $B_{i, t}$ is large because $N_{i, t-1}$ is small
- Optimistic because we pretend the rewards are the plausibly best and then do the greedy thing


## UCB: Analysis

- Define $M_{i}=\left\lceil\frac{12 \log (T)}{\Delta_{i}^{2}}\right\rceil$, the number of pulls of arm $i$ such that $B_{i, t}=\sqrt{\frac{6 \log (t)}{N_{i, t}}} \leq \sqrt{\frac{6 \log (T)}{N_{i, t}}} \leq \frac{\Delta_{i}}{2}$
- The intuition of the proof is

1. Since $\overline{\mathcal{R}_{T}}=\sum_{i} \Delta_{i} \mathbb{E}\left[N_{i, T}\right]$, we bound $\mathbb{E}\left[N_{i, t}\right]$ first.
2. With high probability, we will never pull arm $i$ more than $M_{i}$ times, so

$$
\mathbb{E}\left[N_{i, T}\right]=\mathbb{E} \sum_{t=1}^{T} \mathbb{1}_{\left\{l_{t}=i\right\}} \leq M_{i}+\sum_{t=M_{i}}^{T} \underbrace{\mathbb{E} \mathbb{\{}_{\left\{t=i, N_{i, t}>M_{i}\right\}}}_{\text {we will bound this }}
$$

3. If $\left\{I_{t}=i, N_{i, t}>M_{i}\right\}$ occurs, then the UCB for $i^{*}$ or for $i$ must be wrong (next slide)

## UCB: Analysis

Claim: if $\left\{I_{t}=i, N_{i, t}>M_{i}\right\}$ occurs, then either $\hat{\mu}_{i, t}$ must be too high or $\hat{\mu}_{i^{*}, t}$ must be too low. In a picture:


In an equation: suppose that $N_{i, t}>M_{i}, \hat{\mu}_{i, t}-B_{i, t} \geq \mu_{i}$, and $\hat{\mu}_{i^{*}, t}+B_{i^{*}, t} \geq \mu_{i^{*}}$. Then

$$
\hat{\mu}_{i^{*}, t}+B_{i^{*}, t} \geq \mu_{i^{*}}=\mu_{i}+\Delta_{i} \geq \mu_{i}+\underbrace{2 B_{i, t}}_{\text {by choice of } B_{i, t}} \geq \hat{\mu}_{i, t}+B_{i, t},
$$

so the algorithm will not choose $I_{t}=i$.
If $I_{t}=i$, at least one of the bounds must be wrong, implying

$$
P\left(I_{t}=i, N_{i, t}>M_{i}\right) \leq P\left(\hat{\mu}_{i, t} \leq \mu_{i}+B_{i, t}\right)+P\left(\hat{\mu}_{i^{*}, t}+B_{i^{*}, t} \leq \mu_{i^{*}}\right)
$$

## UCB: Analysis

Using the Hoeffding bound,

$$
\begin{aligned}
P\left(\hat{\mu}_{i, t}-\mu_{i} \leq B_{i, t}\right) & \leq P(\underbrace{\exists s \leq t}: \hat{\mu}_{i, s}-\mu_{i} \leq \sqrt{\frac{6 \log (t)}{s}}) \\
& \leq \sum_{s=1}^{t} P\left(\hat{\mu}_{i, s}-\mu_{i} \leq \sqrt{\frac{6 \log (t)}{s}}\right) \\
& \leq \sum_{s=1}^{t} \exp \left\{-\frac{3 \log (t)}{s}\right\} \leq \sum_{s=1}^{t} t^{-3}=t^{-2} .
\end{aligned}
$$

## UCB: Analysis

Using the Hoeffding bound,

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\end{aligned}
$$

The same inequality holds for $i^{*}$, so

$$
\overline{\mathcal{R}_{T}}=\sum_{i} \Delta_{i} \mathbb{E}\left[N_{i, T}\right] \leq \sum_{i} \Delta_{i}\left(\frac{12 \log (T)}{\Delta_{i}^{2}}+2 \sum_{t=M_{i}+1}^{T} t^{-2}\right) .
$$

## UCB: Analysis

## Theorem (UCB upper bound [Auer, 2002])

The UCB1 algorithm on 1-sub-Gaussian data has

$$
\overline{\mathcal{R}_{T}} \leq \sum_{i} \frac{12 \log (T)}{\Delta_{j}}+o(1) .
$$

## UCB: Analysis

## Theorem (UCB upper bound [Auer, 2002])

The UCB1 algorithm on 1-sub-Gaussian data has

$$
\overline{\mathcal{R}_{T}} \leq \sum_{i} \frac{12 \log (T)}{\Delta_{j}}+o(1)
$$

## Theorem (Lower Bound [Lai and Robbins, 1985])

Suppose we have a parametric family $P_{\theta}$ and $\theta_{1}, \ldots, \theta_{k}$. For any "admissible" algorithm,

$$
\liminf _{T \rightarrow \infty} \frac{\overline{R_{T}}}{\log (T)} \geq \sum_{i \neq i^{*}} \frac{\Delta_{i}}{K L\left(P_{\theta_{i}}, P_{\theta_{i^{*}}}\right)} \approx O\left(\sum_{i \neq i^{*}} \frac{1}{\Delta_{i}}\right)
$$

E.g. if $P_{\theta}$ is Bernoulli, then $\frac{\left(\theta_{i}-\theta_{i}\right)^{2}}{\theta_{i^{*}}\left(1-\theta_{i^{*}}\right)} \geq K L\left(P_{\theta_{i}}, P_{\theta_{i^{*}}}\right) \geq 2\left(\theta_{i}-\theta_{i^{*}}\right)^{2}$.

## Algorithm Design Principle: Probability Matching

- We put a prior $\pi$ over means $\mu_{i}$ and a likelihood $\nu_{i}=P\left(\cdot \mid \mu_{i}\right)$ over rewards
- Choose $P\left(I_{t}=i\right)=P\left(\mu_{i}=\mu_{i^{*}} \mid\right.$ history $)$ (the matching)
- We usually pick conjugate models (e.g. $\mu_{i} \sim N(0,1)$, $\left.X_{t} \sim N\left(\mu_{i}, 1\right)\right)$


## Algorithm Design Principle: Probability Matching

- We put a prior $\pi$ over means $\mu_{i}$ and a likelihood $\nu_{i}=P\left(\cdot \mid \mu_{i}\right)$ over rewards
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## Algorithm: Thompson Sampling

Given: game length $T$, prior $\pi(\mu)$, likelihoods $p(\cdot \mid \mu)$
Initialize posteriors $p_{i, 0}(\mu)=\pi(\mu)$
For $t=1,2, \ldots, T$ :

- Draw $\theta_{i, t} \sim p_{i, t-1}$ for all $i$
- Choose $I_{t}=\arg \max _{i} \theta_{i, t}$ (implements the matching)
- Receive and observe $X_{t} \sim \nu_{l_{t}}$
- Update the posterior $p_{I_{T}, t}(\mu)=p\left(X_{t} \mid \mu\right) p_{I_{t}, t-1}(\mu)$


## Thompson Sampling: Overview



- Not Bayesian: a Bayesian method would maximize the Bayes regret (the expectation under the probability model)
- The regret bound is frequentist
- Arms with small $N_{i, t}$ implies a wide posterior, hence a good probability of being selected
- Generally performs empirically better that UCB (it is much more aggressive)
- Analysis is difficult


## Thompson Sampling: Upper Bound

## Theorem (Agrawal and Goyal [2013])

For binary rewards, Gamma-Beta Thompson sampling has $\mathbb{E}\left[R_{T}\right] \leq(1+\epsilon) \sum_{i \neq i^{*}} \Delta_{i} \frac{\log (T)}{K L\left(\mu_{i}, \mu_{i^{*}}\right)}+O\left(\frac{N}{\epsilon^{2}}\right)$.

- The proof is much more technical that UCB's
- We cannot rely on the upper bounds being correct w.h.p.


For some to-be-tuned $\mu_{i} \leq x_{i} \leq y_{i} \leq \mu_{i^{*}}$, we have

$$
\begin{array}{rlrl}
\mathbb{E}\left[N_{i, T}\right] \leq & \sum_{t=1}^{T} P\left(I_{t}=i\right) \\
\leq & \sum_{t=1}^{T} P\left(I_{t}=i, \hat{\mu}_{i, t-1} \leq x_{i}, \theta_{i, t} \geq y_{i}\right) & \left(O\left(\frac{\log (T)}{k l\left(x_{j}, y_{j}\right)}\right)\right) \\
& +\sum_{t=1}^{T} P\left(I_{t}=i, \hat{\mu}_{i, t-1} \leq x_{i}, \theta_{i, t} \leq y_{i}\right) & & \text { (the tricky case) } \\
& +\sum_{t=1}^{T} P\left(I_{t}=i, \hat{\mu}_{i, t-1} \geq x_{i}\right) & & \text { (Small by concentration) }
\end{array}
$$

## Thompson Sampling: Proof Outline

- The tricky case is $\sum_{t=1}^{T} P\left(I_{t}=i, \hat{\mu}_{i, t-1} \leq x_{i}, \theta_{i, t} \leq y_{i}\right)$
- This happens when we have enough samples of $i$ but not many of $i^{*}$
- A key lemma argues that, on $\hat{\mu}_{i, t-1} \leq x_{i}, \theta_{i, t} \leq y_{i}$, the probability of picking $i$ is a constant less than of picking $i^{*}$ :

$$
\begin{aligned}
& \sum_{t=1}^{T} P\left(I_{t}=i, \hat{\mu}_{i, t-1} \leq x_{i}, \theta_{i, t} \leq y_{i}\right) \\
& \leq \sum_{t=1}^{T} \underbrace{\frac{P\left(\theta_{i^{*}, t} \leq y_{i}\right)}{P\left(\theta_{i^{*}, t}>y_{j}\right)}}_{\text {exponentially small }} P\left(I_{t}=i^{*}, \hat{\mu}_{i, t-1} \leq x_{i}, \theta_{i, t} \leq y_{i}\right)=O(1)
\end{aligned}
$$

- Hence, we will quickly get enough samples of $i^{*}$


## Best of Both Worlds

- The stochastic and adversarial algorithms are quite different
- A natural question: is there an algorithm that
- gets $\mathcal{R}_{T}=O(\sqrt{T K})$ regret for adversarial
- gets $\mathcal{R}_{\mathrm{t}}=O\left(\sum_{i} \log (T) / \Delta_{i}\right)$ regret for stochastic
- without knowing the setting?


## Best of Both Worlds

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- gets $\mathcal{R}_{T}=O(\sqrt{T K})$ regret for adversarial
- gets $\mathcal{R}_{t}=O\left(\sum_{i} \log (T) / \Delta_{i}\right)$ regret for stochastic
- without knowing the setting?
- Bubeck and Slivkins [2012] proposed an algorithm that assumes stochastic but falls back to UCB once adversarial data is detected
- Zimmert and Seldin [2019] showed that (for pseudo-regret), it is possible
- Their algorithm: online mirror descent with $\frac{1}{2}$-Tsallis entropy
- $\Psi(w)=-\sum_{i} 4\left(\sqrt{w_{i}}-\frac{1}{2} w_{i}\right)$


## Pure Exploration

## A New Problem

- What if we only wanted to identify the best arm $i^{*}$ without caring about loss along the way?
- Intuitively, we would explore more; we are happy to accrue less reward if we get more useful samples.
- More similar to hypothesis testing; useful for selecting treatments
- Known as "Best Arm Identification" or "Pure Exploration"


## Two Settings

## Protocol: Best-arm Identification

Given:number of arms $K$, arm distributions $\nu_{1}, \ldots, \nu_{K}$
For $t=1,2, \ldots$,

- The learner picks arm $I_{t} \in\{1, \ldots, K\}$
- The learner observes $X_{t} \sim \nu_{l_{t}}$
- The learner decides whether to stop


## The learner returns arm $A$

Two settings:

|  | fixed-confidence | fixed-budget |
| :--- | :---: | :---: |
| Input | $\delta>0$, | $T$ |
| Goal | $P\left(A=i^{*}\right) \geq 1-\delta$ | maximize $P\left(A=i^{*}\right)$ |
| Stopping | once learner is confident | after $T$ rounds |

- Standard stochastic bandit algorithms under explore (they fail to meet lower bounds on this problem)
- Many can be adapted
- LUCB [Kalyanakrishnan et al., 2012]
- Top-Two Thompson Samping [Russo, 2016]
- Instead, we will describe a new algorithm design principle


## Algorithm Design Principle: Action Elimination

## Algorithm: Successive Elimination

Given: confidence $\delta>0$
Initialize plausibly-best set $S=\{1, \ldots, K\}$
For $t=1,2, \ldots$ :

- Pull all arms in $S$ and update $\hat{\mu}_{i, t}$
- Calculate $B_{t}=\sqrt{2 t^{-1} \log \left(4 K t^{2} / \delta\right)}$
- Remove $i$ from $S$ if $\underbrace{\max _{j \in S} \hat{\mu}_{j, t}-B_{t}}_{\text {Lowest } \mu_{i}^{*} \text { could be }} \geq \underbrace{\hat{\mu}_{i, t}+B_{t}}_{\text {highest } \mu_{i} \text { could be }}$
- If $|S|=1$, stop and return $A=S$.
- $S$ is a list of plausibly-best arms
- Each epoch, all arms that cannot be the best (if the bounds hold) are removed


## Successive Elimination Analysis

- Define the "bad event" $\mathcal{E}=\bigcup_{i, t}\left\{\left|\hat{\mu}_{i, t}-\mu_{i}\right| \geq B_{t}(\delta)\right\}$ : we have

$$
\begin{aligned}
P(\mathcal{E}) & \leq \sum_{i, t} P\left(\left|\hat{\mu}_{i, t}-\mu_{i}\right| \geq \sqrt{2 t^{-1} \log \left(4 K t^{2} / \delta\right)}\right) \leq \sum_{i, t} 2 e^{-\log \left(\frac{4 K t^{2}}{\delta}\right)} \\
& \leq \sum_{i, t} \frac{2 \delta}{4 K t^{2}}=\frac{2 \pi^{2}}{24} \delta \leq \delta
\end{aligned}
$$

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& \leq \sum_{i, t} \frac{2 \delta}{4 K t^{2}}=\frac{2 \pi^{2}}{24} \delta \leq \delta
\end{aligned}
$$

- (Correctness) If $\mathcal{E}$ does not happen,
- $\left|\hat{\mu}_{i^{*}}-\mu_{i^{*}}\right| \leq B_{t}$ and $\left|\mu_{j}-\hat{\mu}_{j}\right| \leq B_{t}$ for all $j$. Thus, for all $j$ $\hat{\mu}_{j}-\hat{\mu}_{i^{*}} \leq\left(\mu_{i^{*}}-\hat{\mu}_{i^{*}}\right)+\left(\mu_{j}-\mu_{i^{*}}\right)+\left(\hat{\mu}_{j}-\mu_{j}\right) \leq 2 B_{t}$
- $i$ is removed if $\max _{j \in S} \hat{\mu}_{j, t}-\hat{\mu}_{i, t} \geq 2 B_{t} \Rightarrow i^{*}$ is never removed
- $\lim _{t \rightarrow \infty} B_{t}(\delta) \rightarrow 0$ : every arm will eventually be removed
- Successive Elimination is correct with probability $1-\delta$


## Successive Elimination Analysis

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\begin{aligned}
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\end{aligned}
$$

- (Correctness) If $\mathcal{E}$ does not happen,
- $\left|\hat{\mu}_{i^{*}}-\mu_{i^{*}}\right| \leq B_{t}$ and $\left|\mu_{j}-\hat{\mu}_{j}\right| \leq B_{t}$ for all $j$. Thus, for all $j$

$$
\hat{\mu}_{j}-\hat{\mu}_{i^{*}} \leq\left(\mu_{i^{*}}-\hat{\mu}_{i^{*}}\right)+\left(\mu_{j}-\mu_{i^{*}}\right)+\left(\hat{\mu}_{j}-\mu_{j}\right) \leq 2 B_{t}
$$

- $i$ is removed if max m $_{j \in S} \hat{\mu}_{j, t}-\hat{\mu}_{i, t} \geq 2 B_{t} \Rightarrow i^{*}$ is never removed
- $\lim _{t \rightarrow \infty} B_{t}(\delta) \rightarrow 0$ : every arm will eventually be removed
- Successive Elimination is correct with probability $1-\delta$
- (Sample Complexity): arm $i$ will be eliminated once $\Delta_{i} \leq 2 B_{t}$
- We can verify that $N_{i}=O\left(\Delta_{i}^{-2} \log \left(K / \delta \Delta_{i}\right)\right)$ is sufficient
- Total sample complexity of $\sum_{i} \Delta_{i}^{-2} \log \left(K / \delta \Delta_{i}\right)$


## Theorem

Successive Elimination is $(0, \delta)$-PAC with sample complexity

$$
O\left(\sum_{i} \Delta_{i}^{-2} \log \left(K / \delta \Delta_{i}\right)\right)
$$

## Theorem

For any best-arm identification algorithm, there is a problem instance that requires

$$
\Omega\left(\sum_{i} \Delta_{i}^{-2} \log \log \left(\frac{1}{\delta \Delta_{i}^{2}}\right)\right)
$$

samples.

## Linear Stochastic Bandits

## Bonus: Linear Contextual Bandits

## Protocol: Contextual Linear Bandit

Given: game length $T$, number of arms $K$
For $t=1,2, \ldots, T$,

- The learner sees one context per arm $c_{1, t}, \ldots, c_{K, t}$
- The learner picks action $I_{t} \in\{1, \ldots, K\}$
- The learner observes and receives reward $X_{t}=\left\langle c_{l_{t}, t}, \theta^{*}\right\rangle+\xi_{t}$

Regret is defined w.r.t. an agent that knows the true $\theta$ :

$$
\overline{\mathcal{R}}_{T}=\sum_{t=1}^{T} \max _{i} x_{i, t}^{\top} \theta^{*}-\sum_{t=1}^{T} x_{l_{t}, t}^{\top} \theta^{*}
$$

## Algorithm Design Principle: Optimism

## Algorithm: OFUL [Abbasi-Yadkori et al., 2011]

Initialize $\hat{\theta}_{0}=0, B_{0}=\mathbb{R}^{d}$
For $t=1,2, \ldots, T$ :

- Receive contexts $c_{1, t}, \ldots, c_{K, t}$
- Choose $\left(I_{t}, \tilde{\theta}_{t}\right)=\arg \max _{i \in\{1, \ldots, K\}, \theta \in B_{t-1}} \theta^{\top} c_{i, t}$ (optimism)
- Observe $X_{t}=c_{I_{t}, t}^{\top} \theta^{*}+\xi_{t}$
- Calculate $V_{t}=\sum_{s=1}^{t} c_{s} c_{s}^{\top}+\lambda /$ and $r_{t}=\sqrt{\log \frac{\operatorname{det}\left(V_{t}\right)}{\delta^{2} \lambda^{d}}}+\sqrt{\lambda}\left\|\theta^{*}\right\|$
- Calculate $\hat{\theta}_{t}=V_{t}^{-1}\left(\sum_{s=1}^{t} c_{s} X_{s}\right)$ (ridge)
- Update $B_{t}=\left\{\theta:\left(\theta-\hat{\theta}_{t}\right)^{\top} V_{t}\left(\theta-\hat{\theta}_{t}\right) \leq r_{t}\right)$
- If $\xi_{t}$ is 1-sub-Gaussian, $\boldsymbol{B}_{t}$ is a confidence sequence with $P\left(\forall t>0: \theta^{*} \in B_{t}\right) \geq 1-\delta$ (more examples in [de la Peña et al., 2009, Howard et al., 2020])


## Analysis

- Regret decomposes over rounds:
- Recall that $\left(I_{t}, \tilde{\theta}_{t}\right)=\arg \max _{i \in\{1, \ldots, K\}, \theta \in B_{t-1}} \theta^{\top} c_{i, t}$

$$
\begin{aligned}
\mathcal{R}_{t}-\mathcal{R}_{t-1} & =c_{i_{t}^{*}}^{\top} \theta^{*}-c_{l_{t}}^{\top} \theta^{*} \\
& \leq c_{l_{t}}^{\top} \tilde{\theta}_{t}-c_{l_{t}}^{\top} \theta^{*} \\
& \leq c_{l_{t}}^{\top}\left(\tilde{\theta}_{t}-\hat{\theta}_{t-1}\right)+c_{l_{t}}^{\top}\left(\hat{\theta}_{t-1}-\theta^{*}\right) \quad \text { (by optimism) } \\
& \leq\left\|c_{l_{t}}\right\| v_{t} \underbrace{\left\|\tilde{\theta}_{t}-\hat{\theta}_{t-1}\right\|_{V_{t}}}_{\leq r_{t}}+\left\|c_{c_{t}}\right\| v_{t} \underbrace{\left\|\hat{\theta}_{t-1}-\theta^{*}\right\|_{V_{t}}}_{\leq r_{t}}
\end{aligned}
$$

- After some algebra, we can show, with probability $\geq 1-\delta$, that

$$
\mathcal{R}_{T}=O\left(\frac{d \log (1 / \delta)}{\Delta}\right)
$$

- The shared structure lets us learn a lot!


## Review

- Setting: adversarial bandits
- Exp3 (exponential weights)
- Setting: stochastic bandits
- UCB (optimism)
- Thompson Sampling (probablity matching)
- Setting: pure exploration
- Successive Elimination (action-elimination)
- Setting: linear contextual bandits
- OFUL (optimism)


## Thanks!

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Extras

## Aside: Lower Bound Reasoning

- Fix a strategy and consider two problem instances:

1. $\nu_{1}, \nu_{2}, \ldots, \nu_{k}$; with $P$ as the joint distribution over $\left(I_{t}, r_{i, t}\right)$
2. $\nu_{1}, \nu_{2}^{\prime}, \ldots, \nu_{K}$; with $P^{\prime}$ as the joint distribution over $\left(I_{t}, r_{i, t}\right)$
3. The optimal arm is different: $\mu_{2}^{\prime} \geq \mu_{1} \geq \mu_{2} \geq \mu_{3} \geq \ldots$
4. The data from $P$ and $P^{\prime}$ will look very similar

- An algorithm that does well on $P$ must not pull arm 2 too many times; hence, it will not do well on $P^{\prime}$
- "Similar" is quantified by a change-of-measure identity; e.g. $P^{\prime}(A)=e^{-\widehat{k I_{N_{2}, T}}} P(A)$, where $\widehat{k l_{t}}=\sum_{s=1}^{t} \log \frac{d \nu_{2}}{d \nu_{2}^{\prime}}\left(X_{2, s}\right)$
- Hence, an algorithm cannot tell if it is $P$ or $P^{\prime}$ and must get high regret under $P^{\prime}$, mistakenly believing it is playing in $P$

Exp3: Analysis Full Detail

## Exp3: Analysis

- Following the EW analysis, $W_{t}$ is a potential function
- For any $i^{*}, e^{-\eta \hat{L}_{T}\left(i^{*}\right)} \leq \sum_{j} e^{-\eta \hat{L}_{T}(j)}=W_{T}=W_{0} \prod_{t=1}^{T} \frac{W_{t}}{W_{t-1}}$.

$$
\begin{aligned}
\frac{W_{t}}{W_{t-1}} & =\frac{\sum_{j} e^{-\eta \hat{L}_{t-1}(j)} e^{-\eta \hat{\ell}_{t}(j)}}{\sum_{j} e^{-\eta \hat{L}_{t-1}(j)}}=\sum_{j} p_{t-1}(j) e^{-\eta \hat{\ell}_{t}(j)} \\
& \leq \underbrace{\sum_{j} p_{t-1}(j)\left(1-\eta \hat{\ell}_{t}(j)+\frac{\eta^{2}}{2} \hat{\ell}_{t}(j)^{2}\right)}_{\text {since } e^{x} \leq 1+x+\frac{1}{2} x^{2} \text { for } x \leq 0} \\
& =1-\eta \sum_{j} p_{t}(j) \hat{\ell}_{t}(j)+\frac{\eta^{2}}{2} \sum_{j} p_{t}(j) \hat{\ell}_{t}(I)^{2} \\
& \leq \underbrace{e^{-\eta \sum_{j} p_{t}(j) \hat{\ell}_{t}\left(j+\frac{\eta^{2}}{2}\right.} \sum_{j} p_{t}(j) \hat{\ell}_{t}(j)^{2}}_{\text {since } 1+x \leq e^{x}}
\end{aligned}
$$

## Exp3: Analysis

$$
\begin{aligned}
& e^{-\eta \hat{L}_{T}\left(i^{*}\right)} \leq W_{0} \prod_{t=1}^{T} \frac{W_{t}}{W_{t-1}} \leq K \prod_{t=1}^{T} e^{-\eta \sum_{j} p_{t}(j) \hat{\ell}_{t}(j)+\frac{\eta^{2}}{2} \sum_{j} p_{t}(j) \hat{\ell}_{t}(j)^{2}} \\
& \Leftrightarrow-\eta \hat{L}_{T}\left(i^{*}\right) \leq \log (K)-\eta \sum_{j} p_{t}(j) \hat{\ell}_{t}(j)+\frac{\eta^{2}}{2} \sum_{j} p_{t}(j) \hat{\ell}_{t}(j)^{2} \\
& \Leftrightarrow \sum_{t=1}^{T} \sum_{j} p_{t}(j) \hat{\ell}_{t}(j)-\hat{L}_{T}\left(i^{*}\right) \leq \frac{\log (K)}{\eta}+\frac{\eta}{2} \sum_{t=1}^{T} \mathbb{E}\left[\sum_{j} p_{t}(j) \hat{\ell}_{t}(j)^{2}\right. \\
& \Rightarrow \sum_{t=1}^{T} \sum_{j} p_{t}(j) \mathbb{E}\left[\hat{\ell}_{t}(j)-\hat{L}_{T}\left(i^{*}\right)\right] \leq \frac{\log (K)}{\eta}+\frac{\eta}{2} \sum_{t=1}^{T} \mathbb{E}\left[\sum_{j} p_{t}\left(j j \hat{\ell}_{t}(j)^{2}\right]\right. \\
& \Leftrightarrow \sum_{t=1}^{T} \mathbb{E}\left[\ell\left(I_{t}\right)\right]-L_{T}\left(i^{*}\right) \leq \frac{\log (K)}{\eta}+\frac{\eta}{2} \sum_{t=1}^{T} \underbrace{\mathbb{E}\left[\sum_{j} p_{t}(j) \frac{\ell_{t}\left(I_{t}\right)^{2}}{p_{t}\left(I_{t}\right)^{2}} \mathbb{1}_{\{I t=i\}}\right]}_{\text {variance term }}
\end{aligned}
$$

## Exp3: Analysis

Bounding the variance term turns out to be easy:

$$
\begin{aligned}
\mathbb{E}\left[\sum_{j} p_{t}(j) \frac{\ell_{t}\left(I_{t}\right)^{2}}{p_{t}\left(I_{t}\right)^{2}} \mathbb{1}_{\left\{I_{t}=i\right\}}\right] & \leq \mathbb{E}\left[\sum_{j} p_{t}(j) \frac{\mathbb{1}_{\left\{I_{t}=i\right\}}}{p_{t}\left(I_{t}\right)^{2}}\right] \\
& =\mathbb{E}\left[\frac{1}{p_{t}\left(I_{t}\right)}\right]=K
\end{aligned}
$$

So, plugging this in, $\sum_{t=1}^{T} \mathbb{E}\left[\ell\left(I_{t}\right)\right]-L_{T}\left(i^{*}\right) \leq \frac{\log (K)}{\eta}+\frac{\eta}{2} T K$
Theorem (Exp3 upper bound [Auer et al., 2002b])
With $\eta=\sqrt{\frac{2 \log (T)}{T K}}$, UCB has $\overline{\mathcal{R}}_{T} \leq \sqrt{2 T K \log (K)}$.
Only get pseudo-Regret bounds because the $i^{*}$ in the proof was fixed, not a function of $I_{1}, \ldots, I_{T}$

