Interactive Machine Learning

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About this monograph: These notes were initially written for myself to refer to while lecturing. Many have found them useful for the course as well as in their research and so we have posted them. There is a large degree of overlap between these notes and the excellent textbook [Lattimore and Szepesvári, 2020]. These notes are not a replacement for the book and many details are omitted. They may contain errors, there will contain typos. I have posted them by request.

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Part I

Probability, Statistics, and Supervised Learning

Chapter 1

Probability and Statistics

Much of this chapter was written as summaries of the excellent notes and books of [Roch, , Pollard, 2002, Lattimore and Szepesvári, 2020]. Please see these resources for clarifications and details.

1.1 Probability theory review

Let us introduce some notations by way of an example. Suppose we toss an unbiased coin twice.

- Sample space: $\Omega = \{TT, TH, HT, HH\}$
- Outcome: $\omega \in \Omega$
- Probability measure: $\mathbb{P}(\omega) = 1/4$ for all $\omega \in \Omega$
- Random variable (function on Ω to the reals): $X(\omega) = \#\mathsf{heads}$ (e.g., $X(TH) = 1$)
- Event (subset of Ω): $A = \{\omega \in \Omega : X(\omega) = 1\} = \{HT, TH\}$, $\mathbb{P}(A) = \mathbb{P}(HT) + \mathbb{P}(TH) = 1/2$
- Expectation: $\mathbb{E}[X] = \sum_{\omega \in \Omega} X(\omega)\mathbb{P}(\omega) = 1$
- Distribution: X is a binomial random variable with $n = 2$ and $p = 1/2$

1.1.1 Basic definitions

Definition 1 (σ-algebra)**.** *A collection $\mathcal{F}$ of subsets of a set Ω is a* σ-algebra *on Ω if*

1. $\Omega \in \mathcal{F}$
2. $F \in \mathcal{F} \implies F^c \in \mathcal{F}$
3. *for a sequence of sets $F_n \in \mathcal{F}$ for all n, $\bigcup_n F_n \in \mathcal{F}$*

Note that the first and second property imply that $\emptyset \in \mathcal{F}$. Also note that for any sequence of sets $F_n \in \mathcal{F}$, we have that $\bigcap_n F_n = \left(\bigcup_n F_n\right)^c \in \mathcal{F}$ by the second and third properties.

The trivial σ-algebra is just the power set of Ω. For example, a σ-algebra of $\Omega = \{TT, TH, HT, HH\}$ is

$$\begin{aligned}\mathcal{F} =& \emptyset, \{TT\}, \{HT\}, \{TH\}, \{HH\}, \{TT, TH\}, \{TT, HH\}, \{HT, TH\}, \{HT, HH\},\\ &\{TT, HT, TH\}, \{TT, HT, HH\}, \{TT, TH, HH\}, \{HT, TH, HH\}, \{TT, TH, HT, HH\}\end{aligned}$$

Definition 2 (Probability measure)**.** *For a σ-algebra $\mathcal{F}$ on Ω, $\mathbb{P}$ is a probability measure if*

1. $\mathbb{P} : \mathcal{F} \to [0, 1]$
2. $\mathbb{P}(\emptyset) = 0$
3. $\mathbb{P}(\Omega) = 1$
4. *for a sequence of sets $F_n \in \mathcal{F}$ with $F_n \cap F_m = \emptyset$ for all n, m, $\mathbb{P}(\bigcup_n F_n) = \sum_n \mathbb{P}(F_n)$*

For our coin example, $\{TT, HT, HH\} \in \mathcal{F}$ and $\{TT, HT, HH\} = \{TT\} \cup \{HT\} \cup \{HH\}$ are disjoint sets. Since all four outcomes are equally likely with probability 1/4 we have

$$\mathbb{P}(\{TT, HT, HH\}) = \mathbb{P}(\{TT\} \cup \{HT\} \cup \{HH\}) = \mathbb{P}(\{TT\}) + \mathbb{P}(\{HT\}) + \mathbb{P}(\{HH\}) = \frac{1}{4} + \frac{1}{4} + \frac{1}{4} = \frac{3}{4}$$

Definition 3 (Probability space)**.** *For a set (sample space) Ω, σ-algebra $\mathcal{F}$ on Ω, and probability measure $\mathbb{P}$, we call $(\Omega, \mathcal{F}, \mathbb{P})$ a probability space.*

Definition 4 (Measurable function)**.** *Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space. For some $h : \Omega \to \mathbb{R}$ define $h^{-1}(A) = \{\omega \in \Omega : h(\omega) \in A\}$. We say h is $\mathcal{F}$-*measurable *if $h^{-1}(B) \in \mathcal{F}$ for all Borel sets B of $\mathbb{R}$.*

Definition 5 (Random variable)**.** *Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space. We call $X : \Omega \to \mathbb{R}$ a* random variable *if X is an $\mathcal{F}$-measurable function.*

For our coin example, let X denote the number of heads of the first two tosses. For any set $A \not\subset \{0, 1, 2\}$ we have that $X^{-1}(A) = \emptyset$ which is in $\mathcal{F}$. Also note that $X^{-1}(0) = \{TT\}$, $X^{-1}(1) = \{HT, TH\}$, and $X^{-1}(2) = \{HH\}$. Moreover, $X^{-1}([-1, 1.5]) = \{TT, HT, TH\}$ which is also in $\mathcal{F}$. We may conclude that X is a random variable on $(\Omega, \mathcal{F}, \mathbb{P})$.

Definition 6 (Natural σ-algebra)**.** *Let X_t for $t \in \mathcal{T}$ be a set of random variables on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$. Let*

$$\sigma(\{X_t\}_{t \in \mathcal{T}})$$

be the smallest σ-algebra on which X_t for all $t \in \mathcal{T}$ are measurable.

For the random variable X denoting the number of heads among the first two flips, note that

$$\sigma(X) = \emptyset, \{TT\}, \{HT, TH\}, \{HH\}, \{TT, HT, TH\}, \{TT, HH\}, \{HT, TH, HH\}, \{TT, HT, TH, HH\}$$

which is a strict subset of $\mathcal{F} = 2^{\Omega}$.

Now let $Y \in \{0, 1\}$ be an indicator that at least one of the two flips of was a head. Then

$$\sigma(Y) = \emptyset, \{TT\}, \{TH, HT, HH\}, \{TT, TH, HT, HH\}$$

for which we note $\sigma(Y) \subset \sigma(X) \subset \mathcal{F}$.

Example 1 (Measurability)**.** *Note that X is $\sigma(X)$-measurable since $\{\omega : X(\omega) \in A\} \subset \sigma(X)$ for all Borel sets $A \subset \mathbb{R}$. However, X is* not *$\sigma(Y)$-measurable since $\{\omega : X(\omega) = 2\} = \{HH\} \notin \sigma(Y)$. Intuitively, X contains information that is not contained in Y and hence, X is not measurable with respect to $\sigma(Y)$.*

1.1.2 Conditional Expectation

For a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ and $A, B \in \mathcal{F}$ we define

$$\mathbb{P}(A|B) = \frac{\mathbb{P}(A \cap B)}{\mathbb{P}(B)}$$

and is read as the probability of event A *given* event B. For our coin example, with X denoting the number of heads in the two tosses, we can compute

$$\mathbb{P}(HT|X=1) = \frac{\mathbb{P}(\{HT\} \cap \{X=1\})}{\mathbb{P}(X=1)} = \frac{\mathbb{P}(\{HT\})}{\mathbb{P}(X=1)} = \frac{1/4}{1/2} = 1/2.$$

Likewise, we can consider the conditional expectation of a random variable X given some $A \in \mathcal{F}$ defined as

$$\mathbb{E}[X|A] = \sum_x x\mathbb{P}(X=x|A).$$

For our coin example, if $Y = \mathbf{1}\{\text{first flip is } H\}$ then we can compute

$$\begin{aligned}\mathbb{E}[X|Y=1] &= 0 \cdot \mathbb{P}(X=0|Y=1) + 1 \cdot \mathbb{P}(X=1|Y=1) + 2 \cdot \mathbb{P}(X=2|Y=1)\\ &= 0 \cdot \frac{\mathbb{P}(X=0 \cap \{Y=1\})}{\mathbb{P}(Y=1)} + 1 \cdot \frac{\mathbb{P}(X=1 \cap \{Y=1\})}{\mathbb{P}(Y=1)} + 2 \cdot \frac{\mathbb{P}(X=2 \cap \{Y=1\})}{\mathbb{P}(Y=1)}\\ &= 0 \cdot \frac{\mathbb{P}(\emptyset)}{1/2} + 1 \cdot \frac{\mathbb{P}(HT)}{1/2} + 2 \cdot \frac{\mathbb{P}(HH)}{1/2} = 3/2.\end{aligned}$$

One can also easily conclude that $\mathbb{E}[X|Y=0] = 1/2$. Observe that we can succinctly write $\mathbb{E}[X|Y=y] = \frac{y+1}{2}$ so that we can say 'the expectation of X given Y is equal to $\frac{Y+1}{2}$.' We can notate this as $\mathbb{E}[X|Y] = \frac{Y+1}{2}$ and note that this itself a random variable, since Y is a random variable. Indeed, since $X : \Omega \to \mathbb{R}$, $Y : \Omega \to \mathbb{R}$, we observe that $\mathbb{E}[X|Y] : \Omega \to \mathbb{R}$ is a valid random variable.

From discrete to continuous spaces Note that the above definition relies critically on the fact that Ω is discrete so that $\mathbb{P}(\omega) > 0$ for all $\omega \in \Omega$ and there are no measurability concerns for discrete outcomes spaces. In general, for any well-defined random variables X, Y defined on $(\Omega, \mathcal{F}, \mathbb{P})$ there exists a definition of $\mathbb{E}[X|Y](\omega)$ that is a valid random variable (in the sense that it is measurable with respect to $\sigma(Y)$) and always exists (we will define it shortly). However, it turns out that there exists pathological cases where there does not exist a measurable function $g : \mathbb{R} \to \mathbb{R}$ such that $g(Y(\omega)) = \mathbb{E}[X|Y](\omega)$. As all valid random variables are measurable, we conclude that $g(Y(\omega))$ is not well-defined. This is because not every $\sigma(Y)$-measurable function is representable by the composition $g \circ Y : \Omega \to \mathbb{R}$. To emphasize this fact, instead of writing $\mathbb{E}[X|Y]$ some authors will write $\mathbb{E}[X|\sigma(Y)]$ to remind the reader that one does not draw $Y(\omega)$ and then compute $\mathbb{E}[X|\sigma(Y)]$ but directly draws from $\mathbb{E}[X|\sigma(Y)]$.

Definition 7. *Let X be a random variable defined on $(\Omega, \mathcal{F}, \mathbb{P})$ and let $\mathcal{H} \subset \mathcal{F}$ be a sub-σ-algebra. Then we say $\mathbb{E}[X|\mathcal{H}] : \mathcal{H} \to \mathbb{R}$ is the conditional expectation of X given $\mathcal{H}$ if*

$$\int_{\omega \in H} \mathbb{E}[X|\mathcal{H}](\omega) d\mathbb{P}(\omega) = \int_{\omega \in H} X(\omega) d\mathbb{P}(\omega) \qquad H \in \mathcal{H}$$

One can show that $\mathbb{E}[X|\mathcal{H}]$ is unique almost surely.

This definition looks funny, so let us verify that when Ω is discrete our natural definition $\mathbb{E}[X|Y](\omega) = \sum_x x\mathbb{P}(X = x|Y = Y(\omega))$ satisfies this definition. Note that for any set $A \in \mathbb{R}$ we have that

$$\begin{aligned}
\sum_{\omega \in Y^{-1}(A)} \mathbb{E}[X|Y](\omega)\mathbb{P}(\omega) &= \sum_{y\in A}\sum_{\omega\in Y^{-1}(A)} \mathbf{1}\{Y(\omega) = y\}\mathbb{E}[X|Y = y]\mathbb{P}(\omega)\\
&= \sum_{y\in A}\mathbb{E}[X|Y = y]\mathbb{P}(Y = y)\\
&= \sum_{y\in A}\sum_{x} x\mathbb{P}(X = x|Y = y)\mathbb{P}(Y = y)\\
&= \sum_{y\in A}\sum_{x} x\mathbb{P}(X = x, Y = y)\\
&= \sum_{y\in A}\sum_{x}\sum_{\omega\in\Omega} X(\omega)\mathbf{1}\{X(\omega) = x, Y(\omega) = y\}\mathbb{P}(\omega)\\
&= \sum_{y\in A}\sum_{\omega\in\Omega} X(\omega)\mathbf{1}\{Y(\omega) = y\}\mathbb{P}(\omega)\\
&= \sum_{\omega\in Y^{-1}(A)} X(\omega)\mathbb{P}(\omega).
\end{aligned}$$

Note that for all $A \subset \mathbb{R}$ we have that $Y^{-1}(A) \in \sigma(Y)$. Thus, our definition of conditional expectation under finite Ω: $\mathbb{E}[X|Y](\omega) = \sum_x x\mathbb{P}(X = x|Y = Y(\omega))$ satisfies

$$\sum_{\omega\in H} \mathbb{E}[X|Y](\omega)\mathbb{P}(\omega) = \sum_{\omega\in H} X(\omega)\mathbb{P}(\omega) \qquad \forall H \in \sigma(Y).$$

In general (i.e., for arbitrary Ω) we will define $\mathbb{E}[X|Y](\omega)$ as any function that satisfies this identity, with each $H \in \sigma(Y)$ providing a constraint on the function.

The benefit of the above definition is that it is always well-defined for both discrete and continuous random variables. The next lemma captures much of the intuition of conditional expectation.

Lemma 1. *Fix any $(\Omega, \mathcal{F}, \mathbb{P})$ and a sub-σ-algebra $\mathcal{G} \subset \mathcal{F}$. If Z is $\mathcal{G}$-measurable R.V. and X is an $\mathcal{F}$-measurable random variable, then*

$$\mathbb{E}[X + Z|\mathcal{G}] = Z + \mathbb{E}[X|\mathcal{G}].$$

Moreover, if Z is a bounded then

$$\mathbb{E}[XZ|\mathcal{G}] = Z\mathbb{E}[X|\mathcal{G}].$$

Proof. The first statement follows by linearity of conditional expectation and that Z is $\mathcal{G}$ measurable so $\mathbb{E}[Z|\mathcal{G}] = Z$.

For the second statement, since Z is assumed bounded, there exists some $L \geq 0$ such that $-L \leq Z(\omega) \leq L$ for all $\omega \in \Omega$. By taking an arbitrarily fine cover of $[-L, L]$ we may assume Z is a discrete random variable taking values $\{z_j\}_j \subset [-L, L]$. For any j we have $G_j = Z^{-1}(z_j) \in \mathcal{G}$ and

$$\begin{aligned}\int_{\omega \in G_j} \mathbb{E}[XZ|\mathcal{G}](\omega) d\mathbb{P}(\omega) &= \int_{\omega \in G_j} X(\omega)Z(\omega) d\mathbb{P}(\omega) \\ &= z_j \int_{\omega \in G_j} X(\omega) d\mathbb{P}(\omega) \\ &= z_j \int_{\omega \in G_j} \mathbb{E}[X|\mathcal{G}](\omega) d\mathbb{P}(\omega)\end{aligned}$$

For any $G \in \mathcal{G}$ there exists an index set $I \subset \mathbb{N}$ such that $G = \bigcup_{j \in I} G_j$. Thus,

$$\begin{aligned}\int_{\omega \in G} \mathbb{E}[XZ|\mathcal{G}](\omega) &= \sum_{j \in I} \int_{\omega \in G_j} \mathbb{E}[XZ|\mathcal{G}](\omega) d\mathbb{P}(\omega) \\ &= \sum_{j \in I} z_j \int_{\omega \in G_j} \mathbb{E}[X|\mathcal{G}](\omega) d\mathbb{P}(\omega) = \int_{\omega \in G} Z(\omega)\mathbb{E}[X|\mathcal{G}](\omega) d\mathbb{P}(\omega).\end{aligned}$$

□

Since $\mathbb{E}[X|Z] = \mathbb{E}[X|\sigma(Z)]$, the above lemma is saying just the intuitive facts that $\mathbb{E}[X + Z|Z] = Z + \mathbb{E}[X|Z]$ and $\mathbb{E}[XZ|Z] = Z\mathbb{E}[X|Z]$.

1.1.3 Filtrations

In our coin example, we have been talking about the event space after both been flipped. But now suppose the coins were drawn sequentially, first observing the first flip, and then the second. Filtrations allow us to incorporate time or a sequence of observations into probability.

Formally, let $X_1, X_2, \dots$ be a sequence of random variables on $(\Omega, \mathcal{F}, \mathbb{P})$. And now imagine that we observe X_t sequentially so that at time t we observe X_t, potentially take some action, and only at the next time observe X_{t+1}. Once we have observed $\{X_s\}_{s=1}^t$ what actions we might potentially are limited to those that depend on measurable random variables, which are precisely those in $\mathcal{F}_t := \sigma(\{X_s\}_{s=1}^t)$. Note that we clearly have $\{\Omega, \emptyset\} = \mathcal{F}_0 \subset \mathcal{F}_1 \subset \cdots \subset \mathcal{F}$. Under this notation, reasoning about, say $\mathbb{E}[X_{t+1}|\{X_s\}_{s=1}^t]$ is exactly equivalent to $\mathbb{E}[X_{t+1}|\mathcal{F}_t]$, as per the discussion on conditional expectation above. The σ-algebra $\mathcal{F}_t$ can be interpreted as the history making a statement like "given all observations of up to t, what is the expectation of X_{t+1}?"

We can also reason about a growing set of σ-algebras that are not necessarily derived from random variables. We say $\mathbb{F} = \{\mathcal{F}_t\}_{t=1}^n$ is a *filtration* of $\mathcal{F}$ if $\mathcal{F}_t \subset \mathcal{F}_{t+1}$ for all t. A sequence of random variables $\{X_t\}_{t=1}^n$ is $\mathbb{F}$-adapted if X_t is $\mathcal{F}_t$ measurable for all $1 \leq t \leq n$. Given a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ and a filtration $\mathbb{F}$ of $\mathcal{F}$, we call the tuple $(\Omega, \mathcal{F}, \mathbb{F}, \mathbb{P})$ a filtered probability space.

1.2 Martingales, Optional stopping, Maximal inequalities

Additional material on this section can be found in [Lattimore and Szepesvári, 2020] and [Howard et al., 2018].

Definition 8. *Fix some filtered probability space $(\Omega, \mathcal{F}, \mathbb{F}, \mathbb{P})$. An $\mathbb{F}$-adapted sequence of random variables is an $\mathbb{F}$-adapted* martingale *if $\mathbb{E}[X_{t+1}|\mathcal{F}_t] = X_t$ for all t and $\mathbb{E}[|X_t|] < \infty$. Furthermore, if*

- *X_t is a super-martingale if $\mathbb{E}[X_{t+1}|\mathcal{F}_t] \leq X_t$*

- *X_t is a sub-martingale if $\mathbb{E}[X_{t+1}|\mathcal{F}_t] \geq X_t$*

Definition 9. *Let $\mathbb{F} = \{\mathcal{F}_t\}_{t\in\mathbb{N}}$ be a filtration. A random variable $\tau \in \mathbb{N}$ is a* stopping time *with respect to $\mathbb{F}$ with values in $\mathbb{N} \cup \{\infty\}$ if $\mathbf{1}\{\tau \leq t\}$ is $\mathcal{F}_t$ measurable for all $t \in \mathbb{N}$.*

Example 2. *Let $Z_1, Z_2, \ldots$ be an $\mathbb{F}$ adapted sequence and define $S_t = \sum_{i=1}^t$. A valid stopping time may be $\tau = \min\{t \in \mathbb{N} : S_t \geq \epsilon\}$ because τ is $\mathcal{F}_t$ measurable: given S_t we can determine whether it is greater than or equal to ϵ or not. An example of a time that is* not *a stopping time is $\tau' = \max\{t \in \mathbb{N} : S_t \geq \epsilon\}$ because given only $\mathcal{F}_t$, the information up to time t, we do not know whether $S_{t'}$ will exceed ϵ again at some future time $t' > t$. Thus, $\mathbf{1}\{\tau' = t\}$ is not measurable with respect to $\mathcal{F}_t$ and thus, is not a stopping time.*

Lemma 2 (Doob's optional stopping)**.** *Let $\mathbb{F} = \{\mathcal{F}_t\}_{t\in\mathbb{N}}$ be a filtration and $\{X_t\}_t$ be an $\mathbb{F}$-adapted martingale and τ be an $\mathbb{F}$-stopping time. If either of the following two events holds*

- *$\exists N \in \mathbb{N}$ such that $\mathbb{P}(\tau \leq N) = 1$, or*
- *$\mathbb{E}[\tau] < \infty$ and $\mathbb{E}[|X_{t+1} - X_t|\,|\mathcal{F}_t] < c$ for all $t < \tau$ for some $c > 0$,*

then X_τ is well-defined and $\mathbb{E}[X_\tau] = \mathbb{E}[X_0]$. Furthermore, if

- *X_t is a super-martingale then $\mathbb{E}[X_\tau] \leq \mathbb{E}[X_0]$*
- *X_t is a sub-martingale then $\mathbb{E}[X_\tau] \geq \mathbb{E}[X_0]$*

Lemma 3 (Maximal inequality)**.** *Let $\{X_t\}_t$ be an $\mathbb{F}$-adapted sequence of random variables with $X_t \geq 0$ almost surely. Then for any $\epsilon > 0$, if*

- *X_t is a super-martingale then $\mathbb{P}(\max_{t\in\mathbb{N}} X_t \geq \epsilon) \leq \mathbb{E}[X_0]/\epsilon$*
- *X_t is a sub-martingale then $\mathbb{P}(\max_{t\in\{1,\ldots,n\}} X_t \geq \epsilon) \leq \mathbb{E}[X_n]/\epsilon$*

Proof. We first present the proof of the super-martingale case, which is thanks to [Lattimore and Szepesvári, 2020]. Fix $n \in \mathbb{N}$ and let $\tau = \min\{n+1, \min\{t : X_t \geq \epsilon\}\}$. Clearly, τ is finite (less than $n+1$) and thus we can apply Doob's optional stopping. Note that $\tau \leq n \iff \exists t \leq n : X_t \geq \epsilon$ Then by optional stopping,

$$\mathbb{E}[X_0] \geq \mathbb{E}[X_\tau] \geq \mathbb{E}[X_\tau \mathbf{1}\{\tau \leq n\}] \geq \epsilon\mathbb{P}(\tau \leq n) = \epsilon\mathbb{P}(\exists t \leq n : X_t \geq \epsilon) = \epsilon\mathbb{P}(A_n)$$

where $A_n := \exists t \leq n : X_t \geq \epsilon$. Note that $A_1 \subset A_2 \subset A_3 \subset \ldots$ so if we define $B_n = A_n \setminus A_{n-1}$ then

$$\begin{aligned}\mathbb{P}(\exists t \in \mathbb{N} : x_t \geq \epsilon) &= \mathbb{P}(\bigcup_{t\in\mathbb{N}} A_n) = \mathbb{P}(\bigcup_{t\in\mathbb{N}} B_n) \\ &= \sum_{t\in\mathbb{N}} \mathbb{P}(B_n) = \lim_{n\to\infty} \sum_{t=1}^n \mathbb{P}(B_n) \\ &= \lim_{n\to\infty} \mathbb{P}(A_n) \leq \frac{\mathbb{E}[X_0]}{\epsilon}.\end{aligned}$$

The following proof of the sub-martingale case is thanks to [Lawler, 2006]. Let $\tau = \min\{t \leq n : X_t \geq \epsilon\}$. Again, τ is finite so we can apply Doob's optional stopping. Using the tower rule of expectations we have

$$\begin{aligned}
\mathbb{E}[X_n] &\geq \mathbb{E}[X_n \mathbf{1}\{\tau \leq n\}] \\
&= \sum_{j=1}^{n} \mathbb{E}[X_n \mathbf{1}\{\tau = j\}] \\
&= \sum_{j=1}^{n} \mathbb{E}[\mathbb{E}[X_n \mathbf{1}\{\tau = j\}|\mathcal{F}_j]] \\
&= \sum_{j=1}^{n} \mathbb{E}[\mathbb{E}[X_n|\mathcal{F}_j] \mathbf{1}\{\tau = j\}] \\
&= \sum_{j=1}^{n} \mathbb{E}[X_j \mathbf{1}\{\tau = j\}] \\
&\geq \epsilon \sum_{j=1}^{n} \mathbb{E}[\mathbf{1}\{\tau = j\}] \\
&= \epsilon \mathbb{P}(\max_{j=1,\dots,n} X_j \geq \epsilon)
\end{aligned}$$

□

Example: Maximal inequality Let $Z_1, Z_2, \dots$ be Bernoulli(1/2) random variables in $\{-1, 1\}$. Verify that $S_t = \sum_{i=1}^t Z_i$ is a martingale. Also note that for any $\lambda > 0$ we have by Jensen's inequality that $\mathbb{E}[\exp(\lambda S_t)|\mathcal{F}_{t-1}] = \mathbb{E}[\exp(\lambda Z_t)|\mathcal{F}_{t-1}] \exp(\lambda S_{t-1}) \geq \exp(\lambda \mathbb{E}[Z_t|\mathcal{F}_{t-1}]) \exp(\lambda S_{t-1}) = \exp(\lambda S_{t-1})$. Thus, $\exp(\lambda S_t)$ is a *sub-martingale*. Applying the maximal inequality for sub-martingales we have for any $N \in \mathbb{N}$ that

$$\begin{aligned}
\mathbb{P}(\max_{t \in \{1,\dots,N\}} S_t \geq \sqrt{2N \log(1/\delta)}) &= \mathbb{P}(\max_{t \in \{1,\dots,N\}} \exp(\lambda S_t) \geq \exp(\lambda \sqrt{2N \log(1/\delta)})) \\
&\leq \exp(-\lambda \sqrt{2N \log(1/\delta)}) \mathbb{E}[\exp(\lambda S_N)] \\
&\leq \exp(-\lambda \sqrt{2N \log(1/\delta)}) \exp(\lambda^2 N/2)
\end{aligned}$$

where the last inequality follows from the fact that S_N is a sum of N IID random variables, so $\mathbb{E}[\exp(\lambda S_N)] \leq \exp(\lambda^2 N/2)$. By setting $\lambda = \sqrt{2 \log(1/\delta)/N}$ we obtain $\mathbb{P}(\max_{t \in \{1,\dots,N\}} S_t \geq \sqrt{2N \log(1/\delta)}) \leq \delta$. Since all we used is that $\mathbb{E}[\exp(\lambda S_N)] \leq \exp(\lambda^2 N/2)$, we could have also applied a standard Chernoff bound at time N to obtain $\mathbb{P}(S_N \geq \sqrt{2N \log(1/\delta)}) \leq \delta$. This above example seems to be getting a guarantee on $t \in \{1, \dots, N-1\}$ for free! It turns out we can do *even better*.

1.3 Anytime concentration inequalities

1.3.1 Linear boundaries

Let $Z_1, Z_2, \dots$ be Bernoulli(1/2) random variables in $\{-1, 1\}$. Define the random walk $S_t = \sum_{i=1}^t Z_i$. If $M_t(\lambda) = \exp(\lambda S_t - t\lambda^2/2)$ then M_t is a super-martingale since

$$\mathbb{E}[M_{t+1}(\lambda)|\mathcal{F}_t] = \mathbb{E}[\exp(\lambda S_{t+1} - (t+1)\lambda^2/2)|\mathcal{F}_t] = \exp(\lambda S_t - t\lambda^2/2)\mathbb{E}[\exp(\lambda Z_{t+1} - \lambda^2/2)|\mathcal{F}_t] \leq M_t(\lambda) \cdot 1$$

Applying the maximal inequality for super-martingales we have

$$\mathbb{P}(\exists t \in \mathbb{N} : S_t \geq t\lambda/2 + \log(1/\delta)/\lambda) = \mathbb{P}(\exists t \in \mathbb{N} : M_t(\lambda) \geq 1/\delta) \leq \delta$$

since $\mathbb{E}[M_0(\lambda)] = 1$. The above holds for any λ and says the random walk S_t, with probability at least $1-\delta$ does not go above the line $t\lambda/2 + \log(1/\delta)/\lambda$ for all $t \in \mathbb{N}$. But if we take $\lambda = \sqrt{2\log(1/\delta)/N}$ then we have that

$$\mathbb{P}(\max_{t\in\{1,\dots,N\}} S_t \geq (t/\sqrt{N} + \sqrt{N})\sqrt{\log(1/\delta)/2}) \leq \delta,$$

a strict improvement over the maximal inequality!

1.3.2 Curved boundaries with a mixing distribution

Let $Z_1, Z_2, \dots$ be Bernoulli(1/2) random variables in $\{-1,1\}$. If $S_t = \sum_{i=1}^t Z_i$ then $M_t(\lambda) = \exp(\lambda S_t - t\lambda^2/2)$ is a super-martingale for any $\lambda \in \mathbb{R}$. Let h be any probability distribution over $\mathbb{R}$. Define $\bar{M}_t = \int_\lambda M_t(\lambda)dh(\lambda)$. Then $\bar{M}_t$ is a super-martingale since

$$\begin{aligned}\mathbb{E}[\bar{M}_{t+1}|\mathcal{F}_t] &= \mathbb{E}\left[\int_\lambda M_{t+1}(\lambda)dh(\lambda)|\mathcal{F}_t\right] \\ &= \int_\lambda \mathbb{E}\left[M_{t+1}(\lambda)|\mathcal{F}_t\right]dh(\lambda) \\ &\leq \int_\lambda M_t(\lambda)dh(\lambda) \\ &= \bar{M}_t.\end{aligned}$$

Suppose we take $h(\lambda) = \frac{1}{\sqrt{2\pi\nu^2}}e^{-\lambda^2/2\nu^2}$. Then

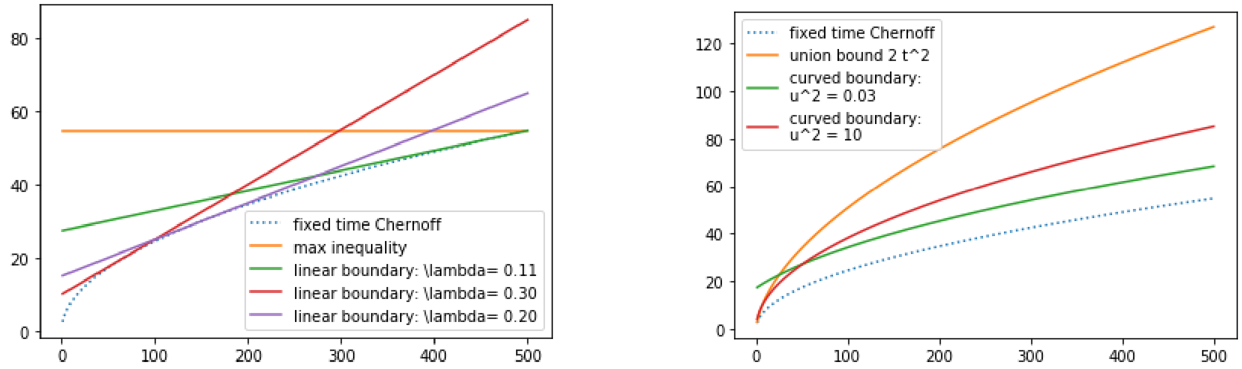
$$\begin{aligned}\bar{M}_t &= \int_\lambda M_t(\lambda)dh(\lambda) = \frac{1}{\sqrt{2\pi\nu^2}}\int \exp(\lambda S_t - t\lambda^2/2 - \lambda^2/2\nu^2)d\lambda \\ &= \frac{1}{\sqrt{2\pi\nu^2}}\int \exp(\lambda S_t - \lambda^2(t+\nu^{-2})/2)d\lambda \\ &= \frac{1}{\sqrt{2\pi\nu^2}}\int \exp(S_t^2(t+\nu^{-2})^{-1}/2 - (S_t(t+\nu^{-2})^{-1} - \lambda)^2/2(t+\nu^{-2})^{-1})d\lambda \\ &= \sqrt{\frac{(t+\nu^{-2})^{-1}}{\nu^2}}\exp(S_t^2(t+\nu^{-2})^{-1}/2) \\ &= \sqrt{\frac{\nu^{-2}}{t+\nu^{-2}}}\exp(S_t^2(t+\nu^{-2})^{-1}/2).\end{aligned}$$

Applying the maximal inequality for super-martingales we have

$$\mathbb{P}(\exists t : |S_t| \geq \sqrt{2(t+\nu^{-2})\left(\log(1/\delta) + \tfrac{1}{2}\log(\frac{t+\nu^{-2}}{\nu^{-2}})\right)}) = \mathbb{P}(\exists t : \bar{M}_t \geq 1/\delta) \leq \delta.$$

A particularly convenient choice for ν is $\nu = 1$ which implies

$$\mathbb{P}\big(\exists t : |S_t| \geq \sqrt{2(t+1)\log(\tfrac{\sqrt{t+1}}{\delta})}\big) \leq \delta.$$



(a) Fix $\delta = 0.05$. The 'fixed time Chernoff' represents $\sqrt{2t\log(1/\delta)}$ which holds at each t but not all $t \leq 500$ simultaneously (which is why it is dotted). The 'max inequality' holds for all $t \leq 500$, and the linear boundaries hold for all $t \in \mathbb{N}$ simultaneously.

(b) Fix $\delta = 0.05$. The 'fixed time Chernoff' represents $\sqrt{2t\log(1/\delta)}$ which holds at each t but not all $t \in \mathbb{N}$ simultaneously (which is why it is dotted). All other curves do hold for all $t \in \mathbb{N}$ simultaneously. "union bound $2t^2$" plots $\sqrt{2\log(2t^2/\delta)}$.

Intuitively, $h(\lambda)$ is a probability distribution over linear boundaries parameterized by λ.

The above Figures compares these linear and curved boundaries. We see that the curved boundary just derived appears much tighter than our naive union bound used in the proofs of the early days of this course. Let us consider a few more interesting examples.

1.3.3 Predictable sequences, Azuma-style inequalities

Let $Z_1, Z_2, \dots$ be an $\mathcal{F}_t$-adapted sequence and assume σ_t is predictable in the sense that σ_t is $\mathcal{F}_{t-1}$-measurable. Furthermore, assume $\mathbb{E}[Z_t|\mathcal{F}_{t-1}] = 0$ and that for any $\lambda > 0$ we have $\mathbb{E}[\exp(\lambda Z_t)|\mathcal{F}_{t-1}] \leq \exp(\lambda^2\sigma_t^2/2)$. Define $S_t = \sum_{i=1}^t Z_i$ and $V_t = \sum_{i=1}^t \sigma_i^2$. Then $M_t(\lambda) = \exp(\lambda S_t - \lambda^2 V_t/2)$ is a super-martingale. Thus,

$$\mathbb{P}(\exists t \in \mathbb{N} : S_t \geq \lambda V_t/2 + \log(1/\delta)/\lambda) = \mathbb{P}(\exists t : M_t(\lambda) \geq 1/\delta) \leq \delta.$$

Likewise, computing $\bar{M}_t$ with $h(\lambda) = \frac{1}{\sqrt{2\pi}}e^{-\lambda^2/2}$ yields

$$\mathbb{P}(\exists t \in \mathbb{N} : |S_t| \geq \sqrt{(V_t+1)\log(\tfrac{V_t+1}{\delta^2})}) = \mathbb{P}(\exists t : \bar{M}_t \geq 1/\delta) \leq \delta.$$

Note that "time" t does not appear anywhere in these bounds explicitly, and has been replaced by V_t.

1.3.4 Vector-valued martingales

Now suppose $Z_1, Z_2, \dots \in \mathbb{R}^d$ is a $\mathcal{F}_t$-adapted random sequence that satisfies $\mathbb{E}[\exp(\langle \lambda, Z_t\rangle)|\mathcal{F}_{t-1}] \leq \exp(\|\lambda\|_{\Sigma_t}^2/2)$ for any $\lambda \in \mathbb{R}^d$ for a Σ_t predictable sequence. Define $S_t = \sum_{i=1}^t Z_i$ and $V_t = \sum_{i=1}^t \Sigma_i$. Then $M_t(\lambda) = \exp(\langle \lambda, S_t\rangle - \|\lambda\|_{V_t}^2/2)$ is a super-martingale. By the same arguments as above, for *any* $\lambda \in \mathbb{R}^d$ we can construct a linear boundary as follows:

$$\mathbb{P}(\exists t \in \mathbb{N} : \langle \lambda, S_t\rangle - \|\lambda\|_{V_t}^2/2 \geq \log(1/\delta)) \leq \delta.$$

Note that $\max_\lambda \langle \lambda, S_t \rangle - \|\lambda\|_{V_t}^2/2 = \|S_t\|_{V_t^{-1}}^2/2$ with the maximizer being $V_t^{-1} S_t$. Let $\mathcal{S}_{r,\epsilon}$ be an ϵ-net of a radius r d-ball and note that $|\mathcal{S}_{r,\epsilon}| \leq (4r/\epsilon)^d$. For any $\lambda \in \mathbb{R}^d$, let $\widetilde{\lambda}$ be in our full cover. Then we have that

$$\langle \lambda, S_t \rangle - \|\lambda\|_{V_t}^2/2 \leq \langle \widetilde{\lambda}, S_t \rangle - \|\widetilde{\lambda}\|_{V_t}^2/2 + \langle \lambda - \widetilde{\lambda}, S_t \rangle - \|\lambda\|_{V_t}^2/2 + \|\widetilde{\lambda}\|_{V_t}^2/2$$

If $h(\lambda) = \frac{1}{(2\pi/\gamma)^{d/2}} \exp(-\|\lambda\|^2 \gamma/2)$ be a mean-zero Gaussian distribution with covariance $\gamma^{-1} I$. If $\bar{M}_t = \int_\lambda M_t(\lambda) dh(\lambda)$ then

$$\begin{aligned}
\bar{M}_t &= \int_\lambda M_t(\lambda) dh(\lambda) \\
&= \frac{1}{(2\pi/\gamma)^{d/2}} \int_\lambda \exp(\langle \lambda, S_t \rangle - \|\lambda\|_{V_t}^2/2 - \|\lambda\|^2 \gamma/2) dh(\lambda) \\
&= \frac{1}{(2\pi/\gamma)^{d/2}} \int_\lambda \exp(\langle \lambda, S_t \rangle - \|\lambda\|_{V_t + \gamma I}^2/2) dh(\lambda) \\
&= \frac{1}{(2\pi/\gamma)^{d/2}} \int_\lambda \exp(\tfrac{1}{2}\|S_t\|_{(V_t+\gamma I)^{-1}}^2 - \tfrac{1}{2}\|(V_t + \gamma I)^{-1} S_t - \lambda\|_{(V_t+\gamma I)}^2) dh(\lambda) \\
&= \frac{|V_t + \gamma I|^{-1/2}}{\gamma^{-d/2}} \exp(\tfrac{1}{2}\|S_t\|_{(V_t+\gamma I)^{-1}}^2)
\end{aligned}$$

then repeating the same steps as above we conclude that

$$\mathbb{P}(\exists t : \|S_t\|_{(V_t+\gamma I)^{-1}} \geq \sqrt{2\log(1/\delta) + \log(\frac{|V_t + \gamma I|}{\gamma^d}})) \leq \delta. \tag{1.1}$$

1.3.5 Application: Online linear regression

Let $x_1, x_2, \dots \in \mathbb{R}^d$ be an $\mathcal{F}_{t-1}$-measurable sequence, and for each $t \in \mathbb{N}$ let $y_t \in \mathbb{R}$ be $\mathcal{F}_t$-measurable. We assume there exists $\theta_* \in \mathbb{R}^d$ such that each $y_t = \langle \theta_*, x_t \rangle + \eta_t$ where η_t is mean-zero, independent of x_t, and $\mathbb{E}[\exp(s\eta_t)|\mathcal{F}_{t-1}] \leq \exp(s^2/2)$ for any $s \in \mathbb{R}$. In the previous example let $Z_i = x_i \eta_i$ so that $S_t = \sum_{i=1}^t x_t \eta_t$ and $V_t = \sum_{i=1}^t x_t x_t^\top$ since

$$\begin{aligned}
\mathbb{E}[\exp(\langle \lambda, x_t \eta_t \rangle)|\mathcal{F}_{t-1}] &= \mathbb{E}[\exp(\langle \lambda, x_t \rangle \eta_t)|\mathcal{F}_{t-1}] \\
&\leq \exp(\langle \lambda, x_t \rangle^2/2) \\
&= \exp(\|\lambda\|_{x_t x_t^\top}^2/2).
\end{aligned}$$

Thus, Equation 1.1 holds for any $\gamma > 0$. Fix some $\gamma > 0$ and define

$$\begin{aligned}
\widehat{\theta}_t &= \arg\min_\theta \sum_{i=1}^t (y_i - \langle x_i, \theta \rangle)^2 + \gamma \|\theta\|_2^2 \\
&= (\sum_{i=1}^t x_i x_i^\top + \gamma I)^{-1} \sum_{i=1}^t x_i y_i \\
&= (V_t + \gamma I)^{-1} V_t \theta_* + (V_t + \gamma I)^{-1} S_t
\end{aligned}$$

Now notice

$$\begin{aligned}
\|\widehat{\theta}_t - \theta_*\|_{(V_t+\gamma I)} &= \|\widehat{\theta}_t - (V_t+\gamma I)^{-1}(V_t+\gamma I)\theta_*\|_{(V_t+\gamma I)} \\
&= \|(V_t+\gamma I)^{-1}S_t - \gamma (V_t+\gamma I)^{-1}\theta_*\|_{(V_t+\gamma I)} \\
&= \|S_t - \gamma\theta_*\|_{(V_t+\gamma^{-1}I)^{-1}} \\
&\leq \|S_t\|_{(V_t+\gamma I)^{-1}} + \gamma\|\theta_*\|_{(V_t+\gamma I)^{-1}} \\
&\leq \|S_t\|_{(V_t+\gamma I)^{-1}} + \sqrt{\gamma}\|\theta_*\|_2.
\end{aligned}$$

We conclude that

$$\begin{aligned}
\mathbb{P}\Big(\exists t : \|\widehat{\theta}_t - \theta_*\|_{(V_t+\gamma I)} \geq & \sqrt{\gamma}\|\theta_*\|_2 + \sqrt{2\log(1/\delta) + \log(\gamma^{-d}|V_t+\gamma I|)}\Big) \qquad (1.2) \\
&\leq \mathbb{P}\Big(\exists t : \|S_t\|_{(V_t+\gamma I)^{-1}} \geq \sqrt{2\log(1/\delta) + \log(\gamma^{-d}|V_t+\gamma I|)}\Big) \leq \delta.
\end{aligned}$$

If we assume $\max_t \|x_t\|_2^2 \leq L$ then we also have by Jensen's inequality

$$\begin{aligned}
\log\left(|V_t+\gamma I|^{1/d}\right) &= \log\left(\prod_{i=1}^d \lambda_i\right)^{1/d} \\
&= \sum_{i=1}^d \frac{1}{d}\log(\lambda_i) \\
&\leq \log\left(\sum_{i=1}^d \frac{1}{d}\lambda_i\right) \\
&= \log\left(\frac{1}{d}\text{Trace}(V_t+\gamma I)\right) \\
&= \log\left(tL/d+\gamma\right)
\end{aligned}$$

so that for all $t \in \mathbb{N}$ we have

$$\|\widehat{\theta}_t - \theta_*\|_{(V_t+\gamma I)} \leq \sqrt{\gamma}\|\theta_*\|_2 + \sqrt{2\log(1/\delta) + d\log(\tfrac{tL}{d\gamma}+1)}$$

Due to its usefulness, we summarize the above discussion in a proposition.

Proposition 1. *Fix $\delta \in (0,1)$, $\gamma \geq 0$, and $\theta_* \in \mathbb{R}^d$. Assume for all $t \geq 1$ that $y_t = \langle \theta_*, x_t \rangle + \eta_t$ and $\mathbb{E}[\exp(s\eta_t)|\mathcal{F}_{t-1}] \leq \exp(s^2/2)$ for any $s \in \mathbb{R}$ where $\mathcal{F}_t$ is such that $x_1, y_1, \dots, x_{t-1}, y_{t-1}, x_t$ are $\mathcal{F}_{t-1}$ measurable. If $S_t = \sum_{i=1}^t x_t\eta_t$, $V_t = \sum_{i=1}^t x_t x_t^\top$, and $\widehat{\theta}_t = (V_t+\gamma I)^{-1}S_t$, then*

$$\|\widehat{\theta}_t - \theta_*\|_{(V_t+\gamma I)} \leq \sqrt{\gamma}\|\theta_*\|_2 + \sqrt{2\log(1/\delta) + \log(\gamma^{-d}|V_t+\gamma I|)}$$

for all $t \geq 1$ simultaneously with probability at least $1-\delta$. Moreover, if $\max_t \|x_t\|_2^2 \leq L$ then $\log(\gamma^{-d}|V_t+\gamma I|) \leq d\log(\frac{tL}{d\gamma}+1)$.

1.4 Wald's identity, Hypothesis testing, Likelihood ratios

Lemma 4 (Wald's identity)**.** *Let Z_t be IID random variables with $\mathbb{E}[Z_t] = \mu$. If τ is a stopping time with $\mathbb{E}[\tau] < \infty$ then $\mathbb{E}[\sum_{t=1}^\tau Z_t] = \mu\mathbb{E}[\tau]$.*

Proof. Note that $X_n = \sum_{t=1}^n Z_t - \mu n$ is a martingale. If $\mu \in \{-\infty, \infty\}$ the result is trivial so assume otherwise. If μ is finite then

$$\mu = \mathbb{E}[Z_t] = \mathbb{E}[\max\{0, Z_{t+1}\}] - \mathbb{E}[\max\{0, -Z_{t+1}\}]$$

implies at most one of these summands could be infinite in magnitude (since $\infty - \infty$ is not defined). But since μ is finite by assumption, neither piece can be infinite in magnitude. Thus, there exists some $c > 0$ such that

$$\mathbb{E}[|X_{t+1} - X_t|\,|\mathcal{F}_t] = \mathbb{E}[|Z_{t+1} - \mu|] \leq |\mu| + \mathbb{E}[\max\{0, Z_{t+1}\}] + \mathbb{E}[\max\{0, -Z_{t+1}\}] \leq c.$$

We can apply Doob's optional stopping to conclude

$$\mathbb{E}[\sum_{t=1}^{\tau} Z_t - \mu\tau] = \mathbb{E}[X_\tau] = \mathbb{E}[X_0] = 0$$

which implies the result by subtracting $\mu\mathbb{E}[\tau]$ from both sides. □

Let $X_1, X_2, \ldots$ be an $\mathcal{F}_t$-adapted sequence of random variables. Consider the hypothesis test

$$\begin{aligned} \mathbf{H}_0 :& X_t \sim p_0 \ \forall t \\ \mathbf{H}_1 :& X_t \sim p_1 \ \forall t. \end{aligned}$$

Define the likelihood ratio $L_t = \prod_{s=1}^t \frac{p_1(X_s)}{p_0(X_s)}$. Let $\mathbb{E}_i[\cdot], \mathbb{P}_i[\cdot]$ denote expectation and probability under $\mathbf{H}_i$. Note that under $\mathbf{H}_0$ we have that L_t is a martingale since

$$\mathbb{E}_0[L_{t+1}|\mathcal{F}_t] = L_t \int_x \frac{p_1(x)}{p_0(x)} p_0(x) dx = L_t \int_x p_1(x) dx = L_t.$$

Similarly, we have that L_t^{-1} is a martingale under $\mathbf{H}_1$. This allows us to apply the maximal inequality to conclude that

$$\max\{\mathbb{P}_0(\exists t \in \mathbb{N} : L_t \geq 1/\delta), \mathbb{P}_1(\exists t \in \mathbb{N} : L_t \leq \delta)\} \leq \delta.$$

We will show that if $\tau := \min\{t \in \mathbb{N} : L_t \notin (\delta, 1/\delta)\}$ then

$$\mathbb{E}_0[\tau] \leq \frac{\log(e/\delta)}{KL(p_0|p_1)} + 1 \qquad \text{and} \qquad \mathbb{E}_1[\tau] \leq \frac{\log(e/\delta)}{KL(p_1|p_0)} + 1.$$

Compare this with our minimax lower bound of above. Since they nearly match, we conclude that this method known as the sequential probability ratio test (SPRT) is optimal.

By Wald's inequality we have

$$\mathbb{E}_0[\log(L_\tau)] = \mathbb{E}_0[\tau]\mathbb{E}_0[\log(\tfrac{p_1(X_1)}{p_0(X_1)})] = -\mathbb{E}_0[\tau] KL(p_0|p_1).$$

But on the other hand, we also have

$$\begin{aligned} \mathbb{E}_0[\log(L_\tau)] &= \mathbb{E}_0[\log(L_\tau)\mathbf{1}\{L_\tau > 1/\delta\}] + \mathbb{E}_0[\log(L_\tau)\mathbf{1}\{L_\tau < \delta\}] \\ &\geq \mathbb{E}_0[\log(L_\tau)\mathbf{1}\{L_\tau < \delta\}] \\ &\geq \mathbb{E}_0[(\log(L_{\tau-1}) + \log(\tfrac{p_1(X_\tau)}{p_0(X_\tau)}))\mathbf{1}\{L_\tau < \delta\}] \\ &\geq \log(\delta) + \mathbb{E}_0[\log(\tfrac{p_1(X_\tau)}{p_0(X_\tau)})\mathbf{1}\{L_\tau < \delta\}] \\ &= \log(\delta) + \mathbb{E}_0[\log(\tfrac{p_1(X_\tau)}{p_0(X_\tau)})\mathbf{1}\{\log(\tfrac{p_1(X_\tau)}{p_0(X_\tau)}) < \log(\delta) - \log(L_{\tau-1})\}] \\ &= \log(\delta) - \mathbb{E}_0[\log(\tfrac{p_0(X_1)}{p_1(X_1)})\mathbf{1}\{p_1(X_1) < p_0(X_1)\}] \\ &\geq \log(\delta) - KL(p_0|p_1) - 1 \end{aligned}$$

where the last line follows from

$$\begin{aligned}
\mathbb{E}_0[\log(\tfrac{p_0(X_1)}{p_1(X_1)})\mathbf{1}\{p_1(X_1) < p_0(X_1)\}] &= \int_x p_0(x)\log(\tfrac{p_0(x)}{p_1(x)})\mathbf{1}\{p_1(x) < p_0(x)\}dx \\
&= \int_{x:p_1(x)<p_0(x)} p_0(x)\log(\tfrac{p_0(x)}{p_1(x)})dx \\
&= \int_x p_0(x)\log(\tfrac{p_0(x)}{p_1(x)})dx - \int_{x:p_1(x)>p_0(x)} p_0(x)\log(\tfrac{p_0(x)}{p_1(x)})dx \\
&= KL(p_0|p_1) + \int_{x:p_1(x)>p_0(x)} p_0(x)\log(\tfrac{p_1(x)}{p_0(x)})dx \\
&= KL(p_0|p_1) + \int_{x:p_1(x)>p_0(x)} p_0(x)\log(1+\tfrac{p_1(x)-p_0(x)}{p_0(x)})dx \\
&\le KL(p_0|p_1) + \int_{x:p_1(x)>p_0(x)} (p_1(x)-p_0(x))dx \\
&\le KL(p_0|p_1) + 1
\end{aligned}$$

where the first inequality follows from $\log(1+x) \le x$. Putting the pieces together, we conclude that $\mathbb{E}_0[\tau] \le \frac{\log(e/\delta)}{KL(p_0|p_1)} + 1$. Repeating the process for $\mathbf{H}_1$ produces an analogous result.

Binary hypothesis test for Gaussians with known variance Let $p_0(x) = \frac{1}{\sqrt{2\pi}}e^{-x^2/2}$ and $p_1(x) = \frac{1}{\sqrt{2\pi}}e^{-(x-\Delta)^2/2}$ so that we are deciding two Gaussian distributions, each with variance 1 and separated by Δ. Note that

$$\begin{aligned}
L_t &= \prod_{s=1}^t \frac{p_1(X_s)}{p_0(X_s)} \\
&= \prod_{s=1}^t \exp(-(X_s-\Delta)^2/2 + X_s^2/2) \\
&= \exp((\sum_{s=1}^t X_s)\Delta - t\Delta^2/2) \\
&= \exp(\Delta S_t - t\Delta^2/2)
\end{aligned}$$

where $S_t = \sum_{s=1}^t X_s$. Applying the maximal inequality of above and rearranging, we have

$$\mathbb{P}_0(\exists t \in \mathbb{N} : S_t \ge t\Delta/2 + \log(1/\delta)/\Delta) = \mathbb{P}_0(\exists t \in \mathbb{N} : L_t \ge 1/\delta) \le \delta.$$

Compare this to the line-crossing super-martingale bound of above. They are equivalent with $\lambda = \Delta$. Because of the optimality of the SPRT, we conclude that a linear boundary is optimal for deciding between two means. Unfortunately, the precise parameterization of λ requires knowledge of the unknown parameter.

1.5 Information theoretic lower bounds

Let $(\mathcal{X}, \mathcal{A})$ be a measurable space and P, Q be two measures over $(\mathcal{X}, \mathcal{A})$. Let ν be a dominating measure so that $p(x) = dP(x)/d\nu(x)$ and $q(x) = dQ(x)/d\nu(x)$ are well-defined.

Definition 10. *The* ***total variation*** *between measures P, Q is defined as*

$$TV(P,Q) = \sup_{A \in \mathcal{A}} |P(A) - Q(A)| = \sup_{A \in \mathcal{A}} \Big| \int_{x \in A} p(x) - q(x) d\nu(x) \Big|.$$

Lemma 5. *[Scheffe's Theorem]* $TV(P,Q) = \frac{1}{2} \int_x |p(x) - q(x)| d\nu(x) = 1 - \int_x \min\{p(x), q(x)\} d\nu(x)$*.*

Lemma 6. *[LeCam's inequality]* $\int_x \min\{p(x), q(x)\} d\nu(x) \geq \frac{1}{2} \left(\int_x \sqrt{p(x)q(x)} d\nu(x) \right)^2$

Proof.

$$\begin{aligned} \left(\int_x \sqrt{p(x)q(x)} d\nu(x) \right)^2 &= \left(\int_{x \in \mathbb{R}^n} \sqrt{\min\{p(x), q(x)\} \max\{p(x), q(x)\}} d\nu(x) \right)^2 \\ &\leq \int_x \min\{p(x), q(x)\} d\nu(x) \int_x \max\{p(x), q(x)\} d\nu(x) && \text{(Cauchy-Schwartz)} \\ &\leq 2 \int_x \min\{p(x), q(x)\} d\nu(x) \end{aligned}$$

by noting that $\int_x \max\{p(x), q(x)\} d\nu(x) \leq \int_x p(x) d\nu(x) + \int_x q(x) d\nu(x) = 2$. □

Definition 11. *The* ***Kullback Liebler divergence*** *between P and Q is*

$$KL(P,Q) = \int_x \log\big(\frac{p(x)}{q(x)}\big) p(x) d\nu(x).$$

Lemma 7 (Pinsker's inequality)**.** $TV(P,Q) \leq \min\left\{ \sqrt{KL(P,Q)/2}, 1 - \frac{1}{2}\exp(-KL(P,Q)) \right\}$*.*

Proof. The first argument is known as Pinsker's inequality, and the following proof is due to Pollard. For random variables X and $Y \geq 0$ Sedrakyan's inequality says $\mathbb{E}[\frac{X^2}{Y}] \geq \frac{\mathbb{E}[|X|]^2}{\mathbb{E}[Y]}$. Define $r(x) = \frac{p(x)}{q(x)} - 1$. Then

$$\begin{aligned} KL(P,Q) &= \int_x \big((1 + r(x)) \log(1 + r(x)) - r(x) \big) q(x) d\nu(x) \\ &\geq \frac{1}{2} \int_x \frac{r(x)^2}{1 + r(x)/3} q(x) d\nu(x) && \text{(Taylor series)} \\ &\geq \frac{1}{2} \frac{\left(\int_x |r(x)| q(x) d\nu(x) \right)^2}{\int_x \big(1 + r(x)/3\big) q(x) d\nu(x)} && \text{(Sedrakyan's inequality)} \\ &= \frac{1}{2} \left(\int_x |p(x) - q(x)| d\nu(x) \right)^2 && (\textstyle\int_x r(x) q(x) d\nu(x) = 0) \\ &= 2\, TV(P,Q)^2. && \text{(Lemma 5)} \end{aligned}$$

The second argument follows by $TV(P,Q) = 1 - \int_x \min\{p(x), q(x)\}d\nu(x)$ and

$$\begin{aligned}
\int_x \min\{p(x), q(x)\}d\nu(x) &\geq \frac{1}{2}\left(\int_x \sqrt{p(x)q(x)}d\nu(x)\right)^2 && \text{(Lemma 6)} \\
&= \frac{1}{2}\exp\left(2\log(\int_x p(x)\sqrt{q(x)/p(x)}d\nu(x))\right) \\
&\geq \frac{1}{2}\exp\left(2\int_x p(x)\log(\sqrt{q(x)/p(x)})d\nu(x)\right) && \text{(Jensen's inequality)} \\
&= \frac{1}{2}\exp\left(-\int_x \log(\tfrac{p(x)}{q(x)})p(x)d\nu(x)\right) \\
&= \frac{1}{2}\exp(-KL(P,Q)).
\end{aligned}$$

□

Lemma 8 (Chain-rule)**.** *Let $P = \prod_{t=1}^n p(\cdot)$ and $Q = \prod_{t=1}^n q(\cdot)$ be product measures with respect to p, q respectively. Then $KL(P,Q) = nKL(p,q)$.*

Proof.

$$KL(P,Q) = \mathbb{E}_P[\log(\prod_{t=1}^n \frac{p(X_t)}{q(X_t)})] = \mathbb{E}_P[\sum_{t=1}^n \log(\frac{p(X_t)}{q(X_t)})] = nKL(p,q)$$

□

Definition 12. *Fix measures P, Q on $(\Omega, \mathcal{F})$ with $Q \gg P$. The Radon-Nikodym derivative of P with respect to Q is a random variable $\frac{dP}{dQ} : \Omega \to \mathbb{R}_+$ such that $P(A) = \int_{\omega \in A} dP(\omega) = \int_{\omega \in A} \frac{dP}{dQ}(\omega)dQ(\omega)$ for all $A \in \mathcal{F}$.*

Lemma 9. *Let P, Q be two probability measures on $(\Omega, \mathcal{F})$. Let Z be a random variable defined on this space and define $P_Z(A) = P(Z \in A) = \int_{\omega \in \Omega : Z(\omega) \in A} dP(\omega)$ and similarly for Q_Z. Then $D(P_Z, Q_Z) = \int \log\left(\frac{dP}{dQ}(Z(\omega))\right)dP(\omega) = \mathbb{E}_P[\log\left(\frac{dP}{dQ}(Z)\right)]$.*

Proof. On the one hand we have

$$\int_{z \in A} dP_Z(z) = \int_{z \in A}\int_{\omega : Z(\omega) = z} dP(\omega) = \int_{z \in A} dP(z) = \int_{z \in A} \frac{dP}{dQ}(z)dQ(z)$$

but on the other we have

$$\begin{aligned}
\int_{z \in A} dP_Z(z) &= \int_{z \in A} \frac{dP_Z}{dQ_Z}(z)dQ_Z(z) \\
&= \int_{z \in A} \frac{dP_Z}{dQ_Z}(z)\int_{\omega : Z(\omega) = z} dQ(\omega) \\
&= \int_{\omega : Z(\omega) \in A} \frac{dP_Z}{dQ_Z}(Z(\omega))dQ(\omega).
\end{aligned}$$

Thus, a valid choice of $\frac{dP_Z}{dQ_Z}(Z(\omega))$ is precisely $\frac{dP}{dQ}(z)$. Now

$$\begin{aligned}
D(P_Z, Q_Z) &= \int_z \log \frac{dP_Z}{dQ_Z}(z) dP_Z(z) \\
&= \int_z \log \frac{dP}{dQ}(z) dP_Z(z) \\
&= \int_z \log \frac{dP}{dQ}(z) \int_{\omega : Z(\omega) = z} dP(\omega) \\
&= \int_\omega \log \frac{dP}{dQ}(Z(\omega)) dP(\omega).
\end{aligned}$$

□

Lemma 10 (A data-processing inequality)**.** *Let P, Q be two probability measures on $(\Omega, \mathcal{F})$. Let Z be a random variable defined on this space and define $P_Z(A) = P(Z \in A) = \int_{\omega \in \Omega : Z(\omega) \in A} dP(\omega)$ and similarly for Q_Z. Then $D(P_Z, Q_Z) \leq D(P, Q)$.*

Proof. We will prove it for Ω discrete. Define $f(x) = x \log(x)$ so that

$$\begin{aligned}
D(P, Q) &= \sum_z \sum_{\omega : Z(\omega) = z} P(\omega) \log(\frac{P(\omega)}{Q(\omega)}) \\
&= \sum_z \sum_{\omega : Z(\omega) = z} Q(\omega) f(\frac{P(\omega)}{Q(\omega)}) \\
&= \sum_z Q_Z(z) \sum_{\omega : Z(\omega) = z} \frac{Q(\omega)}{Q_Z(z)} f(\frac{P(\omega)}{Q(\omega)}) \\
&\geq \sum_z Q_Z(z) f(\sum_{\omega : Z(\omega) = z} \frac{Q(\omega)}{Q_Z(z)} \frac{P(\omega)}{Q(\omega)}) \\
&= \sum_z Q_Z(z) f(\frac{P_Z(z)}{Q_Z(z)}) = D(P_Z, Q_Z)
\end{aligned}$$

where the inequality follows by Jensen's since f is convex. □

To appreciate the significance of the data-processing inequality and chain rule, consider a sequence of random variables $X_1, X_2, \ldots$ where X_t is $\mathcal{F}_t$ measurable. Let τ be a stopping time so that $\{\tau = t\}$ is $\mathcal{F}_t$-measurable, and let Z be an $\mathcal{F}_\tau$ measurable random variable. If P is the probability law of $\{X_t\}_{t=1}^{\tau}$ when $X_t \sim p$ and analogously for Q, q, then

$$\begin{aligned} D(P_Z, Q_Z) &\leq D(P, Q) && \text{(data-processing)} \\ &= \int_\omega \log \frac{dP}{dQ}(\omega) dP(\omega) \\ &= \int_\omega \log \Big(\prod_{t=1}^{\tau(\omega)} \frac{dP}{dQ}(X_t(\omega)) \Big) dP(\omega) && \text{(chain rule)} \\ &= \int_\omega \sum_{t=1}^{\tau(\omega)} \log \Big(\frac{dP}{dQ}(X_t(\omega)) \Big) dP(\omega) \\ &= \mathbb{E}_P[\sum_{t=1}^{\tau} \log(\frac{p(X_t)}{q(X_t)})] \\ &= KL(p,q)\mathbb{E}_P[\tau] \end{aligned}$$

1.5.1 Lower bounds for estimating the mean of a Gaussian

Suppose I get n samples from a Gaussian distribution $\mathcal{N}(\mu, 1)$. You compute the empirical mean $\widehat{\mu} = \frac{1}{n}\sum_{i=1}^n X_i$. We know that $|\widehat{\mu} - \mu| \leq \sqrt{2\log(2/\delta)/n}$. How tight is this? If $\mu \in \{0, \Delta\}$ then we just need $n = 8\Delta^{-2}\log(2/\delta)$[1]

Let $p_\mu(x) = \frac{1}{2\pi}e^{-(x-\mu)^2/2\sigma^2}$ be the Gaussian distribution with mean μ. Under H_0, $X_i \sim p_0$ and under H_1, $X_i \sim p_\Delta$. Let $\phi : \mathbb{R}^n \to \{0,1\}$. Then the minimax probability of error is equal to

$$\begin{aligned} \inf_\phi \max\{\mathbb{P}_0(\phi = 1), \mathbb{P}_1(\phi = 0)\} &\geq \inf_\phi \frac{1}{2}(\mathbb{P}_0(\phi = 1) + \mathbb{P}_1(\phi = 0)) \\ &\geq \frac{1}{2}(1 - \sup_A |\mathbb{P}_0(A) - \mathbb{P}_1(A)|) \\ &\geq \frac{1}{4}\exp(-KL(\mathbb{P}_1, \mathbb{P}_0)) && \text{(Lemma 7)} \end{aligned}$$

Note that

$$\begin{aligned} KL(\mathbb{P}_1|\mathbb{P}_0) &= \int_x \log\left(\prod_{i=1}^n \frac{p_1(x_i)}{p_0(x_i)}\right)\prod_{i=1}^n p_1(x_i)dx \\ &= nKL(p_1|p_0) = n\Delta^2/2 \end{aligned}$$

and that $KL(\mathcal{N}(0,1)|\mathcal{N}(\Delta,1)) = \Delta^2/2$.
We conclude that

$$\inf_\phi \max\{\mathbb{P}_0(\phi = 1), \mathbb{P}_1(\phi = 0)\} \geq \frac{1}{4}\exp\left(-n\Delta^2/2\right)$$

Thus, to determine whether or not n samples are from a Gaussian with mean 0 or Δ with probability of failure less than δ, one needs $n \geq 2\Delta^{-2}\log(1/4\delta)$.

[1] Using the SPRT, as $\delta \to 0$ one needs just an expected number of samples equal to $2\Delta^{-2}\log(2/\delta)$.

Chapter 2

Supervised Learning and Generalization

2.1 Classification and bounded losses

Supervised machine learning is the study of making predictions from labeled data. In the standard paradigm, one is given a dataset of n labeled examples $(x_1, y_1), \dots, (x_n, y_n)$ drawn independently and identically distributed (IID) from some unknown distribution ν over an input space $\mathcal{X}$ and label space $\mathcal{Y} = \{-1, +1\}$. From these examples, one learns a *hypothesis* $h : \mathcal{X} \to \mathcal{Y}$ from a *hypothesis class* $\mathcal{H}$ that can then be applied to predict labels for unseen data.

For a hypothesis $h \in \mathcal{H}$ and distribution ν, define the *population risk*

$$R(h) = \mathbb{P}_{(X,Y)\sim\nu}(h(X) \neq Y),$$

and the *empirical risk* on a sample $(x_1, y_1), \dots, (x_n, y_n)$,

$$R_n(h) = \frac{1}{n}\sum_{i=1}^{n} \mathbf{1}\{h(x_i) \neq y_i\}.$$

Empirical Risk Minimization (ERM) selects

$$\hat{h} = \arg\min_{h\in\mathcal{H}} R_n(h).$$

The goal of learning theory is to bound the population risk $R(\hat{h})$ in terms of the sample size n and properties of $\mathcal{H}$. Often, even the best classifier makes errors so that $\min_{h\in\mathcal{H}} R(h) > 0$ and then we seek to bound the *excess* risk on top of the best performing hypothesis, or $R(\hat{h}) - \min_{h\in\mathcal{H}} R(h)$. If $h_* \in \arg\min_{h\in\mathcal{H}} R(h)$ is an optimal classifier, one way to bound the excess risk is to realize that

$$\begin{aligned} R(\hat{h}) - R(h_*) &= R(\hat{h}) - R_n(\hat{h}) + R_n(\hat{h}) - R_n(h_*) + R_n(h_*) - R(h_*) \\ &\leq \max_{h\in\mathcal{H}} 2|R_n(h) - R(h)| \end{aligned}$$

using the fact that $R_n(\hat{h}) = \min_{h\in\mathcal{H}} R_n(h) \leq R_n(h_*)$ by construction. For a fixed $h \in \mathcal{H}$ note that $R_n(h) - R(h) = \frac{1}{n}\sum_{i=1}^{n}(\mathbf{1}\{h(x_i) \neq y_i\} - R(h))$ is the average of n mean-zero IID random variables bounded in $[-1, 1]$. The next section studies methods of bounding averages like these for more general bounded random variables. We will use classification as a running example.

2.2 Generalization Bounds

We focus on the finite hypothesis class setting, $|\mathcal{H}| < \infty$, which already captures the essential ideas while permitting clean proofs.

2.2.1 The Realizable Case

The *realizable case* assumes the data is generated by some $h^* \in \mathcal{H}$, meaning $y_i = h^*(x_i)$ for all i. Under this assumption ERM is guaranteed to return a hypothesis with small population risk.

Theorem 1 (Realizable ERM). *Let $\mathcal{H}$ be a finite hypothesis class with $|\mathcal{H}| < \infty$, and suppose $h(x) \in \{-1, +1\}$ for all $h \in \mathcal{H}$. Let $(x_1, y_1), \ldots, (x_n, y_n) \overset{\text{iid}}{\sim} \nu$ with $y_i \in \{-1, +1\}$. Assume there exists $h^* \in \mathcal{H}$ with $R(h^*) = 0$. If $\hat{h} = \arg\min_{h \in \mathcal{H}} R_n(h)$, then with probability at least $1 - \delta$,*

$$R(\hat{h}) \leq \frac{\log(|\mathcal{H}|/\delta)}{n}.$$

Proof. Since h^* achieves zero empirical risk, ERM also returns a hypothesis with zero empirical risk: $R_n(\hat{h}) = 0$. For any fixed $h \in \mathcal{H}$ with $R(h) > \epsilon$, since the examples are IID,

$$\mathbb{P}(R_n(h) = 0) = \prod_{i=1}^{n} \mathbb{P}(h(x_i) = y_i) \leq (1 - \epsilon)^n \leq e^{-n\epsilon}.$$

By the union bound over all $h \in \mathcal{H}$,

$$\mathbb{P}\Big(\exists\, h \in \mathcal{H} : R(h) > \epsilon \text{ and } R_n(h) = 0\Big) \leq |\mathcal{H}| \cdot e^{-n\epsilon}.$$

Setting $|\mathcal{H}| e^{-n\epsilon} = \delta$ gives $\epsilon = \log(|\mathcal{H}|/\delta)/n$. Since $\hat{h}$ satisfies $R_n(\hat{h}) = 0$, on the complement of the above event we have $R(\hat{h}) \leq \epsilon$. □

2.2.2 The Agnostic (Non-Realizable) Case

In many settings no hypothesis in $\mathcal{H}$ perfectly explains the data. The *agnostic case* makes no realizability assumption; it asks how well ERM performs relative to the best hypothesis $h^* = \arg\min_{h \in \mathcal{H}} R(h)$ in $\mathcal{H}$. The key probabilistic tool is Hoeffding's inequality.

Lemma 11 (Hoeffding's Lemma). *Let X be a random variable with support in $[a, b]$ almost surely and $\mathbb{E}[X] = 0$. Then*

$$\log \mathbb{E}[\exp(\lambda X)] \leq \frac{(b-a)^2 \lambda^2}{8}.$$

We provide two proofs of this result. Both apply a clever trick followed by derivative calculations.

Proof. This proof is adapted from [Boucheron et al., 2013]. Let P_X denote the distribution of X so that for any function $g : \mathbb{R} \to \mathbb{R}$ we have $\mathbb{E}_X[g(X)] = \int_x g(x) dP(x)$. Define a new random variable Z with distribution P_Z defined as $dP_Z(x) = \frac{1}{\mathbb{E}_X[\exp(\lambda X)]} e^{\lambda x} dP_X(x)$. Note that P_Z is a valid distribution as $dP_Z(x) \geq 0$ for all x and $\int_x dP_Z(x) = \frac{1}{\mathbb{E}_X[\exp(\lambda X)]} \int_x e^{\lambda x} dP_X(x) = \frac{1}{\mathbb{E}_X[\exp(\lambda X)]} \mathbb{E}_X[\exp(\lambda X)] = 1.$

The key observation is to notice that

$$\begin{aligned}
\psi_X(\lambda) :=& \log(\mathbb{E}_X[\exp(\lambda X)]) \\
\psi'_X(\lambda) =& \frac{1}{\mathbb{E}_X[\exp(\lambda X)]}\mathbb{E}_X[X\exp(\lambda X)] \\
\psi''_X(\lambda) =& \frac{1}{\mathbb{E}_X[\exp(\lambda X)]}\mathbb{E}_X[X^2\exp(\lambda X)] - \left(\frac{1}{\mathbb{E}_X[\exp(\lambda X)]}\mathbb{E}_X[X\exp(\lambda X)]\right)^2 \\
=& \mathbb{E}_Z[Z^2] - \mathbb{E}_Z[Z]^2 \\
=& \mathbb{V}ar(Z) \\
\le& (b-a)^2/4
\end{aligned}$$

where the last line follows from the fact that the support of P_Z is contained in $[a,b]$ so that

$$\mathbb{V}ar(Z) = \mathbb{E}_Z[(Z-\mathbb{E}_Z[Z]^2)^2] \le \mathbb{E}_Z[(Z-\tfrac{a+b}{2})^2] \le (b-a)^2/4.$$

By Taylor's remainder theorem, for some $\theta \in [0,\lambda]$ we have

$$\begin{aligned}
\psi_X(\lambda) &= \psi_X(0) + \psi'_X(0)\lambda + \psi''_X(\theta)\lambda^2/2 \\
&= \psi''_X(\theta)\lambda^2/2 \\
&\le (b-a)^2\lambda^2/8
\end{aligned}$$

which completes the proof. □

Proof. Since $X \in [a,b]$, note that if we define $Z = \frac{X-a}{b-a}$ then $Z \in [0,1]$ and $X = (1-Z)a + Zb$. We can then write

$$\begin{aligned}
\mathbb{E}[\exp(\lambda X)] &= \mathbb{E}[\exp\big(\lambda((1-Z)a+Zb)\big)] \\
&\le \mathbb{E}[(1-Z)e^{\lambda a} + Ze^{\lambda b}] \\
&= \frac{b}{b-a}e^{\lambda a} + \frac{-a}{b-a}e^{\lambda b} \\
&= (1-t)e^{-\lambda(b-a)t} + te^{\lambda(b-a)(1-t)} \\
&= e^{-\lambda(b-a)t}\big[1-t+te^{\lambda(b-a)}\big]
\end{aligned}$$

where $t = \frac{-a}{b-a}$. Thus, if $\phi(\lambda) := -\lambda(b-a)t + \log(1-t+te^{\lambda(b-a)})$ then $\log\big(\mathbb{E}[\exp(\lambda X)]\big) \le \phi(\lambda)$. Note that

$$\begin{aligned}
\phi(\lambda) &= -\lambda(b-a)t + \log(1-t+te^{\lambda(b-a)}) \\
\phi'(\lambda) &= -(b-a)t + \frac{t(b-a)e^{\lambda(b-a)}}{1-t+te^{\lambda(b-a)}} \\
\phi''(\lambda) &= \frac{t(b-a)^2e^{\lambda(b-a)}(1-t+te^{\lambda(b-a)}) - t^2(b-a)^2e^{2\lambda(b-a)}}{(1-t+te^{\lambda(b-a)})^2} \\
&= \frac{t(1-t)e^{\lambda(b-a)}}{(1-t+te^{\lambda(b-a)})^2}(b-a)^2 \\
&\le (b-a)^2/4
\end{aligned}$$

where the last inequality follows from the arithmetic-geometric mean inequality: $\frac{\alpha+\beta}{2} \geq \sqrt{\alpha\beta}$ for positive α, β. We apply Taylor's theorem to complete the proof:

$$\phi(\lambda) \leq \phi(0) + \phi'(0)\lambda + \sup_{\tau} \phi''(\tau)\lambda^2/2 \leq \lambda^2(b-a)^2/8.$$

□

Corollary 1 (Hoeffding's Inequality)**.** *Let $Z_1, \dots, Z_n$ be independent random variables with $Z_i \in [a,b]$ almost surely and $\mathbb{E}[Z_i] = \mu$. For any $\epsilon > 0$,*

$$\mathbb{P}\left(\frac{1}{n}\sum_{i=1}^{n} Z_i \geq \mu + \epsilon\right) \leq \exp\left(\frac{-2n\epsilon^2}{(b-a)^2}\right).$$

Proof. Center $X_i = Z_i - \mu \in [a-\mu, b-\mu]$ with $\mathbb{E}[X_i] = 0$ and apply Lemma 11 together with Markov's inequality on $\exp(\lambda \sum_i X_i)$: for any $\lambda > 0$,

$$\mathbb{P}\left(\frac{1}{n}\sum_{i=1}^{n} Z_i \geq \mu + \epsilon\right) = \mathbb{P}\left(e^{\lambda \sum_i X_i} \geq e^{n\lambda\epsilon}\right) \leq e^{-n\lambda\epsilon} \prod_{i=1}^{n} \mathbb{E}[e^{\lambda X_i}] \leq e^{-n\lambda\epsilon} \cdot e^{n(b-a)^2\lambda^2/8}.$$

Optimizing over $\lambda > 0$ by setting $\lambda = 4\epsilon/(b-a)^2$ gives the stated bound. □

Applying Lemma 1 to $Z_i = \mathbf{1}\{h(x_i) \neq y_i\} \in [0,1]$ with mean $R(h)$ and using a union bound over both tails for each of the $|\mathcal{H}|$ hypotheses yields: with probability at least $1-\delta$, for all $h \in \mathcal{H}$ simultaneously,

$$\left|R(h) - R_n(h)\right| \leq \sqrt{\frac{\log(2|\mathcal{H}|/\delta)}{2n}}.$$

Theorem 2 (Agnostic ERM)**.** *Under the same setup as Theorem 1 but without the realizability assumption, let $h^* = \arg\min_{h \in \mathcal{H}} R(h)$. If $\hat{h} = \arg\min_{h \in \mathcal{H}} R_n(h)$, then with probability at least $1-\delta$,*

$$R(\hat{h}) \leq R(h^*) + \sqrt{\frac{2\log(|\mathcal{H}|/\delta)}{n}}.$$

Proof. By a union bound over $\mathcal{H}$ and Hoeffding's inequality, with probability at least $1-\delta$, for all $h \in \mathcal{H}$ simultaneously,

$$|R(h) - R_n(h)| \leq \epsilon_n, \qquad \text{where } \epsilon_n = \sqrt{\frac{\log(2|\mathcal{H}|/\delta)}{2n}}.$$

On this event, since $\hat{h}$ minimizes empirical risk,

$$R(\hat{h}) \leq R_n(\hat{h}) + \epsilon_n \leq R_n(h^*) + \epsilon_n \leq R(h^*) + 2\epsilon_n = R(h^*) + \sqrt{\frac{2\log(2|\mathcal{H}|/\delta)}{n}}.$$

Replacing $2|\mathcal{H}|/\delta$ by $|\mathcal{H}|/\delta$ adjusts the failure probability by at most a constant factor, giving the stated bound. □

Remark 1. *Theorem 2 interpolates with Theorem 1: in the realizable case the excess risk $R(\hat{h}) - R(h^*)$ vanishes at rate $O(\log(|\mathcal{H}|)/n)$, whereas in the agnostic case it vanishes at the slower rate $O(\sqrt{\log(|\mathcal{H}|)/n})$. This slower rate is tight in general; it cannot be improved without additional assumptions on $\mathcal{H}$ or the data-generating process.*

The following Bernstein inequality sharpens Hoeffding's bound when the variance of the random variables is small, and provides a unified view that encompasses both the realizable and agnostic rates.

Lemma 12 (Bernstein's Inequality). *Let $X_1, \ldots, X_n$ be independent random variables such that $\frac{1}{n}\sum_{i=1}^n \mathbb{E}[(X_i - \mathbb{E}[X_i])^2] \le \sigma^2$ and $|X_i| \le B$. Then with probability at least $1-\delta$,*

$$\left|\frac{1}{n}\sum_{i=1}^n X_i - \mathbb{E}[X_i]\right| \le \sqrt{\frac{2\sigma^2 \log(2/\delta)}{n}} + \frac{2B\log(2/\delta)}{3n}.$$

Moreover, if $X_1, \ldots, X_n$ form a martingale difference sequence with $\mathbb{E}[X_i \mid \mathcal{F}_{i-1}] = 0$ and $\frac{1}{n}\sum_{i=1}^n \mathbb{E}[X_i^2 \mid \mathcal{F}_{i-1}] \le \sigma^2$ almost surely, the same bound holds.

Remark 2 (Interpolation between realizable and agnostic rates). *Bernstein's inequality interpolates between the $O(\log|\mathcal{H}|/n)$ realizable rate and the $O(\sqrt{\log|\mathcal{H}|/n})$ agnostic rate as a function of the variance σ^2. To see this, apply Lemma 12 with $X_i = \mathbf{1}\{h(x_i) \ne y_i\}$ and $B = 1$. In the realizable case, $R(h^*) = 0$ implies every h^*-consistent labeling has $X_i \equiv 0$, so $\sigma^2 = 0$ and the bound reduces to $O(\log(1/\delta)/n)$, recovering the fast rate. In the fully agnostic case $\sigma^2 = O(1)$, the $\sqrt{\cdot}$ term dominates and we recover the $O(\sqrt{\log|\mathcal{H}|/\delta)/n})$ slow rate. In between, when $R(h^*) = \rho$ is small but nonzero, the variance $\sigma^2 \le \rho$ is also small, giving an intermediate rate of $O(\sqrt{\rho\log|\mathcal{H}|/n} + \log|\mathcal{H}|/n)$ that smoothly connects the two extremes.*

2.2.3 Infinite Hypothesis Classes

When $|\mathcal{H}| = \infty$—for example, when $\mathcal{H}$ is the class of all linear classifiers in $\mathbb{R}^d$—the bounds above become vacuous. Several tools have been developed to handle this regime. The *VC dimension* $\mathrm{VC}(\mathcal{H})$ is a combinatorial measure of the complexity of $\mathcal{H}$ that replaces $\log|\mathcal{H}|$: a version of Theorem 2 holds with $\log|\mathcal{H}|$ replaced by $\mathrm{VC}(\mathcal{H})$. *Rademacher complexity* and *covering numbers* provide complementary, often tighter, characterizations. We refer the reader to [Shalev-Shwartz and Ben-David, 2014] for a comprehensive treatment of these tools.

2.3 Squared Loss Regression

We now develop generalization bounds for the squared loss, which arises naturally in regression and serves as a bridge to the interactive learning settings studied later in these notes.

Let $\mathcal{X}$ be an input space and let $(X,Y) \sim \nu$ be drawn from an unknown distribution over $\mathcal{X} \times [0,1]$. We consider an arbitrary collection $\mathcal{F}$ of prediction functions $f : \mathcal{X} \to [0,1]$ and measure quality via the squared loss.

Definition 13 (Squared risk). *For $f : \mathcal{X} \to [0,1]$ define the* population risk

$$L(f) = \mathbb{E}_{(X,Y)\sim\nu}\left[(f(X) - Y)^2\right],$$

and the empirical risk *on an IID sample $(x_1, y_1), \ldots, (x_n, y_n) \sim \nu$,*

$$L_n(f) = \frac{1}{n}\sum_{i=1}^n (f(x_i) - y_i)^2.$$

The population-risk minimizer over *all* measurable functions is the conditional mean.

Proposition 2 (Bayes predictor)**.** *Define $f^*(x) = \mathbb{E}[Y \mid X = x]$. For any measurable $f : \mathcal{X} \to [0,1]$,*

$$L(f) \;=\; L(f^*) \;+\; \mathbb{E}\big[(f(X) - f^*(X))^2\big]\,.$$

In particular, $f^* = \arg\min_f L(f)$ and $L(f) \geq L(f^*)$ for every f.

Proof. Write $f(X) - Y = \big(f(X) - f^*(X)\big) + \big(f^*(X) - Y\big)$ and expand the square:

$$L(f) \;=\; \mathbb{E}\big[(f(X) - f^*(X))^2\big] + 2\,\mathbb{E}[(f(X) - f^*(X))(f^*(X) - Y)] + \mathbb{E}\big[(f^*(X) - Y)^2\big]\,.$$

The cross term vanishes by the tower property:

$$\mathbb{E}[(f(X) - f^*(X))(f^*(X) - Y)] \;=\; \mathbb{E}\Big[(f(X) - f^*(X))\,\underbrace{\mathbb{E}[f^*(X) - Y \mid X]}_{=\,0}\Big] \;=\; 0,$$

since $\mathbb{E}[Y \mid X] = f^*(X)$ by definition. Thus $L(f) = L(f^*) + \mathbb{E}[(f(X) - f^*(X))^2] \geq L(f^*)$. □

The identity $L(f) - L(f^*) = \mathbb{E}[(f(X) - f^*(X))^2]$ is a *bias–variance decomposition*: the excess squared risk of f equals the mean-squared deviation from the Bayes predictor.

In the finite-class setting $|\mathcal{F}| < \infty$ the Bayes predictor f^* need not lie in $\mathcal{F}$. Write $f^*_{\mathcal{F}} = \arg\min_{f\in\mathcal{F}} L(f)$ for the best predictor within the class. *Empirical Risk Minimization* (ERM) selects

$$\hat{f} \;=\; \arg\min_{f\in\mathcal{F}} L_n(f).$$

2.3.1 Generalization bounds via Hoeffding's inequality

Since $f(x), y \in [0,1]$, the loss $(f(x) - y)^2$ takes values in $[0,1]$. Boundedness alone is enough to apply the same Hoeffding-plus-union-bound strategy used in Chapter 2.

Theorem 3 (Agnostic ERM, squared loss)**.** *Let $\mathcal{F}$ be a finite class with $|\mathcal{F}| < \infty$, and let $(x_1, y_1), \ldots, (x_n, y_n) \overset{\text{iid}}{\sim} \nu$ with $y_i \in [0,1]$. If $\hat{f} = \arg\min_{f\in\mathcal{F}} L_n(f)$ and $f^*_{\mathcal{F}} = \arg\min_{f\in\mathcal{F}} L(f)$, then with probability at least $1 - \delta$,*

$$L(\hat{f}) - L(f^*_{\mathcal{F}}) \;\leq\; \sqrt{\frac{2\log(2|\mathcal{F}|/\delta)}{n}}.$$

Proof. Fix $f \in \mathcal{F}$. The variables $Z_i = (f(x_i) - y_i)^2$ are IID with $Z_i \in [0,1]$ and $\mathbb{E}[Z_i] = L(f)$. Applying Corollary 1 with $[a,b] = [0,1]$ and a union bound over $f \in \mathcal{F}$ and both tails, with probability at least $1 - \delta$ the following holds simultaneously for all $f \in \mathcal{F}$:

$$|L(f) - L_n(f)| \;\leq\; \sqrt{\frac{\log(2|\mathcal{F}|/\delta)}{2n}} \;=:\; \epsilon_n.$$

On this event, since $\hat{f}$ minimizes L_n:

$$L(\hat{f}) \;\leq\; L_n(\hat{f}) + \epsilon_n \;\leq\; L_n(f^*_{\mathcal{F}}) + \epsilon_n \;\leq\; L(f^*_{\mathcal{F}}) + 2\epsilon_n.$$

□

Remark 3. *Comparing with Theorem 2, the squared-loss bound is identical in form to the classification bound: both scale as $O(\sqrt{\log(|\mathcal{F}|/\delta)/n})$. This is because both losses lie in $[0,1]$, and the Hoeffding proof uses only boundedness.*

2.3.2 Fast rates via variance control

The $O(n^{-1/2})$ rate of Theorem 3 can be improved when $L(f^*_{\mathcal{F}})$ is small, by exploiting the specific structure of the squared loss through Bernstein's inequality (Lemma 12). The key observation is that the variance of $(f(X)-Y)^2$ is bounded by its mean.

Lemma 13 (Self-bounding variance)**.** *For any $f : \mathcal{X} \to [0,1]$ and $(X,Y) \sim \nu$ with $Y \in [0,1]$,*

$$\operatorname{Var}\big[(f(X)-Y)^2\big] \;\le\; L(f).$$

Proof. Since $f(x), y \in [0,1]$ we have $(f(x)-y)^2 \in [0,1]$, and therefore $(f(x)-y)^4 \le (f(x)-y)^2$. Thus

$$\operatorname{Var}\big[(f(X)-Y)^2\big] \;=\; \mathbb{E}\big[(f(X)-Y)^4\big] - \mathbb{E}\big[(f(X)-Y)^2\big]^2 \;\le\; \mathbb{E}\big[(f(X)-Y)^4\big] \;\le\; \mathbb{E}\big[(f(X)-Y)^2\big] \;=\; L(f).$$

□

When $L(f)$ is small, the variance is small, and Bernstein's inequality gives a tighter concentration bound than Hoeffding's. Combining with a union bound over $\mathcal{F}$ yields a *variance-dependent* uniform convergence result.

Proposition 3 (Bernstein uniform convergence, squared loss)**.** *With probability at least $1-\delta$, for all $f \in \mathcal{F}$ simultaneously,*

$$|L(f) - L_n(f)| \;\le\; \sqrt{\frac{2\,L(f)\,\log(2|\mathcal{F}|/\delta)}{n}} \;+\; \frac{2\log(2|\mathcal{F}|/\delta)}{3n}.$$

Proof. For fixed $f \in \mathcal{F}$, set $Z_i = (f(x_i)-y_i)^2$. These are IID with $Z_i \in [0,1]$, $\mathbb{E}[Z_i] = L(f)$, and $\operatorname{Var}[Z_i] \le L(f)$ by Lemma 13. Applying Lemma 12 with $\sigma^2 = L(f)$ and $B = 1$, then taking a union bound over $f \in \mathcal{F}$, gives the result. □

Notice that the right-hand side of Proposition 3 depends on $L(f)$ itself: when f achieves small risk, its empirical risk concentrates at a rate closer to $O(1/n)$ than $O(1/\sqrt{n})$. This is the mechanism behind the following fast-rate bound for ERM.

Theorem 4 (Fast-rate ERM, squared loss)**.** *Under the same setup as Theorem 3, with probability at least $1-\delta$,*

$$L(\hat{f}) - L(f^*_{\mathcal{F}}) \;\le\; 4\sqrt{\frac{2\,L(f^*_{\mathcal{F}})\,\log(2|\mathcal{F}|/\delta)}{n}} \;+\; \frac{8\log(2|\mathcal{F}|/\delta)}{n}.$$

In particular, when $L(f^*_{\mathcal{F}}) = 0$ the excess risk is $O(\log(|\mathcal{F}|/\delta)/n)$.

Proof. Let $\beta = \log(2|\mathcal{F}|/\delta)$. By Proposition 3, on an event of probability at least $1-\delta$, the following hold simultaneously for all $f \in \mathcal{F}$:

$$L(\hat{f}) \le L_n(\hat{f}) + \sqrt{\tfrac{2\beta\,L(\hat{f})}{n}} + \tfrac{2\beta}{3n}, \tag{2.1}$$

$$L_n(f^*_{\mathcal{F}}) \le L(f^*_{\mathcal{F}}) + \sqrt{\tfrac{2\beta\,L(f^*_{\mathcal{F}})}{n}} + \tfrac{2\beta}{3n}. \tag{2.2}$$

Using $L_n(\hat{f}) \le L_n(f^*_{\mathcal{F}})$ and combining (2.1)–(2.2):

$$L(\hat{f}) \;\le\; L(f^*_{\mathcal{F}}) + \sqrt{\tfrac{2\beta\,L(f^*_{\mathcal{F}})}{n}} + \sqrt{\tfrac{2\beta\,L(\hat{f})}{n}} + \tfrac{4\beta}{3n}. \tag{2.3}$$

Set $a = L(\hat{f})$, $b = L(f^*_{\mathcal{F}})$, $\alpha = \sqrt{2\beta/n}$, and $c = 4\beta/(3n)$. Then (2.3) reads $a \le b + \alpha\sqrt{b} + \alpha\sqrt{a} + c$, i.e.

$$\sqrt{a}^2 - \alpha\sqrt{a} \ \le \ b + \alpha\sqrt{b} + c.$$

Completing the square in $u = \sqrt{a}$ and recognizing the right-hand side:

$$\left(u - \tfrac{\alpha}{2}\right)^2 \ \le \ \left(\sqrt{b} + \tfrac{\alpha}{2}\right)^2 + c.$$

Taking square roots and using $\sqrt{A^2 + c} \le A + \sqrt{c}$ for $A, c \ge 0$:

$$u \ \le \ \sqrt{b} + \alpha + \sqrt{c}.$$

Therefore $a = u^2 \le (\sqrt{b} + \alpha + \sqrt{c})^2$, giving

$$L(\hat{f}) - L(f^*_{\mathcal{F}}) \ \le \ 2\sqrt{b}(\alpha + \sqrt{c}) + (\alpha + \sqrt{c})^2.$$

Since $c = 4\beta/(3n)$ and $\alpha^2 = 2\beta/n$, we have $\sqrt{c} = 2\sqrt{\beta/(3n)} \le \sqrt{2\beta/n} = \alpha$, so $\alpha + \sqrt{c} \le 2\alpha$. Substituting:

$$L(\hat{f}) - L(f^*_{\mathcal{F}}) \ \le \ 4\alpha\sqrt{b} + 4\alpha^2 \ = \ 4\sqrt{\frac{2\beta\, L(f^*_{\mathcal{F}})}{n}} + \frac{8\beta}{n}.$$

□

Remark 4 (Rate interpolation for squared loss)**.** *Theorem 4 parallels the Bernstein interpolation discussed in Chapter 2. When $L(f^*_{\mathcal{F}}) = \rho$ is small, the leading term $O(\sqrt{\rho \log|\mathcal{F}|/n})$ lies strictly between the $O(\sqrt{\log|\mathcal{F}|/n})$ slow rate (large ρ) and the $O(\log|\mathcal{F}|/n)$ fast rate ($\rho = 0$). Crucially, the fast rate here requires only that the best predictor in $\mathcal{F}$ achieves zero squared risk, not that f^* itself belongs to $\mathcal{F}$. The self-bounding property of the squared loss (Lemma 13) is the key structural fact:* $\mathrm{Var}[(f(X) - Y)^2] \le L(f)$ *is precisely the analogue of* $\mathrm{Var}[\mathbf{1}\{h(X) \ne Y\}] \le R(h)$ *that drives fast rates in classification.*

Part II

Online Learning and Adversarial Games

Chapter 3

Online Learning for bounded losses, classification

The generalization guarantees in Chapter 2 depend critically on the IID assumption. In many real-world settings this assumption fails: email spam evolves as spammers adapt to our filters; financial returns are influenced by participants' actions; in a game-playing context, an opponent actively works to defeat our strategy. *Online learning* is a paradigm that yields nontrivial performance guarantees even when examples are chosen by an adversary.

Online learning proceeds in rounds. On round $t = 1, 2, \ldots, T$:

1. An input $x_t \in \mathcal{X}$ arrives.
2. The player selects (possibly at random) a hypothesis $h_t \in \mathcal{H}$.
3. The true label $y_t \in \{-1, +1\}$ is revealed.
4. The player suffers loss $\ell_t = \mathbf{1}\{h_t(x_t) \neq y_t\}$.

We consider two regimes:

- **IID**: $(x_t, y_t) \overset{\text{iid}}{\sim} \nu$ for an unknown fixed ν.
- **Adversarial**: (x_t, y_t) are chosen by an adversary that may know the player's algorithm (but not future random choices).

The adversarial setting is strictly more general: any guarantee under adversarial inputs implies the same guarantee in the IID setting.

3.1 Realizable Case: Mistake-Bounded Learning

Assume there exists $h^* \in \mathcal{H}$ with $h^*(x_t) = y_t$ for all t. The *mistake bound* is the total number of rounds on which $h_t(x_t) \neq y_t$. In the IID realizable case, running ERM on all past examples at each round works well: after $t - 1$ examples, the ERM hypothesis has population risk at most $O(\log(|\mathcal{H}|)/t)$, so the expected number of new mistakes is small. Summing over t gives an expected total of $O(\log(T) \log(|\mathcal{H}|))$ mistakes.

In the adversarial realizable case, ERM breaks down. Since many hypotheses may be consistent with past data, an adversary can choose x_t to be a point where consistent hypotheses disagree, then set y_t to contradict our specific prediction. A smarter approach maintains the *version space* $V_t = \{h \in \mathcal{H} : h(x_s) = y_s,\ s < t\}$ of all hypotheses consistent with all past observations and predicts by majority vote.

```
Halving Algorithm
Input: Hypothesis class $\mathcal{H}$ with $|\mathcal{H}| < \infty$.
Initialize version space $V_1 = \mathcal{H}$.
for $t = 1, 2, \ldots$ do
    Observe $x_t$.
    Predict $\hat{y}_t = \mathrm{sign}\Big( \sum_{h \in V_t} h(x_t) \Big)$ (majority vote over $V_t$).
    Observe $y_t$.
    Update $V_{t+1} = \{h \in V_t : h(x_t) = y_t\}$.
```

Theorem 5 (Halving Algorithm)**.** *Suppose the data satisfies $y_t = h^*(x_t)$ for all t for some fixed $h^* \in \mathcal{H}$, with (x_t, y_t) chosen adversarially. The Halving algorithm makes at most $\lfloor \log_2(|\mathcal{H}|) \rfloor$ mistakes.*

Proof. Note that $h^* \in V_t$ for all t, since h^* is consistent with every observation. When the algorithm makes a mistake at round t—meaning $\hat{y}_t \neq y_t = h^*(x_t)$—strictly more than half the hypotheses in V_t predicted $\hat{y}_t \neq y_t$ (because $\hat{y}_t$ is the majority). All such hypotheses are excluded from V_{t+1}, so

$$|V_{t+1}| \leq \frac{|V_t|}{2}.$$

If m mistakes have occurred by time t, then $|V_t| \leq |\mathcal{H}|/2^m$. Since $h^* \in V_t$ always, we need $|V_t| \geq 1$, which requires $|\mathcal{H}|/2^m \geq 1$, giving $m \leq \log_2(|\mathcal{H}|)$. □

Remark 5. *The Halving algorithm achieves a mistake bound of* $\log_2(|\mathcal{H}|)$ *that is* independent of T *and holds against an adversary. One can show this is optimal: no algorithm can guarantee fewer than* $\log_2(|\mathcal{H}|)$ *mistakes in the worst case. When the hypothesis class is infinite but has finite Littlestone dimension d (a combinatorial dimension analogous to VC dimension for the online setting), a generalization of the Halving algorithm achieves a mistake bound of $O(d)$ [Littlestone, 1988].*

3.2 Non-Separable Case: Regret Minimization

When no hypothesis perfectly classifies all examples—either because the problem is noisy or because an adversary can force mistakes on any algorithm—the mistake-bound framework is no longer meaningful. Instead, we measure performance via *regret*: the excess number of mistakes compared to the best fixed hypothesis in hindsight.

Define the *regret* after T rounds as

$$\mathrm{Regret}_T = \sum_{t=1}^{T} \mathbb{E}[\mathbf{1}\{h_t(x_t) \neq y_t\}] - \min_{h \in \mathcal{H}} \sum_{t=1}^{T} \mathbf{1}\{h(x_t) \neq y_t\},$$

where the expectation is over any internal randomness of the algorithm. The goal is to design an algorithm with $\mathrm{Regret}_T = o(T)$, meaning the algorithm is competitive in the long run with the best fixed hypothesis selected in hindsight.

Remark 6. *Against an adversary, a deterministic algorithm can suffer $\Omega(T)$ regret. Randomization is essential: by sampling h_t from a distribution over $\mathcal{H}$, the player can hedge against adversarial label choices.*

3.2.1 Exponential Weights

The *Exponential Weights* algorithm (also known as Hedge or the multiplicative weights update method) is a fundamental algorithm that achieves near-optimal regret.

```
Exponential Weights Algorithm (Hedge)
Input: Hypothesis class $\mathcal{H}$ with $|\mathcal{H}| < \infty$, learning rate $\eta > 0$.
Initialize $w_1(h) = 1$ for all $h \in \mathcal{H}$.
for $t = 1, 2, \dots, T$ do
    Let $W_t = \sum_{h \in \mathcal{H}} w_t(h)$ and $p_t(h) = w_t(h)/W_t$.
    Observe $x_t$; sample $h_t \sim p_t$ and predict $h_t(x_t)$.
    Observe $y_t$; compute $\ell_t(h) = \mathbf{1}\{h(x_t) \neq y_t\}$ for all $h \in \mathcal{H}$.
    Update $w_{t+1}(h) = w_t(h) \cdot e^{-\eta \ell_t(h)}$ for all $h \in \mathcal{H}$.
```

Theorem 6 (Exponential Weights Regret Bound)**.** *For any sequence $(x_1, y_1), \dots, (x_T, y_T)$ chosen adversarially with $y_t \in \{-1, +1\}$, the Exponential Weights algorithm with $\eta = \sqrt{8 \log(|\mathcal{H}|)/T}$ satisfies*

$$\text{Regret}_T \leq \sqrt{\frac{T \log(|\mathcal{H}|)}{2}}.$$

Proof. Let $\ell_t(h) = \mathbf{1}\{h(x_t) \neq y_t\} \in [0, 1]$ and $W_t = \sum_{h \in \mathcal{H}} w_t(h)$. We bound $\log(W_{T+1}/W_1)$ from two directions.

Upper bound. Using $w_{t+1}(h) = w_t(h) e^{-\eta \ell_t(h)}$,

$$W_{t+1} = \sum_{h \in \mathcal{H}} w_t(h) e^{-\eta \ell_t(h)} = W_t \cdot \mathbb{E}_{h \sim p_t}\left[e^{-\eta \ell_t(h)}\right].$$

Since $\ell_t(h) \in [0, 1]$, by Hoeffding's lemma (Lemma 11 applied to the distribution p_t),

$$\log \mathbb{E}_{h \sim p_t}\left[e^{-\eta \ell_t(h)}\right] \leq -\eta \mathbb{E}_{h \sim p_t}[\ell_t(h)] + \frac{\eta^2}{8}.$$

Therefore $\log W_{t+1} \leq \log W_t - \eta \mathbb{E}_{h \sim p_t}[\ell_t(h)] + \eta^2/8$. Telescoping from $t = 1$ to T and using $W_1 = |\mathcal{H}|$:

$$\log W_{T+1} \leq \log |\mathcal{H}| - \eta \sum_{t=1}^{T} \mathbb{E}_{h \sim p_t}[\ell_t(h)] + \frac{\eta^2 T}{8}. \tag{3.1}$$

Lower bound. For any fixed $h^* \in \mathcal{H}$,

$$W_{T+1} \geq w_{T+1}(h^*) = \exp\left(-\eta \sum_{t=1}^{T} \ell_t(h^*)\right),$$

so $\log W_{T+1} \geq -\eta \sum_{t=1}^{T} \ell_t(h^*)$.

Combining. Chaining the two bounds and rearranging,

$$\sum_{t=1}^{T} \mathbb{E}_{h \sim p_t}[\ell_t(h)] - \sum_{t=1}^{T} \ell_t(h^*) \leq \frac{\log |\mathcal{H}|}{\eta} + \frac{\eta T}{8}.$$

Since this holds for any $h^* \in \mathcal{H}$, taking the minimum over h^* gives

$$\text{Regret}_T \leq \frac{\log |\mathcal{H}|}{\eta} + \frac{\eta T}{8}.$$

Setting $\eta = \sqrt{8 \log(|\mathcal{H}|)/T}$ balances the two terms:

$$\text{Regret}_T \leq 2\sqrt{\frac{T \log(|\mathcal{H}|)}{8}} = \sqrt{\frac{T \log(|\mathcal{H}|)}{2}}.$$

□

Remark 7. *The regret bound $\sqrt{T \log |\mathcal{H}|/2}$ is optimal up to constants; no algorithm can guarantee $o(\sqrt{T \log |\mathcal{H}|})$ regret in the worst case. Note that $\text{Regret}_T/T \to 0$ as $T \to \infty$, meaning the algorithm is asymptotically as good per-round as the best fixed hypothesis in $\mathcal{H}$, even against an adversary. The per-round computational cost is $O(|\mathcal{H}|)$.*

The Exponential Weights algorithm is one of the most broadly applicable ideas in machine learning. It extends naturally to arbitrary convex losses, to portfolio optimization, and to game theory. The following sections develop these extensions, moving from finite hypothesis classes to continuous action sets.

Chapter 4

Universal Portfolio Optimization

A beautiful application of online learning is to stock market portfolio management, where OGD and Exponential Weights yield algorithms with provable worst-case guarantees—even against adversarially chosen returns.

Consider d stocks. Let $r_t(i) = S_{t+1}(i)/S_t(i) \geq 0$ denote the *gross return* of stock i at time t (the ratio of tomorrow's price to today's price). A portfolio at time t is a distribution $p_t \in \triangle_d$ over stocks. Starting with wealth v_1, the investor rebalances daily, so after T rounds the total wealth is

$$v_{T+1} = v_1 \prod_{t=1}^{T} \langle p_t, r_t \rangle.$$

The goal is to maximize the cumulative log-return $\log(v_{T+1}/v_1) = \sum_{t=1}^{T} \log\langle p_t, r_t \rangle$.

Classical approach. Markowitz (1952) assumes returns r_t are IID with mean $\mu = \mathbb{E}[r_t]$ and covariance $\Sigma = \mathbb{E}[(r_t - \mu)(r_t - \mu)^\top]$, and solves the mean-variance optimization

$$\min_{p \in \triangle_d} p^\top \Sigma p \quad \text{subject to} \quad p^\top \mu \geq \bar{r}.$$

In practice, μ and Σ must be estimated from data, and the IID assumption fails catastrophically during market disruptions.

Online approach. We treat the return sequence $r_1, r_2, \ldots$ as adversarially chosen and measure *regret* relative to the best *fixed* portfolio in hindsight:

$$\text{Regret}_T = \max_{p \in \triangle_d} \sum_{t=1}^{T} \log\langle p, r_t \rangle - \sum_{t=1}^{T} \log\langle p_t, r_t \rangle.$$

4.1 Competing with the Best Single Stock

As a first result, we show that Exponential Weights (with the log-loss) competes with the best *single* stock.

Theorem 7. *Run Exponential Weights with $\eta = 1$ and loss $\ell_t(p) = -\log\langle p, r_t \rangle$. Then*

$$\max_{i \in [d]} \sum_{t=1}^{T} \log r_t(i) - \sum_{t=1}^{T} \log\langle p_t, r_t \rangle \leq \log d.$$

Proof. Apply the Exponential Weights analysis of Theorem 6 with $|\mathcal{H}| = d$ experts (pure portfolios e_i) and loss $z_t(i) = -\log r_t(i) \in [0, \infty)$. The weight update is $w_{t+1}(i) \propto w_t(i) \cdot r_t(i)$, so $p_t(i) = w_t(i)/W_t$. Observe that $\langle p_t, r_t \rangle = W_{t+1}/W_t$, so $\log(W_{T+1}/W_1) = \sum_{t=1}^{T} \log\langle p_t, r_t \rangle$. Since $W_{T+1} \geq w_{T+1}(i^*) = \prod_{t=1}^{T} r_t(i^*)$ for the best stock i^*, and $W_1 = d$,

$$\sum_{t=1}^{T} \log\langle p_t, r_t \rangle = \log(W_{T+1}/W_1) \geq \log\left(\frac{\prod_{t=1}^{T} r_t(i^*)}{d} \right) = \sum_{t=1}^{T} \log r_t(i^*) - \log d.$$

□

4.2 Competing with the Best Fixed Portfolio

The bound above is unsatisfying: the best fixed portfolio $p^* \in \triangle_d$ can dramatically outperform any single stock by rebalancing between alternating stocks.

Example 3. *Consider $d = 2$ stocks with alternating returns: $r_t = (2, \frac{1}{2})$ for odd t and $r_t = (\frac{1}{2}, 2)$ for even t. Each single stock has return 1 after every two steps. But the uniform portfolio $p = (\frac{1}{2}, \frac{1}{2})$ earns $\langle p, r_t \rangle = \frac{5}{4}$ at every step, giving $\prod_{t=1}^{T} \langle p, r_t \rangle = (5/4)^T \to \infty$.*

To compete with any $p^* \in \triangle_d$, we need an algorithm over a *continuous* action set, which brings us to the Continuous Exponential Weights algorithm of the next section.

4.3 Continuous Exponential Weights

The Exponential Weights algorithm generalizes from a finite set of experts to a continuous convex action set via a Gibbs distribution.

```
Continuous Exponential Weights (CEW)
Input: Convex set $\mathcal{A} \subseteq \mathbb{R}^d$, learning rate $\eta > 0$, reference measure $\nu$ on $\mathcal{A}$.
for $t = 1, 2, \ldots, T$ do
Sample $a_t \sim p_t$, where $p_t(a) \propto \exp\Big(-\eta \sum_{s=1}^{t-1} \ell_s(a)\Big)\, d\nu(a)$.
Observe loss $\ell_t$ and suffer $\ell_t(a_t)$.
```

Theorem 8 (Continuous Exponential Weights Regret)**.** *Let $\mathcal{A} \subseteq \mathbb{R}^d$ be a convex set and $\ell_t : \mathcal{A} \to [0, 1]$ be convex for each t. With Lebesgue measure ν on $\mathcal{A}$, for any $\eta > 0$,*

$$\mathrm{Regret}_T = \max_{a \in \mathcal{A}} \sum_{t=1}^{T} \ell_t(a_t) - \ell_t(a) \leq \frac{d \log T}{\eta} + \frac{\eta T}{8} + 1.$$

Setting $\eta = \sqrt{8d \log T/T}$ gives $\mathrm{Regret}_T \leq \sqrt{dT \log T/2} + 1$.

The proof follows from a continuous analogue of the finite Exponential Weights argument; see [Bubeck, 2015] for a full treatment. The key difference from the finite case is that the entropy term $\log|\mathcal{H}|$ is replaced by the *differential entropy* of the prior ν relative to the posterior, which for a d-dimensional convex body scales as $O(d \log T)$ after T rounds.

Remark 8 (Comparison to OGD)**.** *Theorem 8 gives a regret bound of $O(\sqrt{dT \log T})$, slightly worse than OGD's $O(\sqrt{T})$ by a $\sqrt{d \log T}$ factor. However, Continuous Exponential Weights is* randomized *and requires no gradient computation—only loss evaluations. This makes it applicable in* bandit *settings where the learner observes $\ell_t(a_t)$ but not the full function ℓ_t.*

4.3.1 Application: Universal Portfolio

Applying Continuous Exponential Weights to portfolio optimization with $\mathcal{A} = \triangle_d$ and $\ell_t(p) = -\log\langle p, r_t\rangle$ yields:

Corollary 2 (Universal Portfolio)**.** *The Continuous Exponential Weights algorithm with* $\eta = 1$ *and* $\ell_t(p) = -\log\langle p, r_t\rangle$ *satisfies*

$$\max_{p\in\triangle_d} \sum_{t=1}^{T} \log\langle p, r_t\rangle - \sum_{t=1}^{T} \log\langle p_t, r_t\rangle \leq 1 + d\log T.$$

This is Cover's (1991) *Universal Portfolio* algorithm [Cover, 1991]: the regret grows only as $O(d\log T)$ regardless of the return sequence, improving on the $O(\log d)$ bound of Theorem 7 which only competes with the best single stock. The term $d\log T$ reflects the complexity of the continuous d-dimensional simplex: it takes $O(d\log T)$ bits to identify the best portfolio to within T^{-1} precision.

Chapter 5

Online Learning with Squared Loss

We now consider a natural extension of the Exponential Weights framework to regression with a finite function class. The protocol is as follows: at each round $t = 1, 2, \ldots, T$,

1. Nature reveals context $x_t \in \mathcal{X}$.
2. The learner plays a prediction $\hat{y}_t \in [0, 1]$.
3. Nature reveals label $y_t \in [0, 1]$.
4. The learner suffers squared loss $(\hat{y}_t - y_t)^2$.

The learner has access to a finite function class $\mathcal{F}$ of predictors $f : \mathcal{X} \to [0, 1]$. The goal is to minimize the *regret*

$$\mathrm{Regret}_T = \sum_{t=1}^{T} (\hat{y}_t - y_t)^2 - \min_{f \in \mathcal{F}} \sum_{t=1}^{T} (f(x_t) - y_t)^2.$$

No distributional assumption is made on (x_t, y_t); the sequence may be adversarially chosen.

5.1 Averaged Exponential Weights

Rather than playing a single function, the learner maintains a distribution over $\mathcal{F}$ and predicts with its weighted average. Let $w_t(f) > 0$ be the weight on function f at time t, initialized to $w_1(f) = 1$ for all f. After observing (x_t, y_t), weights are updated as

$$w_{t+1}(f) = w_t(f) \cdot e^{-\eta (f(x_t) - y_t)^2},$$

and the prediction at round t is the weighted average

$$\hat{y}_t = \frac{\sum_{f \in \mathcal{F}} w_t(f)\, f(x_t)}{\sum_{f \in \mathcal{F}} w_t(f)}.$$

```
Averaged Exponential Weights for Regression
Input: Function class $\mathcal{F}$, learning rate $\eta > 0$.
Initialize $w_1(f) = 1$ for all $f \in \mathcal{F}$.
for $t = 1, 2, \ldots, T$ do
    Observe $x_t$.
    Predict $\hat{y}_t = \frac{\sum_{f\in\mathcal{F}} w_t(f)\, f(x_t)}{\sum_{f\in\mathcal{F}} w_t(f)}$.
    Observe $y_t$; update $w_{t+1}(f) = w_t(f) \cdot e^{-\eta(f(x_t)-y_t)^2}$ for all $f \in \mathcal{F}$.
```

5.2 Regret Bound

Theorem 9 (Averaged Exponential Weights Regret)**.** *Let $\mathcal{F}$ be a finite function class with each $f : \mathcal{X} \to [0,1]$. Running Averaged Exponential Weights with $\eta = \frac{1}{2}$ yields, for every adversarial sequence $(x_1, y_1), \ldots, (x_T, y_T)$ with $y_t \in [0,1]$,*

$$\mathrm{Regret}_T = \sum_{t=1}^{T} (\hat{y}_t - y_t)^2 - \min_{f\in\mathcal{F}} \sum_{t=1}^{T} (f(x_t) - y_t)^2 \le 2 \ln |\mathcal{F}|.$$

Proof. The proof has two ingredients: a potential function argument and the *mixability* of the squared loss.

Step 1: Potential function. Define $W_t = \sum_{f\in\mathcal{F}} w_t(f)$ and $p_t(f) = w_t(f)/W_t$. Note $W_1 = |\mathcal{F}|$ and p_1 is uniform over $\mathcal{F}$. The update rule gives $W_{t+1} = W_t \cdot \mathbb{E}_{f\sim p_t}\big[e^{-\eta(f(x_t)-y_t)^2}\big]$, so telescoping yields

$$\ln \frac{W_{T+1}}{W_1} = \sum_{t=1}^{T} \ln \mathbb{E}_{f\sim p_t}\Big[e^{-\eta(f(x_t)-y_t)^2}\Big]. \tag{5.1}$$

Step 2: Lower bound by the best function. For any $f^* \in \mathcal{F}$, since $W_{T+1} \ge w_{T+1}(f^*) = e^{-\eta \sum_t (f^*(x_t)-y_t)^2}$,

$$\ln \frac{W_{T+1}}{W_1} \ge -\eta \sum_{t=1}^{T} (f^*(x_t) - y_t)^2 - \ln |\mathcal{F}|. \tag{5.2}$$

Step 3: Upper bound via mixability. We claim that for $\eta \le \frac{1}{2}$,

$$\ln \mathbb{E}_{f\sim p_t}\Big[e^{-\eta(f(x_t)-y_t)^2}\Big] \le -\eta(\hat{y}_t - y_t)^2. \tag{5.3}$$

Define $g(z) = e^{-\eta z^2}$. Computing $g''(z) = (4\eta^2 z^2 - 2\eta)e^{-\eta z^2}$, we see $g''(z) \le 0$ if and only if $|z| \le \frac{1}{\sqrt{2\eta}}$. For $\eta \le \frac{1}{2}$, we have $\frac{1}{\sqrt{2\eta}} \ge 1$, so g is *concave* on $[-1,1]$. Since $f(x_t) - y_t \in [-1,1]$ for all $f \in \mathcal{F}$ and $y_t \in [0,1]$, Jensen's inequality gives

$$\mathbb{E}_{f\sim p_t}[g(f(x_t) - y_t)] \le g(\mathbb{E}_{f\sim p_t}[f(x_t) - y_t]) = g(\hat{y}_t - y_t) = e^{-\eta(\hat{y}_t - y_t)^2}.$$

Taking logarithms (monotone, so the inequality is preserved) yields (5.3).

Step 4: Combining. Summing (5.3) over $t = 1, \ldots, T$ and applying (5.2) with $f^* = \arg\min_{f\in\mathcal{F}} \sum_t (f(x_t) - y_t)^2$:

$$-\eta \sum_{t=1}^{T} (f^*(x_t) - y_t)^2 - \ln |\mathcal{F}| \;\le\; \sum_{t=1}^{T} \ln \mathbb{E}_{f\sim p_t}\Big[e^{-\eta(f(x_t)-y_t)^2}\Big] \;\le\; -\eta \sum_{t=1}^{T} (\hat{y}_t - y_t)^2.$$

Rearranging and setting $\eta = \frac{1}{2}$ (the maximum value permitted by the concavity condition):

$$\sum_{t=1}^{T}(\hat{y}_t - y_t)^2 - \min_{f\in\mathcal{F}}\sum_{t=1}^{T}(f(x_t) - y_t)^2 \le \frac{\ln|\mathcal{F}|}{\eta} = 2\ln|\mathcal{F}|. \qquad \square$$

Remark 9 (Comparison to supervised learning)**.** *The regret bound $O(\log|\mathcal{F}|)$ is strikingly better than the $O(\sqrt{T\log|\mathcal{F}|})$ bound from Exponential Weights for bounded losses. The improvement is possible because the squared loss is mixable with parameter $\eta = 1/2$: the averaged prediction $\hat{y}_t$ suffers less squared loss than any mixture. Classification with the $0/1$ loss is not mixable and requires the $\sqrt{T}$ factor.*

Chapter 6

Online Convex Optimization and Online Gradient Descent

The Exponential Weights algorithm is restricted to finite hypothesis classes and the 0/1 loss. In practice, hypothesis classes are often parameterized by a continuous vector $\theta \in \mathcal{K} \subseteq \mathbb{R}^d$, and losses are smooth and convex. *Online Convex Optimization* (OCO) is the natural generalization: the player repeatedly picks a point a_t from a convex set $\mathcal{K} \subseteq \mathbb{R}^d$ and then suffers a convex loss $\ell_t(a_t)$, where the adversary may choose the convex loss function $\ell_t : \mathcal{K} \to \mathbb{R}$ after a_t is revealed. The regret is

$$\mathrm{Regret}_T = \sum_{t=1}^{T} \ell_t(a_t) - \min_{a \in \mathcal{K}} \sum_{t=1}^{T} \ell_t(a).$$

Remark 10. *The finite Exponential Weights setting is a special case: take $\mathcal{K} = \triangle_d$ (the d-simplex), $a_t = p_t \in \triangle_d$ a distribution over d experts, and $\ell_t(p) = \langle p, z_t \rangle$ where $z_t(i) \in [0, 1]$ is the loss of expert i.*

The key insight enabling efficient optimization over continuous sets is that one only needs *local* gradient information. Recall that for a differentiable convex function f, the first-order inequality gives $f(y) \geq f(x) + \nabla f(x)^\top (y - x)$ for all x, y. This means gradient information at x provides a global linear lower bound on f.

```
Online Gradient Descent (OGD)
Input: Convex set $\mathcal{K} \subseteq \mathbb{R}^d$, step sizes $\eta_t > 0$.
Initialize $a_1 \in \mathcal{K}$ arbitrarily.
for $t = 1, 2, \ldots, T$ do
Play $a_t \in \mathcal{K}$.
Observe loss $\ell_t$ and compute (sub)gradient $g_t \in \partial \ell_t(a_t)$.
Update $a_{t+1} = \Pi_{\mathcal{K}}(a_t - \eta_t g_t)$, where $\Pi_{\mathcal{K}}(v) = \arg\min_{a \in \mathcal{K}} \|a - v\|_2$.
```

Theorem 10 (OGD Regret Bound)**.** *Let $\mathcal{K} \subseteq \mathbb{R}^d$ be a convex set with diameter $D = \sup_{a,b \in \mathcal{K}} \|a - b\|_2$, and suppose $\|g_t\|_2 \leq G$ for all t. With step sizes $\eta_t = \eta = D/(G\sqrt{T})$, Online Gradient Descent satisfies*

$$\mathrm{Regret}_T \leq DG\sqrt{T}.$$

Proof. Fix any $a^* \in \mathcal{K}$. By convexity of ℓ_t,

$$\ell_t(a_t) - \ell_t(a^*) \leq g_t^\top (a_t - a^*).$$

Write $a'_{t+1} = a_t - \eta g_t$ (before projection). By the Pythagorean property of projections,

$$\|a_{t+1} - a^*\|^2 \leq \|a'_{t+1} - a^*\|^2 = \|a_t - \eta g_t - a^*\|^2 = \|a_t - a^*\|^2 - 2\eta g_t^\top (a_t - a^*) + \eta^2 \|g_t\|^2.$$

Rearranging,

$$g_t^\top (a_t - a^*) \leq \frac{\|a_t - a^*\|^2 - \|a_{t+1} - a^*\|^2}{2\eta} + \frac{\eta \|g_t\|^2}{2}.$$

Summing from $t = 1$ to T and telescoping,

$$\text{Regret}_T \leq \sum_{t=1}^{T} g_t^\top (a_t - a^*) \leq \frac{\|a_1 - a^*\|^2}{2\eta} + \frac{\eta}{2} \sum_{t=1}^{T} \|g_t\|^2 \leq \frac{D^2}{2\eta} + \frac{\eta G^2 T}{2}.$$

Setting $\eta = D/(G\sqrt{T})$ balances these terms and gives $\text{Regret}_T \leq DG\sqrt{T}$. □

Remark 11. *The $O(\sqrt{T})$ rate matches the Exponential Weights bound (up to constants) and is optimal for OCO in the worst case. Online Gradient Descent is computationally tractable for large hypothesis classes: each step costs only one gradient evaluation and one projection, making it practical for neural network training, online regression, and reinforcement learning. When $\mathcal{K} = \mathbb{R}^d$ (unconstrained) and ℓ_t is the squared loss, OGD reduces to the well-known* least mean squares *(LMS) online algorithm.*

Chapter 7

Adversarial bandits

In adversarial bandits, at each time t the adversary plays a loss $\ell_t \in [-1,1]^n$ and simultaneously the player plays an arm $I_t \in [n]$ and receives the observed loss ℓ_{t,I_t}. We will begin by considering only oblivious adversaries: the entire loss sequence $\{\ell_t\}_{t=1}^T$ is chosen *before* the start of the game, that is, they are $\mathcal{F}_0$ measurable if (ℓ_t, I_t) are an $\mathbb{F} = \{\mathcal{F}_t\}_t$ adapted sequence. This is in contrast to adaptive adversaries that can decide the next loss sequence based on both the previous losses and the player's actions–ℓ_t is $\mathcal{F}_{t-1}$ measurable.

7.1 EXP3

The first algorithm we will consider is a generalization of the exponential weights, or Hedge, algorithm to bandit feedback. As only ℓ_{t,I_t} is observed, and not the full loss vector $\ell_t \in [-1,1]^n$, the algorithm constructs an unbiased estimator $\widehat{\ell}_{t,i} = \frac{\mathbf{1}\{I_t=i\}}{q_{t,i}}\ell_{t,i}$ for each arm i, where $I_t \sim q_t \in \triangle_n$. It is straightforward to check that $\mathbb{E}[\widehat{\ell}_{t,i}|q_t] = \ell_{t,i}$. We define regret as

$$\max_i \mathbb{E}\Big[\sum_{t=1}^T \ell_{t,I_t} - \ell_{t,i}\Big]$$

where we emphasize that the expectation is only with respect to the random plays I_t as the adversary chose the losses ℓ_t prior to the start of the game, by assumption. The adversary is unaware of the player's source of randomness, so the random choice of $I_t \sim q_t$ enables the player to surprise the adversary. Convince yourself that any deterministic algorithm must suffer linear regret against some adversary.

Below we present a slight generalization of the famous EXP3 algorithm known as the EXP3(γ) algorithm.

```
EXP3($\gamma$): Exponential Weights for Exploration Exploitation
Input: Time horizon $T$, $n$ arms, $\eta > 0$, $\gamma \in [0,1]$
Initialize: Player sets $p_1 = (1/n, \dots, 1/n) \in \triangle_n$. Adversary chooses $\{\ell_t\}_{t=1}^T \subset [-1,1]^n$.
for: $t = 1, \cdots, T$
    Player defines $\lambda_t \in \triangle_n$ and plays $I_t \sim q_t := (1-\gamma)p_t + \gamma\lambda_t$
    Player suffers (and observes) loss $\ell_{t,I_t}$ (but does not observe $\ell_{t,i}$ for $i \neq I_t$)
    Player computes loss estimator $\widehat{\ell}_{t,i}$ for all $i \in [n]$
    Update iterates:
        $w_{t+1,i} = w_{t,i} \exp(-\eta \widehat{\ell}_{t,i}) \qquad p_{t+1,i} = w_{t+1,i} / \sum_{j=1}^n w_{t+1,j}$.
```

Theorem 11. *Fix any sequence $\ell_t \in [-1,1]$ for all t. For any $\widehat{\ell}_{t,i}$ and $\eta, \gamma \geq 0$ that satisfy $\mathbb{E}[\widehat{\ell}_{t,i} | \mathcal{F}_{t-1}] = \ell_{t,i}$ and $-\eta\widehat{\ell}_{t,i} \leq 1$ for all i, t we have*

$$\max_{i=1,\dots,n} \mathbb{E}\Big[\sum_{t=1}^T \ell_{t,I_t} - \ell_{t,i}\Big] \leq 2\gamma T + \frac{\log(n)}{\eta} + (1-\gamma)\eta\mathbb{E}\Big[\sum_{t=1}^T \sum_{j=1}^n p_{t,j}\widehat{\ell}_{t,j}^2\Big].$$

Proof. First note that since $\mathbb{E}[\widehat{\ell}_{t,i}] = \ell_{t,i}$ we have that

$$\begin{aligned}
\mathbb{E}\Big[\sum_{t=1}^T \ell_{t,I_t} - \ell_{t,i}\Big] &= \mathbb{E}\Big[\sum_{t=1}^T \Big(\sum_{j=1}^n q_{t,j}\ell_{t,j}\Big) - \ell_{t,i}\Big] \\
&\leq \gamma T + \mathbb{E}\Big[\sum_{t=1}^T \Big(\sum_{j=1}^n (1-\gamma) p_{t,j}\ell_{t,j}\Big) - \ell_{t,i}\Big] \\
&\leq 2\gamma T + (1-\gamma)\mathbb{E}\Big[\sum_{t=1}^T \Big(\sum_{j=1}^n p_{t,j}\ell_{t,j}\Big) - \ell_{t,i}\Big] \\
&= 2\gamma T + (1-\gamma)\mathbb{E}\Big[\sum_{t=1}^T \Big(\sum_{j=1}^n p_{t,j}\widehat{\ell}_{t,j}\Big) - \widehat{\ell}_{t,i}\Big]
\end{aligned}$$

Define $W_t = \sum_{i=1}^n w_{t,i}$ with the convention that $w_{1,i} = 1$. Then for any $i \in [n]$ we have

$$\log(\frac{W_{T+1}}{W_1}) \geq \log(w_{T+1,i}) - \log(n) \geq -\eta \sum_{t=1}^T \widehat{\ell}_{t,i} - \log(n).$$

On the other hand, by assumption $-\eta\widehat{\ell}_{t,i} \leq 1$ so

$$\begin{aligned}
\log(\frac{W_{T+1}}{W_1}) &= \sum_{t=1}^{T} \log(\frac{W_{t+1}}{W_t}) \\
&= \sum_{t=1}^{T} \log(\sum_{i=1}^{n} \frac{w_{t,i}}{W_t} \exp(-\eta\widehat{\ell}_{t,i})) \\
&= \sum_{t=1}^{T} \log(\sum_{i=1}^{n} p_{t,i} \exp(-\eta\widehat{\ell}_{t,i})) \\
&\leq \sum_{t=1}^{T} \log(1 - \eta\Big(\sum_{j=1}^{n} p_{t,j}\widehat{\ell}_{t,j}\Big) + \Big(\eta^2 \sum_{j=1}^{n} \widehat{\ell}_{t,j}^{2}\Big)) \\
&\leq -\eta \sum_{t=1}^{T} \Big(\sum_{j=1}^{n} p_{t,j}\widehat{\ell}_{t,j}\Big) + \eta^2 \sum_{t=1}^{T}\sum_{j=1}^{n} p_{t,j}\widehat{\ell}_{t,j}^{2}
\end{aligned}$$

where the first inequality holds by $\exp(x) \leq 1 + x + x^2$ for $x \leq 1$, and the second inequality holds by $1 + x \leq e^x$ for all x. Thus, rearranging we have

$$\sum_{t=1}^{T} \Big(\sum_{j=1}^{n} p_{t,j}\widehat{\ell}_{t,j}\Big) - \widehat{\ell}_{t,i} \leq \frac{\log(n)}{\eta} + \eta \sum_{t=1}^{T}\sum_{j=1}^{n} p_{t,j}\widehat{\ell}_{t,j}^{2}.$$

□

7.2 Multi-armed bandits

Corollary 3. *Consider an n-armed bandit and define $\widehat{\ell}_{t,i} = \frac{\mathbf{1}\{I_t=i\}}{q_{t,i}}\ell_{t,i}$ where $I_t \sim q_t$. If $\lambda = (1/n, \dots, 1/n)$, $\eta = \sqrt{\frac{\log(n)}{3nT}}$, and $\gamma = \eta n$ then $\max_{i=1,\dots,n} \mathbb{E}\Big[\sum_{t=1}^{T} \ell_{t,I_t} - \ell_{t,i}\big] \leq \sqrt{12nt\log(n)}$.*

$|\eta\widehat{\ell}_{t,j}| = \eta\frac{\mathbf{1}\{I_t=j\}}{q_{t,j}}|\ell_{t,j}| \leq \eta\frac{\mathbf{1}\{I_t=j\}}{\gamma/n}|\ell_{t,j}| \leq 1$ if $\gamma = \eta n$.

$$\mathbb{E}\Big[\sum_{t=1}^{T}\sum_{j=1}^{n} p_{t,j}\widehat{\ell}_{t,j}^{2}\Big] \leq \mathbb{E}\Big[\sum_{t=1}^{T} p_{t,I_t}\frac{\ell_{t,I_t}^{2}}{q_{t,I_t}^{2}}\Big] \leq \frac{1}{1-\gamma}\mathbb{E}\Big[\sum_{t=1}^{T} \frac{\ell_{t,I_t}^{2}}{q_{t,I_t}}\Big] = \frac{1}{1-\gamma}\sum_{t=1}^{T}\sum_{j=1}^{n} \ell_{t,j}^{2} \leq \frac{nT}{1-\gamma}.$$

This implies a regret bound of

$$\max_{i=1,\dots,n} \mathbb{E}\Big[\sum_{t=1}^{T} \ell_{t,I_t} - \ell_{t,i}] \leq 2\gamma T + \frac{\log(n)}{\eta} + (1-\gamma)\eta\mathbb{E}\Big[\sum_{t=1}^{T}\sum_{j=1}^{n} p_{t,j}\widehat{\ell}_{t,j}^{2}\Big] \leq 2\eta nT + \frac{\log(n)}{\eta} + \eta nT.$$

Choosing $\eta = \sqrt{\frac{\log(n)}{3nT}}$ obtains a regret of $\sqrt{12nT\log(n)}$.

7.3 Linear bandits

Consider the following game where an adversary chooses a sequence $\theta_t \in \mathbb{R}^d$ for all t in advance, and then at each time the player picks an index $I_t \in [n]$ and observes the loss $\ell_{t,I_t} := \langle x_{I_t}, \theta_t\rangle$ where

$\mathcal{X} = (x_1, \ldots, x_n)$ are a set of known linear vectors. We measure regret just as before, but now we have the side knowledge of linear loss structure. Specifically,

$$R_T(\mathcal{X}) = \max_{i=1,\ldots,n} \Big[\sum_{t=1}^{n} \langle x_{I_t} - x_i, \theta_t \rangle \Big].$$

As before, we assume $\ell_{t,i} \in [-1, 1]$ which amounts to $\max_i |\langle x_i, \theta_t \rangle| \leq 1$.

Corollary 4. *Fix $\mathcal{X} = (x_1, \ldots, x_n) \subset \mathbb{R}^d$ and define $\ell_{t,i} := \langle x_i, \theta_t \rangle$, assuming $|\ell_{t,i}| \leq 1$ for all t, i. Furthermore, define $\widehat{\ell}_{t,i} = x_i^\top A^{-1}(q_t) x_{I_t} \ell_{t,I_t}$ where $A(q) := \sum_{i=1}^n q_i x_i x_i^\top$ and $I_t \sim q_t$. If $\lambda_t = \arg\min_{\lambda \in \triangle_n} \max_{i=1,\ldots,n} \|x_i\|^2_{A(\lambda)^{-1}}$, $\eta = \sqrt{\frac{\log(n)}{3nT}}$, and $\gamma = \eta n$ then $\max_{i=1,\ldots,n} \mathbb{E}\Big[\sum_{t=1}^T \ell_{t,I_t} - \ell_{t,i}] = \max_{i=1,\ldots,n} \mathbb{E}\Big[\sum_{t=1}^T \langle x_{I_t} - x_i, \theta_t \rangle \Big] \leq \sqrt{12nt\log(n)}$.*

Note that

$$\mathbb{E}[\widehat{\ell}_{t,i} | \mathcal{F}_{t-1}] = x_i^\top A^{-1}(q_t) \mathbb{E}[x_{I_t} \ell_{t,I_t}] = x_i^\top A^{-1}(q_t) \sum_{j=1}^n q_{t,j} x_j x_j^\top \theta_t = x_i^\top \theta_t = \ell_{t,i}.$$

To apply the above theorem we need $\max_i |\eta \widehat{\ell}_{t,i}| \leq 1$. Observe that by Cauchy-Schwartz we have

$$\max_i |\eta \widehat{\ell}_{t,i}| \leq \max_i |\eta x_i^\top A^{-1}(q_t) x_{I_t}| \leq \max_i \eta \|x_i\|_{A(q_t)^{-1}} \|x_{I_t}\|_{A(q_t)^{-1}} \leq \max_i \frac{\eta}{\gamma} \|x_i\|^2_{A(\lambda)^{-1}}.$$

As λ is our choice, it is natural to choose is to minimize the right hand side. Note that this precisely prescribes λ to be the G-optimal design so that $\max_i \|x_i\|^2_{A(\lambda)^{-1}} = d$. This then suggests $\gamma = \eta d$. We are then just left to compute

$$\begin{aligned}
\mathbb{E}\Big[\sum_{t=1}^T \sum_{j=1}^n p_{t,j} \widehat{\ell}^2_{t,j} \Big] &= \mathbb{E}\Big[\sum_{t=1}^T \sum_{j=1}^n p_{t,j} x_j^\top A^{-1}(q_t) x_{I_t} x_{I_t}^\top A^{-1}(q_t) x_j \ell^2_{t,I_t} \Big] \\
&\leq \mathbb{E}\Big[\sum_{t=1}^T \sum_{j=1}^n p_{t,j} x_j^\top A^{-1}(q_t) x_{I_t} x_{I_t}^\top A^{-1}(q_t) x_j \Big] \\
&\leq \sum_{t=1}^T \sum_{j=1}^n p_{t,j} x_j^\top A^{-1}(q_t) x_j \\
&\leq \frac{1}{1-\gamma} \sum_{t=1}^T \sum_{j=1}^n p_{t,j} x_j^\top A^{-1}(p_t) x_j \\
&= \frac{1}{1-\gamma} \sum_{t=1}^T \mathrm{Trace}\Big(A^{-1}(p_t) \sum_{j=1}^n p_{t,j} x_j x_j^\top \Big) \\
&= \frac{dT}{1-\gamma}
\end{aligned}$$

where the first inequality follows by each summand being non-negative, and the next line follows from $\mathbb{E}\Big[x_{I_t} x_{I_t}^\top \Big] = A(q_t)$. Choosing $\eta = \sqrt{\frac{\log(n)}{3dT}}$ obtains a regret of $\sqrt{12dT\log(n)}$.

7.4 Experts and Contextual bandits

In the contextual bandits setting, at the start of each round the adversary discloses a context $c_t \in \mathcal{C}$, the player chooses a policy $\pi_t \in \Pi$ which is a probability distribution over actions $[d]$ and plays $a_t \sim \pi_t(c_t) \in \triangle_d$ in response, and receives loss $\ell(c_t, a_t)$. The objective is to minimize expected regret

$$R_T(\Pi) := \sum_{t=1}^{T} \mathbb{E}_{a_t \sim \pi_t(c_t)}\big[\ell(c_t, a_t)\big] - \min_{\pi \in \Pi} \sum_{t=1}^{T} \mathbb{E}_{a \sim \pi(c_t)}\big[\ell(c_t, a)\big]$$

where the expectation is with respect to the potential randomness in the selection of π_t and the random actions. We will prove the following corollary in this section.

Corollary 5. *Fix a loss function $\ell : \mathcal{C} \times [d] \to [-1, 1]$ and suppose an adversary chooses a sequence of contexts $\{c_t\}_{t=1}^T \subset \mathcal{C}$. Given a collection of policies $\Pi = (\pi_1, \dots, \pi_n)$ such that $\pi_i : \mathcal{C} \to \triangle_d$ and a loss estimator $\widehat{\ell}_{t,i} = \frac{\pi_i(a_t|c_t)}{\sum_{i'=1}^n q_{t,i'}\pi_{i'}(a_t|c_t)}\ell_t(a_t)$ where $a_t \sim \sum_{i=1}^n q_{t,i}\pi_i(c_t)$. If $\lambda_t = \arg\min_{\lambda \in \triangle_n} \max_{i=1,\dots,n} \sum_{j=1}^d \frac{\pi_i(j|c_t)}{\sum_{k=1}^n \lambda_k \pi_k(j|c_t)}$, $\eta = \sqrt{\frac{\log(n)}{3nT}}$, and $\gamma = \eta n$ then $R_T(\Pi) \le \sqrt{12nt\log(n)}$.*

More abstractly, we can discard with the notion of the context and assume we have $n = |\Pi|$ experts where at the start of each round the ith expert suggests a distribution $E_{t,i} \in \triangle_d$ to play over the d actions. That is, $E_{t,i} = \pi_i(c_t)$. In this way, we define a distribution $q_t \in \triangle_n$ over our experts and at each round draw an expert $I_t \sim q_t$ and then play action $a_t \sim E_{t,I_t} \in \triangle_d$ and receive loss $\ell_t(a_t)$. If $\ell_{t,i} := \mathbb{E}_{a \sim E_{t,i}}\big[\ell_t(a)\big]$ then in this setting we define the regret as

$$\max_{i \in [n]} \mathbb{E}[\sum_{t=1}^{T} \ell_{t,I_t} - \ell_{t,i}] = \sum_{t=1}^{T} \mathbb{E}_{a_t \sim E_{t,I_t}}\big[\ell_t(a_t)\big] - \min_{i \in [n]} \sum_{t=1}^{T} \mathbb{E}_{a \sim E_{t,i}}\big[\ell_t(a)\big].$$

Define the loss of the ith expert at time t as

$$\widehat{\ell}_{t,i} := \sum_{j=1}^{d} [E_{t,i}]_j \frac{\mathbf{1}\{a_t = j\}}{\sum_{i'=1}^n q_{t,i'}[E_{t,i'}]_j} \ell_t(a_t) = \frac{[E_{t,i}]_{a_t}}{\sum_{i'=1}^n q_{t,i'}[E_{t,i'}]_{a_t}} \ell_t(a_t)$$

Note that

$$\begin{aligned}
\mathbb{E}[\mathbf{1}\{a_t = j\}\ell_t(a_t)] &= \sum_{a=1}^{d} \mathbb{P}(a_t = a)\mathbf{1}\{a = j\}\ell_t(a) \\
&= \sum_{a=1}^{d}\sum_{i=1}^{n} \mathbb{P}(I_t = i)\mathbb{P}(a_t = a | I_t = i)\mathbf{1}\{a = j\}\ell_t(a) \\
&= \sum_{a=1}^{d}\sum_{i=1}^{n} q_{t,i}[E_{t,i}]_a \mathbf{1}\{a = j\}\ell_t(a) \\
&= \sum_{i=1}^{n} q_{t,i}[E_{t,i}]_j \ell_t(j)
\end{aligned}$$

so that

$$\mathbb{E}[\widehat{\ell}_{t,i}] = \sum_{j=1}^{d} [E_{t,i}]_j \ell_t(j) = \mathbb{E}_{a \sim E_{t,i}} \ell_t(a) = \ell_{t,i}.$$

Moreover,

$$\begin{aligned}
-\eta\widehat{\ell}_{t,i} &\leq \eta \sum_{j=1}^{d} [E_{t,i}]_j \frac{1}{\sum_{i'=1}^{n} q_{t,i'}[E_{t,i'}]_j} \\
&\leq \frac{\eta}{\gamma} \sum_{j=1}^{d} [E_{t,i}]_j \frac{1}{\sum_{i'=1}^{n} \lambda_{t,i'}[E_{t,i'}]_j} \\
&= \frac{\eta}{\gamma} d
\end{aligned}$$

where the last line holds for the minimum λ by a Kiefer-Wolfowitz-like result:

Proposition 4. *For $i = 1, \dots, n$ let $p_i \in \triangle_d$. Then $\min_{\lambda \in \triangle_n} \max_{i=1,\dots,n} \sum_{j=1}^{d} \frac{p_{i,j}}{\sum_{k=1}^{n} \lambda_k p_{k,j}} = d$.*

Proof. Let $f(\lambda) = \sum_{j=1}^{d} \log\left(\sum_{k=1}^{n} \lambda_k p_{k,j}\right)$ and let $\lambda_* = \arg\max_{\lambda \in \triangle_n} f(\lambda)$. By concavity, for any λ we have $f(\lambda) \leq f(\lambda_*) + \langle \nabla f(\lambda_*), \lambda - \lambda_* \rangle$ and so if $f(\lambda^*) \geq f(\lambda)$ this implies

$$\begin{aligned}
0 &\geq \langle \nabla f(\lambda^*), \lambda - \lambda^* \rangle \\
&= \sum_{i=1}^{n} \sum_{j=1}^{d} \frac{p_{i,j}}{\sum_{k=1}^{n} \lambda_k^* p_{k,j}} (\lambda_i - \lambda_i^*) \\
&= \sum_{i=1}^{n} \sum_{j=1}^{d} \frac{\lambda_i p_{i,j}}{\sum_{k=1}^{n} \lambda_k^* p_{k,j}} - d.
\end{aligned}$$

Thus, taking $\lambda = \mathbf{e}_i$ we have $\min_{\lambda \in \triangle_n} \sum_{j=1}^{d} \frac{p_{i,j}}{\sum_{k=1}^{n} \lambda_k p_{k,j}} \leq \sum_{j=1}^{d} \frac{p_{i,j}}{\sum_{k=1}^{n} \lambda_k^* p_{k,j}} \leq d$ for all $i \in [n]$. On the other hand, we have

$$\min_{\lambda \in \triangle_n} \max_{i=1,\dots,n} \sum_{j=1}^{d} \frac{p_{i,j}}{\sum_{k=1}^{n} \lambda_k p_{k,j}} \geq \min_{\lambda \in \triangle_n} \sum_{i=1}^{n} \lambda_i \sum_{j=1}^{d} \frac{p_{i,j}}{\sum_{k=1}^{n} \lambda_k p_{k,j}} = d$$

which demonstrates equality. □

Thus, we choose $\gamma = \eta d$ to ensure $-\eta\widehat{\ell}_{t,i} \leq 1$.

Continuing,

$$\begin{aligned}
\mathbb{E}\Big[\sum_{t=1}^{T}\sum_{i=1}^{n} p_{t,i}\widehat{\ell}_{t,i}^{2}\Big] &= \mathbb{E}\Big[\sum_{t=1}^{T}\sum_{i=1}^{n} p_{t,i}\Big(\frac{[E_{t,i}]_{a_t}}{\sum_{i'=1}^{n} q_{t,i'}[E_{t,i'}]_{a_t}}\ell_t(a_t)\Big)^2\Big] \\
&\leq \mathbb{E}\Big[\sum_{t=1}^{T}\sum_{i=1}^{n} p_{t,i}\Big(\frac{[E_{t,i}]_{a_t}}{\sum_{i'=1}^{n} q_{t,i'}[E_{t,i'}]_{a_t}}\Big)^2\Big] \\
&= \mathbb{E}\Big[\sum_{t=1}^{T}\sum_{i=1}^{n} p_{t,i}\sum_{j=1}^{d}\frac{[E_{t,i}]_{j}^{2}}{\sum_{i'=1}^{n} q_{t,i'}[E_{t,i'}]_{j}}\Big] \\
&\leq \mathbb{E}\Big[\sum_{t=1}^{T}\sum_{i=1}^{n} p_{t,i}\sum_{j=1}^{d}\frac{[E_{t,i}]_{j}}{\sum_{i'=1}^{n} q_{t,i'}[E_{t,i'}]_{j}}\Big] \\
&\leq \frac{1}{1-\gamma}\mathbb{E}\Big[\sum_{t=1}^{T}\sum_{i=1}^{n} p_{t,i}\sum_{j=1}^{d}\frac{[E_{t,i}]_{j}}{\sum_{i'=1}^{n} p_{t,i'}[E_{t,i'}]_{j}}\Big] \\
&= \frac{dT}{1-\gamma}.
\end{aligned}$$

Choosing $\eta = \sqrt{\frac{\log(n)}{3dT}}$ obtains a regret of $\sqrt{12dT\log(n)}$.

Chapter 8

Stochastic online mirror descent

```
Protocal for Linear Bandits
Input: Time horizon $T$, action set $\mathcal{A} \subset \mathbb{R}^d$.
Initialize: Adversary chooses $\{z_t\}_{t=1}^T \subset \mathbb{R}^d$.
for: $t = 1, \cdots, T$
    Player chooses action $A_t \in \mathcal{A}$
    Player suffers (and observes) loss $\ell(A_t, z_t) = A_t^\top z_t$
```

8.0.1 Preliminaries

This presentation of mirror descent follows [Bubeck et al., 2012, Ch. 5].

For any open convex set $\mathcal{D} \subset \mathbb{R}^d$ and its closure denoted $\bar{\mathcal{D}}$, for any Legendre F on $\bar{\mathcal{D}}$ define $F^*(x) := \sup_{y \in \bar{\mathcal{D}}} x^\top y - F(y)$.

Define $D_F(x, y) = F(x) - F(y) - (x - y)^\top \nabla F(y)$.

Let the Mirror Descent iterations satisfy, $a_1 = \arg\min_{a \in \mathcal{A}} F(a)$ then

$$\widetilde{a}_{t+1} = \nabla F^*(\nabla F(a_t) - \eta \nabla \ell(a_t, z_t)) \tag{8.1}$$

$$a_{t+1} = \arg\min_{a \in \mathcal{A}} D_F(a, \widetilde{a}_{t+1}) \tag{8.2}$$

where we have assumed the iterates exist.

Theorem 12 (Online Mirror Descent). *Let $\mathcal{A} \subset \mathbb{R}^d$ be a closed convex action set, ℓ a subdifferentiable loss, and F a Legendre function defined on $\mathcal{A} \subset \bar{\mathcal{D}}$, such that $\nabla F(a) - \eta z \in dom(\nabla F(\mathcal{D}))$ for all $(a, z) \in \mathcal{A} \times \mathcal{Z}$ is satisfied. Then OMD satisfies*

$$\sup_{a \in \mathcal{A}} \sum_{t=1}^{T} \ell(a_t, z_t) - \ell(a, z_t) \leq \frac{\sup_{a \in \mathcal{A}} F(a) - F(a_1)}{\eta} + \frac{1}{\eta} \sum_{t=1}^{T} D_{F^*}\left(\nabla F(a_t) - \eta \nabla \ell(a_t, z_t), \nabla F(a_t)\right).$$

```
Online Mirror Descent with Linear Losses
Input: Time horizon $T$, convex action set $\mathcal{A} \subset \mathbb{R}^d$.
Initialize: Player sets $a_1 = \arg\min_{a\in\mathcal{A}} F(a)$. Adversary chooses $\{z_t\}_{t=1}^T \subset [0,1]^d$.
for: $t = 1, \cdots, T$
    Player suffers (and observes) loss $\ell(a_t, z_t) = a_t^\top z_t$
    Player observes $z_t$
    Update mirror descent iterates:
        $\widetilde{a}_{t+1} = \nabla F^*(\nabla F(a_t) - \eta z_t)$
        $a_{t+1} = \arg\min_{a\in\mathcal{A}} D_F(a, \widetilde{a}_{t+1})$
```

Corollary 6 (Online Mirror Descent with Linear Losses)**.** *Let $\mathcal{A} \subset \mathcal{D} \subset \mathbb{R}^d$ be a closed convex action set, $\{z_t\}_{t=1}^T \subset \mathcal{Z}$, $\ell(a,z) = a^\top z$, and F a Legendre function defined on $\mathcal{A} \subset \bar{\mathcal{D}}$, such that $\nabla F(a) - \eta z \in \nabla F(\mathcal{D})$ for all $(a,z) \in \mathcal{A} \times \mathcal{Z}$ is satisfied. Then OMD satisfies*

$$\sup_{a\in\mathcal{A}} \sum_{t=1}^T (a_t - a)^\top z_t \leq \frac{\sup_{a\in\mathcal{A}} F(a) - F(a_1)}{\eta} + \frac{1}{\eta}\sum_{t=1}^T D_{F^*}\left(\nabla F(a_t) - \eta z_t, \nabla F(a_t)\right).$$

```
Stochastic Online Mirror Descent with Linear Losses
Input: Time horizon $T$, action set $\mathcal{A} \subset \mathbb{R}^d$.
Initialize: Player sets $a_1 = \arg\min_{a\in\mathcal{A}} F(a)$. Adversary chooses $\{z_t\}_{t=1}^T \subset [0,1]^d$.
for: $t = 1, \cdots, T$
    Player chooses distribution $P_t$ over $\mathcal{A}$ with $a_t = \mathbb{E}[A_t|P_t] = \sum_{a\in\mathcal{A}} aP_t(a)$
    Player samples $A_t$ from $P_t$ and suffers (and observes) loss $\ell(A_t, z_t) = A_t^\top z_t$
    Player computes estimate $\widehat{z}_t$ with $\mathbb{E}[\widehat{z}_t|P_t] = z_t$
    Update mirror descent iterates:
        $\widetilde{a}_{t+1} = \nabla F^*(\nabla F(a_t) - \eta\widehat{z}_t)$
        $a_{t+1} = \arg\min_{a\in\text{convhull}(\mathcal{A})} D_F(a, \widetilde{a}_{t+1})$
```

Corollary 7 (Stochastic Online Mirror Descent with Linear Losses)**.** *Let $\mathcal{A} \subset \mathcal{D} \subset \mathbb{R}^d$ be a finite action set, $\{\widehat{z}_t\}_{t=1}^T \subset \mathcal{Z}$, $\ell(a,z) = a^\top z$, and F a Legendre function defined on $\mathcal{A} \subset \bar{\mathcal{D}}$, such that $\nabla F(a) - \eta z \in \nabla F(\mathcal{D})$ for all $(a,z) \in \mathcal{A} \times \mathcal{Z}$ is satisfied. Then OMD satisfies*

$$\sup_{a\in\mathcal{A}} \mathbb{E}\left[\sum_{t=1}^T (A_t - a)^\top z_t\right] \leq \frac{\sup_{a\in\mathcal{A}} F(a) - F(a_1)}{\eta} + \frac{1}{\eta}\sum_{t=1}^T \mathbb{E}\left[D_{F^*}\left(\nabla F(a_t) - \eta\widehat{z}_t, \nabla F(a_t)\right)\right].$$

Proof. Applying Corollary 1 with $\widehat{z}_t$ we have

$$\sup_{a\in\mathcal{A}} \sum_{t=1}^T (a_t - a)^\top \widehat{z}_t \leq \frac{\sup_{a\in\mathcal{A}} F(a) - F(a_1)}{\eta} + \frac{1}{\eta}\sum_{t=1}^T D_{F^*}\left(\nabla F(a_t) - \eta\widehat{z}_t, \nabla F(a_t)\right).$$

Taking the expectation on both sides yields the result by noting that

$$\mathbb{E}\left[\sum_{t=1}^T z_t^\top (A_t - a)\right] = \mathbb{E}\left[\sum_{t=1}^T z_t^\top (a_t - a)\right] = \mathbb{E}\left[\sum_{t=1}^T \mathbb{E}[z_t^\top (a_t - a)|P_t]\right] = \mathbb{E}\left[\sum_{t=1}^T \mathbb{E}[\widehat{z}_t^\top (a_t - a)|P_t]\right] = \mathbb{E}\left[\sum_{t=1}^T \widehat{z}_t^\top (a_t -\right.$$

□

8.1 Simplex games with unnormalized negative entropy

Example 1 Let $\mathcal{A} = \{x \in \mathbb{R}^d : x_i \geq 0, \sum_{i=1}^{d} = 1\}$, $F(x) = \sum_{i=1}^{n} x_i \log(x_i) - x_i$ with $\mathcal{D} = (0, \infty)^d$. F is Legendre and

$$
\begin{aligned}
[\nabla F(x)]_i &= \log(x_i) \\
D_F(x, y) &= \sum_{i=1}^{d} x_i \log(\tfrac{x_i}{y_i}) - \sum_{i=1}^{d} (x_i - y_i) \\
F^*(x) &= \sum_{i=1}^{d} \exp(x_i) \\
[\nabla F^*(x)]_i &= \exp(x_i) \\
D_{F^*}(x, y) &= \sum_{i=1}^{d} \exp(y_i)(\exp(x_i - y_i) - 1 - (x_i - y_i))
\end{aligned}
$$

8.1.1 Full information game, simplex action set

Assume the setting of Example 1. The following algorithm implements the updates of Mirror Descent above for the particular loss $\ell(a, z) = a^\top z$.

```
Exponential Weights
Input: Time horizon $T$.
Initialize: Player sets $a_1 = (1/d, \dots, 1/d)$. Adversary chooses $\{z_t\}_{t=1}^{T} \subset [0,1]^d$.
for: $t = 1, \cdots, T$
    Player chooses $a_t \in \mathcal{A}$
    Player suffers (and observes) loss $\ell(a_t, z_t) = a_t^\top z_t$
    Player observes $z_t$
    Update mirror descent iterates:
        $\widetilde{a}_{t+1,i} = \exp(-\eta \sum_{s=1}^{t} z_{s,i}) \qquad a_{t,i} = \widetilde{a}_{t+1,i} / \sum_{j=1}^{d} \widetilde{a}_{t+1,j}.$
```

Corollary 8 (Exponential weights)**.** *Under the conditions of Example 1 with let $\ell(a, z) = a^\top z$, the exponential weights algorithm satisfies*

$$
\sup_{a \in \mathcal{A}} \sum_{t=1}^{T} \ell(a_t, z_t) - \ell(a, z_t) \leq \frac{\log(d)}{\eta} + \frac{\eta T}{2} \leq \sqrt{2T \log(d)}
$$

Proof. Note $\nabla_a \ell(a, z) = z$. Plug in quantities of the example to obtain for any $a \in \mathcal{A}$

$$\begin{aligned}
\sum_{t=1}^{T} \ell(a_t, z_t) - \ell(a, z_t) &= \sum_{t=1}^{T} z_t^\top (a_t - a) \\
&\leq \frac{\log(d)}{\eta} + \frac{1}{\eta} \sum_{t=1}^{T} \sum_{i=1}^{d} a_{t,i} (\exp(-\eta z_{t,i}) - 1 + \eta z_{t,i}) \\
&\leq \frac{\log(d)}{\eta} + \frac{\eta}{2} \sum_{t=1}^{T} \sum_{i=1}^{d} a_{t,i} z_{t,i}^2 \\
&\leq \frac{\log(d)}{\eta} + \frac{\eta T}{2}
\end{aligned}$$

where the second line uses $F(x) \leq 0$ and $F(a_1) = \log(d)$, the third line uses $\exp(-x) \leq 1 - x + \frac{1}{2}x^2$ for $x \geq 0$, and the last line follows from $z_{t,i} \in [0, 1]$ and a_t is a probability distribution. □

8.1.2 Full information game, finite action set

Analogous to the categorial weather prediction problem in class, we now consider the case where the player can only play from a distinct set $\{1, \dots, d\}$ (i.e., predict rain, snow, sunny). As discussed in class, any deterministic algorithm will suffer linear regret, so instead, at time t we choose a probability distribution $a_t \in \mathcal{A}$ (in the setting of Example 1), choose distinct action I_t drawn according to a_t so that $A_t := \mathbf{e}_{I_t}$, and then suffer loss $\ell(A_t, z_t) = A_t^\top z_t = z_{t,I_t}$. Note that $\mathbb{E}[A_t] = \mathbb{E}[\mathbf{e}_{I_t}] = \sum_{i=1}^d \mathbf{e}_i a_{t,i} = a_t$ so that $\mathbb{E}[\ell(A_t, z_t)] = \mathbb{E}[A_t^\top z_t] = a_t^\top z_t$. Thus, the expected regret relative to any probability distribution $a \in \mathcal{A}$ over distinct items in hindsight is

$$\begin{aligned}
\mathbb{E}\left[\sum_{t=1}^{T} \ell(A_t, z_t) - \ell(a, z_t)\right] &= \mathbb{E}\left[\sum_{t=1}^{T} z_t^\top (A_t - a)\right] \\
&= \mathbb{E}\left[\sum_{t=1}^{T} z_t^\top (a_t - a)\right] \\
&= \mathbb{E}\left[\sum_{t=1}^{T} \ell(a_t, z_t) - \ell(a, z_t)\right]
\end{aligned}$$

where the expectation is with to the random selection of each I_t from a_t. Alternatively, we can directly apply Corollary 2 with $\widehat{z}_t = z_t$ since we are in the full information setting.

```
Exponential Weights over finite actions
Input: Time horizon $T$.
Initialize: Player sets $a_1 = (1/d, \dots, 1/d)$. Adversary chooses $\{z_t\}_{t=1}^{T} \subset [0,1]^d$.
for: $t = 1, \cdots, T$
    Player chooses $a_t \in \mathcal{A}$
    Player draws $I_t \sim a_t$, sets $A_t = \mathbf{e}_{I_t}$ and suffers (and observes) loss $\ell(A_t, z_t) = A_t^\top z_t = z_{t,I_t}$
    Player observes $z_t$
    Update mirror descent iterates:
        $\widetilde{a}_{t+1,i} = \exp(-\eta \sum_{s=1}^{t} z_{s,i}) \qquad a_{t,i} = \widetilde{a}_{t+1,i} / \sum_{j=1}^{d} \widetilde{a}_{t+1,j}.$
```

Corollary 9 (Exponential weights over finite actions)**.** *Under the conditions of Example 1 where the player can only play $\mathbf{e}_i$ for $i \in \{1, \dots, d\}$ with let $\ell(a,z) = a^\top z$, the exponential weights over finite actions algorithm satisfies*

$$\mathbb{E}\left[\sup_{a \in \mathcal{A}} \sum_{t=1}^{T} \ell(\mathbf{e}_{I_t}, z_t) - \ell(a, z_t)\right] \le \frac{\log(d)}{\eta} + \frac{\eta T}{2} \le \sqrt{2T \log(d)}$$

Proof. Immediate from reduction described above and the previous corollary since the iterates are identical in the full information game. Due to the oblivious adversary we have

$$\sup_{a \in \mathcal{A}} \mathbb{E}\left[\sum_{t=1}^{T} \ell(a_t, z_t) - \ell(a, z_t)\right] = \mathbb{E}\left[\sup_{a \in \mathcal{A}} \sum_{t=1}^{T} \ell(a_t, z_t) - \ell(a, z_t)\right]$$

Note, as we did in class, one can also prove a high probability bound that would apply to a general reactive adversary [**?**, Ch. 2.7] □

8.1.3 Bandit feedback, finite action set

This setting is identical to the previous setting, but now we do not observe the entire vector z_t at each time t, we only observe the element we played z_{t,I_t}. Using this single value, the player constructs an unbiased estimate of z_t with $\widehat{z}_{t,i} = \frac{\mathbf{1}\{I_t = i\} z_{t,i}}{a_{t,i}}$ for all i. Note that

$$\begin{aligned}
\mathbb{E}[\widehat{z}_{t,i} | a_1, I_1, \dots, a_{t-1}, I_{t-1}, a_t] &= \mathbb{E}[\frac{\mathbf{1}\{I_t = i\} z_{t,i}}{a_{t,i}} | a_1, I_1, \dots, a_{t-1}, I_{t-1}, a_t] \\
&= \sum_{j=1}^{d} a_{t,j} \frac{\mathbf{1}\{j = i\} z_{t,i}}{a_{t,i}} \\
&= z_{t,i}.
\end{aligned}$$

Also note that $\mathbb{E}[A_t] = \mathbb{E}[\mathbf{e}_{I_t}] = \sum_{i=1}^{d} \mathbf{e}_i a_{t,i} = a_t$.

```
EXP3: Exponential Weights for Exploration Exploitation
Input: Time horizon $T$, $\mathcal{A} = \{x \in \mathbb{R}^d : x_i \geq 0, \sum_{i=1}^d = 1\}$.
Initialize: Player sets $a_1 = (1/d, \dots, 1/d)$. Adversary chooses $\{z_t\}_{t=1}^T \subset [0,1]^d$.
for: $t = 1, \cdots, T$
    Player draws $I_t \sim a_t$ and suffers (and observes) loss $\ell(\mathbf{e}_{I_t}, z_t) = z_{t,I_t}$
    Player sets $\widehat{z}_{t,i} = \frac{\mathbf{1}\{I_t=i\} z_{t,i}}{a_{t,i}}$
    Update mirror descent iterates:

        $\widetilde{a}_{t+1,i} = \exp(-\eta \sum_{s=1}^{t} \widehat{z}_{s,i}) \qquad a_{t,i} = \widetilde{a}_{t+1,i} / \sum_{j=1}^{d} \widetilde{a}_{t+1,j}.$
```

Corollary 10 (EXP3)**.** *Under the conditions of Example 1 where the player can only play* $\mathbf{e}_i$ *for* $i \in \{1, \dots, d\}$ *with* $\ell(a,z) = a^\top z$ *and only observe bandit feedback, the EXP3 algorithm satisfies*

$$\begin{aligned}
\sup_{a \in \mathcal{A}} \mathbb{E}\left[\sum_{t=1}^{T} \ell(A_t, z_t) - \ell(a, z_t)\right] &\leq \frac{\log(d)}{\eta} + \frac{\eta}{2} \sum_{t=1}^{T} \mathbb{E}\left[\sum_{i=1}^{d} a_{t,i} \widehat{z}_{t,i}^2\right] \\
&\leq \frac{\log(d)}{\eta} + \frac{\eta T d}{2} \leq \sqrt{2dT \log(d)}
\end{aligned}$$

Proof. We can directly apply Corollary 2:

$$\begin{aligned}
\mathbb{E}\left[\sup_{a \in \mathcal{A}} \sum_{t=1}^{T} (A_t - a)^\top z_t\right] &\leq \frac{\sup_{a \in \mathcal{A}} F(a) - F(a_1)}{\eta} + \frac{1}{\eta} \sum_{t=1}^{T} \mathbb{E}\left[D_{F^*}\left(\nabla F(a_t) - \eta \widehat{z}_t, \nabla F(a_t)\right)\right] \\
&= \frac{\log(d)}{\eta} + \frac{1}{\eta} \sum_{t=1}^{T} \mathbb{E}\left[\sum_{i=1}^{d} a_{t,i} (\exp(-\eta \widehat{z}_{t,i}) - 1 + \eta \widehat{z}_{t,i})\right] \\
&\leq \frac{\log(d)}{\eta} + \frac{\eta}{2} \sum_{t=1}^{T} \mathbb{E}\left[\sum_{i=1}^{d} a_{t,i} \widehat{z}_{t,i}^2\right] \\
&= \frac{\log(d)}{\eta} + \frac{\eta}{2} \sum_{t=1}^{T} \mathbb{E}\left[\sum_{i=1}^{d} a_{t,i} \frac{\mathbf{1}\{I_t = i\} z_{t,i}^2}{a_{t,i}^2}\right] \\
&= \frac{\log(d)}{\eta} + \frac{\eta}{2} \sum_{t=1}^{T} \sum_{i=1}^{d} z_{t,i}^2 \\
&\leq \frac{\log(d)}{\eta} + \frac{\eta d T}{2}
\end{aligned}$$

□

For an alternative proof of EXP3, see [Lattimore and Szepesvári, 2020, Ch. 11]

8.2 Other action sets

The previous section addressed the case of the action set being equal to the simplex: $\mathcal{A} = \{x \in \mathbb{R}^d : x_i \geq 0, \sum_{i=1}^d = 1\}$. As our Legendre potential we chose unnormalize negative entropy $F(x) =$

$\sum_{i=1}^{d} x_i \log(x_i) - x_i$. Consider what the guarantee would be from Corollary 2 if we chose a different function, say, $F(x) = \frac{1}{2}\|x\|_2^2$ then:

$$\begin{aligned}
\mathbb{E}\left[\sup_{a\in\mathcal{A}} \sum_{t=1}^{T} (A_t - a)^\top z_t\right] &\le \frac{\sup_{a\in\mathcal{A}} F(a) - F(a_1)}{\eta} + \frac{1}{\eta}\sum_{t=1}^{T} \mathbb{E}\left[D_{F^*}\left(\nabla F(a_t) - \eta \widehat{z}_t, \nabla F(a_t)\right)\right] \\
&\le \frac{1}{\eta} + \frac{\eta}{2}\sum_{t=1}^{T} \mathbb{E}\left[\|\widehat{z}_t\|_2^2\right] \\
&= \frac{1}{\eta} + \frac{\eta}{2}\sum_{t=1}^{T} \mathbb{E}\left[\sum_{i=1}^{d} \widehat{z}_{t,i}^2\right] \\
&= \frac{1}{\eta} + \frac{\eta}{2}\sum_{t=1}^{T} \mathbb{E}\left[\sum_{i=1}^{d} \frac{z_{t,i}^2}{a_{t,i}}\right].
\end{aligned}$$

The issue here is that $a_{t,i}$ can become arbitrarily close to 0 and blow up the bound. If we mix in unfirom exploration at each round, one can show that the regret bound is $O((dT)^{2/3})$ which is significantly worse than $O(\sqrt{dT\log(d)})$ of EXP3 above. So given an action set $\mathcal{A}$ how do we choose F? The next proposition sheds some light on this question.

Proposition 5. *If F is twice continuously differntiable, and if its Hessian $\nabla^2 F(x)$ is invertible $\forall x \in \mathcal{D}$, then $\forall x, y \in \mathcal{D}$, there exists $\zeta \in \mathcal{D}$ such that $\nabla F(\zeta) \in [\nabla F(x), \nabla F(y)]$ and*

$$D_{F^*}(\nabla F(x), \nabla F(y)) = \frac{1}{2}\|\nabla F(x) - \nabla F(y)\|^2_{(\nabla^2 F(\zeta))^{-1}}.$$

The implication of the above proposition is that $\exists \nabla F(\zeta_t) \in [\nabla F(a_t) - \eta\widehat{z}_t, \nabla F(a_t)]$ and

$$D_{F^*}\left(\nabla F(a_t) - \eta\widehat{z}_t, \nabla F(a_t)\right) = \frac{\eta^2}{2}\|\widehat{z}_t\|^2_{(\nabla^2 F(\zeta_t))^{-1}}$$

For the choice of $F(x) = \frac{1}{2}\|x\|_2^2$ we have $\nabla^2 F(\zeta_t) = I$ for any ζ_t so that the Hessian is flat across the action set. On the other hand, with the choice $F(x) = \sum_{i=1}^{d} x_i \log(x_i) - x_i$, we have $\nabla^2 F(x) = \operatorname{diag}(1/x_1, \ldots, 1/x_d)$ which blows up as a component of x approaches 0. But this is perfect, since then

$$\begin{aligned}
\mathbb{E}\left[D_{F^*}\left(\nabla F(a_t) - \eta\widehat{z}_t, \nabla F(a_t)\right)\right] &= \mathbb{E}\left[\frac{\eta^2}{2}\|\widehat{z}_t\|^2_{(\nabla^2 F(\zeta_t))^{-1}}\right] \\
&= \mathbb{E}\left[\frac{\eta^2}{2}\sum_{i=1}^{d} \widehat{z}_{t,i}^2 \zeta_{t,i}\right] \\
&= \mathbb{E}\left[\frac{\eta^2}{2}\sum_{i=1}^{d} \frac{z_{t,i}^2}{a_{t,i}} \zeta_{t,i}\right] \\
&\approx \frac{\eta^2}{2}\sum_{i=1}^{d} z_{t,i}^2
\end{aligned}$$

where we have used the approximation that $\zeta_t \approx a_t$. The hessian of F is blowing up precisely at the locations where $\widehat{z}_t$ blows up, essentially cancelling each other! We'll see another example of this in the next subsection.

8.2.1 Bandit feedback, unit ball action set

Here we address the action set $\mathcal{A} = \{x \in \mathbb{R}^d : \|x\|_2 \leq 1\}$. To use Corollary 2, we need to define P_t (or equivalently, A_t) to make sure that $\mathbb{E}[A_t] = a_t$ and we need to define $\widehat{z}_t$ with $\mathbb{E}[\widehat{z}_t] = z_t$. Consider the following choices:

- $\mathcal{X}_t \sim \text{Bernoulli}(\|a_t\|_2)$, $I_t \sim \text{uniform}([d])$, $\epsilon_t \in \{-1, 1\}$ with equal probability
- $A_t = (1 - \mathcal{X}_t)\epsilon_t \mathbf{e}_{I_t} + \mathcal{X}_t \frac{a_t}{\|a_t\|_2}$
- $\widehat{z}_t = (1 - \mathcal{X}_t)\frac{d}{1-\|a_t\|_2} A_t A_t^\top z_t$

It is straightforward to verify that $\mathbb{E}[A_t|a_t] = a_t$ and $\mathbb{E}[\widehat{z}_t|a_t] = z_t$. Following the intuition of the previous section, we need to choose F to make $\mathbb{E}\left[\frac{\eta^2}{2}\|\widehat{z}_t\|^2_{(\nabla^2 F(\zeta_t))^{-1}}\right]$ small. Let $F(x) = -\log(1 - \|x\|_2) - \|x\|_2$. Note that

$$\begin{aligned}
\mathbb{E}\left[\|\widehat{z}_t\|^2_{(\nabla^2 F(\zeta_t))^{-1}}\right] &= \mathbb{E}\left[\|(1-\mathcal{X}_t)\frac{d}{1-\|a_t\|_2} A_t A_t^\top z_t\|^2_{(\nabla^2 F(\zeta_t))^{-1}}\right] \\
&= \mathbb{E}\left[\frac{d^2}{1-\|a_t\|_2}\|A_t A_t^\top z_t\|^2_{(\nabla^2 F(\zeta_t))^{-1}} | \mathcal{X}_t = 0\right] \\
&= \sum_{i=1}^d \frac{1}{d}\frac{d^2}{1-\|a_t\|_2}\|e_i e_i^\top z_t\|^2_{(\nabla^2 F(\zeta_t))^{-1}} \\
&= \frac{d}{1-\|a_t\|_2}\|z_t\|^2_{(\nabla^2 F(\zeta_t))^{-1}} \\
&\leq \frac{d}{1-\|a_t\|_2}(1-\|\zeta_t\|_2)\|z_t\|_2^2 \\
&\leq 2d
\end{aligned}$$

where we have used the fact that $\nabla^2 F(x) \succeq I/(1-\|x\|_2)$ and $\frac{1-\|z_t\|_2}{1-\|a_t\|_2} \leq 2$ (see [Lattimore and Szepesvári, 2020] for second fact).

Using a shrunken action set, one can prove that the regret is bounded by $O(\sqrt{dT})$ (see [Lattimore and Szepesvári, 20

Chapter 9

Matrix games

9.1 The sample complexity of two-player zero-sum matrix games

We begin with the simplest of all games: two-player zero-sum matrix games. In this problem setting, there is an arbitrary input matrix $A \in [-1,1]^{n\times m}$ which is unknown to the learner. The learner can sample an entry (i,j) of A and observe the random variable $X_{i,j} = A_{i,j} + \eta$ where η is a zero-mean 1-sub-Gaussian noise (typically we will assume $A_{i,j} + \eta \in [-1,1]$).

The aim of this section to identify an ϵ-approximate Nash equilibria:

Definition 14 (Nash Equilibrium)**.** *We say a pair $(x,y) \in \triangle_m \times \triangle_n$ is an ϵ-approximate Nash equilibria if both*

$$\langle x, Ay\rangle \geq \langle x', Ay\rangle - \epsilon \quad \textit{and} \quad \langle x, Ay'\rangle \geq \langle x, Ay\rangle - \epsilon \tag{9.1}$$

hold for all $(x',y') \in \triangle_m \times \triangle_n$. If a pair (x,y) satisfies this condition with $\epsilon = 0$, we say it is a Nash equilibria.

Note that if a pair $(x,y) \in \triangle_m \times \triangle_n$ satisfies

$$\max_{(x',y')\in\triangle_m\times\triangle_n} \langle x', Ay\rangle - \langle x, Ay'\rangle \leq \epsilon \tag{9.2}$$

then this assumption says that it is an ϵ-approximate Nash equilibria.

For example, for the rock-paper-scissors game given by

$$A = \begin{bmatrix} 0 & -1 & 1 \\ 1 & 0 & -1 \\ -1 & 1 & 0 \end{bmatrix}$$

one can verify that (x,y) is an ϵ-Nash equilibria if $\|x - \frac{1}{3}\mathbf{1}\|_1 + \|y - \frac{1}{3}\mathbf{1}\|_1 \leq \epsilon$ using (9.2).

Nash proved that a Nash equilibria (and hence an ϵ-approximate Nash equilbria) always exists for finite matrix games of this sort, but they need not be unique (consider the set of Nash equilibria for the all zeros matrix). We now introduce an important sub-class of Nash equilibria.

Definition 15 (Pure Strategy Nash Equilibrium)**.** *An element (i^*,j^*) is a Pure Strategy Nash Equilibrium (PSNE) of the game induced by the matrix $A \in \mathbb{R}^{m\times n}$ if $A_{i^*j^*} = \max_{i\in[m]} A_{i,j^*}$ and $A_{i^*,j^*} = \min_{j\in[n]} A_{i^*,j}$. Moreover, a Nash equilibrium $(x,y) \in \triangle_m \times \triangle_n$ where support$(x) = \{i\}$ and support$(y) = \{j\}$ corresponds to a PSNE (i,j).*

Not every game admits a PSNE, for example, the rock-paper-scissors game of above.

How do we find an approximate Nash equilibria? Given the true matrix A, one observes that a Nash equilibria is a solution to a linear program. However, if we only have access to A through noisy bandit feedback, what can we do?

Theorem 13. *Initialize two independent versions of EXP3(γ) defined above, one for the max/x player and the other for the min/y player where they are trying to maximize or minimize their cumulative observations, respectively. When the max player plays $I_t \in [m]$ and the min player plays $J_t \in [n]$, both players observe the outcomes $A_{I_t,J_t} + \eta_t \in [-1,1]$ where $\mathbb{E}[\eta_t] = 0$. If $\widehat{x} = \frac{1}{T}\sum_{t=1}^T \mathbf{e}_{I_t}$ and $\widehat{y} = \frac{1}{T}\sum_{t=1}^T \mathbf{e}_{J_t}$ then $\widehat{x}, \widehat{y}$ is an ϵ-approximate Nash equilibria, in expectation, if $T \geq 24(m+n)\epsilon^{-2}\log(n)$.*

Proof. At each time $t = 1,2,\dots,T$ the min player chooses $J_t \in [n]$ and observes loss y_{t,J_t} for the loss vector $y_t := A^\top \mathbf{e}_{I_t} + \eta_t \in [-1,1]^n$. Applying Proposition **??** we have that for any $q \in \triangle_n$

$$\begin{aligned}\mathbb{E}[\sum_{t=1}^T \mathbf{e}_{I_t} A(\mathbf{e}_{J_t} - q)] &= \mathbb{E}[\sum_{t=1}^T y_t^\top (\mathbf{e}_{J_t} - q)] \\ &\leq \max_{j\in[m]} \mathbb{E}[\sum_{t=1}^T y_{t,J_t} - y_{t,j}] \leq \sqrt{12nT\log(n)}.\end{aligned}$$

so that

$$\begin{aligned}\mathbb{E}[\sum_{t=1}^T \mathbf{e}_{I_t}^\top A\mathbf{e}_{J_t}] &= \mathbb{E}[\sum_{t=1}^T \mathbf{e}_{I_t}^\top Aq] + \mathbb{E}[\sum_{t=1}^T \mathbf{e}_{I_t}^\top A(\mathbf{e}_{J_t} - q)] \\ &= T\cdot\mathbb{E}[\widehat{x}^\top Aq] + \mathbb{E}[\sum_{t=1}^T \mathbf{e}_{I_t}^\top A(\mathbf{e}_{J_t} - q)] \\ &\leq T\cdot\mathbb{E}[\widehat{x}^\top Aq] + \sqrt{12nT\log(n)}\end{aligned}$$

By the same logic, we have for any $p \in \triangle_m$ that

$$\mathbb{E}[\sum_{t=1}^T \mathbf{e}_{I_t}^\top A\mathbf{e}_{J_t}] \geq T\cdot\mathbb{E}[p^\top A\widehat{y}] - \sqrt{12nT\log(n)}.$$

Rearranging these inequalities, we conclude that

$$\max_{(p,q)\in\triangle_m\times\triangle_n} \mathbb{E}[p^\top A\widehat{y}] + \mathbb{E}[\widehat{x}^\top Aq] \leq \sqrt{12n\log(n)/T} + \sqrt{12m\log(n)/T} \leq \sqrt{48(m+n)T\log(n)}.$$

□

Part III

Stochastic Bandits

Chapter 10

Multi-armed Bandits

10.1 Introduction

Machine learning, and in particular, supervised learning, is the study of making statistical inferences from previously collected data. Multi-armed bandits is more about an interaction between an agent (algorithm) and an environment where one simultaneously collects data and makes inferences in a closed-loop.

You have n "arms" or actions, representing distributions. "Pulling" an arm represents requesting a sample from that arm.

At each time $t = 1, 2, 3, \dots$

- Algorithm chooses an action $I_t \in \{1, \dots, n\}$
- Observes a reward $X_{I_t,t} \sim P_{I_t}$ where $P_1, \dots, P_n$ are unknown distributions

That is, playing arm i and time s results in a reward $X_{i,s}$ from the ith distribution. In these lectures, all distributions will be Gaussian (or sub-Gaussian) with variance 1 unless otherwise specified. An example of a sub-Gaussian distribution is bounded distributions on $[-1, 1]$ or Gaussian $\mathcal{N}(0, 1)$. Formally, a distribution of X is 1-sub-Gaussian if $\mathbb{E}[\exp(\lambda X)] \leq \exp(\lambda^2/2)$.

We will find that the means of the distribution are the most pertinent parameters of these distributions. Let $\theta_i^* = \mathbb{E}_{X \sim P_i}[X]$ be the mean of the ith distribution. Define $\Delta_i = \max_{j=1,\dots,n} \theta_j^* - \theta_i^*$. We measure performance of an algorithm in two ways: 1) how much total reward is accumulated, and 2) how many total pulls are required to identify the best mean.

10.1.1 Regret Minimization

After T time steps, define the *regret* as

$$\begin{aligned} R_T &= \max_{j=1,\dots,n} \mathbb{E}\left[\sum_{t=1}^{T} X_{j,t} - \sum_{t=1}^{T} X_{I_t,t}\right] \\ &= \max_{j=1,\dots,n} \theta_j^* T - \mathbb{E}\left[\sum_{t=1}^{T} X_{I_t,t}\right] \end{aligned}$$

The goal is to have $R(T) = o(T)$ to achieve sub-linear regret (e.g., $R(T) \leq \sqrt{T}$).

If at time T the ith arm has been played T_i times, then

$$\begin{aligned}
R_T &= \max_{j=1,\dots,n} \theta_j^* T - \mathbb{E}\left[\sum_{t=1}^{T} X_{I_t,t}\right] \\
&= \max_{j=1,\dots,n} \theta_j^* T - \sum_{t=1}^{T} \mathbb{E}\left[\sum_{i=1}^{n} X_{i,t} \mathbf{1}\{I_t = i\}\right] \\
&= \max_{j=1,\dots,n} \theta_j^* T - \sum_{i=1}^{n} \theta_i^* \mathbb{E}\left[\sum_{t=1}^{T} \mathbf{1}\{I_t = i\}\right] \\
&= \max_{j=1,\dots,n} \theta_j^* T - \sum_{i=1}^{n} \theta_i^* \mathbb{E}\left[T_i\right] \\
&= \sum_{i=1}^{n} \Delta_i \mathbb{E}\left[T_i\right]
\end{aligned}$$

Thus, we want to minimize the number of times we play sub-optimal arms.

10.1.2 Best-arm identification

Given a $\delta \in (0,1)$ identify the best arm with probability at least $1-\delta$ using as few total pulls as possible.

While related, these objectives are at odds with one another. Sometimes called the (ϵ,δ)-PAC setting, but for simplicity we'll take $\epsilon = 0$.

10.1.3 Warm-up: A/B testing

Suppose $n = 2$. How long would it take to decide one arm was better than another using sub-gaussian bounds? Consider the trivial algorithm:

Input: 2 arms, time $\tau \in \mathbb{N}$.
Pull each arm $i \in \{1,2\}$ exactly τ times and compute empirical mean $\widehat{\theta}_i$.
For all $t > 2\tau$ play arm $\arg\max_i \widehat{\theta}_i$

Without loss of generality, assume $\theta_1^* > \theta_2^*$. If $\widehat{\theta}_i$ is the empirical mean of arm i after pulling it τ times, it is a random variable that intuitively should be "close" to θ_i^*. Suppose we could guarantee that $\widehat{\theta}_1 > \widehat{\theta}_2$ with probability $1-\delta$. If this were true then we have an algorithm for identifying the best arm with probability at least $1-\delta$ using at most 2τ pulls. Moreover, with probability at least $1-\delta$ the sub-optimal arm is pulled at most τ times incurring a regret of at most $\tau\Delta$ where $\Delta := \theta_1^* - \theta_2^*$. To make this argument rigorous, we need to be able to build a confidence interval on each $\widehat{\theta}_i - \theta_i^*$ with high probability. By the central limit theorem (CLT) we know that $\widehat{\theta}_i - \theta_i^* \sim \mathcal{N}(0, \frac{\mathbb{V}\mathrm{ar}(Z)}{\tau})$ where $\mathbb{V}\mathrm{ar}(Z)$ denotes the variance of each individual observation (assumed the same for each arm). This suggests that $\frac{\widehat{\theta}_i - \theta_i^*}{\sqrt{\mathbb{V}\mathrm{ar}(Z))}} \in [-1.96, 1.96]$ with probability at least .95 using a standard Normal distribution look up. But this is asymptotic, can we get non-asymptotic and mathematically convenient quantities?

10.1.4 Finite-sample confidence intervals

Proposition 6 (Chernoff Bounding technique)**.** *Fix ϵ, δ. If $Z_1, Z_2, \dots$ are independent mean-zero random variables with $\psi_Z(\lambda) := \log(\mathbb{E}[\exp(\lambda Z_i)])$ then $\mathbb{P}(\frac{1}{\tau}\sum_{t=1}^{\tau} Z_t > \epsilon) \leq \inf_\lambda \exp(-\tau\epsilon\lambda + \tau\psi_Z(\lambda))$.*

Proof.

$$\begin{aligned}
\mathbb{P}(\frac{1}{\tau}\sum_{t=1}^{\tau} Z_t > \epsilon) &= \mathbb{P}(\exp\left(\lambda\sum_{t=1}^{\tau} Z_t\right) > \exp(\lambda\tau\epsilon)) \\
&\leq e^{-\lambda\tau\epsilon}\mathbb{E}\left[\exp\left(\lambda\sum_{t=1}^{\tau} Z_t\right)\right] && \text{(Markov's)} \\
&= e^{-\lambda\tau\epsilon}\prod_{t=1}^{\tau}\mathbb{E}\left[\exp\left(\lambda Z_t\right)\right] && \text{(Independence)} \\
&= \exp\left(-\lambda\tau\epsilon + \tau\psi_Z(\lambda)\right)
\end{aligned}$$

□

Corollary 11. *Let $Z_1, Z_2, \dots$ be independent mean-zero σ^2-sub-Gaussian random variables so that $\psi_Z(\lambda) := \log(\mathbb{E}[\exp(\lambda Z_t)]) \leq \exp(\lambda^2\sigma^2/2)$, then for $\tau = \lceil 2\sigma^2\epsilon^{-2}\log(1/\delta)\rceil$ we have $\mathbb{P}(\frac{1}{\tau}\sum_{t=1}^{\tau} Z_t \leq \epsilon) \geq 1-\delta$.*

Lemma 14 (Hoeffding's Lemma)**.** *Let X be an independent random variable with support in $[a,b]$ almost surely and $\mathbb{E}[X] = 0$. Then $\log(\mathbb{E}[\exp(\lambda X)]) \leq (b-a)^2\lambda^2/8$.*

Two proofs of this result are given in Chapter 2 (Lemma 11).

10.1.5 A/B testing solution

Set $\tau = \lceil 8\Delta^{-2}\log(4/\delta)\rceil$ and let $\widehat{\theta}_i = \frac{1}{\tau}\sum_{s=1}^{\tau} X_{i,s}$ for $i = 1, 2$. Define the event

$$\mathcal{E}_i := \left\{ |\widehat{\theta}_i - \theta_i^*| \leq \sqrt{\frac{2\log(4/\delta)}{\tau}} \right\}.$$

Then $\mathbb{P}(\mathcal{E}_1^c \cup \mathcal{E}_2^c) \leq \mathbb{P}(\mathcal{E}_1^c) + \mathbb{P}(\mathcal{E}_2^c) \leq \delta$. Thus, if we pull each arm τ times then on $\mathcal{E}_1 \cap \mathcal{E}_2$ we have

$$\begin{aligned}
\widehat{\theta}_1 &> \theta_1^* - \sqrt{\frac{2\log(4/\delta)}{\tau}} \\
&> \theta_1^* - \Delta/2 \\
&\geq \theta_2^* + \Delta/2 \\
&\geq \widehat{\theta}_2 - \sqrt{\frac{2\log(4/\delta)}{\tau}} + \Delta/2 \\
&> \widehat{\theta}_2
\end{aligned}$$

so that we have determined the best-arm. And we can play it forever.

After any T total plays such that arm i has been played T_i times and $T = T_1 + T_2$, the expected regret is at most

$$\begin{aligned}
\theta_1^* T - \mathbb{E}\left[\sum_{s=1}^{T} X_{I_s,s}\right] &= \theta_1^* T - \mathbb{E}\left[(T_1\theta_1^* + T_2\theta_2^*)\right] \\
&= \mathbb{E}\left[T_2\Delta\right] \\
&= \mathbb{E}\left[T_2\Delta\mathbf{1}\{\mathcal{E}_1 \cap \mathcal{E}_2\} + T_2\Delta\mathbf{1}\{\mathcal{E}_1^c \cup \mathcal{E}_2^c\}\right] \\
&\leq \mathbb{E}\left[\tau\Delta\mathbf{1}\{\mathcal{E}_1 \cap \mathcal{E}_2\} + T\Delta\mathbf{1}\{\mathcal{E}_1^c \cup \mathcal{E}_2^c\}\right] \\
&\leq 8\Delta^{-1}\log(4/\delta) + \Delta T \mathbb{P}(\mathcal{E}_1^c \cup \mathcal{E}_2^c) \\
&\leq 8\Delta^{-1}\log(4/\delta) + \Delta T\delta.
\end{aligned}$$

If we take $\delta = 1/T$ then the expected regret is less than $\Delta + 8\Delta^{-1}\log(4T)$. On the other hand, the regret can't possibly be greater than ΔT, thus the total regret is bounded by

$$\begin{aligned}
\theta_1^* T - \mathbb{E}\left[\sum_{s=1}^{T} X_{I_s,s}\right] &= \min\{T\Delta, \Delta + 8\Delta^{-1}\log(4T)\} \\
&\leq 1 + 2\sqrt{8T\log(4T)}
\end{aligned}$$

where the last step takes the worst case $\Delta = \sqrt{8\log(4T)/T}$.

Takeaway: For very small Δ we lose almost nothing, for very large Δ its easy to distinguish, its maximized at around $1/\sqrt{T}$. We'll see this again.

10.2 Elimination Algorithm for Pure exploration

```
Input: $n$ arms $\mathcal{X} = \{1, \ldots, n\}$, confidence level $\delta \in (0,1)$.
Let $\mathcal{X}_1 \leftarrow \mathcal{X}, \ell \leftarrow 1$
while $|\mathcal{X}_\ell| > 1$ do
  $\epsilon_\ell = 2^{-\ell}$
  Pull each arm in $\mathcal{X}_\ell$ exactly $\tau_\ell = \lceil 2\epsilon_\ell^{-2}\log(\frac{4\ell^2|\mathcal{X}|}{\delta})\rceil$ times
  Compute the empirical mean of these rewards $\widehat{\theta}_{i,\ell}$ for all $i \in \mathcal{X}_\ell$
 $\mathcal{X}_{\ell+1} \leftarrow \mathcal{X}_\ell \setminus \left\{i \in \mathcal{X}_\ell : \max_{j\in\mathcal{X}_\ell} \widehat{\theta}_{j,\ell} - \widehat{\theta}_{i,\ell} > 2\epsilon_\ell\right\}$
 $\ell \leftarrow \ell + 1$
Output: $\mathcal{X}_{\ell+1}$ (or play the last arm forever in the regret setting)
```

Lemma 15. *Assume that* $\max_{i\in\mathcal{X}} \Delta_i \leq 4$. *With probability at least* $1 - \delta$, *we have* $1 \in \mathcal{X}_\ell$ *and* $\max_{i\in\mathcal{X}_\ell} \Delta_i \leq 8\epsilon_\ell$ *for all* $\ell \in \mathbb{N}$.

Proof. For any $\ell \in \mathbb{N}$ and $i \in [n]$ define

$$\mathcal{E}_{i,\ell} = \left\{|\widehat{\theta}_{i,\ell} - \theta_i^*| \leq \epsilon_\ell\right\}$$

and $\mathcal{E} = \bigcap_{i=1}^{n} \bigcap_{\ell=1}^{\infty} \mathcal{E}_{i,\ell}$. Noting that $\epsilon_\ell = \sqrt{\frac{2\log(4n\ell^2/\delta)}{\tau_\ell}}$ we have

$$\mathbb{P}(\mathcal{E}^c) = \mathbb{P}\left(\bigcup_{i=1}^{n}\bigcup_{\ell=1}^{\infty} \mathcal{E}_{i,\ell}^c\right) \leq \sum_{i=1}^{n}\sum_{\ell=1}^{\infty} \frac{\delta}{2n\ell^2} \leq \delta.$$

In what follows assume $\mathcal{E}$ holds.
Fix any ℓ for which $1 \in \mathcal{X}_\ell$ (note $1 \in \widehat{\mathcal{X}}_1$). Then for any $j \in \mathcal{X}_\ell$ we have

$$\begin{aligned} \widehat{\theta}_{j,\ell} - \widehat{\theta}_{1,\ell} &= (\widehat{\theta}_{j,\ell} - \theta_j^*) - (\widehat{\theta}_{1,\ell} - \theta_1^*) - \Delta_\ell \\ &\overset{\mathcal{E}}{\le} 2\epsilon_\ell \end{aligned}$$

which implies $1 \in \mathcal{X}_{\ell+1}$. Thus, $1 \in \mathcal{X}_\ell$ for all ℓ. On the other hand, any i for which $\Delta_i = \theta_1^* - \theta_i^* > 4\epsilon_\ell$ we have

$$\begin{aligned} \max_{j \in \mathcal{X}_\ell} \widehat{\theta}_{j,\ell} - \widehat{\theta}_{i,\ell} &\ge \widehat{\theta}_{1,\ell} - \widehat{\theta}_{i,\ell} \\ &= (\widehat{\theta}_{1,\ell} - \theta_1) - (\widehat{\theta}_{i,\ell} - \theta_i) + \Delta_i \\ &> -2\epsilon_\ell + 4\epsilon_\ell = 2\epsilon_\ell \end{aligned}$$

which implies this $\max_{j \in \mathcal{X}_{\ell+1}} \theta_j^* \ge \theta_1^* - 4\epsilon_\ell = \theta_1^* - 8\epsilon_{\ell+1}$. □

Theorem 14. *Assume that* $\max_{i \in \mathcal{X}} \Delta_i \le 4$. *Then with probability at least* $1 - \delta$, 1 *is returned from the algorithm at a time* τ *that satisfies*

$$\tau \le c \sum_{i=2}^{n} \Delta_i^{-2} \log(n \log(\Delta_i^{-2})/\delta)$$

Proof. Assume $\mathcal{E}$ holds, as it does with probability at least $1 - \delta$. If $\Delta = \min_{i \neq 1} \Delta_i$ then $\mathcal{X}_\ell = \{1\}$ for $t \ge \lceil \log_2(8\Delta^{-1}) \rceil$ since all other arms would have been removed. Note that

$$\begin{aligned} T_i &= \sum_{\ell=1}^{\lceil \log_2(8\Delta^{-1}) \rceil} \tau_\ell \mathbf{1}\{i \in \mathcal{X}_\ell\} \\ &\le \sum_{\ell=1}^{\lceil \log_2(8\Delta^{-1}) \rceil} \tau_\ell \mathbf{1}\{\Delta_i \le 8\epsilon_\ell\} \\ &= \sum_{\ell=1}^{\lceil \log_2(8\Delta_i^{-1}) \rceil} \tau_\ell \\ &= \sum_{\ell=1}^{\lceil \log_2(8\Delta_i^{-1}) \rceil} \lceil 2\epsilon_\ell^{-2} \log(\tfrac{4\ell^2 |\mathcal{X}|}{\delta}) \rceil \\ &\le \lceil 2 \log(\tfrac{4 \log_2^2(16\Delta_i^{-2}) |\mathcal{X}|}{\delta}) \rceil \sum_{\ell=1}^{\lceil \log_2(8\Delta_i^{-1}) \rceil} 4^\ell \\ &\le c\Delta_i^{-2} \log(\tfrac{4 \log_2^2(16\Delta_i^{-2}) |\mathcal{X}|}{\delta}). \end{aligned}$$

Thus, the total number of samples taken before $\mathcal{X}_\ell = \{1\}$ is equal to

$$\begin{aligned} \sum_{i=1}^{n} T_i &\le T_1 + \sum_{i=1}^{n} c\Delta_i^{-2} \log(\tfrac{4 \log_2^2(16\Delta_i^{-2}) |\mathcal{X}|}{\delta}) \\ &\le 2 \sum_{i=1}^{n} c\Delta_i^{-2} \log(\tfrac{4 \log_2^2(16\Delta_i^{-2}) |\mathcal{X}|}{\delta}) \end{aligned}$$

which implies that one can identify the best arm after no more than $\sum_{i=2}^{n} \Delta_i^{-2} \log(n \log(\Delta_i^{-2})/\delta)$. □

10.3 Elimination Algorithm for Regret minimization

We will use the same algorithm and Lemma as above, but now analyze the regret of the algorithm.

Theorem 15. *Assume that* $\max_{i\in\mathcal{X}} \Delta_i \le 4$. *For any* $T \in \mathbb{N}$, *with probability at least* $1-\delta$

$$\sum_{i:\Delta_i>0} T_i\Delta_i \le \inf_{\nu\ge 0} \nu T + \sum_{i=1}^n c(\Delta_i \vee \nu)^{-1}\log(\tfrac{\log((\Delta_i\vee\nu)^{-1})|\mathcal{X}|}{\delta}).$$

Moreover, if the algorithm is run with $\delta = 1/T$ *then* $R_T \le c\sum_{i=2}^n \Delta_i^{-1}\log(T)$ *and* $R_T \le c\sqrt{nT\log(T)}$.

Suppose you run for T timesteps. For any $\nu \ge 0$ the regret is bounded by:

$$\begin{aligned}
\sum_{i=2}^n \Delta_i T_i &= \sum_{i:\Delta_i\le\nu} \Delta_i T_i + \sum_{i:\Delta_i>\nu} \Delta_i T_i \\
&\le \nu T + \sum_{i:\Delta_i>\nu} \Delta_i T_i \\
&= \nu T + \sum_{i:\Delta_i>\nu}\sum_{\ell=1}^{\infty} \Delta_i \tau_\ell \mathbf{1}\{i \in \mathcal{X}_\ell\} \\
&\le \nu T + \sum_{i:\Delta_i>\nu}\sum_{\ell=1}^{\infty} \Delta_i \tau_\ell \mathbf{1}\{\Delta_i \le 8\epsilon_\ell\} \\
&\le \nu T + \sum_{i=2}^{n}\sum_{\ell=1}^{\infty} \Delta_i \tau_\ell \mathbf{1}\{\Delta_i \vee \nu \le 8\epsilon_\ell\} \\
&\le \nu T + \sum_{i=2}^{n}\sum_{\ell=1}^{\lceil\log_2(8(\Delta_i\vee\nu)^{-1})\rceil} 8\epsilon_\ell\tau_\ell \\
&= \nu T + \sum_{i=2}^{n}\sum_{\ell=1}^{\lceil\log_2(8(\Delta_i\vee\nu)^{-1})\rceil} 8\epsilon_\ell\lceil 2\epsilon_\ell^{-2}\log(\tfrac{4\ell^2|\mathcal{X}|}{\delta})\rceil \\
&\le \nu T + \sum_{i=2}^{n} c\log(\tfrac{4\log_2^2(8(\Delta_i\vee\nu)^{-2})|\mathcal{X}|}{\delta})\sum_{\ell=1}^{\lceil\log_2(8(\Delta_i\vee\nu)^{-1})\rceil} 2^\ell \\
&\le \nu T + \sum_{i=2}^{n} c(\Delta_i \vee \nu)^{-1}\log(\tfrac{\log((\Delta_i\vee\nu)^{-1})|\mathcal{X}|}{\delta})
\end{aligned}$$

where the second inequality follows from Lemma 15. Setting $\nu = 0$ yields a regret of $\sum_{i=2}^n \Delta_i^{-1}\log(n\log(\Delta_i^{-1})/\delta)$. On the other hand, using $\Delta_i \vee \nu \ge \nu$ and minimizing over ν yields a regret of $\sqrt{nT\log(n\log(T)/\delta)}$.
The expected regret, of course, is then bounded by

$$\begin{aligned}
\sum_{i=2}^n \Delta_i \mathbb{E}[T_i] &= \mathbb{E}\left[\sum_{i=2}^n \Delta_i T_i\right] \\
&\le \sum_{i=2}^n \Delta_i^{-1}\log(n\log(\Delta_i^{-1})/\delta) + T\mathbb{P}(\mathcal{E}^c)
\end{aligned}$$

Setting $\delta = 1/T$ implies the regret is less than $\sum_{i=2}^n c\Delta_i^{-1}\log(T)$.
Some remarks:

- This analysis doesn't reuse samples from previous rounds, it is easy to make this change.
- Regret bound requires knowledge of T a priori. One can avoid knowing this by using a double trick: guess a value of T, then when you reach this value double T and restart using this value of T.

10.4 Lower bounds for Multi-armed Bandits

Let us briefly pause to consider how far off from optimal we are, and then think about an algorithm that could get us to optimality. How do we know we're doing okay?

Using the measure-theoretic tools developed in Chapter 1, we can establish the following key decomposition for bandit problems.

Lemma 16. *Let $\nu = (\nu_1, \ldots, \nu_n)$ be the reward distributions associated with one n-armed bandit, and let $\nu' = (\nu'_1, \ldots, \nu'_n)$ be the reward distributions associated with another n-armed bandit. Fix some policy π and let $\mathbb{P}_\nu$ be the probability measures induced by the T-round interaction of π and ν (respectively, π and ν'). Then,*

$$\mathrm{KL}(\mathbb{P}_\nu, \mathbb{P}_{\nu'}) = \sum_{i=1}^{n} \mathbb{E}_\nu[T_i(T)]\,\mathrm{KL}(\nu_i, \nu'_i).$$

Proof. For simplicity, assume ν_i, ν'_i are continuous densities with the same support (the lemma holds more generally). Consider a sample path $(I_1, X_1, I_2, X_2, \ldots, I_T, X_T)$. Note that the likelihood of this sample path under ν is given as

$$\prod_{t=1}^{T} \nu_{I_t}(X_t)\pi(I_t|\{I_s, X_s\}_{s<t})$$

with an analogous expression holding for ν'. Thus,

$$\begin{aligned}
\mathrm{KL}(\mathbb{P}_\nu, \mathbb{P}_{\nu'}) &= \mathbb{E}_\nu[\log \prod_{t=1}^{T} \frac{\nu_{I_t}(X_t)\pi(I_t|\{I_s, X_s\}_{s<t})}{\nu'_{I_t}(X_t)\pi(I_t|\{I_s, X_s\}_{s<t})}] \\
&= \mathbb{E}_\nu[\sum_{t=1}^{T} \log\big(\frac{\nu_{I_t}(X_t)}{\nu'_{I_t}(X_t)}\big)] \\
&= \sum_{i=1}^{n}\sum_{t=1}^{T} \mathbb{E}_\nu[\mathbf{1}\{I_t = i\} \log\big(\frac{\nu_i(X_t)}{\nu'_i(X_t)}\big)] \\
&= \sum_{i=1}^{n}\sum_{t=1}^{T} \mathbb{P}_\nu(I_t = i)\mathbb{E}_{\nu_i}[\log\big(\frac{\nu_i(X_t)}{\nu'_i(X_t)}\big)] \\
&= \sum_{i=1}^{n} \mathbb{E}_\nu[T_i(T)]KL(\nu_i|\nu'_i)
\end{aligned}$$

where we've used the fact that the policy acts identically under the same observations (and thus cancels with itself) in the first step, and that X_t is conditionally independent given I_t. □

10.4.1 Identification

An algorithm for best-arm identification at time t is described by given a history $(I_s, X_s)_{s<t}$ for each time t is described by a

- **selection rule** $I_t \in [n]$ is $\mathcal{F}_{t-1}$ measurable where $\mathcal{F}_t = \sigma(I_1, X_1, I_2, X_2, \ldots, I_{t-1}, X_{t-1})$
- **stopping time** τ is $\mathcal{F}_t$ measurable, and
- **recommendation rule** $\widehat{i} \in [n]$ invoked at time τ which is $\mathcal{F}_\tau$-measurable.

Definition 16. *We say that an algorithm for best-arm identification is δ-PAC if for all $\theta^* \in \mathbb{R}^n$ we have $\mathbb{P}_{\theta^*}(\widehat{i} = \arg\max_{i\in[n]} \theta_i^*) \geq 1 - \delta$.*

The following is due to [Kaufmann et al., 2016], a strengthening of the first time it appeared in [Mannor and Tsitsiklis, 2004].

Theorem 16 (Best-arm identification lower bound)**.** *Any algorithm that is δ-PAC on $\{P : P_i = \mathcal{N}(\theta_i, 1), \theta_1 > \max_{i\neq 1} \theta_i, \theta \in [0,1]^n\}$ for $\delta < 0.15$ satisfies $\mathbb{E}_{\theta^*}[\tau] \geq 2\log(\frac{1}{2.4\delta}) \sum_{i=1}^n \Delta_i^{-2}$.*

Proof sketch: The original instance has $P_i = \mathcal{N}(\theta_i^*, 1)$. Pick some $j \in [n]$ and define an alternative mean vector $\theta^{(j)} \in [0,1]^n$ such that $\theta_i^{(j)} = \theta_i^*$ if $i \neq j$ and $\theta_i^{(j)} = \theta_1 + \epsilon$ for $j = i$ for some arbitrarily small number ϵ. Note that under $\theta^{(j)}$, arm j is the best arm.

Because the algorithm claims to be δ-PAC, it has to output arm 1 under θ^* and arm j under $\theta^{(j)}$. But these two bandit games only differ on arm j so to tell the difference between them its only natural to sample arm j until one can figure out which instance is being played (i.e., is its mean θ_j or $\theta_1 + \epsilon$?) The discussion above suggests that to make this distinction with probability at least $1 - \delta$, it is necessary to sample arm j at least $2(\theta_1 - \theta_j + \epsilon)^{-2}\log(1/4\delta)$ times. Taking ϵ to zero and noticing that j was arbitrary completes the sketch.

This is *not* a proof, however, because the number of times the algorithm samples arm j is random whereas in the above argument it was fixed. The proof of [Kaufmann et al., 2016] provides convenient tools to prove general lower bounds for δ-PAC settings.

10.4.2 Regret, minimax

Theorem 17 (Minimax regret lower bound)**.** *For every $T \geq n$ there exists a set of instances $P_\theta = \mathcal{N}(\theta, I)$ such that $\sup_{P_\theta} \mathbb{E}_\theta[R_T] \geq \sqrt{(n-1)T/256}$.*

Proof. Let $\theta = (\Delta, 0, \ldots, 0)$. For any algorithm, by the pigeon hole principle, there exists an arm $\widehat{i} \in [n] \setminus \{1\}$ such that $\mathbb{E}[T_{\widehat{i}}] \leq T/(n-1)$. Define θ' to be identical to θ except set $\theta_{\widehat{i}} = 2\Delta$. Let $\nu = \prod_{i=1}^n \mathcal{N}(\theta_i, 1)$ and $\nu' = \prod_{i=1}^n \mathcal{N}(\theta_i', 1)$.

Note that

$$\mathbb{E}_{\nu'}[\text{Regret}] = \sum_{i=1}^n (\theta'_{\widehat{i}} - \theta'_i)\mathbb{E}_{\nu'}[T_i] \geq (\theta'_{\widehat{i}} - \theta'_1)\mathbb{E}_{\nu'}[T_1] = \Delta\mathbb{E}_{\nu'}[T_1] \geq \Delta\mathbb{P}_{\nu'}(T_1 \geq T/2)T/2$$

by Markov's inequality, and similarly we have

$$\mathbb{E}_{\nu}[\text{Regret}] = \sum_{i=1}^n (\theta_1 - \theta_i)\mathbb{E}_{\nu}[T_i] = \Delta(\mathbb{E}_\nu[\sum_{i\neq 1} T_i]) \geq \Delta\mathbb{P}\big(\sum_{i\neq 1} T_i \geq T/2\big)T/2 = \Delta(1 - \mathbb{P}_\nu(T_1 \geq T/2))T/2.$$

We observe that

$$
\begin{aligned}
\max_{\mu \in \{\nu, \nu'\}} \mathbb{E}_\mu[\text{Regret}] &\geq (\mathbb{E}_{\nu'}[\text{Regret}] + \mathbb{E}_\nu[\text{Regret}])/2 \\
&= \frac{\Delta T}{4}(1 + \mathbb{P}_{\nu'}(T_1 \geq T/2) - \mathbb{P}_\nu(T_1 \geq T/2)) \\
&\geq \frac{\Delta T}{4}(1 - \sup_E |\mathbb{P}_{\nu'}(E) - \mathbb{P}_\nu(E)|) \\
&\geq \frac{\Delta T}{4}(1 - \sqrt{KL(\mathbb{P}_\nu|\mathbb{P}_{\nu'})/2}) && \text{(Lemma 7)} \\
&\geq \frac{\Delta T}{4}(1 - \sqrt{KL(\mathcal{N}(\theta_{\widehat{i}}, 1)|\mathcal{N}(\theta'_{\widehat{i}}, 1))\mathbb{E}_\nu[T_{\widehat{i}}]/2}) && \text{(Lemma 16)} \\
&= \frac{\Delta T}{4}(1 - \sqrt{\Delta^2 \mathbb{E}_\nu[T_{\widehat{i}}]}) \\
&\geq \frac{\Delta T}{4}(1 - \sqrt{\Delta^2 T/(n-1)}).
\end{aligned}
$$

Taking $\Delta = \sqrt{\frac{n-1}{4T}}$ completes the proof. □

10.4.3 Gap-dependent regret

Lemma 17. *Any strategy that satisfies* $\mathbb{E}[T_i(t)] = o(t^a)$ *for any arm* i *with* $\Delta_i > 0$ *and* $a \in (0,1)$*, we have that* $\liminf_{T\to\infty} \frac{\bar{R}_T}{\log(T)} = \sum_{i=2}^n \frac{2}{\Delta_i}$.

Takeaway: This is what his field does: prove an initial upper, then lower, then chase it.

10.4.4 Revisiting MAB with Optimism

Why go beyond action elimination algorithms? Because they will never hit the asymptotic lower bound, for one thing, since if we look at when the second to last arm exits, the lowerbounds are the same.

α-UCB which is $\arg\max_i \widehat{\theta}_{i,T_i(t)} + \sqrt{\frac{2\alpha\log(t)}{T_i(t)}}$ as $\alpha \to 1$ achieves the lower bound.

Any sub-linear regret algorithm plays arm 1 an infinite number of times, so assume $\widehat{\mu}_1 \approx \mu_1$. Minimizing the maximum upper bound. Thus, we expect the number of times the ith arm is pulled is $2\Delta_i^{-2}\log(T)$, which is optimal.

UCB1 in its most popular form was developed by [Auer et al., 2002].

MOSS first achieved $\sqrt{nT}$ regret [Audibert and Bubeck, 2009].

KL-UCB is finite-time analysis with optimal constants for asymptotic regret [Cappé et al., 2013].

The recent work of [Lattimore, 2018] defined a UCB-based algorithm that achieves asymptotic optimal constants, and finite regret bounds of $\sum_i \frac{\log(T)}{\Delta_i^{-1}}$ and $\sqrt{nT}$.

Chapter 11

Linear bandits

11.1 Problem statement

Now suppose each arm $i = 1, \ldots, n$ has a feature vector $x_i \in \mathbb{R}^d$. And more over, there exists some $\theta^* \in \mathbb{R}^d$ such that a pull of arm $I_t \in [n]$ results in a reward $y_t = \langle x_{I_t}, \theta^* \rangle + \eta_t$ where $\eta_t \sim \mathcal{N}(0, 1)$.

Applications: Drug-discovery, Spotify, Netflix, ads

In the previous setup, pulling arm i provided no information about arm j, but now suddenly it does.

11.2 Review of least squares

Given a sequence of arm choices and observed rewards let $\{x_t, y_t, \eta_t\}_{t=1}^{\tau}$ we denote the stacked sequences of each as $X \in \mathbb{R}^{\tau \times d}, Y \in \mathbb{R}^{\tau}$, and $\eta \in \mathbb{R}^{\tau}$ respectively where $Y = X\theta^* + \eta$. Using this information we can derive a least-squares estimate of θ_* given as follows

$$\hat{\theta} = (X^T X)^{-1} X^T Y = (X^T X)^{-1} X^T (X\theta_* + \eta) = \theta_* + (X^T X)^{-1} X^T \eta.$$

Fix any $z \in \mathbb{R}^d$, then Thus

$$z^\top (\hat{\theta} - \theta_*) = z^\top (X^\top X)^{-1} X^\top \eta.$$

Note that $\eta \sim \mathcal{N}(0, I)$. For any $W \sim \mathcal{N}(\mu, \Sigma)$ we have $AW + b \sim \mathcal{N}(A\mu + b, A\Sigma A^\top)$. Thus

$$z^\top (\hat{\theta} - \theta_*) \sim \mathcal{N}(0, z^\top (X^\top X)^{-1} z).$$

so that

$$\mathbb{P}\left(z^\top (\hat{\theta} - \theta_*) \geq \sqrt{2 z^\top (X^\top X)^{-1} z \log(1/\delta)} \right) \leq \delta.$$

We will use the notation $\|z\|_A^2 = z^\top A z$ so that with probability at least $1 - \delta$

$$z^\top (\hat{\theta} - \theta_*) \leq \|z\|_{(X^\top X)^{-1}} \sqrt{2 \log(1/\delta)}$$

Aside: Gaussian to sub-Gaussian

For an arbitrary constant μ,

$$\begin{aligned}
P(x^T(\hat{\theta}-\theta_*) > \mu) &= P(w^T\eta > \mu) \\
&\leq \exp(-\lambda\mu)\mathbb{E}[\exp(\lambda w^T\eta)], \quad \text{let } \lambda > 0 && \text{Chernoff Bound} \\
&= \exp(-\lambda\mu)\mathbb{E}[\exp(\lambda\sum_{i=1}^{t} w_i\eta_i)] \\
&= \exp(-\lambda\mu)\prod_{i=1}^{t}\mathbb{E}[\exp(\lambda w_i\eta_i)] && \text{independence of } w_i\eta_i \\
&\leq \exp(-\lambda\mu)\prod_{i=1}^{t}\exp(\lambda^2 w_i^2/2) && \text{sub-Gaussian assumption} \\
&= \exp(-\lambda\mu)\exp(\frac{\lambda^2}{2}||w||_2^2) \\
&\leq \exp(-\frac{\mu^2}{2||w||_2^2}) && \lambda = \frac{\mu}{||w||_2^2} \\
&= \exp(-\frac{\mu^2}{2x^T(X^TX)^{-1}x}) = \delta,
\end{aligned}$$

where in the final step we made use of the following equality

$$||w||_2^2 = x^T(X^TX)^{-1}X^TX(X^TX)^{-1}x = x^T(X^TX)^{-1}x.$$

Thus with probability at least $1-\delta$,

$$\begin{aligned}
x^T(\hat{\theta}-\theta_*) &\leq \sqrt{2x^T(X^\top X)^{-1}x\log(\frac{1}{\delta})} \\
&=: \|x\|_{(X^\top X)^{-1}}\sqrt{2\log(1/\delta)}
\end{aligned}$$

11.3 Experimental design and Kiefer-Wolfowitz

Note that if I take measurements $(x_1,\dots,x_n) \in \mathcal{X}$ and observe their corresponding observations $y_i = \langle x_i, \theta^*\rangle + \eta_i$ where $\eta_i \sim \mathcal{N}(0,1)$, then $\mathbb{E}[(\widehat{\theta}-\theta)(\widehat{\theta}-\theta)^\top] = \sigma^2(X^TX)^{-1}$ and also, $\widehat{\theta}-\theta^* \sim \mathcal{N}(0,\sigma^2(X^\top X)^{-1})$. We can visualize this as a confidence ellipsoid for each choice of X. And we can even think of optimizing the choice. Recall that the PDF of a Gaussian is $\phi(x) = \frac{1}{(2\pi|\Sigma|)^{d/2}}e^{-x^\top\Sigma^{-1}x/2}$. With entropy $\frac{1}{2}\log(2\pi e|\Sigma|)$.

When the number of selected points is large, its more convenient to think of sampling n points from a distribution placed over $\mathcal{X}$. Define

$$A_\lambda = \sum_{x\in\mathcal{X}}\lambda_x xx^\top$$

so that for every $X \in \mathbb{R}^{\tau\times d}$ there exists some $\lambda \in \triangle_{\mathcal{X}}$ such that $X^\top X = \sum_{x\in\mathcal{X}}\lceil\lambda_x\tau\rceil xx^\top = A_\lambda$. This A_λ can then be used to shape the covariance $\widehat{\theta}$:

- **A-optimality**: minimize $f_A(\lambda) = \mathrm{Tr}(A_\lambda^{-1})$ minimizes $\mathbb{E}[\|\widehat{\theta} - \theta\|_2^2]$

- **E-optimality**: minimize $f_E(\lambda) = \max_{u:\|u\|\leq 1} u^\top A_\lambda^{-1} u$ minimizes $\max_{u:\|u\|\leq 1} \mathbb{E}[(\langle u, \widehat{\theta} - \theta\rangle)^2]$

- **D-optimality**: maximize $g_D(\lambda) = \log(|A_\lambda|)$ maximizes the entropy of distribution. Also, if $\mathcal{E}_\lambda = \{x : x^\top A_\lambda^{-1} x \leq d\}$ then D-optimality is the minimum volume ellipsoid that contains $\mathcal{X}$.

- **G-optimality**: minimize $f_G(\lambda) = \max_{x\in\mathcal{X}} x^\top A_\lambda^{-1} x$ minimizes $\max_{x\in\mathcal{X}} \mathbb{E}[(\langle x, \widehat{\theta} - \theta^*\rangle)^2]$

Lemma 18 (Kiefer-Wolfowitz (1960))**.** *For any $\mathcal{X}$ with $d = dim(span(\mathcal{X}))$, there exists a $\lambda^* \in \triangle_\mathcal{X}$ that*

- $\max_\lambda g_D(\lambda) = g_D(\lambda^*)$

- $\min_\lambda f_G(\lambda) = f_G(\lambda^*)$

- $f_G(\lambda^*) = d$

- *support*$(\lambda^*) = (d+1)d/2$

Proposition 7. *If λ^* is the G-optimal design for $\mathcal{X}$ then if we pull arm $x \in \mathcal{X}$ exactly $\lceil \tau\lambda_x^* \rceil$ times for some $\tau > 0$ and compute the least squares estimator $\widehat{\theta}$. Then for each $x \in \mathcal{X}$ we have with probability at least $1-\delta$*

$$\begin{aligned}
\langle x, \widehat{\theta} - \theta^*\rangle &\leq \|x\|_{(\sum_{x\in\mathcal{X}} \lceil \tau\lambda_x^* \rceil x x^\top)^{-1}} \sqrt{2\log(1/\delta)} \\
&\leq \frac{1}{\sqrt{\tau}} \|x\|_{(\sum_{x\in\mathcal{X}} \lambda_x^* x x^\top)^{-1}} \sqrt{2\log(1/\delta)} \\
&\leq \sqrt{\frac{2d\log(1/\delta)}{\tau}}
\end{aligned}$$

and we have taken at most $\tau + \frac{d(d+1)}{2}$ pulls. Thus, for any $\delta' \in (0,1)$ we have $\mathbb{P}(\bigcup_{x\in\mathcal{X}}\{|\langle x, \widehat{\theta} - \theta^*\rangle| > \sqrt{\frac{2d\log(2|\mathcal{X}|/\delta')}{\tau}}\}) \leq \delta'$.

Notes:

- The support size of $(d+1)d/2$ is trivial application of Caratheodory's theorem. Many algorithms to find this efficiently.

- Note that one can find a λ^* with a constant approximation with just support $O(d)$.

- Leverage scores if V-optimality

- John's ellipsoid is equivalent to G/D-optimality

[Pukelsheim, 2006, Yu et al., 2006]. [Yu et al., 2006, Soare et al., 2014, Soare, 2015, Lattimore and Szepesvari, 201

11.3.1 Frank-Wolfe for D/G-optimal design

Define $g(\lambda) = \text{logdet}(\sum_{x\in\mathcal{X}} \lambda_x x x^\top)$. Recall that for any $\lambda \in \triangle_{\mathcal{X}}$ we have by Kiefer-Wolfowitz that $[\nabla g(\lambda)]_{x'} = \|x'\|^2_{(\sum_{x\in\mathcal{X}} \lambda_x x x^\top)^{-1}} \geq d$.

```
**Input**: Finite set $(x_1, \dots, x_n) \subset \mathbb{R}^d$, $\lambda^1 \in \triangle_n$.
**for** $k = 1, 2, \dots$
    $I_k = \arg\max_i \|x_i\|^2_{(\sum_{j=1}^n \lambda_j^k x_j x_j^\top)^{-1}}$
    $\lambda^{k+1} = (1-\gamma_k)\lambda^k + \gamma_k [\nabla g(\lambda)]_{I_k}$ where
        $\gamma_k = \arg\max_{\gamma} g\left((1-\gamma)\lambda^k + \gamma \mathbf{e}_{I_k}\right)$
    **If** $\max_i \|x_i\|^2_{(\sum_{j=1}^n \lambda_j^{k+1} x_j x_j^\top)^{-1}} \leq 2d$ **Terminate**
```

The analysis of the algorithm critically leverages the step size selection. Let $A(\lambda) = \sum_{i=1}^n \lambda_i x_i x_i^\top$ so that $g(\lambda) = \text{logdet}(A(\lambda))$. Note that for some step size γ and $i \in [n]$ we have

$$\begin{aligned}
g\left((1-\gamma)\lambda + \gamma \mathbf{e}_i\right) &= g\left((1-\gamma)[\lambda + \tfrac{\gamma}{1-\gamma}\mathbf{e}_i]\right) \\
&= d\log(1-\gamma) + \text{logdet}(A(\lambda) + \tfrac{\gamma}{1-\gamma} x_i x_i^\top) \\
&= d\log(1-\gamma) + \text{logdet}(A(\lambda)(I + \tfrac{\gamma}{1-\gamma} A(\lambda)^{-1} x_i x_i^\top)) \\
&= d\log(1-\gamma) + \text{logdet}(A(\lambda)) + \log(1 + \tfrac{\gamma}{1-\gamma}\|x_i\|^2_{A(\lambda)^{-1}})
\end{aligned}$$

which means, plugging in the definition of γ_k and I_k,

$$\begin{aligned}
g(\lambda^{k+1}) - g(\lambda^k) &= \max_{\gamma} d\log(1-\gamma) + \log(1 + \tfrac{\gamma}{1-\gamma}\|x_{I_k}\|^2_{A(\lambda^k)^{-1}}) \\
&= \max_{\tau} -d\log(1+\tau) + \log(1 + \tau\|x_{I_k}\|^2_{A(\lambda^k)^{-1}}) \\
&\geq \max_{\tau} -d\tau + \tau\|x_{I_k}\|^2_{A(\lambda)^{-1}} - \tau^2\|x_{I_k}\|^4_{A(\lambda^k)^{-1}}/2 \\
&= \frac{(\|x_{I_k}\|^2_{A(\lambda)^{-1}} - d)^2}{2\|x_{I_k}\|^4_{A(\lambda^k)^{-1}}}
\end{aligned}$$

where we have taken the reparameterization $\tau = \frac{\gamma}{1-\gamma}$ which implies $\gamma = \tau/(1+\tau)$, and the fact $\log(1+x) \geq x - x^2/2$ for $x \geq 0$.

Let K be the final iterate of the algorithm when it terminates. By the definition of the termination condition and I_k, for all $k \leq K$ we have that $\|x_{I_k}\|^2_{A(\lambda^k)^{-1}} > 2d$. Thus,

$$\begin{aligned}
g(\lambda^{K+1}) &\geq g(\lambda^K) + \frac{(\|x_{I_K}\|^2_{A(\lambda^K)^{-1}} - d)^2}{2\|x_{I_K}\|^4_{A(\lambda^K)^{-1}}} \\
&\geq g(\lambda^1) + \sum_{k=1}^K \frac{(\|x_{I_k}\|^2_{A(\lambda)^{-1}} - d)^2}{2\|x_{I_k}\|^4_{A(\lambda^k)^{-1}}} \\
&= g(\lambda^1) + \sum_{k=1}^K (1 - \frac{d}{\|x_{I_K}\|^2_{A(\lambda)^{-1}}})^2/2 \\
&\geq g(\lambda^1) + K/8
\end{aligned}$$

which implies $K \leq 8(\max_\lambda g(\lambda) - g(\lambda^1))$.

There exists an algorithm to produce an initialization with $|\text{support}(\lambda^1)| = 2d$ and $\max_\lambda g(\lambda) - g(\lambda^1) \leq 5d\log(d)$ [**?**]. This implies that $|\text{support}(\lambda^{(K+1)})| \leq 40d\log(d)$. But our above analysis is actually quite weak, one can improve this result to $O(d\log\log(d))$ with a more careful Taylor series upper bound.

11.4 Elimination algorithm for Regret Minimization

This section is inspired by [Lattimore and Szepesvári, 2020].

```
Input: Finite set $\mathcal{X} \subset \mathbb{R}^d$, confidence level $\delta \in (0,1)$.
Let $\mathcal{X}_1 \leftarrow \mathcal{X}, \ell \leftarrow 1$
while $|\mathcal{X}_\ell| > 1$ do
  Let $\widehat{\lambda}_\ell \in \triangle_{\mathcal{X}_\ell}$ be a $\frac{d(d+1)}{2}$-sparse minimizer of $f(\lambda) = \max_{x \in \mathcal{X}_\ell} \|x\|^2_{(\sum_{x \in \mathcal{X}_\ell} \lambda_x x x^\top)^{-1}}$
  $\epsilon_\ell = 2^{-\ell}$, $\tau_\ell = 2d\epsilon_\ell^{-2}\log(4\ell^2|\mathcal{X}|/\delta)$
  Pull arm $x \in \mathcal{X}$ exactly $\lceil \widehat{\lambda}_{\ell,x}\tau_\ell \rceil$ times and construct the least squares estimator $\widehat{\theta}_\ell$ using only the observations of this round
  $\mathcal{X}_{\ell+1} \leftarrow \mathcal{X}_\ell \setminus \left\{x \in \mathcal{X}_\ell : \max_{x' \in \mathcal{X}_\ell}\langle x' - x, \widehat{\theta}_\ell \rangle > 2\epsilon_\ell\right\}$
  $\ell \leftarrow \ell + 1$
Output: $\mathcal{X}_\ell$
```

After T time steps, define the *regret* as

$$R_T = \langle x^\star, \theta^* \rangle - \mathbb{E}\left[\sum_{t=1}^T \langle x_t, \theta^* \rangle\right]$$
$$= \mathbb{E}\left[\sum_{x \neq x^\star} T_x \Delta_x\right]$$

where $\Delta_x = \langle x^\star - x, \theta^* \rangle$.

Lemma 19. *Assume that* $\max_{x \in \mathcal{X}} \langle x^\star - x, \theta^* \rangle \leq 4$. *With probability at least* $1 - \delta$, *we have* $x^\star \in \mathcal{X}_\ell$ *and* $\max_{x \in \mathcal{X}_\ell} \langle x^\star - x, \theta^* \rangle \leq 8\epsilon_\ell$ *for all* $\ell \in \mathbb{N}$.

Proof. For any $\mathcal{V} \subseteq \mathcal{X}$ and $x \in \mathcal{V}$ define

$$\mathcal{E}_{x,\ell}(\mathcal{V}) = \{|\langle x, \widehat{\theta}_\ell(\mathcal{V}) - \theta^* \rangle| \leq \epsilon_\ell\}$$

where it is implicit that $\widehat{\theta}_\ell := \widehat{\theta}_\ell(\mathcal{V})$ is the G-optimal design constructed in the algorithm at stage ℓ with respect to $\mathcal{X}_\ell = \mathcal{V}$. Note that this is precisely the analogous events of multi-armed bandits.

The key piece of the analysis is that

$$\begin{aligned}
\mathbb{P}\left(\bigcup_{\ell=1}^{\infty}\bigcup_{x\in\mathcal{X}_\ell}\{\mathcal{E}_{x,\ell}^c(\mathcal{X}_\ell)\}\right) &\leq \sum_{\ell=1}^{\infty}\mathbb{P}\left(\bigcup_{x\in\mathcal{X}_\ell}\{\mathcal{E}_{x,\ell}^c(\mathcal{X}_\ell)\}\right)\\
&= \sum_{\ell=1}^{\infty}\sum_{\mathcal{V}\subseteq\mathcal{X}}\mathbb{P}\left(\bigcup_{x\in\mathcal{V}}\{\mathcal{E}_{x,\ell}^c(\mathcal{V})\}, \mathcal{X}_\ell = \mathcal{V}\right)\\
&= \sum_{\ell=1}^{\infty}\sum_{\mathcal{V}\subseteq\mathcal{X}}\mathbb{P}\left(\bigcup_{x\in\mathcal{V}}\{\mathcal{E}_{x,\ell}^c(\mathcal{V})\}\right)\mathbb{P}(\mathcal{X}_\ell = \mathcal{V})\\
&\leq \sum_{\ell=1}^{\infty}\sum_{\mathcal{V}\subseteq\mathcal{X}}\tfrac{\delta|\mathcal{V}|}{2\ell^2|\mathcal{X}|}\mathbb{P}(\mathcal{X}_\ell = \mathcal{V}) \leq \delta
\end{aligned}$$

Thus, in what follows, assume $\mathcal{E} := \bigcap_{x\in\mathcal{X}}\bigcap_{\ell=1}^{\infty}\{\mathcal{E}_{x,\ell}(\mathcal{X}_\ell)\}$ holds.

Fix any ℓ for which $x^\star \in \mathcal{X}_\ell$ (note $x^\star \in \mathcal{X}_1$). Then for any $x \in \mathcal{X}_\ell$ we have

$$\begin{aligned}
\langle x - x^\star, \widehat{\theta}_\ell\rangle &= \langle x, \widehat{\theta}_\ell - \theta^*\rangle - \langle x^\star, \widehat{\theta}_\ell - \theta^*\rangle + \langle x - x^\star, \theta^*\rangle\\
&\leq 2\epsilon_\ell
\end{aligned}$$

which implies $x^\star \in \mathcal{X}_{\ell+1}$. Thus, $x^\star \in \mathcal{X}_\ell$ for all ℓ. On the other hand, any x for which $\langle x^\star - x, \theta^*\rangle > 4\epsilon_\ell$ we have

$$\begin{aligned}
\max_{x'\in\mathcal{X}_\ell}\langle x' - x, \widehat{\theta}_\ell\rangle &\geq \langle x^\star - x, \widehat{\theta}_\ell\rangle\\
&= \langle x^\star, \widehat{\theta}_\ell - \theta^*\rangle - \langle x, \widehat{\theta}_\ell - \theta^*\rangle + \langle x^\star - x, \theta^*\rangle\\
&> 2\epsilon_\ell
\end{aligned}$$

which implies $\max_{x\in\mathcal{X}_{\ell+1}}\langle x, \theta^*\rangle \geq \langle x^\star, \theta^*\rangle - 4\epsilon_\ell = \langle x^\star, \theta^*\rangle - 8\epsilon_{\ell+1}$. □

For any $\ell \geq \lceil \log_2(8\Delta^{-1})\rceil$ we have that $\mathcal{X}_\ell = \{x^\star\}$. Suppose you run for T timesteps. Then for any $\nu \geq 0$ the regret is bounded by:

$$\begin{aligned}
\sum_{x\in\mathcal{X}\setminus x^\star}\Delta_x T_x &= \sum_{x\in\mathcal{X}\setminus x^\star:\Delta_x\leq\nu}\Delta_x T_x + \sum_{x\in\mathcal{X}\setminus x^\star:\Delta_x>\nu}\Delta_x T_x\\
&\leq \nu T + \sum_{\ell=1}^{\infty}\sum_{x\in\mathcal{X}_\ell\setminus x^\star:\Delta_x>\nu}\Delta_x\lceil\tau_\ell\widehat{\lambda}_{\ell,x}\rceil\\
&\leq T\nu + \sum_{\ell=1}^{\lceil\log_2(8(\Delta\vee\nu)^{-1})\rceil} 8\epsilon_\ell(|\text{support}(\widehat{\lambda}_\ell)| + \tau_\ell)\\
&= T\nu + \sum_{\ell=1}^{\lceil\log_2(8(\Delta\vee\nu)^{-1})\rceil} 8\epsilon_\ell(\tfrac{(d+1)d}{2} + 2d\epsilon_\ell^{-2}\log(4\ell^2|\mathcal{X}|/\delta))\\
&\leq T\nu + 4(d+1)d\lceil\log_2(8(\Delta\vee\nu)^{-1})\rceil + \sum_{\ell=1}^{\lceil\log_2(8(\Delta\vee\nu)^{-1})\rceil} 16d\epsilon_\ell^{-1}\log(4\ell^2|\mathcal{X}|/\delta)\\
&\leq T\nu + 4(d+1)d\lceil\log_2(8(\Delta\vee\nu)^{-1})\rceil + 16d\log(4\log_2^2(16(\Delta\vee\nu)^{-1})|\mathcal{X}|/\delta)\sum_{\ell=1}^{\lceil\log_2(8(\Delta\vee\nu)^{-1})\rceil} 2^\ell\\
&\leq T\nu + 4(d+1)d\lceil\log_2(8(\Delta\vee\nu)^{-1})\rceil + 512d(\Delta\vee\nu)^{-1}\log(4\log_2^2(16(\Delta\vee\nu)^{-1})|\mathcal{X}|/\delta)
\end{aligned}$$

Setting $\nu = 0$ yields a regret bound of $O(d\Delta^{-1}\log(|\mathcal{X}|\log(\Delta^{-1})/\delta))$ which implies $R_T \leq c\frac{d}{\Delta}\log(|\mathcal{X}|T)$. Minimizing over $\nu > 0$ yields a regret bound of $O(\sqrt{dT\log(\log(T/d)|\mathcal{X}|/\delta)})$ which implies $R_T \leq c\sqrt{dT\log(|\mathcal{X}|T)}$.

Remarks:

- Let $\mathcal{X} = \{\mathbf{e}_i : i \in [d]\}$. Then for this action set, this bound is nearly minimax according to our lower bounds!

- However, this is also concerning: we know that in the bandit setting the regret scales like $\sum_{i=2}^d \Delta_i^{-1}\log(T)$ but this scales $d\Delta^{-1}\log(T)$, which is significantly worse. Can we achieve this?

- For **pure-exploration**, an analogous analysis shows that one can identify the best-arm in $\frac{d}{\Delta^2}\log(1/\delta)$ pulls. But this is exactly the same rate we would have gotten if we did G-optimal *once* in the beginning and sample according to that!

- **Optimism won't help here**

11.5 Elimination algorithm for Pure exploration

This section is inspired by [Fiez et al., 2019].

Showing that $x^\star$ is the best arm is equivalent to showing that $\langle x^\star - x, \theta^*\rangle > 0$ for all $x \in \mathcal{X} \setminus x^\star$. Given a finite number of observations, we have an estimate $\widehat{\theta}$ and a confidence set for θ^*.

$$\begin{aligned}\langle x^\star - x, \widehat{\theta}\rangle &= \langle x^\star - x, \widehat{\theta} - \theta^*\rangle + \langle x^\star - x, \theta^*\rangle \\ &= \langle x^\star - x, \widehat{\theta} - \theta^*\rangle + \Delta_x\end{aligned}$$

Recalling above, we have for any vector $z \in \mathbb{R}^d$ that $|\langle z, \widehat{\theta} - \theta^*\rangle| \leq \|z\|_{(X^\top X)^{-1}}\sqrt{2\log(1/\delta)}$ w.p. $\geq 1-\delta$.

We need to show that this confidence set is completely inside the $x^\star$ region. Where we need to decrease uncertainty is in the directions $x - x^\star$, clearly, which is not the G-optimal design. The most realistic optimization program

$$\begin{aligned}\rho^\star := &\inf_{\lambda\in\triangle\mathcal{X},\tau\in\mathbb{N}} \tau \\ &\text{subject to} \quad \max_{x\in\mathcal{X}} \frac{\|x^\star - x\|^2_{(\sum_{x\in\mathcal{X}}\tau\lambda_x xx^\top)^{-1}}}{\Delta_x^2} \leq \frac{1}{2} \\ = &\inf_{\lambda\in\triangle\mathcal{X}} \max_{x\in\mathcal{X}} \frac{\|x^\star - x\|^2_{(\sum_{x\in\mathcal{X}}\lambda_x xx^\top)^{-1}}}{\Delta_x^2}\end{aligned}$$

One can prove a lower bound of $\log(1/2.4\delta)\rho^\star$.

```
Input: Finite set $\mathcal{X} \subset \mathbb{R}^d$, confidence level $\delta \in (0, 1)$.
Let $\mathcal{X}_1 \leftarrow \mathcal{X}, t \leftarrow 1$
while $|\mathcal{X}_\ell| > 1$ do
  Let $\widehat{\lambda}_\ell \in \triangle_{\mathcal{X}}$ be a $\frac{d(d+1)}{2}$-sparse minimizer of $f(\lambda; \mathcal{X}_\ell)$ where
      $f(\mathcal{V}) = \inf_{\lambda \in \mathcal{X}} f(\lambda; \mathcal{V}) = \inf_{\lambda \in \mathcal{X}} \max_{x, x' \in \mathcal{V}} \|x - x'\|^2_{(\sum_{x \in \mathcal{X}} \lambda_x x x^\top)^{-1}}$
  Set $\epsilon_\ell = 2^{-\ell}$, $\tau_\ell = 2\epsilon_\ell^{-2} f(\mathcal{X}_\ell) \log(4\ell^2|\mathcal{X}|/\delta)$
  Pull arm $x \in \mathcal{X}$ exactly $\lceil \tau_\ell \widehat{\lambda}_{\ell,x} \rceil$ times and construct $\widehat{\theta}_\ell$
  $\mathcal{X}_{\ell+1} \leftarrow \mathcal{X}_\ell \setminus \left\{x \in \mathcal{X}_\ell : \max_{x' \in \mathcal{X}_\ell} \langle x' - x, \widehat{\theta}_t \rangle > \epsilon_\ell \right\}$
  $t \leftarrow t + 1$
Output: $\mathcal{X}_{t+1}$
```

Lemma 20. *Assume that* $\max_{x \in \mathcal{X}} \langle x^\star - x, \theta^* \rangle \leq 2$. *With probability at least* $1 - \delta$, *we have* $x^\star \in \mathcal{X}_\ell$ *and* $\max_{x \in \mathcal{X}_\ell} \langle x^\star - x, \theta^* \rangle \leq 4\epsilon_\ell$ *for all* $\ell \in \mathbb{N}$.

Proof. For any $\mathcal{V} \subseteq \mathcal{X}$ and $x \in \mathcal{V}$ define

$$\mathcal{E}_{x,\ell}(\mathcal{V}) = \{|\langle x - x^\star, \widehat{\theta}_\ell(\mathcal{V}) - \theta^* \rangle| \leq \epsilon_\ell\}$$

where it is implicit that $\widehat{\theta}_\ell := \widehat{\theta}_\ell(\mathcal{V})$ is the design constructed in the algorithm at stage ℓ with respect to $\mathcal{X}_\ell = \mathcal{V}$. Given $\mathcal{X}_\ell$, with probability at least $1 - \frac{\delta}{2\ell^2|\mathcal{X}|}$

$$\begin{aligned}
|\langle x - x^\star, \widehat{\theta}_\ell - \theta^* \rangle| &\leq \|x - x^\star\|_{(\sum_{x \in \mathcal{V}} \lceil \tau_\ell \lambda_{\ell,x}(\mathcal{V}) \rceil x x^\top)^{-1}} \sqrt{2 \log(4\ell^2|\mathcal{X}|/\delta)} \\
&\leq \frac{\|x - x^\star\|_{(\sum_{x \in \mathcal{V}} \lambda_{\ell,x}(\mathcal{V}) x x^\top)^{-1}}}{\sqrt{\tau_\ell}} \sqrt{2 \log(4\ell^2|\mathcal{X}|/\delta)} \\
&\leq \sqrt{\frac{\|x - x^\star\|^2_{(\sum_{x \in \mathcal{V}} \lambda_{\ell,x}(\mathcal{V}) x x^\top)^{-1}}}{2\epsilon_\ell^{-2} f(\mathcal{V}) \log(4\ell^2|\mathcal{X}|/\delta)}} \sqrt{2 \log(4\ell^2|\mathcal{X}|/\delta)} \\
&= \epsilon_\ell
\end{aligned}$$

By exactly the same sequence of steps as above, we have $\mathbb{P}(\bigcap_{\ell=1}^\infty \bigcap_{x \in \mathcal{X}_\ell} \{|\langle x - x^\star, \widehat{\theta}_t - \theta^* \rangle| > \epsilon_t\}) = \mathbb{P}\left(\bigcap_{x \in \mathcal{X}} \bigcap_{\ell=1}^\infty \mathcal{E}_{x,\ell}(\mathcal{X}_\ell)\right) \geq 1 - \delta$, so assume these events hold. Consequently, for any $x' \in \mathcal{X}_\ell$

$$\begin{aligned}
\langle x' - x^\star, \widehat{\theta}_\ell \rangle &= \langle x' - x^\star, \widehat{\theta}_\ell - \theta^* \rangle + \langle x' - x^\star, \theta^* \rangle \\
&\leq \langle x' - x^\star, \widehat{\theta}_\ell - \theta^* \rangle \\
&\leq \epsilon_\ell
\end{aligned}$$

so that $x^\star$ would survive to round $\ell + 1$. And for any $x \in \mathcal{X}_\ell$ such that $\langle x^\star - x, \theta^* \rangle > 2\epsilon_\ell$ we have

$$\begin{aligned}
\max_{x' \in \mathcal{X}_\ell} \langle x' - x, \widehat{\theta}_\ell \rangle &\geq \langle x^\star - x, \widehat{\theta}_\ell \rangle \\
&= \langle x^\star - x, \widehat{\theta}_\ell - \theta^* \rangle + \langle x^\star - x, \theta^* \rangle \\
&> -\epsilon_\ell + 2\epsilon_\ell \\
&= \epsilon_\ell
\end{aligned}$$

which implies this x would be kicked out. Note that this implies that $\max_{x \in \mathcal{X}_{\ell+1}} \langle x^\star - x, \theta^* \rangle \leq 2\epsilon_\ell = 4\epsilon_{\ell+1}$. □

Theorem 18. *Assume that $\max_{x\in\mathcal{X}}\langle x^\star - x, \theta^*\rangle \leq 2$. Then with probability at least $1-\delta$, $x^\star$ is returned from the algorithm at a time τ that satisfies*

$$\tau \leq c\rho^\star \log(\Delta^{-1})[\log(1/\delta) + \log(\log(\Delta^{-1})) + \log(|\mathcal{X}|)].$$

Proof. Define $S_\ell = \{x \in \mathcal{X} : \langle x^\star - x, \theta^*\rangle \leq 4\epsilon_\ell\}$. Note that by assumption $\mathcal{X} = \mathcal{X}_1 = S_1$. The above lemma implies that with probability at least $1-\delta$ we have $\bigcap_{\ell=1}^\infty\{\mathcal{X}_\ell \subseteq S_\ell\}$. This implies that

$$\begin{aligned} f(\mathcal{X}_\ell) &= \min_{\lambda\in\triangle_{\mathcal{X}}} \max_{x,x'\in\mathcal{X}_\ell} \|x-x'\|^2_{(\sum_{x\in\mathcal{X}}\lambda_x xx^\top)^{-1}} \\ &\leq \min_{\lambda\in\triangle_{\mathcal{X}}} \max_{x,x'\in S_\ell} \|x-x'\|^2_{(\sum_{x\in\mathcal{X}}\lambda_x xx^\top)^{-1}} \\ &= f(S_\ell) \end{aligned}$$

For $\ell \geq \lceil\log_2(4\Delta^{-1})\rceil$ we have that $S_\ell = \{x^\star\}$, thus, the sample complexity to identify $x^\star$ is equal to

$$\begin{aligned} \sum_{\ell=1}^{\lceil\log_2(4\Delta^{-1})\rceil} \sum_{x\in\mathcal{X}} \lceil \tau_\ell \widehat{\lambda}_{\ell,x}\rceil &= \sum_{\ell=1}^{\lceil\log_2(4\Delta^{-1})\rceil} \left(\tfrac{(d+1)d}{2} + \tau_\ell\right) \\ &= \sum_{\ell=1}^{\lceil\log_2(4\Delta^{-1})\rceil} \left(\tfrac{(d+1)d}{2} + 2\epsilon_\ell^{-2} f(\mathcal{X}_\ell)\log(4\ell^2|\mathcal{X}|/\delta)\right) \\ &\leq \tfrac{(d+1)d}{2}\lceil\log_2(4\Delta^{-1})\rceil + \sum_{\ell=1}^{\lceil\log_2(4\Delta^{-1})\rceil} 2\epsilon_\ell^{-2} f(S_\ell)\log(4\ell^2|\mathcal{X}|/\delta) \\ &\leq \tfrac{(d+1)d}{2}\lceil\log_2(4\Delta^{-1})\rceil + 4\log\left(\tfrac{4\log_2^2(8\Delta^{-1})|\mathcal{X}|}{\delta}\right) \sum_{\ell=1}^{\lceil\log_2(4\Delta^{-1})\rceil} 2^{2\ell} f(S_\ell). \end{aligned}$$

We now note that

$$\begin{aligned} \rho^\star &= \inf_{\lambda\in\triangle_{\mathcal{X}}} \max_{x\in\mathcal{X}} \frac{\|x-x^\star\|^2_{(\sum_{x\in\mathcal{X}}\lambda_x xx^\top)^{-1}}}{(\langle x-x^\star,\theta^*\rangle)^2} \\ &= \inf_{\lambda\in\triangle_{\mathcal{X}}} \max_{\ell\leq\lceil\log_2(4\Delta^{-1})\rceil} \max_{x\in S_\ell} \frac{\|x-x^\star\|^2_{(\sum_{x\in\mathcal{X}}\lambda_x xx^\top)^{-1}}}{(\langle x-x^\star,\theta^*\rangle)^2} \\ &\geq \frac{1}{\lceil\log_2(4\Delta^{-1})\rceil} \inf_{\lambda\in\triangle_{\mathcal{X}}} \sum_{\ell=1}^{\lceil\log_2(4\Delta^{-1})\rceil} \max_{x\in S_\ell} \frac{\|x-x^\star\|^2_{(\sum_{x\in\mathcal{X}}\lambda_x xx^\top)^{-1}}}{(\langle x-x^\star,\theta^*\rangle)^2} \\ &\geq \frac{1}{16\lceil\log_2(4\Delta^{-1})\rceil} \sum_{\ell=1}^{\lceil\log_2(4\Delta^{-1})\rceil} 2^{2\ell} \inf_{\lambda\in\triangle_{\mathcal{X}}} \max_{x\in S_\ell} \|x-x^\star\|^2_{(\sum_{x\in\mathcal{X}}\lambda_x xx^\top)^{-1}} \\ &\geq \frac{1}{64\lceil\log_2(4\Delta^{-1})\rceil} \sum_{\ell=1}^{\lceil\log_2(4\Delta^{-1})\rceil} 2^{2\ell} \inf_{\lambda\in\triangle_{\mathcal{X}}} \max_{x,x'\in S_\ell} \|x-x'\|^2_{(\sum_{x\in\mathcal{X}}\lambda_x xx^\top)^{-1}} \\ &\geq \frac{1}{64\lceil\log_2(4\Delta^{-1})\rceil} \sum_{\ell=1}^{\lceil\log_2(4\Delta^{-1})\rceil} 2^{2\ell} f(S_\ell) \end{aligned}$$

where we have used the fact that $\max_{x,x'\in S_t}\|x-x'\|^2_{(\sum_{x\in\mathcal{X}}\lambda_x xx^\top)^{-1}} \leq 4\max_{x\in S_t}\|x-x^\star\|^2_{(\sum_{x\in\mathcal{X}}\lambda_x xx^\top)^{-1}}$ by the triangle inequality. □

11.6 Regret minimization revisited

Okay, now that we know how to do optimal pure exploration, how do we turn this into an algorithm that is optimal?
Let $R_T(\mathcal{X},\theta) = \mathbb{E}_\theta[\sum_{t=1}^T \Delta_{X_t}]$, $\qquad \Delta_x = \max_{x'\in\mathcal{X}}\langle x'-x,\theta\rangle$
The next theorem is from [Lattimore and Szepesvári, 2020].

Theorem 19. *Fix any $\mathcal{X}\subset\mathbb{R}^d$ that spans $\mathbb{R}^d$ and $\theta^*\in\mathbb{R}^d$ such that $\arg\max_{x\in\mathcal{X}}\langle x,\theta^*\rangle$ is unique. Any policy for which $R_T(\mathcal{X},\theta^*) = o(T^a)$ for any $a>0$ also satisfies $\liminf_{T\to\infty}\frac{R_T(\mathcal{X},\theta^*)}{\log(T)} \geq r^\star$ where*

$$\begin{aligned} r^\star := & \inf_{\alpha\in[0,\infty)^{\mathcal{X}}} \sum_{x\in\mathcal{X}} \alpha_x\Delta_x \\ \textit{subject to} \quad & \max_{x\in\mathcal{X}} \frac{\|x^\star - x\|^2_{(\sum_{x\in\mathcal{X}}\alpha_x x x^\top)^{-1}}}{\Delta_x^2} \leq \frac{1}{2} \end{aligned}$$

Note that

$$\begin{aligned} \rho^\star := & \inf_{\alpha\in[0,\infty)^{\mathcal{X}}} \frac{1}{2}\sum_{x\in\mathcal{X}} \alpha_x \\ \text{subject to} \quad & \max_{x\in\mathcal{X}} \frac{\|x^\star - x\|^2_{(\sum_{x\in\mathcal{X}}\alpha_x x x^\top)^{-1}}}{\Delta_x^2} \leq \frac{1}{2} \end{aligned}$$

Notes

- There exists an asymptotic algorithm [Lattimore and Szepesvari, 2016], but no satisfying finite-time algorithm as of yet.
- Information directed sampling may be near-optimal and very high performance.

Chapter 12

Contextual Bandits

12.1 Introduction

This section is inspired by [Lattimore and Szepesvári, 2020]
For $t = 1, 2, \dots$

- Nature reveals $c_t \overset{iid}{\sim} \mathcal{D}$
- Player chooses $a_t \in \mathcal{A}$ and observes $y_t = v(c_t, a_t) + \epsilon_t$

which models users showing up to websites, or patients showing up to the doctor with different symptoms.

12.1.1 Finite contexts

Suppose the space of contexts, denoted $\mathcal{C}$, is finite. Then a natural algorithm would be to run an individual multi-armed bandit algorithm (action elimination, UCB, etc.) per context. We know that after T time steps, such a strategy applied to context $c \in \mathcal{C}$ would satisfy

$$\max_{a \in \mathcal{A}} \sum_{t=1}^{T} \mathbf{1}\{c_t = c\} v(c, a) - \sum_{t=1}^{T} \mathbf{1}\{c_t = c\} v(c, a_t) \lesssim \sqrt{T_c |\mathcal{A}| \log(T_c |\mathcal{A}|/\delta)} \leq \sqrt{T_c |\mathcal{A}| \log(T|\mathcal{A}|/\delta)}.$$

where $T_c := \sum_{t=1}^{T} \mathbf{1}\{c_t = c\}$. Summing over contexts we have

$$\begin{aligned}\sum_{c \in \mathcal{C}} \max_{a \in \mathcal{A}} \sum_{t=1}^{T} \mathbf{1}\{c_t = c\} \left(v(c, a) - v(c, a_t)\right) &\lesssim \sum_{c \in \mathcal{C}} \sqrt{T_c |\mathcal{A}| \log(T|\mathcal{A}|/\delta)} \\ &\leq \sqrt{|\mathcal{C}| \; |\mathcal{A}| T \log(T|\mathcal{A}|/\delta)} \qquad (12.1)\end{aligned}$$

by Cauchy-Schwartz.

The clear problem with this strategy is that this regret is trivial if $|\mathcal{C}|$ is very large. Indeed, if we had just *ignored* the context altogether at each time t, we could just play a multi-armed bandit algorithm to achieve

$$\max_{a \in \mathcal{A}} \sum_{t=1}^{T} \left(v(c_t, a) - v(c_t, a_t)\right) \lesssim \sqrt{|\mathcal{A}| T \log(T|\mathcal{A}|/\delta)}. \qquad (12.2)$$

While the right hand side of (12.2) appears much smaller than the right hand side of (12.1) (by a factor of $\sqrt{|\mathcal{C}|}$) we point out that the left had sides are not equivalent – they're using a different benchmark of regret! The first compares to the best single action *per context* whereas the latter compares itself to the single best action with respect to *all contexts.* The first is a much higher standard. The next section formalizes a unifying benchmark, which we denote as policy regret.

12.1.2 Policy Regret

A policy $\pi : \mathcal{C} \to \mathcal{A}$ maps contexts to actions. The value of a policy π is defined as

$$V(\pi) = \mathbb{E}_{C,\epsilon}[v(C, \pi(C)) + \epsilon] = \mathbb{E}_C[v(C, \pi(C))].$$

We assume at the start of the game the learner has access to a set of policies Π which may be infinite, but for simplicity we will assume it is finite. At each time, we assume the action taken is according to some policy $\pi_t \in \Pi$ so that the regret is defined as

$$R_T = T \cdot \max_{\pi \in \Pi} V(\pi) - \mathbb{E}[\sum_{t=1}^{T} V(\pi_t)]$$

and for convenience, we will fix a $\pi^\star := \arg\max_{\pi\in\Pi} V(\pi)$.
Connecting to the previous section, $|\Pi| = |\mathcal{A}|^{|\mathcal{C}|}$ and $|\Pi| = |\mathcal{A}|$ respectively.

12.2 Policy evaluation

Suppose for each policy $\pi \in \Pi$ we wished to estimate $V(\pi)$ up to tolerance $\epsilon > 0$ with probability at least $1 - \delta$. A naive strategy would be to simply play policy π for some number of trials to estimate its value. That is, for some $\tau \in \mathbb{N}$, play each $\pi \in \Pi$ for τ trials in response to the IID contexts. For each π this would result in a set of rewards $\{r_t^\pi\}_{t=1}^\tau$ each in $[0, 1]$ which we can use to define $\widehat{V}(\pi) = \frac{1}{\tau}\sum_{t=1}^{\tau} r_t^\pi$. By Hoeffding's inequality and a union bound, we have that

$$\mathbb{P}\left(\bigcup_{\pi\in\Pi}\{|\widehat{V}(\pi) - V(\pi)| \geq \sqrt{\log(2|\Pi|/\delta)/2\tau}\right) \leq \delta.$$

Thus, if $\tau \geq \epsilon^{-2}\log(2|\Pi|/\delta)/2$ samples were taken for each policy $\pi \in \Pi$ we can estimate each $V(\pi)$ up to tolerance ϵ with probability at least $1 - \delta$ using $\epsilon^{-2}|\Pi|\log(2|\Pi|/\delta)/2$. But this linear scaling in $|\Pi|$ is awful if $|\Pi|$ is large! Can we do better?

12.2.1 Logging policy

The core difficulty of model evaluation in contextual bandits is that if I take action i and receive a reward with mean $v(c_t, i)$, I don't observe $v(c_t, j)$ for some $j \neq i$. But if every context appears very rarely so that I cannot rely on seeing the same context multiple times, how can I predict what I should have done? We will employ the use of a randomized logging policy to help us solve this riddle.

For any context c fix an exploration distribution $\mu(a|c) \in \triangle_{\mathcal{A}}$ such that $\mu(a|c) > 0$ for all a, c. The distribution $\mu(a|c)$ will act as our randomized logging policy to collect data in aid of estimating each $V(\pi)$ efficiently. We can define $\mu(a|c)$ independently of Π, or we can perform "proper learning" so that $\mu(a|c)$ is actually playing a random policy $\pi \in \Pi$ at each time. To do this, fix some distribution over policies $\lambda \in \triangle_\Pi$, and then at each time t, draw $\pi_t \sim \lambda$ and play $a_t = \pi_t(c_t)$. Here, $\mu(a|c) = \sum_{\pi\in\Pi} \lambda_\pi \mathbf{1}\{\pi(c) = a\}$.

If we play the logging policy for $\tau \in \mathbb{N}$ rounds, at each time $t = 1, \dots, \tau$ nature reveals a context $c_t \sim \mathcal{D}$, the logging policy plays $a_t \sim \mu(\cdot|c_t)$, and receives reward $r_t = v(c_t, a_t) + \epsilon_t \in [0, 1]$ where $\mathbb{E}[\epsilon_t] = 0$, by assumption. This results in a dataset $\{(c_t, a_t, r_t, p_t)\}_{t=1}^\tau$ where $p_t := \mu(a_t|c_t)$. Given this dataset, we wish to estimate each $V(\pi)$. We describe two ways to do so described as *model the bias* and *model the world*. We will also consider a hybrid of the two.

12.2.2 Model the bias

If we just naively estimated $V(\pi)$ with $\frac{1}{\tau}\sum_{t=1}^\tau r_t \mathbf{1}\{\pi(c_t) = a_t\}$ this would be a biased estimator: its expectation may not converge to $V(\pi)$ no matter how large τ is. We now define an unbiased estimator for $V(\pi)$. Define the *inverse propensity scoring* estimator as

$$\widehat{v}(c_t, a) := r_t \frac{\mathbf{1}\{a_t = a\}}{p_t}, \qquad \text{and} \qquad \widehat{V}(\pi) = \frac{1}{\tau}\sum_{t=1}^{\tau} \widehat{v}(c_t, \pi(c_t)).$$

Note that $\widehat{V}(\pi)$ is unbiased since

$$\mathbb{E}[\widehat{V}(\pi)] = \frac{1}{\tau}\sum_{t=1}^{\tau} \mathbb{E}[\widehat{v}(c_t, \pi(c_t))] = \frac{1}{\tau}\sum_{t=1}^{\tau} \mathbb{E}[\mathbb{E}[\widehat{v}(c_t, \pi(c_t))|c_t]] = \mathbb{E}_{C\sim\mathcal{D}}[v(C, \pi(C))] = V(\pi)$$

and

$$\begin{aligned}
\mathbb{E}[\widehat{v}(c_t, a)|c_t] &= \mathbb{E}\left[r_t \frac{\mathbf{1}\{a_t = a\}}{p_t}|c_t\right] \\
&= \sum_{a'\in\mathcal{A}} \mu(a'|c_t)\mathbb{E}\left[r_t \frac{\mathbf{1}\{a_t = a\}}{\mu(a_t|c_t)}|c_t, a_t = a'\right] \\
&= \sum_{a'\in\mathcal{A}} \mu(a'|c_t) v(c_t, a') \frac{\mathbf{1}\{a' = a\}}{\mu(a'|c_t)} \\
&= v(c_t, a).
\end{aligned}$$

The variance of $\widehat{V}(\pi)$ is

$$\mathbb{E}[(\widehat{V}(\pi) - V(\pi))^2] = \frac{1}{\tau^2}\sum_{t=1}^{\tau} \mathbb{E}[\mathbb{E}[(\widehat{v}(c_t, \pi(x)) - v(c_t, \pi(x)))^2|c_t]] \leq \frac{1}{\tau}\mathbb{E}_{C\sim\mathcal{D}}\left[\frac{1}{\mu(\pi(C)|C)}\right]$$

due to

$$\begin{aligned}
\mathbb{E}[(\widehat{v}(c_t, a) - v(c_t, a))^2|c_t] &\leq \mathbb{E}[(\widehat{v}(c_t, a))^2|c_t] \\
&\leq \mathbb{E}\left[\frac{\mathbf{1}\{a_t = a\}}{\mu(a_t|c_t)^2}|c_t\right] \qquad\qquad (r_t \in [0, 1]) \\
&\leq \sum_{a'\in\mathcal{A}} \mu(a'|c_t) \frac{\mathbf{1}\{a' = a\}}{\mu(a'|c_t)^2} \\
&= \frac{1}{\mu(a|c_t)}.
\end{aligned}$$

We will use Bernstein's inequality (Lemma 12 in Chapter 2), which states that for independent random variables $X_1, \dots, X_m$ with $\frac{1}{m}\sum_{i=1}^m \mathbb{E}[(X_i - \mathbb{E}[X_i])^2] \leq \sigma^2$ and $|X_i| \leq B$, with probability at least $1-\delta$,

$$\left| \frac{1}{m}\sum_{i=1}^m X_i - \mathbb{E}[X_i] \right| \leq \sqrt{\frac{2\sigma^2 \log(2/\delta)}{m}} + \frac{2B\log(2/\delta)}{3m},$$

and the same bound holds when $X_1, \dots, X_m$ form a martingale difference sequence.

If $v_{\max} := \max_c \max_{\pi\in\Pi} \frac{1}{\mu(\pi(c)|c)}$ and

$$C_\tau(\pi) := \sqrt{\frac{2\log(2|\Pi|/\delta)}{\tau}\mathbb{E}_{C\sim\mathcal{D}}\left[\frac{1}{\mu(\pi(C)|C)}\right]} + \frac{2\widehat{v}_{\max}\log(2|\Pi|/\delta)}{3\tau}$$

then by Bernstein's inequality we have $\mathbb{P}\left(\bigcup_{\pi\in\Pi}\{|V(\pi) - \widehat{V}(\pi)| \leq C_\tau(\pi)\}\right) \leq \delta$. We can also derive a data-dependent bound by defining $\mathcal{F}_{i-1} = (c_1, a_1, r_1, \dots, c_{i-1}, a_{i-1}, r_{i-1}, c_i, a_i\}$ so that (c_i, a_i) are $\mathcal{F}_{i-1}$ measurable and

$$\widehat{C}_\tau(\pi) := \sqrt{\frac{2\log(2|\Pi|/\delta)}{\tau}\sum_{t=1}^{\tau}\frac{1/\tau}{p_t}} + \frac{2\widehat{v}_{\max}\log(2|\Pi|/\delta)}{3\tau}$$

to conclude that $\mathbb{P}\left(\bigcup_{\pi\in\Pi}\{|V(\pi) - \widehat{V}(\pi)| \leq \widehat{C}_\tau(\pi)\}\right) \leq \delta$.

In particular, if we set $\mu(a|c) = \frac{1}{|\mathcal{A}|}$ for all a, c then for any $\tau \geq 2|\mathcal{A}|\log(2|\Pi|/\delta)$ we have

$$|V(\pi) - \widehat{V}(\pi)| \leq \sqrt{\frac{2|\mathcal{A}|\log(2|\Pi|/\delta)}{\tau}} + \frac{2|\mathcal{A}|\log(2|\Pi|/\delta)}{3\tau} \leq \sqrt{\frac{4|\mathcal{A}|\log(2|\Pi|/\delta)}{\tau}}$$

for all $\pi \in \Pi$ with probability at least $1-\delta$. Thus, it suffices to take $\tau = 4\epsilon^{-2}|\mathcal{A}|\log(2|\Pi|/\delta)$ samples to estimate every $V(\pi)$ up to tolerance ϵ with probability at least $1-\delta$.

12.2.3 Principle of Pessimism for Off-policy optimization

Frequently, μ will not be uniform but some arbitrary logging policy that has been running for a while to collect data. If one had to output a best guess of the best policy, a natural choice is $\widehat{\pi}_{mle} := \arg\max_\pi \widehat{V}(\pi)$ which satisfies

$$\begin{aligned} V(\widehat{\pi}_{mle}) &= \widehat{V}(\widehat{\pi}_{mle}) - V(\widehat{\pi}_{mle}) + \widehat{V}(\widehat{\pi}_{mle}) \\ &\geq \widehat{V}(\pi_*) - C_\tau(\widehat{\pi}_{mle}) \\ &\geq V(\pi_*) - C_\tau(\pi_*) - C_\tau(\widehat{\pi}_{mle}) \\ &\geq V(\pi_*) - \max_{\pi\in\Pi} 2C_\tau(\pi_*) \end{aligned}$$

which suggests we need to estimate *every* policy uniformly well for $\widehat{\pi}_{mle}$ to perform well since we don't know how to bound $C_\tau(\widehat{\pi}_{mle})$.

Alternatively, define $\widehat{\pi}_{pess} = \arg\max_{\pi\in\Pi} \widehat{V}(\pi) - C_\tau(\pi)$ that penalizes policies that are poorly estimated. Then

$$\begin{aligned} V(\widehat{\pi}_{mle}) &= \widehat{V}(\widehat{\pi}_{mle}) - V(\widehat{\pi}_{mle}) + \widehat{V}(\widehat{\pi}_{mle}) \\ &\geq \widehat{V}(\widehat{\pi}_{mle}) - C_\tau(\widehat{\pi}_{mle}) \\ &\geq \widehat{V}(\pi_*) - C_\tau(\pi_*) \\ &\geq V(\pi_*) - 2C_\tau(\pi_*) \end{aligned}$$

which suggests we only need to estimate π_* well, which could lead to a much better output policy!

12.2.4 Model the world

Consider a function class $\mathcal{F}$ such that for each $f \in \mathcal{F}$ we have $f : \mathcal{C} \times \mathcal{A} \to \mathbb{R}$. The idea is that some function $f_* \in \mathcal{F}$ is close enough to $v(c, a)$ to be useful, and that we can identify f_* or some function close to it using our collected dataset $\{(c_t, a_t, r_t, p_t)\}_{t=1}^{\tau}$. Let

$$\widehat{f} = \arg\min_{f\in\mathcal{F}} \sum_{t=1}^{\tau} (r_t - f(c_t, a_t))^2.$$

We can then estimate $V(\pi)$ with $\widehat{V}(\pi) = \frac{1}{\tau}\sum_{t=1}^{\tau} \widehat{f}(c_t, \pi(c_t))$. This incurs an expected error of

$$\begin{aligned} \mathbb{E}|V(\pi) - \widehat{V}(\pi)| &= \mathbb{E}|\mathbb{E}_C[v(C, \pi(C)) - \widehat{f}(C, \pi(C))]| \\ &\leq |\mathbb{E}_C[v(C, \pi(C)) - f_*(C, \pi(C))]| + \mathbb{E}|\mathbb{E}_C[f_*(C, \pi(C)) - \widehat{f}(C, \pi(C))]| \\ &\leq \underbrace{|\mathbb{E}_C[v(C, \pi(C)) - f_*(C, \pi(C))]|}_{bias} + \sqrt{\underbrace{\mathbb{E}|\mathbb{E}_C[f_*(C, \pi(C)) - \widehat{f}(C, \pi(C))]|^2}_{variance}}. \end{aligned}$$

The bias is unavoidable if $f_* \neq v$ which happens if $v \notin \mathcal{F}$. However, if $\mu(a|c) > 0$ for all a, c then as $\tau \to \infty$ the variance term goes to zero and we have that $\widehat{f} \to f_*$. Below we will see how the variance term behaves as a function of $\mu(a|c)$ for linear functions.

We say the contextual bandit instance is *realizable* if $v \in \mathcal{F}$, and a great number of works have taken advantage of this fact. If $v \notin \mathcal{F}$ then this technique is biased and no matter how much data you collect, you may never get accurate estimates for the true value of a policy $\pi \in \Pi$. Nevertheless, this method is extremely popular in practice because its so easy to solve a least squares problem like the above for arbitrary function classes, like neural networks. Then people will just use $a_t = \arg\max_{a\in\mathcal{A}} f(c_t, a)$, totally bypassing the definition of the policy class Π.

12.2.5 Doubly robust estimators

The *model the bias* approach potentially has high variance and the *model the world* approach potentially has high bias. Doubly robust methods get the best of both worlds: unbiased but if the model $\widehat{f}$ is close to the true v then the variance is reduced [Dudík et al., 2011]. Technically, $\widehat{f}$ should be trained using data independent of our dataset $\{(c_t, a_t, r_t, p_t)\}_{t=1}^{\tau}$, like a hold-out set, but in practice people will often just reuse the dataset. Define

$$\widehat{v}_{DR}(c_t, a) = \widehat{f}(c_t, a) + (r_t - \widehat{f}(c_t, a))\frac{\mathbf{1}\{a_t = a\}}{p_t}.$$

It is easy to check this is unbiased with expectation $v(c_t, a)$. In the variance calculation of IPS we simply used the fact that r_t was bounded in magnitude by 1. Here, we will take advantage of the possibility that r_t may be close to $\widehat{f}(c_t, a)$. If r_t still has lots of intrinsic variance, this method won't help much, but if $|r_t - \widehat{f}(c_t, a)|$ is small, it can help a lot.

12.3 Stochastic Linear model

Consider a very special case of *model the world* where we assume that $v(c, a) = \langle \phi(c, a), \theta_* \rangle$ for some $\theta_* \in \mathbb{R}^d$ and Π is induced by all possible $\theta \in \mathbb{R}^d$ with $\pi(c) = \arg\max_{a \in \mathcal{A}} \langle \phi(c, a), \theta_* \rangle$ We can restate the above models as For $t = 1, 2, \dots$

- Nature reveals $(x_{t,1}, \dots, x_{t,n}) = \mathcal{X}_t \subset \mathbb{R}^d$
- Player chooses $I_t \in [n]$ and observes $y_t = \langle x_{t,I_t}, \theta^* \rangle + \epsilon_t$

When we had a fixed action set, we built confidence intervals on $\langle x_i, \widehat{\theta} - \theta^* \rangle$. Now that we don't know what action sets to expect, a natural to assume $\max_{i,t} \|x_{i,t}\| \leq 1$ and build confidence intervals on $\sup_{u:\|u\|_2 \leq 1} \langle u, \widehat{\theta} - \theta^* \rangle = \|\widehat{\theta} - \theta^*\|_2$, or equivalently, define a set C_t with the guarantee that $\theta^* \in C_t$ for all t. When an action set $\mathcal{X}_t$ shows up, we could eliminate all provably sub-optimal arms by setting $\mathcal{X}_t = \mathcal{X} \setminus \{x : \max_{x' \in \mathcal{X}} \langle x' - x, \theta \rangle < 0 \; \forall \theta \in C_t\}$ and play uniformly in this set. An alternative is to run UCB, defining:

$$UCB_t(x) = \max_{\theta \in C_t} \langle x, \theta \rangle$$

and play $x_t = \arg\max_{x \in \mathcal{X}_t} UCB_t(x)$. If $x_t^\star = \arg\max_{x \in \mathcal{X}_t} \langle x, \theta^* \rangle$ then

$$\langle x_t^\star, \theta^* \rangle \leq UCB_t(x_t^\star) \leq UCB_t(x_t) = \langle x_t, \widetilde{\theta} \rangle$$

where $\widetilde{\theta} = \arg\max_{\theta \in C_t} \langle x_t, \theta \rangle$. Thus, the instantaneous regret at time t satisfies

$$\begin{aligned} r_t &= \langle x_t^\star - x_t, \theta^* \rangle \\ &\leq \langle x_t, \widetilde{\theta} - \theta^* \rangle \\ &\leq \|x_t\|_{A_{t-1}^{-1}} \|\widetilde{\theta} - \theta^*\|_{A_{t-1}} \\ &\leq 2\|x_t\|_{A_{t-1}^{-1}} \sqrt{\beta_{t-1}} \end{aligned}$$

Thus, the random regret satisfies

$$\widehat{R}_T = \sum_{t=1}^T r_t \leq \sqrt{T \sum_{t=1}^T r_t^2} \approx \sqrt{2T\beta_T \sum_{t=1}^T \|x_t\|^2_{A_{t-1}^{-1}}}$$

Let $\hat{\theta}_t$ be the ℓ^2-regularized least-squares estimate of θ_* with regularization parameter $\lambda > 0$ given by

$$\hat{\theta}_t = \arg\min_\theta \|\mathbf{X}_{1:t}\theta - \mathbf{Y}_{1:t}\| + \lambda \|\theta\|_2^2 = (\mathbf{X}_{1:t}^T \mathbf{X}_{1:t} + \lambda I)^{-1} \mathbf{X}_{1:t}^T \mathbf{Y}_{1:t}$$

where we are denoting $\mathbf{X}_{1:t}$ as a matrix with rows $X_1^T, X_2^T, \dots, X_t^T$ and $\mathbf{Y}_{1:t}$ as the vector $(Y_1, \dots, Y_t)^T$. The following theorem says that with high probability θ_* lies with high probability in an ellipsoid with center at $\hat{\theta}_t$.

Theorem 20. *Confidence Ellipsoid. Assume the same as in Theorem **??**, let $V = I\lambda, \lambda > 0$, define $Y_t = \langle X_t, \theta_t \rangle + \eta_t$ and assume that $\|\theta_*\| \leq S$. Then for any $\delta > 0$, with probability at least $1-\delta$, for all $t \geq 0, \theta_*$ lies in the set*

$$C_t = \left\{ \theta \in \mathbb{R}^d : \|\hat{\theta} - \theta\|_{\overline{V}_t} \leq R\sqrt{2\log(\frac{\det(\overline{V}_t)^{1/2})\det(\lambda I)^{-1/2}}{\delta})} + \lambda^{1/2}S \right\}.$$

Furthermore, if for all $t \geq 1, \|X_t\|_2 \leq L$ then with probability at least $1-\delta$, for all $t \geq 0, \theta_*$ lies in the set

$$C'_t = \left\{ \theta \in \mathbb{R}^d : \|\hat{\theta} - \theta\|_{\overline{V}_t} \leq R\sqrt{d\log(\frac{1+tL^2/\lambda}{\delta})} + \lambda^{1/2}S \right\}.$$

12.4 Stochastic Contextual Bandits for General policy classes

Let's return to the general setting of trying to minimize policy regret without assuming a parametric structure on $v(c,a)$. Fix some policy set Π.

12.4.1 τ-greedy

Consider running the uniform exploration logging policy of above for τ steps. If $\epsilon_\tau := \sqrt{\frac{4|\mathcal{A}|\log(2|\Pi|/\delta)}{\tau}}$ and $\widehat{\pi} = \arg\max_{\pi\in\Pi}\widehat{V}(\pi)$ then

$$\begin{aligned} V(\widehat{\pi}) &= \underbrace{V(\widehat{\pi}) - \widehat{V}(\widehat{\pi})}_{\geq -\epsilon_\tau} + \underbrace{\widehat{V}(\widehat{\pi}) - \widehat{V}_t(\pi^\star)}_{\geq 0} + \underbrace{\widehat{V}(\pi^\star) - V(\pi^\star)}_{\geq -\epsilon_\tau} + V(\pi^\star) \\ &\geq V(\pi^\star) - 2\epsilon_\tau \end{aligned}$$

If we explore uniformly for τ rounds according to our logging policy and then exploit for $T-\tau$ rounds then we achieve a regret of at most

$$1\cdot\tau + 2\epsilon_\tau\cdot(T-\tau) \leq \tau + T\sqrt{\frac{4|\mathcal{A}|\log(2|\Pi|/\delta)}{\tau}}$$

which is minimized at $\tau = (|\mathcal{A}|T^2\log(2|\Pi|/\delta))^{1/3}$ which yields a regret of $O(T^{2/3}(|\mathcal{A}|\log(2|\Pi|/\delta))^{1/3})$ regret.

12.4.2 Reduction to cost-sensitive classification

The above τ-greedy procedure requires a solution to the optimization problem $\widehat{\pi} = \arg\max_{\pi\in\Pi}\widehat{V}(\pi)$. Note that

$$\begin{aligned} \arg\max_{\pi\in\Pi}\widehat{V}(\pi) &= \arg\max_{\pi\in\Pi}\frac{1}{\tau}\sum_{t=1}^{\tau}\frac{\mathbf{1}\{a_t = \pi(c_t)\}}{p_t}r_t \\ &= \arg\max_{\pi\in\Pi}\frac{1}{\tau}\sum_{t=1}^{\tau}(1 - \mathbf{1}\{a_t \neq \pi(c_t)\})\frac{r_t}{p_t} \\ &= \arg\min_{\pi\in\Pi}\frac{1}{\tau}\sum_{t=1}^{\tau}\mathbf{1}\{a_t \neq \pi(c_t)\}\frac{r_t}{p_t}. \end{aligned}$$

where the last line is empirical risk minimization of the 0/1-loss with example-label pairs (c_t, a_t) weighted by $\frac{r_t}{p_t}$.

Example 4. *Let $\phi : \mathcal{C} \times \mathcal{A} \to \mathbb{R}^d$ be a feature map and assume Π is parameterized by $\mathbb{R}^d$ so that for every $\theta \in \mathbb{R}^d$ there exists a $\pi \in \Pi$ such that $\pi(c_t) = \arg\max_{a \in \mathcal{A}} \langle \theta, \phi(c_t, a) \rangle$. Note, unlike Section 12.3, we are not assuming anything about the relationship between $\langle \theta, \phi(c, a) \rangle$ and $v(c, a)$. A natural convex relaxation of $\mathbf{1}\{a_t \neq \pi(c_t)\}$ is cross-entropy loss $-\log(\frac{\exp(\langle \theta, \phi(c_t, a_t) \rangle)}{\sum_{a \in \mathcal{A}} \exp(\langle \theta, \phi(c_t, a) \rangle)})$. We can approximate $\widehat{\pi} = \arg\max_{\pi \in \Pi} \widehat{V}(\pi)$ with an iterative algorithm where $\theta_{k+1} = \theta_k + \eta_k \sum_{t=1}^{\tau} \frac{r_t}{p_t} \nabla_\theta \log(\frac{\exp(\langle \theta, \phi(c_t, a_t) \rangle)}{\sum_{a \in \mathcal{A}} \exp(\langle \theta, \phi(c_t, a) \rangle)}$ for some step size sequence η_k.*

12.4.3 Elimination algorithm

We will make the strong assumption that the distribution of contexts $\mathcal{D}$ is known a priori. This is not so implausible due to historical data, and often one can proceed in stages where the previous stage's data can be used to approximate the context distribution. The algorithm and analysis is inspired by [Dudik et al., 2011].

Recall the value of a policy $\pi \in \Pi$ as $V(\pi) = \mathbb{E}_{C \sim \mathcal{D}}[v(C, \pi(C))]$. Taking our G-optimality approach, we aim to sequentially define a distribution λ over policies Π and at each time play according to $\pi_t \sim \lambda$. Given an active set of policies still under consideration, we wish to identify the distribution that minimizes

$$\min_{\lambda \in \Delta_{\widehat{\Pi}}} \max_{\pi \in \widehat{\Pi}} \mathbb{E}[(\widehat{V}_t(\pi) - V(\pi))^2]$$

for some active set $\widehat{\Pi} \subset \Pi$.

```
**Input**: Policy set $\Pi$ such that $\pi : \mathcal{C} \to \mathcal{A}$ for all $\pi \in \Pi$, $n = |\mathcal{A}|$, confidence level $\delta \in (0, 1)$.
Let $\widehat{\Pi}_1 \leftarrow \Pi, \ell \leftarrow 1, T_0 \leftarrow 0$
**while** $|\widehat{\Pi}_\ell| > 1$ **do**
  $\epsilon_\ell = 2^{-\ell}$, $\tau_\ell = \lceil 16 n \epsilon_\ell^{-2} \log(2|\Pi|T/\delta) \rceil$, $\gamma_\ell = \min\{\frac{1}{2n}, \sqrt{\frac{\log(2|\Pi|T/\delta)}{9n\tau_\ell}}\}$, $T_\ell = T_{\ell-1} + \tau_\ell$
  $Q_\ell = \arg\min_{Q \in \triangle_{\widehat{\Pi}_\ell}} \max_{\pi \in \widehat{\Pi}_\ell} \mathbb{E}_C \left[ \frac{1}{Q^{\gamma_\ell}(\pi(C)|C)} \right]$
                 s.t. $Q^\gamma(a|c) = \gamma + (1 - \gamma n) \sum_{\pi \in \widehat{\Pi}_\ell : \pi(c) = a} Q(\pi)$
  **for** $t = T_{\ell-1} + 1, \ldots, T_\ell$
    Observe context $c_t$
    Play $a_t \sim Q^\gamma(\cdot|c_t)$, set $p_t = Q^\gamma(a_t|c_t)$ and observe reward $r_t = v(c_t, a_t) + \eta_t$
  Set $\widehat{V}_\ell(\pi) = \frac{1}{T_\ell - T_{\ell-1}} \sum_{t \in (T_{\ell-1}, T_\ell]} r_t \frac{\mathbf{1}\{\pi(c_t) = a_t\}}{p_t}$
  $\widehat{\Pi}_{\ell+1} \leftarrow \widehat{\Pi}_\ell \setminus \{\pi \in \widehat{\Pi}_\ell | \max_{\pi' \in \widehat{\Pi}_\ell} \widehat{V}_\ell(\pi') - \widehat{V}_\ell(\pi) \geq 2\epsilon_\ell\}$
  $t \leftarrow t + 1$
**Output**: $\Pi_{t+1}$
```

The following lemma is somewhat of a generalization of Kiefer-Wolfowitz.

Lemma 21. *Let $\xi \in \Xi$ be a random variable and let $\phi : \mathcal{A} \times \Xi \to \mathbb{R}^d$. Then*

$$\min_{\lambda \in \triangle_{\mathcal{A}}} \max_{a \in \mathcal{A}} \mathbb{E}_\xi \left[\phi(a, \xi)^\top \left(\sum_{a' \in \mathcal{A}} \lambda_{a'} \phi(a', \xi) \phi(a', \xi)^\top \right)^\dagger \phi(a, \xi) \right] \leq d,$$

with equality if $\dim\mathrm{span}(\{\phi(a, \xi) : a \in \mathcal{A}\}) = d$ *for all* $\xi \in \Xi$.

Proof. Define $f(\lambda) = \mathbb{E}_\xi\left[f(\lambda;\xi)\right]$ and $f(\lambda;\eta) = \operatorname{logdet}\left(\sum_{a\in\mathcal{A}} \lambda_a V_\eta \phi(a,\eta)\phi(a,\eta)^\top V_\eta^\top\right)$ where $V_\eta \in \mathbb{R}^{k\times d}$ satisfies $V_\eta^\top V_\eta \phi(a;\eta) = \phi(a;\eta)$ and $k = \operatorname{dimspan}(\{\phi(a,\eta) : a \in \mathcal{A}\})$. First note that for any $A : \mathbb{R} \to \mathbb{R}^{k\times k}$ we have $\frac{d}{dt}\operatorname{logdet}\left(A(t)\right)|_{t=t_0} = \operatorname{Trace}(A(t_0)^{-1}\frac{dA(t)}{dt}|_{t=t_0})$. Thus

$$
\begin{aligned}
\frac{\partial f(\lambda;\xi)}{\partial \lambda_a} &= \operatorname{Trace}\left(\left(\sum_{a'\in\mathcal{A}} \lambda_{a'} V_\xi \phi(a',\xi)\phi(a',\xi)^\top V_\xi^\top\right)^{-1} V_\xi\phi(a,\xi)\phi(a,\xi)^\top V_\xi^\top\right)\\
&= \phi(a,\xi)^\top V_\xi^\top \left(\sum_{a'\in\mathcal{A}} \lambda_{a'} V_\xi \phi(a',\xi)\phi(a',\xi)^\top V_\xi^\top\right)^{-1} V_\xi\phi(a,\xi)\\
&= \phi(a,\xi)^\top \left(\sum_{a'\in\mathcal{A}} \lambda_{a'} \phi(a',\xi)\phi(a',\xi)^\top\right)^{\dagger} \phi(a,\xi)
\end{aligned}
$$

Note that for any λ we have $\langle \nabla f(\lambda;\xi), \lambda\rangle = \operatorname{dimspan}(\phi(a',\xi) : a' \in \mathcal{A})$. Let $\lambda^* = \arg\min_{\lambda\in\triangle_{\mathcal{A}}} f(\lambda)$ and fix any $a \in \mathcal{A}$. Then by first order conditions,

$$
\begin{aligned}
0 &\geq \langle \nabla f(\lambda^*), \mathbf{e}_a - \lambda^*\rangle\\
&= \mathbb{E}_\xi\left[\langle \nabla f(\lambda^*;\xi), \mathbf{e}_a\rangle - \operatorname{dimspan}(\phi(a',\xi) : a' \in \mathcal{A})\right]\\
&\geq \mathbb{E}_\xi\left[\phi(a,\xi)^\top \left(\sum_{a'\in\mathcal{A}} \lambda^*_{a'} \phi(a',\xi)\phi(a',\xi)^\top\right)^{\dagger} \phi(a,\xi)\right] - \max_{\eta\in\Xi} \operatorname{dimspan}(\phi(a',\eta) : a' \in \mathcal{A})
\end{aligned}
$$

Because $a \in \mathcal{A}$ was arbitrary, this completes the first part of the proof. Now suppose $d = \max_{\eta\in\Xi} \operatorname{dimspan}(\phi(a',\eta) : a' \in \mathcal{A})$. Then by the previous display we have

$$
\begin{aligned}
d &\geq \max_{a\in\mathcal{A}} \mathbb{E}_\xi\left[\phi(a,\xi)^\top \left(\sum_{a'\in\mathcal{A}} \lambda^*_{a'} \phi(a',\xi)\phi(a',\xi)^\top\right)^{\dagger} \phi(a,\xi)\right]\\
&\geq \min_{\lambda\in\triangle_{\mathcal{A}}} \max_{a\in\mathcal{A}} \mathbb{E}_\xi\left[\phi(a,\xi)^\top \left(\sum_{a'\in\mathcal{A}} \lambda_{a'} \phi(a',\xi)\phi(a',\xi)^\top\right)^{\dagger} \phi(a,\xi)\right]\\
&\geq \min_{\lambda\in\triangle_{\mathcal{A}}} \sum_{a\in\mathcal{A}} \lambda_a \mathbb{E}_\xi\left[\phi(a,\xi)^\top \left(\sum_{a'\in\mathcal{A}} \lambda_{a'} \phi(a',\xi)\phi(a',\xi)^\top\right)^{\dagger} \phi(a,\xi)\right]\\
&= d
\end{aligned}
$$

which completes the proof. □

However, the original proof in [Dudik et al., 2011] proves this result in a very different way, appealing to Sion's minimax theorem.

Lemma 22. *For any finite policy set* Π *we have*

$$
\min_{Q\in\triangle_\Pi} \max_{\pi\in\Pi} \mathbb{E}_C\left[\frac{1}{Q(\pi(C)|C)}\right] \leq |\mathcal{A}|,
$$

with equality if $|\cup_{\pi\in\Pi}\pi(c)| = |\mathcal{A}|$ *for all* c. *Moreover, for any finite policy set* Π *and* $\gamma \leq \frac{1}{2|\mathcal{A}|}$ *we have*

$$
\min_{Q\in\triangle_\Pi} \max_{\pi\in\Pi} \mathbb{E}_C\left[\frac{1}{Q^\gamma(\pi(C)|C)}\right] = \min_{Q\in\triangle_\Pi} \max_{\pi\in\Pi} \mathbb{E}_C\left[\frac{1}{\gamma + (1-\gamma|\mathcal{A}|)Q(\pi(C)|C)}\right] \leq 2|\mathcal{A}|.
$$

Proof. Consider $i = 1, \dots, |\mathcal{A}|$ actions and for each $c \in \mathcal{C}$ define $\pi_c := \mathbf{e}_{\pi(c)} \in \{0,1\}^{|\mathcal{A}|}$. For any $Q \in \triangle_\Pi$

$$\pi_c^\top \left(\sum_{\pi' \in \Pi} Q(\pi') \pi'_c \pi'^\top_c \right)^\dagger \pi_c = \frac{1}{\sum_{\pi' \in \Pi : \pi'(c) = \pi(c)} Q(\pi')} = \frac{1}{Q(\pi(c)|c)}$$

Applying the above lemma we have

$$\min_{q \in \triangle_\Pi} \max_{\pi \in \Pi} \mathbb{E}_C \left[\pi_C^\top \left(\sum_{\pi' \in \Pi} q_{\pi'} \pi'_C \pi'^\top_C \right)^\dagger \pi_C \right] \leq |\mathcal{A}|.$$

□

Remark 12. *In light of the connection to Kiefer-Wolfowitz, where one appealed to Caratheodory's theorem to find a sparse solution that grew only quadratically in the dimension, one may wonder if Q can also be sparse in this setting. If $|\mathcal{C}| < \infty$ then by constructing a sparse solution via Caratheodory for each $c \in \mathcal{C}$ we can always find a solution Q that is $|\mathcal{C}|\,|\mathcal{A}|$ sparse. Can we do better? Unfortunately, for some absolute constant $\alpha \gg 2$, [Agarwal et al., 2014] prove that for sufficiently small $\gamma > 0$ there exists a contextual bandit instance with $|\mathcal{C}| = \frac{1}{2\sqrt{2}\alpha|\mathcal{A}|\gamma}$ such that if a $Q \in \triangle_\Pi$ satisfies $\max_{\pi \in \Pi} \mathbb{E}_C \left[\frac{1}{\gamma + (1-\gamma n) Q(\pi(C)|C)} \right] \leq \alpha |\mathcal{A}|$, then $|support(Q)| \geq (|\mathcal{C}|-1)|\mathcal{A}| = \frac{1}{4\sqrt{2}\alpha\gamma}$. They also show how to obtain a $O(1/\gamma)$-sparse solution for a very similar optimization problem for any contextual bandit instance.*

Lemma 23. *For all $\ell = 1, 2, \dots$ we have $\pi^\star \in \widehat{\Pi}_\ell$ and $\max_{\pi \in \widehat{\Pi}_\ell} V(\pi) \geq V(\pi^\star) - 8\epsilon_\ell$.*

Proof. Let $\tau_\ell = T_\ell - T_{\ell-1}$. Noting that the variance of $\widehat{V}_\ell(\pi)$ is bounded by $\max_{\pi \in \widehat{\Pi}_\ell} \mathbb{E}_C \left[\frac{1}{Q_\ell^\gamma(\pi(C)|C)} \right]$, we apply Bernstein's inequality at each stage ℓ to find

$$\begin{aligned} |V(\pi) - \widehat{V}_\ell(\pi)| &\leq \sqrt{\frac{4n \log(2|\Pi|T/\delta)}{\tau_\ell}} + \frac{2\log(2|\Pi|T/\delta)}{3\gamma_\ell \tau_\ell} \\ &\leq \sqrt{\frac{16n \log(2|\Pi|T/\delta)}{\tau_\ell}} \end{aligned}$$

for the choice of $\gamma_\ell = \min\{\frac{1}{2n}, \sqrt{\frac{\log(2|\Pi|T/\delta)}{9n\tau_\ell}}\}$ to equalize the terms for large τ_ℓ. The last inequality holds if $\tau_\ell \geq n \log(2|\Pi|T/\delta)$. To make the right hand side less than ϵ_ℓ, it suffices to take $\tau_\ell = \lceil 16 n \epsilon_\ell^{-2} \log(2|\Pi|T/\delta) \rceil$.

For any fixed $\widehat{\Pi}_\ell$ with $\pi^\star \in \widehat{\Pi}_\ell$, we have that any $\pi \in \widehat{\Pi}_\ell$ satisfies

$$\begin{aligned} \widehat{V}_\ell(\pi) - \widehat{V}_\ell(\pi^\star) &= \widehat{V}_\ell(\pi) - V(\pi) + \underbrace{V(\pi) - V(\pi^\star)}_{\leq 0} + V(\pi^\star) - \widehat{V}_\ell(\pi^\star) \\ &\leq 2\epsilon_\ell. \end{aligned}$$

On the other hand, for any π such that $V(\pi^\star) - V(\pi) > 4\epsilon_\ell$

$$\begin{aligned} \max_{\pi' \in \widehat{\Pi}_\ell} \widehat{V}_\ell(\pi') - \widehat{V}_\ell(\pi) &\geq \widehat{V}_\ell(\pi^\star) - \widehat{V}_\ell(\pi) \\ &= \widehat{V}_\ell(\pi^\star) - V(\pi^\star) + \underbrace{V(\pi^\star) - V(\pi)}_{> 4\epsilon_\ell} + V(\pi) - \widehat{V}_\ell(\pi) \\ &> 2\epsilon_\ell \end{aligned}$$

which implies this π will be kicked out. This means that $\max_{\pi\in\widehat{\Pi}_{\ell+1}} V(\pi) \geq V(\pi^\star) - 4\epsilon_\ell \geq V(\pi^\star) - 8\epsilon_{\ell+1}$.

Extending the proof to all ℓ and random $\widehat{\Pi}_\ell$ is identical to above for linear bandits. □

Suppose you run for T timesteps. Let $\Delta = \min_{\pi\neq\pi^\star} V(\pi^\star) - V(\pi)$. Then for any $\nu \geq 0$ the regret is bounded by:

$$\begin{aligned}
T\nu + & \sum_{\ell=1}^{\lceil \log_2(4(\Delta\vee\nu)^{-1})\rceil} (\gamma_\ell n + 8\epsilon_\ell(1-\gamma_\ell n))\tau_\ell \\
&= T\nu + \sum_{\ell=1}^{\lceil \log_2(4(\Delta\vee\nu)^{-1})\rceil} (n\sqrt{\tfrac{\log(2|\Pi|T/\delta)}{9n\tau_\ell}} + 8\epsilon_\ell)\tau_\ell \\
&= T\nu + \sum_{\ell=1}^{\lceil \log_2(4(\Delta\vee\nu)^{-1})\rceil} n\sqrt{\lceil 16n\epsilon_\ell^{-2}\log(2|\Pi|T/\delta)\rceil \log(2|\Pi|T/\delta)/9n} + 8\epsilon_\ell\lceil 16n\epsilon_\ell^{-2}\log(2|\Pi|T/\delta)\rceil \\
&\leq T\nu + \sum_{\ell=1}^{\lceil \log_2(4(\Delta\vee\nu)^{-1})\rceil} 2n\epsilon_\ell^{-1}\log(4|\Pi|T/\delta) + 128n\epsilon_\ell^{-1}\log(4|\Pi|T/\delta) \\
&\leq T\nu + 8 + 130n\log(2|\Pi|T/\delta) \sum_{t=1}^{\lceil \log_2(4(\Delta\vee\nu)^{-1})\rceil} 2^t \\
&\leq T\nu + 8 + 2080n(\Delta\vee\nu)^{-1}\log(2|\Pi|T/\delta).
\end{aligned}$$

As before, using the upper bound $(\Delta\vee\nu) \leq \nu$ and optimizing over ν we have that the regret is no greater than $O(\sqrt{nT\log(|\Pi|T/\delta)})$.

Notes: [Dudik et al., 2011] compute a different Q_t every time a new context c_t arrives instead of our algorithm, above, which computes it only once per stage. Also, when estimating the value of a policy, they use all the observed data up to the current time, whereas our algorithm only uses the data from that round. Reusing data introduces dependencies that are easily handled by the martingale-based bounds of above since we can define our filtration as $\mathcal{F}_{t-1} = (c_1, x_1, r_1, \dots, c_{t-1}, x_{t-1}, r_{t-1}, c_t)$ so that $c_t \in \mathcal{F}_{t-1}$ which makes p_t a predictable sequence.

While the τ-greedy algorithm is computationally efficient via a reduction to cost-sensitive classification, it is unclear how to make the above elimination algorithm computationally efficient. Fortunately, [Agarwal et al., 2014] did precisely that by approximately solving the optimization problem over $\triangle_\Pi$ using an iterative algorithm which results in a finite cover over Π.

12.4.4 A $\sqrt{T}$ computationally efficient algorithm

In this section we will propose an algorithm analogous to [Agarwal et al., 2014], but presented a bit differently.

```
**Input**: Policy set $\Pi$ such that $\pi : \mathcal{C} \to [n]$ for all $\pi \in \Pi$, confidence level $\delta \in (0,1)$.
Let $\widehat{\Pi}_1 \leftarrow \Pi, \ell \leftarrow 1, T_0 \leftarrow 0$
**for** $\ell = 1, 2, \dots$
    $\epsilon_\ell = 2^{-\ell}$, $\tau_\ell = \lceil 16 n \epsilon_\ell^{-2} \log(2|\Pi|T/\delta) \rceil$, $\gamma_\ell = \min\{\frac{1}{2n}, \sqrt{\frac{\log(2|\Pi|T/\delta)}{9n\tau_\ell}}\}$, $T_\ell = T_{\ell-1} + \tau_\ell$
    Let $Q_\ell$ be any $Q \in \triangle_\Pi$ that satisfies both
        $\sum_{\pi\in\Pi} \widehat{\Delta}_{\ell-1}(\pi) Q(\pi) \le c_0 \epsilon_\ell$    (12.3)
        $\mathbb{E}_C\left[\frac{1}{Q^{\gamma_\ell}(\pi(C)|C)}\right] \le n + \frac{\widehat{\Delta}_{\ell-1}(\pi)}{\gamma_\ell} \qquad \forall \pi \in \Pi$    (12.4)
        where $Q^\gamma(x|c) = \gamma + (1-\gamma n) \sum_{\pi\in\Pi:\pi(c)=x} Q(\pi)$
    **for** $T_\ell$ steps
        Observe context $c_t$
        Play $x_t \sim Q_\ell^{\gamma_\ell}(\cdot|c_t)$, set $p_t = Q_\ell^{\gamma_\ell}(x_t|c_t)$ and observe reward $r_t = v(c_t, x_t) + \eta_t$
    Set $\widehat{V}_\ell(\pi) = \frac{1}{T_\ell - T_{\ell-1}} \sum_{t\in(T_{\ell-1},T_\ell]} r_t \frac{\mathbf{1}\{\pi(c_t)=c_t\}}{p_t}$ and $\widehat{\Delta}_\ell(\pi) = \max_\pi \widehat{V}_\ell(\pi') - \widehat{V}_\ell(\pi)$
    $\ell \leftarrow \ell + 1$
**Output**: $\Pi_{t+1}$
```

On stage ℓ, for any $\lambda < \gamma_\ell$ and $\pi \in \Pi$, we have by Equation **??** that with probability at least $1-\delta$ that $S \le \frac{\lambda V}{2(1-c\lambda)} + \log(|\Pi|/\delta)/\lambda$ where $S = \sum_{t\in(T_{\ell-1},T_\ell]} r_t \frac{\mathbf{1}\{\pi(c_t)=c_t\}}{p_t}$, $V = \tau_\ell \mathbb{E}_C\left[\frac{1}{Q^{\gamma_\ell}(\pi(C)|C)}\right]$, and $c = 1/3\gamma_\ell$. Thus, taking $\lambda = \gamma_\ell/2$ we have with probability at least $1-\delta$ that for all $\pi \in \Pi$

$$\begin{aligned} |\widehat{V}_\ell(\pi) - V(\pi)| &\le \lambda \mathbb{E}_C\left[\frac{1}{Q^{\gamma_\ell}(\pi(C)|C)}\right] + \frac{\log(2|\Pi|T/\delta)}{\tau_\ell \lambda} \\ &= \frac{\gamma_\ell}{2} \mathbb{E}_C\left[\frac{1}{Q^{\gamma_\ell}(\pi(C)|C)}\right] + \frac{\log(2|\Pi|T/\delta)}{\tau_\ell \gamma_\ell/2}. \end{aligned}$$

Since $\gamma_\ell \approx \frac{\epsilon_\ell}{n}$, $\frac{\log(2|\Pi|T/\delta)}{\tau_\ell\gamma_\ell/2} \lesssim \epsilon_\ell$, and there always exists a Q to with $\mathbb{E}_C\left[\frac{1}{Q^{\gamma_\ell}(\pi(C)|C)}\right] \le 2n$, we have that we will have that $|\widehat{V}_1(\pi) - V(\pi)| \le \epsilon_1$. By an inductive argument, one can show that Equation 12.4 guarantees that $\widehat{V}_\ell(\pi) - V(\pi) \le c(\epsilon_\ell + \Delta(\pi))$ for some small $c < 1$. In particular, it implies that

$$\begin{aligned} \widehat{\Delta}_\ell(\pi) &= \max_\pi \widehat{V}_\ell(\pi') - \widehat{V}_\ell(\pi) \\ &\ge \widehat{V}_\ell(\pi^*) - \widehat{V}_\ell(\pi) \\ &= \Delta(\pi) + \widehat{V}_\ell(\pi^*) - V(\pi^*) + V(\pi) - \widehat{V}_\ell(\pi) \\ &= \Delta(\pi) - c(2\epsilon_\ell + \Delta(\pi)) \end{aligned}$$

which is at least $\Delta(\pi)/2$ when $\epsilon_\ell \le \Delta(\pi)/2$. This, in turn, implies that Equation 12.3 is using accurate estimates of $\widehat{\Delta}_\ell(\pi)$. Thus, approximating $\widehat{\Delta}_\ell(\pi) \approx \max\{\Delta(\pi), \epsilon_\ell$, if a feasible Q_ℓ is identified at each round, then during round ℓ one will incur an average regret of at most $c_0(\epsilon_\ell + \gamma_\ell n)$ since $\mathbb{P}(x_t = x) = \gamma_\ell + (1-\gamma_\ell n)\mathbf{1}\{\pi_t(c_t) = x\}$ and $\pi_t \sim Q_\ell$. Then the regret analysis of above follows identically. Now all that remains is to show that (i) there exists a feasible Q_ℓ at each round with high probability, and (ii) such a Q_ℓ can be identified using a computationally efficient procedure.

To solve (i) we will explicitly construct a feasible Q_ℓ. For $j \le \ell$ define $\Pi_j = \{\pi \in \Pi : \Delta(\pi) \le \epsilon_\ell\}$ and

$$P_j = \arg \min_{P\in\triangle_\Pi:\text{support}(P)\subset\Pi_j} \max_{\pi\in\Pi_j} \mathbb{E}_C\left[\frac{1}{P^{\gamma_j}(\pi(C)|C)}\right]$$

where $P^{\gamma}(x|c) = \gamma + (1-\gamma n)\sum_{\pi\in\Pi_j:\pi(c)=x} P(\pi)$. With τ_j and γ_j defined as above, let $\bar{P}_\ell = \frac{1}{T_\ell}\sum_{j=1}^{\ell} P_j\tau_j$ where we recall that $T_\ell = \sum_{j=1}^{\ell}\tau_j$. Note that P_j is essentially the distribution identified in the computationally inefficient algorithm at each round j. Thus, Equation 12.4 will be satisfied almost immediately, since for any π such that $\Delta(\pi) \leq \epsilon_j$ we have $\bar{P}_\ell^{\gamma_\ell}(\pi(c)|c)T_\ell \geq P_j^{\gamma_j}(\pi(c)|c)\tau_j$ which makes the LHS less than $O(\epsilon_j)$. To show that Equation 12.3 is satisfied, we observe that

$$\begin{aligned}
\sum_{\pi\in\Pi}\widehat{\Delta}_{\ell-1}(\pi)\bar{P}_\ell(\pi) &\approx \sum_{\pi\in\Pi}\Delta(\pi)\bar{P}_\ell(\pi)\\
&= \sum_{j=0}^{\ell}\sum_{\pi\in\Pi:\Delta(\pi)\leq\epsilon_j}\Delta(\pi)\bar{P}_\ell(\pi)\\
&\leq \frac{1}{T_\ell}\sum_{j=0}^{\ell}\sum_{\pi\in\Pi:\Delta(\pi)\leq\epsilon_j}\epsilon_j P_j(\pi)\tau_j\\
&\lesssim \frac{1}{T_\ell}\sum_{j=0}^{\ell}\sum_{\pi\in\Pi:\Delta(\pi)\leq\epsilon_j}\epsilon_j P_j(\pi) n\epsilon_j^{-2}\log(2|\Pi|T/\delta)\\
&= \frac{1}{T_\ell}\sum_{j=0}^{\ell} n\epsilon_j^{-1}\log(2|\Pi|T/\delta)\\
&\lesssim \frac{1}{T_\ell} n\epsilon_\ell^{-1}\log(2|\Pi|T/\delta)\\
&\lesssim \frac{1}{\tau_\ell} n\epsilon_\ell^{-1}\log(2|\Pi|T/\delta)\\
&\lesssim \epsilon_\ell
\end{aligned}$$

where we have used the inequality $\sum_{j=0}^{\ell} a^j \leq 2a^\ell$ for $a \geq 2$.

To solve (ii) we employ the use of a Frank-Wolfe style algorithm, as used in [Agarwal et al., 2014]. In particular, at each step we find some π that invalidates Equation 12.4 (which can be cast as a cost-sensitive classification problem) increase $Q(\pi)$, and then renormalize Q so that Equation 12.3 is satisfied. The process will eventually terminate with a Q that doesn't necessarily sum to one (but does not exceed it). To make the policy sum to 1, use the empirical best policy.

12.4.5 Frank-Wolfe

```
Frank-Wolfe for contextual bandits
Input: $\phi : [n] \times \Xi \rightarrow \mathbb{R}^d$, $\gamma > 0$, $\alpha \in \mathbb{R}_+^n$, $\lambda^{(0)} \in \triangle_n$
Set: $t = 1$, $\omega_j(\lambda) = \mathbb{E}\left[\phi(j,\xi)^\top(\sum_{i=1}^n \lambda_i\phi(i,\xi)\phi(i,\xi)^\top + \gamma I)^{-1}\phi(j,\xi)\right]$
do
    $k = \arg\max_{i=1,\dots,n} \omega_i(\lambda^{(t-1)}) - \alpha_i$
    $\eta = \frac{\omega_i(\lambda^{(t-1)})-\alpha_i}{\omega_i(\lambda^{(t-1)})^2}$
    $\lambda^{(t)} = \lambda^{(t-1)} + \eta\mathbf{e}_k$
    if $\sum_{j=1}^n \alpha_j\lambda_j^{(t)} > d$
        $\lambda^{(t)} = \lambda^{(t)} \cdot \frac{d}{\sum_{j=1}^n \alpha_j\lambda_j^{(t)}}$
    $t = t + 1$
until $\max_{i=1,\dots,n} \omega_i - 2\alpha_i \leq 0$
Output: Single element in $V$
```

$$f(\lambda) = -\mathbb{E}_\xi[\text{logdet}(\sum_{i=1}^n \lambda_i \phi(i,\xi)\phi(i,\xi)^\top + \gamma I)] + \sum_{i=1}^n \lambda_i \alpha_i$$

$$\begin{aligned}
\frac{\partial f(\lambda)}{\partial \lambda_j} &= -\mathbb{E}\left[\text{Trace}\left((\sum_{i=1}^n \lambda_i \phi(i,\xi)\phi(i,\xi)^\top + \gamma I)^{-1} \phi(j,\xi)\phi(j,\xi)^\top \right)\right] + \alpha_j \\
&= -\mathbb{E}\left[\phi(j,\xi)^\top (\sum_{i=1}^n \lambda_i \phi(i,\xi)\phi(i,\xi)^\top + \gamma I)^{-1} \phi(j,\xi)\right] + \alpha_j \\
&=: -\omega_j + \alpha_j
\end{aligned}$$

For some λ and $k \in [n]$ such that $\omega_k \geq 2\alpha_k$ consider

$$\begin{aligned}
f(\lambda + \eta \mathbf{e}_k) &= -\mathbb{E}_\xi[\text{logdet}(\sum_{i=1}^n \lambda_i \phi(i,\xi)\phi(i,\xi)^\top + \gamma I + \eta \phi(k,\xi)\phi(k,\xi)^\top)] + \sum_{i=1}^n \lambda_i \alpha_i + \eta \alpha_k \\
&= f(\lambda) - \log(1 + \eta \omega_k) + \eta \alpha_k \\
&\leq f(\lambda) - \eta \omega_k + \eta^2 \omega_k^2 / 2 + \eta \alpha_k \\
&= f(\lambda) - \frac{(\omega_k - \alpha_k)^2}{2\omega_k^2} \\
&\leq f(\lambda) - 1/2
\end{aligned}$$

using the fact that $\log(1+x) \geq x - x^2/2$ and the prescribed step size.

Fix λ and let $g(c) = f(c\lambda)$ so that

$$g(c) = -\mathbb{E}_\xi[\text{logdet}(\sum_{i=1}^n c\lambda_i \phi(i,\xi)\phi(i,\xi)^\top + \gamma I)] + \sum_{i=1}^n c\lambda_i \alpha_i$$

$$\begin{aligned}
g'(c) &= -\mathbb{E}\left[\text{Trace}\left((\sum_{i=1}^n c\lambda_i \phi(i,\xi)\phi(i,\xi)^\top + \gamma I)^{-1} \sum_{j=1}^n \lambda_j \phi(j,\xi)\phi(j,\xi)^\top \right)\right] + \sum_{j=1}^n \alpha_j \lambda_j \\
&= -\frac{1}{c}\mathbb{E}\left[\text{Trace}\left((\sum_{i=1}^n c\lambda_i \phi(i,\xi)\phi(i,\xi)^\top + \gamma I)^{-1} (c\sum_{j=1}^n \lambda_j \phi(j,\xi)\phi(j,\xi)^\top + \gamma I - \gamma I) \right)\right] + \sum_{j=1}^n \alpha_j \lambda_j \\
&= -\frac{1}{c}\mathbb{E}\left[\text{Trace}\left(I - \gamma(\sum_{i=1}^n c\lambda_i \phi(i,\xi)\phi(i,\xi)^\top + \gamma I)^{-1} \right)\right] + \sum_{j=1}^n \alpha_j \lambda_j \\
&\geq -\frac{d}{c} + \sum_{j=1}^n \alpha_j \lambda_j.
\end{aligned}$$

Thus, $g(1) \geq g(c)$ if $c = \frac{d}{\sum_{j=1}^n \alpha_j \lambda_j}$. So if at some point in the algorithm, if $\sum_{j=1}^n \alpha_j \lambda_j > d$ then $\lambda \mapsto c\lambda$. Thus, the projection step does not increase the objective.

If $\lambda^{(0)} = 0$ then the algorithm terminates after $O(n \log(1/\gamma_L))$ steps.

12.5 Stochastic Contextual Bandits with General Function Approximation

This presentation closely follows lecture notes of Dylan Foster and Sasha Rakhlin based on `arXiv:2312.16730`. One major difference between the previous sections is that now we make no assumptions on the sequence of contexts $c_1, c_2, \dots$ and, in fact, they may be chosen adversarially. However, we still assume that rewards $y_t \in [0,1]$ given (c_t, a_t) are still conditionally IID.

12.5.1 Online regression Oracles

Fix a class $\mathcal{F} \subseteq \{f : \mathcal{C} \times [A] \to [0,1]\}$ and assume there exists $f^\star \in \mathcal{F}$ such that $\mathbb{E}[y_t \mid c_t, a_t] = f^\star(c_t, a_t)$ for all t. At each round t, after observing the history $(c_s, a_s, y_s)_{s<t}$, an online regression oracle returns a predictor $\widehat{f}_t \in \mathcal{F}$. We say the oracle has squared-error guarantee $\mathrm{EstSq}(\mathcal{F}, T, \delta)$ if, with probability at least $1-\delta$,

$$\sum_{t=1}^{T} \mathbb{E}_{a_t \sim p_t(\cdot|c_t)} \left[\left(\widehat{f}_t(c_t, a_t) - f^\star(c_t, a_t) \right)^2 \,\middle|\, c_t, \mathcal{H}_{t-1} \right] \le \mathrm{EstSq}(\mathcal{F}, T, \delta),$$

where $p_t(\cdot \mid c_t)$ is the action distribution used by the bandit algorithm at round t. This section will show that if online regression in $\mathcal{F}$ is easy, then contextual bandits in $\mathcal{F}$ are also easy provided we explore in the right way.

12.5.2 ε-greedy exploration

Before introducing inverse gap weighting, it is instructive to consider the simpler ε-greedy strategy. At round t, given a predictor $\widehat{f}_t \in \mathcal{F}$, the learner acts greedily with probability $1-\varepsilon$ and explores uniformly with probability ε.

```
**$\varepsilon$-Greedy for Contextual Bandits**
**Input**: $\varepsilon \in (0,1)$.
For $t = 1, 2, \dots, T$:
    obtain $\widehat{f}_t$ from the online regression oracle using $(c_s, a_s, y_s)_{s<t}$;
    observe context $c_t$;
    with probability $\varepsilon$, choose $a_t \sim \mathrm{unif}([A])$;
    with probability $1-\varepsilon$, choose $a_t = \widehat{a}_t$;
    observe reward $y_t$.
```

Let $a^\star(c) \in \arg\max_{a \in [A]} f^\star(c, a)$ and write

$$\mathrm{Regret}_T = \sum_{t=1}^{T} \left(f^\star(c_t, a^\star(c_t)) - f^\star(c_t, a_t) \right).$$

Theorem 21. *Assume $f^\star \in \mathcal{F}$ and that the online regression oracle satisfies the squared-error guarantee*

$$\sum_{t=1}^{T} \mathbb{E}_{a_t \sim p_t(\cdot|c_t)} \left[\left(\widehat{f}_t(c_t, a_t) - f^\star(c_t, a_t) \right)^2 \right] \le \mathit{EstSq}(\mathcal{F}, T, \delta)$$

with probability at least $1-\delta$, where $p_t(\cdot \mid c_t)$ is the action distribution used at round t. Then, for a suitable choice of ε, the ε-greedy algorithm satisfies, with probability at least $1-\delta$,

$$\mathit{Regret}_T \lesssim A^{1/3} T^{2/3} \mathit{EstSq}(\mathcal{F}, T, \delta)^{1/3}.$$

Proof. Let p_t denote the action distribution used on round t. Since the algorithm explores uniformly with probability ε, we may write

$$\mathbb{E}\big[f^\star(c_t, a^\star(c_t)) - f^\star(c_t, a_t)\big] \le f^\star(c_t, a^\star(c_t)) - f^\star(c_t, \widehat{a}_t) + \varepsilon.$$

Summing over t gives

$$\mathrm{Regret}_T \le \sum_{t=1}^{T} \Big(f^\star(c_t, a^\star(c_t)) - f^\star(c_t, \widehat{a}_t) \Big) + \varepsilon T.$$

Fix t and abbreviate $a^\star = a^\star(c_t)$. Since $\widehat{a}_t$ is greedy for $\widehat{f}_t(c_t, \cdot)$,

$$\widehat{f}_t(c_t, a^\star) - \widehat{f}_t(c_t, \widehat{a}_t) \le 0,$$

and therefore

$$f^\star(c_t, a^\star) - f^\star(c_t, \widehat{a}_t) \le \sum_{a \in \{a^\star, \widehat{a}_t\}} \big| f^\star(c_t, a) - \widehat{f}_t(c_t, a) \big|.$$

Since $p_t(a) \ge \varepsilon/A$ for every $a \in [A]$, we have

$$\sum_{a \in \{a^\star, \widehat{a}_t\}} \big| f^\star(c_t, a) - \widehat{f}_t(c_t, a) \big| \le \sum_{a \in \{a^\star, \widehat{a}_t\}} \frac{1}{\sqrt{p_t(a)}} \sqrt{p_t(a)} \big| f^\star(c_t, a) - \widehat{f}_t(c_t, a) \big|.$$

Applying Cauchy–Schwarz,

$$f^\star(c_t, a^\star) - f^\star(c_t, \widehat{a}_t) \le \sqrt{\frac{2A}{\varepsilon}} \left(\mathbb{E}_{a_t \sim p_t(\cdot|c_t)} \big[\big(\widehat{f}_t(c_t, a_t) - f^\star(c_t, a_t) \big)^2 \big] \right)^{1/2}.$$

Summing over t and applying Cauchy–Schwarz once more yields

$$\sum_{t=1}^{T} \Big(f^\star(c_t, a^\star(c_t)) - f^\star(c_t, \widehat{a}_t) \Big) \lesssim \sqrt{\frac{AT}{\varepsilon}} \left(\sum_{t=1}^{T} \mathbb{E}_{a_t \sim p_t(\cdot|c_t)} \big[\big(\widehat{f}_t(c_t, a_t) - f^\star(c_t, a_t) \big)^2 \big] \right)^{1/2}.$$

On the high-probability event of the oracle guarantee, this is at most

$$\sqrt{\frac{AT}{\varepsilon} \mathrm{EstSq}(\mathcal{F}, T, \delta)}.$$

Hence

$$\mathrm{Regret}_T \lesssim \sqrt{\frac{AT}{\varepsilon} \mathrm{EstSq}(\mathcal{F}, T, \delta)} + \varepsilon T.$$

Choosing

$$\varepsilon \asymp \left(\frac{A \, \mathrm{EstSq}(\mathcal{F}, T, \delta)}{T} \right)^{1/3}$$

yields

$$\mathrm{Regret}_T \lesssim A^{1/3} T^{2/3} \mathrm{EstSq}(\mathcal{F}, T, \delta)^{1/3}.$$

□

Thus ε-greedy gives a general reduction from contextual bandits to online regression, but the resulting regret is suboptimal. The issue is that the distribution p_t puts mass at least ε/A on every action, including clearly suboptimal ones. The inverse gap weighting strategy introduced next corrects this and leads to the optimal SquareCB guarantee.

12.5.3 Inverse gap weighting, SquareCB

Definition 17 (Inverse gap weighting). *Fix $\gamma > 0$ and a score vector $g \in \mathbb{R}^A$. Let $\hat{a} \in \arg\max_{a\in[A]} g(a)$. The inverse gap weighting distribution $p = \mathrm{IGW}_\gamma(g)$ is defined by*

$$p(a) = \frac{1}{\lambda + 2\gamma(g(\hat{a}) - g(a))},$$

where $\lambda \in [1, A]$ is chosen so that $\sum_{a=1}^A p(a) = 1$.

Thus actions with smaller estimated gap are sampled more often, while clearly suboptimal actions receive less mass. The key point is that this particular distribution converts instantaneous regret into squared prediction error.

Proposition 8. *Fix $g \in \mathbb{R}^A$ and let $p = \mathrm{IGW}_\gamma(g)$. Then for every reward vector $g^\star \in \mathbb{R}^A$,*

$$\mathbb{E}_{a\sim p}[g^\star(a^\star) - g^\star(a)] \le \frac{A}{\gamma} + \gamma\mathbb{E}_{a\sim p}\left[(g(a) - g^\star(a))^2\right],$$

where $a^\star \in \arg\max_{a\in[A]} g^\star(a)$.

Proof. Let $\hat{a} \in \arg\max_a g(a)$. Write

$$\mathbb{E}_{a\sim p}[g^\star(a^\star) - g^\star(a)] = \mathbb{E}_{a\sim p}[g(\hat{a}) - g(a)] + \mathbb{E}_{a\sim p}[g(a) - g^\star(a)] + g^\star(a^\star) - g(\hat{a}).$$

For the first term,

$$\mathbb{E}_{a\sim p}[g(\hat{a}) - g(a)] = \sum_{a=1}^A \frac{g(\hat{a}) - g(a)}{\lambda + 2\gamma(g(\hat{a}) - g(a))} \le \sum_{a=1}^A \frac{1}{2\gamma} \le \frac{A}{2\gamma}.$$

For the second term, by $u \le \frac{1}{2\gamma} + \frac{\gamma}{2}u^2$,

$$\mathbb{E}_{a\sim p}[g(a) - g^\star(a)] \le \frac{1}{2\gamma} + \frac{\gamma}{2}\mathbb{E}_{a\sim p}\left[(g(a) - g^\star(a))^2\right].$$

For the third term, we use $u \le \frac{1}{2\gamma} + \frac{\gamma}{2}u^2$ again to obtain

$$\begin{aligned}
g^\star(a^\star) - g(\hat{a}) &= g^\star(a^\star) - g(a^\star) - \big(g(\hat{a}) - g(a^\star)\big) \\
&\le \frac{1}{2\gamma p(a^\star)} + \frac{\gamma}{2}p(a^\star)(g(a) - g^\star(a))^2 - \big(g(\hat{a}) - g(a^\star)\big) \\
&= \frac{\lambda + 2\gamma(g(\hat{a}) - g(a^\star))}{2\gamma} + \frac{\gamma}{2}p(a^\star)(g(a) - g^\star(a))^2 - \big(g(\hat{a}) - g(a^\star)\big) \\
&= \frac{\lambda}{2\gamma} + \frac{\gamma}{2}p(a^\star)(g(a) - g^\star(a))^2 \\
&\le \frac{A}{2\gamma} + \frac{\gamma}{2}\mathbb{E}_{a\sim p}\left[(g(a) - g^\star(a))^2\right]
\end{aligned}$$

Summing the three bounds proves the claim. □

This leads to the following algorithm.

```
SquareCB
Input: exploration parameter $\gamma > 0$.
For $t = 1, 2, \ldots, T$:
    obtain $\widehat{f}_t$ from the online regression oracle using $(c_s, a_s, y_s)_{s<t}$;
    observe context $c_t$;
    set $p_t = \mathrm{IGW}_\gamma(\widehat{f}_t(c_t, 1), \ldots, \widehat{f}_t(c_t, A))$;
    sample $a_t \sim p_t$ and observe reward $y_t$.
```

Let $\pi^\star(c) \in \arg\max_{a\in[A]} f^\star(c, a)$ and define the regret

$$R_T = \sum_{t=1}^{T} \big(f^\star(c_t, \pi^\star(c_t)) - f^\star(c_t, a_t)\big).$$

Theorem 22. *Assume the online regression oracle satisfies the above squared-error guarantee. Then, with probability at least $1 - \delta$, SquareCB satisfies*

$$R_T \le \frac{AT}{\gamma} + \gamma \, \mathrm{EstSq}(\mathcal{F}, T, \delta).$$

Consequently, taking

$$\gamma = \sqrt{\frac{AT}{\mathrm{EstSq}(\mathcal{F}, T, \delta)}}$$

gives

$$R_T \le 2\sqrt{AT \, \mathrm{EstSq}(\mathcal{F}, T, \delta)}.$$

Proof. Condition on the high-probability event in the oracle guarantee. For each round t, apply Proposition 8 with $g(a) = \widehat{f}_t(c_t, a)$ and $g^\star(a) = f^\star(c_t, a)$ to obtain

$$\mathbb{E}[f^\star(c_t, \pi^\star(c_t)) - f^\star(c_t, a_t) \mid c_t, \mathcal{H}_{t-1}] \le \frac{A}{\gamma} + \gamma \mathbb{E}\left[\big(\widehat{f}_t(c_t, a_t) - f^\star(c_t, a_t)\big)^2 \,\middle|\, c_t, \mathcal{H}_{t-1}\right].$$

Summing over t and using the oracle bound yields

$$R_T \le \frac{AT}{\gamma} + \gamma \, \mathrm{EstSq}(\mathcal{F}, T, \delta).$$

Optimizing over γ gives the second display. □

In particular, if $\mathcal{F}$ is finite and one uses the standard exponential-weights regression oracle, then $\mathrm{EstSq}(\mathcal{F}, T, \delta) \lesssim \log(|\mathcal{F}|/\delta)$ and hence

$$R_T \lesssim \sqrt{AT \log(|\mathcal{F}|/\delta)}.$$

Part IV

Active Learning

Chapter 13

Active Learning for Classification

This chapter is concerned learning a binary classifier while requesting as few labels as possible. Specifically, for an example space $\mathcal{X}$ and label space $\{0,1\}$ let $\mathcal{H}$ be a *hypothesis class* such that for each $h \in \mathcal{H}$ we have $h : \mathcal{X} \to \{0,1\}$. For example, $\mathcal{X}$ could be a set of images in some database, and each image $x \in \mathcal{X}$ either contains a man-made object $y = 1$ or not $y = 1$. After labels for examples in a subset of $\mathcal{X}$ are observed, one can construct $\widehat{h} \in \mathcal{H}$ which can then be applied to every image in the database $\mathcal{X}$ to predict their unknown labels.

In the *pool-based* setting, at any point we can choose any $x \in \mathcal{X}$ and then request its label $y \in \{0,1\}$. We evaluate an algorithm by the number of labels requested and the number of errors the learned classifier $\widehat{h}$ makes over the entire pool $\mathcal{X}$, whether they were queried or not. In the *streaming* setting, there exists a distribution $\mathcal{D}$ over $\mathcal{X}$ and we can only obtain samples $x \sim \mathcal{D}$. In this setting, we evaluate an algorithm based on how many total examples are drawn from $\mathcal{D}$ (amount of unlabeled data), the number of labels that are requested, and the error of the classifier over $\mathcal{X}$ with respect to $\mathcal{D}$. Note, by taking $\mathcal{D}$ to be a uniform distribution over $\mathcal{X}$, one can always apply an algorithm for the streaming setting to the pool-based setting. On the other hand, if we had no restriction on the amount of unlabeled data, one could keep sampling from $\mathcal{D}$ until any desired $x \in \text{support}(\mathcal{D}) \subset \mathcal{X}$ eventually is returned (though this could take a very long time).

13.1 Separable, pool-based setting

We say a problem is *separable* if there exists an $h^* \in \mathcal{H}$ such that for every $x \in \mathcal{X}$ and its corresponding label $y \in \{0,1\}$, $h^*(x) = y$. The goal of *exact learning* in the pool-based setting is to identify h^* using as few queries as possible. In this section, we propose different strategies for accomplishing this. For a deterministic algorithm $\mathcal{A}$, let $\mathfrak{S}(\mathcal{X}, \mathcal{H}, h, \mathcal{A})$ be the number of labels that algorithm $\mathcal{A}$ requests before identifying the true hypothesis $h^* = h$, and let $\mathfrak{S}(\mathcal{X}, \mathcal{H}, \mathcal{A}) = \max_{h \in \mathcal{H}} \mathfrak{S}(\mathcal{X}, \mathcal{H}, h, \mathcal{A})$. In the pool-based setting, $|\mathcal{X}| < \infty$ which implies $|\mathcal{H}| < \infty$. Thus, any deterministic algorithm can be thought of as a binary tree where each node specifies which $x \in \mathcal{X}$ to request the label for, and each child node to move to depends on the label $y \in \{0,1\}$. The leaves of this tree correspond to a unique $h \in \mathcal{H}$. Because a binary tree with $|\mathcal{H}|$ leaves has depth at least $\lceil \log_2(|\mathcal{H}|) \rceil$ we have the immediate proposition.

Proposition 9. *For any hypothesis space $\mathcal{H}$ defined over $\mathcal{X}$, any algorithm $\mathcal{A}$ satisfies $\mathfrak{S}(\mathcal{X}, \mathcal{H}, \mathcal{A}) \geq \lceil \log_2 \mathcal{H} \rceil$.*

Note that for some hypothesis classes, this lower bound is achievable:

Example 5 (Binary search)**.** *Let $n \in \mathbb{N}$ be a power of two, $\mathcal{X} = \{1, \dots, n\}$, and $\mathcal{H}_{thresholds} = \{h(x) = \mathbf{1}\{x \in \{1, \dots, k\}\} : k \in \{1, \dots, n\}\}$. Each $h \in \mathcal{H}$ corresponds to a unique index $k \in [n]$ and the label for each query $i \in \mathcal{X} = [n]$ is equivalent to asking whether $i \leq k$ or $i > k$. Performing bisection/binary search identifies the correct hypothesis after exactly $\log_2(n) = \log_2(|\mathcal{H}|)$. Thus, $\min_{\mathcal{A}} \mathfrak{S}(\mathcal{X}, \mathcal{H}_{thresholds}, \mathcal{A}) = \lceil \log_2 |\mathcal{H}_{thresholds}| \rceil$.*

However, clearly $\log_2(|\mathcal{H}|)$ is not always possible:

Example 6 (Needle in a haystack)**.** *Fix $n \in \mathbb{N}$, $\mathcal{X} = \{1, \dots, n\}$, and $\mathcal{H}_{needle} = \{h(x) = \mathbf{1}\{x = k\} : k \in \{1, \dots, n\}\}$. Exhaustive search is clearly the best one could hope for here, which takes $n - 1 = |\mathcal{H}| - 1$ queries. Thus, $\min_{\mathcal{A}} \mathfrak{S}(\mathcal{X}, \mathcal{H}_{needle}, \mathcal{A}) = |\mathcal{H}_{needle}| - 1$*

Moreover, its easy to see that $\min_{\mathcal{A}} \mathfrak{S}(\mathcal{X}, \mathcal{H}, \mathcal{A}) \leq |\mathcal{H}| - 1$ in general since without loss of generality we have $|\mathcal{X}| \leq |\mathcal{H}|$, otherwise queries in $\mathcal{X}$ are equivalent. The above two examples show that $\min_{\mathcal{A}} \mathfrak{S}(\mathcal{X}, \mathcal{H}, \mathcal{A})$ lies somewhere between $\lceil \log_2 |\mathcal{H}| \rceil$ and $|\mathcal{H}| - 1$. Can we get a bit tighter?

13.1.1 Extended teaching dimension and the Halving algorithm

Here we introduce a combinatorial quantity called the extended teaching dimension that describes the complexity of exact learning [Hegedus, 1995]. First, some definitions. Let $n = |\mathcal{X}|$.

Definition 18. *We say $S \subset \mathcal{X}$ is a* specifying set for $b \in \{0, 1\}^n$ *(with respect to $\mathcal{H}$) if $|\{h \in \mathcal{H} : h(x) = b(x) \ \forall x \in S\}| \leq 1$.*

Definition 19. *For any $\mathcal{X}$ and hypothesis class $\mathcal{H}$ over $\mathcal{X}$, define extended teaching dimension* Ext-TD($\mathcal{H}$) *as* Ext-TD$(\mathcal{H}) = \min\{k : \forall b \in \{0, 1\}^{|\mathcal{X}|}, \exists$ *specifying set S for b with $|S| \leq k\}$.*

Examples make these definitions clearer.

Example 7 (Thresholds)**.** *If $b = \mathbf{0}$ then $S = \{1\}$ suffices since $h(1) = 1$ for all $h \in \mathcal{H}$. If $b \in \{0, 1\}^n$ such that $b \notin \mathcal{H}_{thresholds}$ and $b \neq \mathbf{0}$ then there exists some $1 \leq i < j \leq n$ such that $b(i) = 0$ and $b(j) = 1$ so $S = \{i, j\}$ suffices. Finally, if $b \in \mathcal{H}$ then there exists an index i such that $b(i) = 1$ and $b(i + 1) = 0$ and so $S = \{i, i + 1\}$ suffices. Thus* Ext-TD$(\mathcal{H}_{thresholds}) = 2$.

Example 8 (Needle in a Haystack)**.** *Take S to be any subset of $[n]$ with $|S| = n - 1$. Fix any $b \in \{0, 1\}^n$. If $b(i) = 0$ for all $i \in S$ then the remaining index either uniquely specifies an $h \in \mathcal{H}$ or is equal to 0, in which no $h \in \mathcal{H}$ is consistent. If $|\{b(i) = 1 : i \in S\}| \geq 1$ then either no $h \in \mathcal{H}$ is consistent or the correct h is specified (since b cannot contain multiple 1s). Finally, if $b = \mathbf{0}$ and $|S| < n - 2$ then there are two hypotheses in $\mathcal{H}$ that are consistent with any $S \subset \mathcal{X}$. Together, these cases imply that* Ext-TD$(\mathcal{H}_{needle}) = |S| - 1$.

Theorem 23. *For any $\mathcal{H}$ we have* Ext-TD$(\mathcal{H}) \leq \min_{\mathcal{A}} \mathfrak{S}(\mathcal{X}, \mathcal{H}, \mathcal{A}) \leq$ Ext-TD$(\mathcal{H}) \lceil \log_2(|\mathcal{H}|) \rceil$*. Moreover, the upper bound is achieved by the* Halving *algorithm.*

Proof. Suppose $\mathcal{A}$ is an algorithm that takes at most $\mathfrak{S}(\mathcal{X}, \mathcal{H}, \mathcal{A})$ queries when run on any instance $h \in \mathcal{H}$. Without loss of generality, we may assume that after receiving a label in each round, $\mathcal{A}$ checks whether there exists more than one hypothesis consistent with the observations. If so it continues, if not it stops. Moreover, assume that if $\mathcal{A}$ is played on some $b \notin \mathcal{H}$ and it encounters a query that is inconsistent with any $h \in \mathcal{H}$ it also stops and outputs Fail. Note that this algorithm takes no more than $\mathfrak{S}(\mathcal{X}, \mathcal{H}, \mathcal{A})$ queries when it is run on any $b \in \{0, 1\}^n$. Thus, when run on any

$b \in \{0,1\}^n$, the set of measured example, label pairs is a specifying set for b with respect to $\mathcal{H}$. This proves the lower bound.

The upper bound follows from the Halving algorithm. At each round, if $b(x) = h^*(x)$ for all $x \in S$ then $V = \{h^*\}$ by the definition of the specifying set. If there exists an $x \in S$ such that $b(x) \neq h^*(x)$ then at least half of the hypotheses in V at the start of the round are removed, due to majority vote. Because this can occur at most $\lceil \log_2(|\mathcal{H}|) \rceil$ times and the size of each specifying set is at most Ext-TD($\mathcal{H}$), the result follows. □

```
Halving Algorithm for exact learning
Input: Finite hypothesis set $\mathcal{H}$ such that each $h : \mathcal{X} \to \{0,1\}$.
Initialize: version space $V = \mathcal{H}$
while $|V| > 1$
    Set $b(x) = \textsc{MajorityVote}(h(x) : h \in V)$ for all $x \in \mathcal{X}$
    Let $S \subset \mathcal{X}$ be a minimal specifying set for $b \in \{0,1\}^{|\mathcal{X}|}$ with respect to $\mathcal{H}$ and request $h^*(x)$ for all $x \in S$
    Update $V = \{h \in V : h(x) = h^*(x)\}$
Output: Single element in $V$
```

The result of Theorem 23 sheds light on the sample complexity of exact learning. However, the Halving algorithm and its analysis has many downsides. First, its not clear how to compute a minimal specifying set. Second, even if one could, the computational complexity of the algorithm scales like $|\mathcal{X}|\,|\mathcal{H}|$ which is almost always intractable. Finally, even as a theoretical result alone, the definition of Ext-TD($\mathcal{H}$) is very combinatorial and can be difficult to bound.

13.1.2 Generalized binary search

There have been many variants of greedy information gain algorithms that have been proposed and analyzed. They go by names like query by committee, splitting algorithm, or generalized binary search [Freund et al., 1997, Dasgupta, 2005a, Nowak, 2011, Golovin and Krause, 2011]. These generalized binary search algorithms define a probability distribution p over $\mathcal{H}$ and take queries to remove as much mass as possible.

```
Generalized Binary Search (GBS) for exact learning
Input: Finite hypothesis set $\mathcal{H}$ such that each $h : \mathcal{X} \to \{0,1\}$. Probability distribution $p \in \triangle_{\mathcal{H}}$
Initialize: Version space $V = \mathcal{H}$
while $|V| > 1$
    Set $x' \leftarrow \arg\min_{x\in\mathcal{X}} \left|\frac{1}{2} - \sum_{h\in V} p(h)\, h(x)\right|$
    Request $h^*(x')$ and update $V = \{h \in V : h(x') = h^*(x')\}$
Output: Single element in $V$
```

Theorem 24 ([Dasgupta, 2005a])**.** *Fix any finite hypothesis class $\mathcal{H}$ and $p \in \triangle_{\mathcal{H}}$. Let* OPT $= \min_{\mathcal{A}} \mathbb{E}_{h\sim p}\left[\mathfrak{S}(\mathcal{X},\mathcal{H},h,\mathcal{A})\right]$*. The GBS algorithm satisfies* $\mathbb{E}_{h\sim p}\left[\mathfrak{S}(\mathcal{X},\mathcal{H},h,\mathcal{A}_{GBS})\right] \leq 4\text{OPT}\max_{h\in\mathcal{H}} \log(1/p(h))$.

When p is taken to be the uniform distribution over $\mathcal{H}$ this amounts to a $\log(|\mathcal{H}|)$ approximation ratio. Note that while the previous section has been considering $\mathfrak{S}(\mathcal{X},\mathcal{H},\mathcal{A}) \max_{h\in\mathcal{H}} \mathfrak{S}(\mathcal{X},\mathcal{H},h,\mathcal{A})$, this theorem is concerned with the average case sample complexity $\mathbb{E}_{h\sim p}\left[\mathfrak{S}(\mathcal{X},\mathcal{H},h,\mathcal{A})\right]$.

For some special classes of $\mathcal{H}$, or those that possess certain geometrical properties, this average-case approximation ratio can be shown to be a constant [Nowak, 2011]. A related greedy approach attempts to remove as many pairs of hypotheses that cannot be distinguished between. Its sample complexity is given in terms of the *splitting index* [Dasgupta, 2005b].

13.1.3 Open problems

All of the above algorithms are computationally infeasible since they scale like $|\mathcal{X}|\,|\mathcal{H}|$. If $\mathcal{X} \subset \mathbb{R}^d$ and $\mathcal{H}$ is the space of linear half-spaces then $O(|\mathcal{X}|^d)$. Ideally, an algorithm for this setting would only require calls to an oracle of the form $\arg\min_{h\in\mathcal{H}} \sum_{x\in S} \mathbf{1}\{h(x) \neq h^*(x)\}$ for any $S \in \mathcal{X}$. In special cases, such as the space of half-space classifiers, one can efficiently approximate the volume of the version space thereby making algorithms like GBS with a uniform prior potentially runnable.

For this pool-based setting, the extended teaching dimension is the only result that I am aware of that provides a nearly matching upper and lower bound that quantifies the sample complexity (i.e., not a non-constructive OPT). [Dasgupta, 2005b] proves an upper bound in terms of the splitting index. However, the lower bound relies on either the number of unlabeled data being large *or* the number of labels needed being large–this is vacuous in the pool-based setting. Reducing the gap between the upper and lower bound of Theorem 23 is a great open problem. Especially if the new bounds are in terms of efficiently computable quantities.

The extended teaching dimension bounds are worst-case over the class of $\mathcal{H}$. Which means that if I embed a set of hard instances in $\mathcal{H}$, the teaching dimension and thus the sample complexity of this appended class is at least as hard as learning the hard instances. Is there some notion of segmenting $\mathcal{H}$ into equivalence classes of instances of difficulty such that some instances are learnable with very queries while others may require a lot, and this is reflected in the sample complexity?

13.2 Separable, streaming setting

While in the pool-based setting we assumed that $|\mathcal{X}| < \infty$ and can be enumerated over, when we move to the streaming setting we make no such restriction. Here $\mathcal{X}$ can be uncountable and we assume we have access to a sampling oracle such that we can query an $x_t \sim \mathcal{D}_X$ over $\mathcal{X}$. If we request a corresponding label $y_t \in \{0,1\}$ we assume that the pair $(x_t, y_t) \sim \mathcal{D}$. For simplicity we will still assume $\mathcal{H}$ is finite.

Define the *risk* of any $h \in \mathcal{H}$ with respect to $\mathcal{D}$ as $R(h) := \mathbb{E}_{(X,Y)\sim\mathcal{D}}[\mathbf{1}\{h(X) \neq Y\}$. We do not assume that we know $\mathcal{D}$ directly, but we can collect an iid dataset $\{(x_i, y_i)\}_{i=1}^n$ from drawn from $\mathcal{D}$. Hence, define the *empirical risk* as $\widehat{R}_n(h) = \frac{1}{n}\sum_{i=1}^n \mathbf{1}\{h(x_i) \neq y_i\}$. For i.i.d. draws $\{x_i, y_i\}_{i=1}^n$, the empirical risk $\widehat{R}(h)$ is an unbiased estimator of the true risk $R(h)$ for any hypothesis $h \in \mathcal{H}$. Let $h^* = \arg\min_{h\in\mathcal{H}} R(h)$ be a hypothesis of minimum true risk in $\mathcal{H}$. Then, the goal of the learner is to return a hypothesis $h \in \mathcal{H}$ with true risk $R(h)$ as close as possible to the minimum true risk $R(h^*)$.

13.2.1 Review of passive learning

We start with the problem of passive learning for binary classification. Herein, we have a set of data points and labels $\{(x_i, y_i)\}_{i=1}^n$ drawn i.i.d. from distribution $\mathcal{D}$. Our goal is to find how fast the true risk goes down as a function of n. Intuitively, the lower the risk we want, the more data points we need to sample. Further, there must be a positive relationship between the number of hypotheses we have in the hypothesis space and the number of data points we need to identify the hypothesis with the minimum true risk almost surely. The following theorem characterizes these relationships:

Theorem 25. *Fix a distribution $\mathcal{D}$ over $\mathcal{X} \times \{0,1\}$ and a finite set of hypotheses $\mathcal{H}$ (i.e., $|\mathcal{H}| < \infty$). We assume that the data is separable so that*$\min_{h\in\mathcal{H}} \mathbb{P}_{(X,Y)\sim\mathcal{D}}(h(X) \neq Y) = 0$. *Given n IID* *draws from $\mathcal{D}$, $\{(x_i, y_i)\}_{i=1}^n$, let $\hat{h}_n = \arg\min_{h\in\mathcal{H}} \hat{R}_n(h)$ be the empirical risk minimizer. For any $\epsilon, \delta \in (0,1)$, we have $\mathbb{P}\big(R(\hat{h}_n) > \epsilon\big) \leq \delta$ whenever $n \geq \epsilon^{-1}\log(\frac{|\mathcal{H}|}{\delta})$. In other words, for any $\epsilon, \delta \in (0,1)$, with probability $1-\delta$, we have $R(\hat{h}_n) \leq \frac{\log(\frac{|\mathcal{H}|}{\delta})}{n}$*

Before going over the proof, it is worth noting that the theorem assumes a finite set of hypotheses in the hypothesis class $\mathcal{H}$. Such assumption, besides being practical from an optimization point of view, also simplifies the theory. Given that an infinite hypothesis class applied to a finite number of points observations yields a finite number of labellings, intuitively, assuming a finite hypothesis should not be too restrictive. We refer the interested reader to Boucheron et al. [Boucheron, 2005] in order to better understand how to make this argument rigorous by appealing to quantities like the Vapnik-Chervonenkis (VC) dimension and Rademacher complexity.

Proof. First note that $\hat{R}_n(\hat{h}_n) = 0$ since $\hat{R}_n(\hat{h}_n) = \min_{h\in\mathcal{H}} \hat{R}_n(h) \leq \hat{R}_n(h^*) = 0$. Now we can write:

$$\Pr\big(R(\hat{h}_n) > \epsilon\big) = \Pr\Big(\bigcup_{h\in\mathcal{H}}\{R(h) > \epsilon \wedge\ \hat{R}_n(h) = 0\}\Big) \leq \sum_{h\in\mathcal{H}} \Pr\big(\{R(h) > \epsilon \wedge\ \hat{R}_n(h) = 0\}\big), \quad (13.1)$$

where we performed a union bound to obtain the inequality. We can now find a bound for each element—$\Pr\big(\{R(h) > \epsilon,\ \hat{R}_n(h) = 0\}\big)$. This is the probability that a hypothesis with true risk greater than ϵ shows zero empirical risk in n points drawn i.i.d. from $\mathcal{D}$. Since the true risk for this hypothesis is greater than ϵ, the probability that this hypothesis correctly identifies a random point is lower than $1-\epsilon$. Thus, we can write:

$$\Pr\big(R(\hat{h}_n) > \epsilon\big) \leq \sum_{h\in\mathcal{H}} \Pr\big(\{R(h) > \epsilon \wedge\ \hat{R}_n(h) = 0\}\big) \leq \sum_{h\in\mathcal{H}}(1-\epsilon)^n \leq |\mathcal{H}|e^{-n\epsilon}$$

using the approximation $1 - x \leq e^{-x}$ for $x \geq 0$. Thus, $\Pr\big(R(\hat{h}_n) > \epsilon\big) \leq |\mathcal{H}|e^{-\epsilon n} = \delta$. Solving for n, we find $n \geq \epsilon^{-1}\log(\frac{|\mathcal{H}|}{\delta})$, and this completes the proof. □

Example 9. *As a concrete example, let us assume x being uniform on $[0,1]$, and that the hypothesis class is defined as $\mathcal{H} = \{\mathbf{1}\{x \leq \frac{i-1}{m-1}\} : i = 1, ..., m\}$; that is, there are m classifiers uniformly spaced in our hypothesis class (i.e., $|\mathcal{H}| = m$). If $y = h^*(x)$ for some $h^* \in \mathcal{H}$ (i.e., the perfect classifier exists in the hypothesis class), then we can apply Theorem* **??** *and say that after n observations with probability at least $1-\delta$ we have $R(\hat{h}_n) \leq \frac{\log(m/\delta)}{n}$.*

13.2.2 CAL, Disagreement-based learning

Now we will attempt to reduce the number of labels that are requested while achieving the same performance as passive learning. The style of algorithm we consider here is known as a disagreement-based learner. [Hanneke et al., 2014] provides an excellent survey of these methods.

Definition 20. *For some hypothesis class $\mathcal{H}$ and subset $V \subset \mathcal{H}$ where for each $h \in \mathcal{H}, h : \mathcal{X} \to \{0,1\}$, the* region of disagreement *is defined as*

$$DIS(V) = \{x \in \mathcal{X} : \exists\ h, h' \in \mathcal{H}\ s.t.\ h(x) \neq h'(x)\}$$

which is the set of unlabeled examples x for which there are hypotheses in V that disagree on how to label x.

The CAL[1] algorithm [Cohn et al., 1994] (see Algorithm 3) at time t, in response to Nature revealing $x_t \sim \mathcal{D}_X$, decides to request y_t if and only if $x_t \in DIS(V_{t-1})$ where V_t represents the subset of hypotheses in $\mathcal{H}$ that is consistent with all data requested up to time t. Note that if $x_t \notin DIS(V_{t-1})$ then *all* $h \in V_{t-1}$ agree on its label. Because $h^* \in V_t$ for all t on the assumption that $y_t = h^*(x_t)$, if $x_t \notin DIS(V_{t-1})$ then we can conclude that $y_t = h(x_t)$ for all $h \in V_{t-1}$. Thus, after n unlabeled examples, CAL has the same performance guarantee as the passive learning algorithm that observes all n labels. All that is left to do is bound how many samples CAL takes.

Computational efficiency Note, the check "$x_t \in DIS(V_{t-1})$" can often be computed efficiently. To see how, note that $x_t \in DIS(V_{t-1})$ if and only if there exists an $h \in V_{t-1}$ such that $h(x_t) \neq h^*(x_t)$. Now, $h \in V_{t-1}$ if and only if $h(x_s) = h^*(x_s)$ for all $s \in Z_{t-1}$. Thus, an equivalent check to $x_t \in DIS(V_{t-1})$ is a check if there exist an $h_1 \in \mathcal{H}$ such that $h_1(x_s) = y_s$ for all $(x_s, y_s) \in Z_{t-1} \cup (x_t, 1)$ *and* and an $h_0 \in \mathcal{H}$ such that $h_0(x_s) = y_s$ for all $(x_s, y_s) \in Z_{t-1} \cup (x_t, 0)$. This inspires the algorithm efficient CAL. This idea was first introduced in [Dasgupta et al., 2008]. If $\mathcal{H}$ is the set of linear halfspaces, such a check is a linear program.

Algorithm 1 CAL

```
Initialize: $Z_0 = \emptyset$, $V_0 = \mathcal{H}$
for $t = 1, 2 ... n$ do
    Nature reveals unlabeled data point $x_t$
    if $x_t \in DIS(V_{t-1})$ then
        Query $y_t$, and set $Z_t = Z_{t-1} \cup (x_t, y_t)$
    else
        $Z_t = Z_{t-1}$
    end if
    $V_t = \{h \in \mathcal{H} : h(x_i) = y_i \ \ \forall (x_i, y_i) \in Z_t\}$
end for
return any $h \in V_n$
```

Algorithm 2 Efficient CAL

```
Initialize: $Z_0 = \emptyset$
for $t = 1, 2 ... n$ do
    Nature reveals unlabeled data point $x_t$
    if for $\widehat{y} \in \{0, 1\}$ $\exists h_{\widehat{y}} \in \mathcal{H} : h_{\widehat{y}}(x_s) = y_s$, $\forall (x_s, y_s) \in Z_{t-1} \cup (x_t, \widehat{y})$ then
        Query $y_t$, and set $Z_t = Z_{t-1} \cup (x_t, y_t)$
    else
        $Z_t = Z_{t-1}$
    end if
end for
return $\arg\min_{h \in \mathcal{H}} \sum_{(x,y) \in Z_t} \mathbf{1}\{h(x) \neq y\}$.
```

CAL (and other disagreement-based methods) use a concept called the *disagreement coefficient* for analyzing the label complexity. Define the disagreement (pseudo) metric ρ on $\mathcal{H}$ as $\rho(h, h') := \mathbb{P}_{X \sim \mathcal{D}_X}(h(X) \neq h'(X))$. Let $B(h, r) := \{h' \in \mathcal{H} : \rho(h, h') \leq r\}$ denote the closed ball centered at $h \in \mathcal{H}$ with radius r.

Definition 21. *The* disagreement coefficient *of $h \in \mathcal{H}$ with respect to a hypothesis class $\mathcal{H}$ and distribution $\mathcal{D}_X$ is defined as*

$$\theta_h = \sup_r \frac{\mathbb{P}_{X \sim \mathcal{D}_X}(X \in DIS(B(h, r)))}{r}$$

As we will see, a small disagreement coefficient is a sufficient condition for efficient active learning algorithms. Essentially, it says that as the version space collapses around h^*, there is always sufficient mass between some sub-optimal h and h^* to rule out h in a bounded amount of time.

As an example, consider our example of before with $\mathcal{D}_X$ uniform on $[0, 1]$ and $\mathcal{H}$ as thresholds. Then, interpreting h^* as a number in $[0, 1]$ denoting the threshold location, $DIS(B(h^*, r)) = [h^* - r, h^* + r]$ and so $\mathbb{P}_{X \sim \mathcal{D}_X}(X \in DIS(B(h^*, r))) = 2r$. Therefore, the disagreement coefficient is equal to $\theta_{h^*} = \sup_r \frac{Pr(DIS(B(h^*, r)))}{r} = \frac{2r}{r} = 2$. With the exception of very nice situations (uniform distribution, symmetric geometry, etc.) the disagreement coefficient is often very difficult to calculate. Some

[1] Named for its inventors Cohn, Atlas, and Ladner

"nice" classes include i) homogeneous hyperplanes in $\mathbb{R}^d$ with data uniformly distributed on a sphere: $\theta \leq \sqrt{d}$, ii) general hyperplanes in $\mathbb{R}^d$ with the data density bounded below: $\theta = O(d)$, and iii) intervals $[a, b]$ on $\mathbb{R}$: $\theta = \infty$.

Theorem 26. *Let $h^* = \arg\min_{h\in\mathcal{H}} R(h)$ and assume $R(h^*) = 0$. Suppose n iid labeled examples $\{(x_i, y_i)\}_{i=1}^n$ are drawn from $\mathcal{D}$ and $V_n = \{h \in \mathcal{H} : h(x_i) = y_i \ \forall i \in [n]\}$. If we request λ additional labels only when the samples lie in the disagreement region $DIS(V_n)$, where $\lambda = 2\theta_{h^*} \log(|\mathcal{H}|/\delta)$, then, with probability greater than $1 - \delta$ we have $\sup_{h\in V_{n+\lambda}} R(h) \leq \sup_{h\in V_n} \frac{1}{2}R(h)$.*

Proof. The disagreement coefficient allows for a bound that relates the region of disagreement to the true risk of any $h \in V_n$. First, observe that:

$$\begin{aligned}\frac{\mathbb{P}_{X\sim\mathcal{D}_X}(X \in DIS(V_n))}{\sup_{h\in V_n} R(h)} &\leq \frac{\mathbb{P}_{X\sim\mathcal{D}_X}(X \in DIS(B(h^*, \sup_{h\in V_n} R(h))))}{\sup_{h\in V_n} R(h)} \\ &\leq \theta_{h^*}\end{aligned}$$

where the first inequality follows from the fact that in the RHS we replace V_n with a bigger set. To see this, for any $h \in V_n$ we have that $\rho(h, h^*) = \mathbb{P}_{X\sim\mathcal{D}_X}(h(X) \neq h^*(X)) = \mathbb{P}_{X\sim\mathcal{D}_X}(h(X) \neq Y) = R(h) \leq \max_{h\in V_n} R(h)$, which implies $h \in B(h^*, \sup_{h\in V_n} R(h))$. The second inequality follows by the definition of the disagreement coefficient.
By the definition of risk we have:

$$\begin{aligned}\sup_{h\in V_{n+\lambda}} R(h) &= \sup_{h\in V_{n+\lambda}} \mathbb{P}(h(X) \neq Y) \\ &= \sup_{h\in V_{n+\lambda}} \mathbb{P}(h(X) \neq Y|X \in DIS(V_n))\mathbb{P}(X \in DIS(V_n)) \\ &\leq \sup_{h\in V_{n+\lambda}} \mathbb{P}(h(X) \neq Y|X \in DIS(V_n))\, \theta_{h^*} \sup_{h\in V_n} R(h)\end{aligned}$$

where the second equality exploits the fact that $\mathbb{P}(h(X) \neq Y|X \notin DIS(V_n)) = 0$ since $h^*, h \in V_n$ and $Y = h^*(X)$. To bound, $\mathbb{P}(h(X) \neq Y|X \in DIS(V_n))$ note that it only looks at λ points that land in the disagreement region of V_n. This is like a brand new problem, where we can do passive learning only with points that land in $DIS(V_n)$. If we apply Theorem **??** and condition on the new version space $V_{n+\lambda}$, then the risk of any classifier in the new version space if we see only λ samples satisfies:

$$Pr(h(X) \neq Y|X \in DIS(V_n)) \leq \frac{\log(|V_{n+\lambda}|/\delta)}{\lambda} \leq \frac{\log(|\mathcal{H}|/\delta)}{\lambda}$$

Thus, for our specified value of λ, we conclude that $\sup_{h\in V_{n+\lambda}} R(h) \leq \frac{1}{2} \sup_{h\in V_n} R(h)$. □

Finally, we need to do the previous procedure $\log_2(1/\epsilon)$ times in order to achieve ϵ-error, meaning that the bound holds simultaneously for all epochs. By taking a union bound over $\lambda, 2\lambda, ..., \lceil\log_2(1/\epsilon)\rceil/\lambda$, we have that after $n \geq \lambda\lceil\log_2(1/\epsilon)\rceil$ labels, the true risk of any classifier satisfies $R(h) \leq \epsilon$, and the total number of requested labels is bounded by $2\theta_{h^*} \log(|\mathcal{H}|/\delta) \log(1/\epsilon)$ with probability at least $1 - \delta$. Compare this to passive learning which requires $O(\log(|\mathcal{H}|)/\epsilon)$ labels to reach an ϵ risk.

13.2.3 Splitting index

The CAL algorithm is very mellow in the sense that it will request the label of any example that will remove at least one hypothesis from the current version space. It is intuitive that it may be more advantageous for the learner to pass on some examples in favor of waiting for future examples to cut off a more substantial chunk of the version space. If we only have access to a sample oracle $x \sim \mathcal{D}$, this naturally leads to the question of what is the fundamental trade off between labeled data and unlabeled data?

A hard instance [Dasgupta, 2005b]. For some $\tau \in (0,1)$ let the distribution over $\mathcal{X}$ be denoted as $(1-\tau)\Gamma + \tau\Gamma'$ where Γ is the uniform distribution on the set $\{x \in \mathbb{R}^d : x_1^2 + x_2^2 = 1, x_3 = 0\}$ and Γ' is the uniform distribution on the set $\{x \in \mathbb{R}^d : x_1^2 + x_2^2 = 1, x_3 = 1\}$. Consider the set of tilted half-spaces that go through the origin so that they bisect Γ', and capture just a fraction ϵ of Γ. Assume $h^* \in \mathcal{H}$. Recall at each time Nature reveals $x \sim (1-\tau)\Gamma + \tau\Gamma'$, assume τ is very tiny. Note that by construction, if we only request labels that land on Γ', CAL would find an ϵ-close hypothesis to h^* using just $\log(1/\epsilon)$ queries. But it would only get a sample from Γ' every $1/\tau$ unlabeled examples. If τ is tiny and one seeks to minimize the amount of unlabeled data, it is better to run CAL on the full stream where the vast amount of data comes from Γ. This will find an ϵ-good classifier after $1/\epsilon$ labeled and unlabeled data. Can we formalize this trade off?

Consider a finite hypothesis space $\mathcal{H}$ and consider any $Q \subset \binom{\mathcal{H}}{2}$ where $(h,h') \in Q$ can be considered an edge connecting any two hypotheses. For any $\widehat{y} \in \{0,1\}$ define $\mathcal{H}_{(x,\widehat{y})} = \{h \in \mathcal{H} : h(x) = \widehat{y}\}$. We say an example x *ρ-splits Q* if requesting its label reduces the number of edges by at least a fraction $\rho \in (0,1)$:

$$\max\{|Q \cap \mathcal{H}_{(x,0)}|, |Q \cap \mathcal{H}_{(x,1)}|\} \leq (1-\rho)|Q|.$$

We are now ready to introduce the splitting index.

Definition 22. *Fix any subset $S \subset \mathcal{H}$ and $Q \subset \binom{S}{2}$ such that $\mathbb{P}(h(X) \neq h'(X)) \geq \epsilon, \forall (h,h') \in Q$. Then we say S is (ρ,ϵ,τ)-*splittable *if $\mathbb{P}(X$ splits $Q) \geq \tau$.*

Basically, the definition is saying that to reduce the number of pairs of hypotheses that differ by at least ϵ by a fraction at least ρ, requires $1/\tau$ unlabeled data. If $\mathcal{H}$ is finite, and $\mathcal{H}$ is (ρ,ϵ,τ)-splittable, then it is almost immediate that there exists an algorithm that requires $1/(\tau\rho)$ unlabeled data and $1/\rho$ labels to identify an ϵ-good classifier ([Dasgupta, 2005b] suggests one, though it is computationally intractable). What is more important is the reproduced lower bound:

Theorem 27 ([Dasgupta, 2005b]). *Fix any hypothesis space $\mathcal{H}$ and distribution $\mathcal{D}$ over $\mathcal{X} \times \{0,1\}$. Suppose that for some $\rho \in (0,1)$, $\epsilon \in (0,1)$ and some $\tau \in (0,1/2)$, the set $S \subset \mathcal{H}$ is not (ρ,ϵ,τ)-splittable. Then any active learning strategy that achieves an accuracy of $\epsilon/2$ on all target hypotheses in S must, with probability at least $3/4$ (taken over the random sampling of data), either draw $\geq 1/\tau$ unlabeled samples, or must request $\geq 1/\rho$ labels.*

The above theorem characterizes the trade off between the streaming sampling oracle from $\mathcal{X}$ and the pool-based setting. In the streaming setting, one may be able to use as few labels as the learner in the pool-based setting, but they may have to wade through an arbitrarily large amount of unlabeled data first.

13.2.4 Lower bounds

The somewhat trivial covering lower bound of Proposition 9 for the separable, pool-based setting can be extended to the separable, streaming setting by replacing finite cardinality classes with ϵ-covers with respect to the underlying distribution [Kulkarni et al., 1993]. Just like in the pool-based setting, this style of lower bound is unlikely to be achieved by an algorithm in all cases because it is not considering how little information each query may provide. The splitting-index lower bound of Theorem 27 is one of the only results I am aware of that has a corresponding upper bound for a fixed instance of $\mathcal{D}_X$ and $\mathcal{H}$, indicating that it may be fundamental. Hanneke developed a framework in the streaming setting inspired by Hegedus's extended teaching dimension. Essentially, the extended teaching dimension is now a random quantity based on data, and is bounded with high probability. The sample complexity is upper and lower bounded by quantities that match in limiting cases, but is not as strong as the same quantity appearing in both the upper and lower bounds like in the pool-based case. There are *minimax* lower bounds known for the separable setting which considers a worst-case choice of $\mathcal{D}_X$ for each choice of $\mathcal{H}$. As described in the lower bounds section below, these can be misleading.

13.2.5 Open problems

The algorithm in [Dasgupta, 2005b] that achieves the lower bound is computationally intractable. Recent work has demonstrated that if one has access to a sampling distribution over $\mathcal{H}$, one can use rejection sampling to write down an algorithm that can be run, though it may still have unbounded computation [Tosh and Dasgupta, 2017]. A significant advancement would be an algorithm that achieves the same performance but only uses empirical risk oracles, like those used in the efficient version of CAL. It is much more natural to efficiently minimize a loss than define a favorable distribution over hypotheses.

13.3 Agnostic, sampling-oracle setting

In contrast to the separable setting, in the agnostic setting we now make minimal assumptions on how labels related to our hypothesis class $\mathcal{H}$. Specifically, in this setting we assume that when we request the label of some $x \in \mathcal{X}$ we observe a Bernoulli random variable $Y \in \{0,1\}$ with $\mathbb{P}(Y = 1|X = x) = \eta(x)$ where $\eta : \mathcal{X} \to [0,1]$ is arbitrary. Define $R(h) = \mathbb{E}_{X\sim\nu, Y\sim\eta(X)}[\mathbf{1}\{h(X) \neq Y\}]$.

13.3.1 Passive learning

First, let us establish the baseline of a passive learning algorithm that observes the label of every $x \sim \nu$. Let $\{(x_t, y_t)\}_{t=1}^n$ be a dataset such that $x_t \sim \nu$ and $y_t \sim \eta(x_t)$. Let $\widehat{R}_n(h) = \frac{1}{n}\sum_{t=1}^n \mathbf{1}\{h(x_t) \neq y_t\}$ and $\widehat{h}_n = \arg\min_{h\in\mathcal{H}} \widehat{R}_n(h)$. Note that for any $h \in \mathcal{H}$ we have

$$\begin{aligned}
\mathbb{E}_{X\sim\nu}[(\mathbf{1}\{h(X) \neq Y\} - \mathbf{1}\{h^*(X) \neq Y\})^2] &= \mathbb{E}_{X\sim\nu}[\mathbf{1}\{h(X) \neq h^*(X)\}] \\
&= \mathbb{E}_{X\sim\nu}[\mathbf{1}\{h(X) = Y, h^*(X) \neq Y\} + \mathbf{1}\{h(X) \neq Y, h^*(X) = Y\}] \\
&\leq R(h) + R(h^*) \\
&\leq 2\max\{R(h) - R(h^*), 2R(h^*)\}
\end{aligned}$$

By Bernstein's inequality, we have with probability at least $1-\delta$

$$\begin{aligned}
R(\widehat{h}_n) - R(h^*) &\leq \widehat{R}_n(\widehat{h}_n) - \widehat{R}_n(h^*) + \sqrt{\mathbb{E}_{X\sim\nu}[\mathbf{1}\{\widehat{h}_n(X) \neq h^*(X)\}]\,\frac{2\log(|\mathcal{H}|/\delta)}{n}} + \frac{\log(|\mathcal{H}|/\delta)}{n} \\
&\leq \sqrt{\max\{R(\widehat{h}_n) - R(h^*), 2R(h^*)\}\,\frac{4\log(|\mathcal{H}|/\delta)}{n}} + \frac{\log(|\mathcal{H}|/\delta)}{n} \\
&\leq \max\{\frac{8\log(|\mathcal{H}|/\delta)}{n}, \sqrt{\frac{4R(h^*)\log(|\mathcal{H}|/\delta)}{n}} + \frac{\log(|\mathcal{H}|/\delta)}{n}\} \\
&\leq \frac{8\log(|\mathcal{H}|/\delta)}{n} + \sqrt{\frac{4R(h^*)\log(|\mathcal{H}|/\delta)}{n}}
\end{aligned}$$

where the third inequality follows from the quadratic equation. We summarize our findings in the following theorem.

Theorem 28. *Fix a distribution $\mathcal{D}$ over $\mathcal{X}\times\{0,1\}$ and a finite set of hypotheses $\mathcal{H}$ (i.e., $|\mathcal{H}|<\infty$). Given n IID draws from $\mathcal{D}$, $\{(x_i,y_i)\}_{i=1}^n$, let $\hat{h}_n = \arg\min_{h\in\mathcal{H}}\hat{R}_n(h)$ be the empirical risk minimizer. Let $h^*\in\arg\min_{h\in\mathcal{H}}R(h)$ be the true risk minimizer. For any $\epsilon,\delta\in(0,1)$, we have $\mathbb{P}\big(R(\hat{h}_n) - R(h^*) > \epsilon\big) \leq \delta$ whenever $n \geq \left(\frac{R(h^*)}{\epsilon^2} + \frac{1}{\epsilon}\right) 8\log(|\mathcal{H}|/\delta)$. In other words, for any $\delta\in(0,1)$, with probability $1-\delta$, we have $R(\hat{h}_n) \leq R(h^*) + \sqrt{\frac{4R(h^*)\log(|\mathcal{H}|/\delta)}{n}} + \frac{8\log(|\mathcal{H}|/\delta)}{n}$.*

13.3.2 Robust CAL

Our strategy will be to use disagreement-based learning. This algorithm and its analysis is based on [Dasgupta et al., 2008]. While the argument here is somewhat coherent, I encourage you to go and read the paper because like most works Sanjoy Dasgupta is involved in, it is an exemplar of technical writing.

Algorithm 3 Robust CAL

```
Initialize: $Z_0 = \emptyset$, $V_1 = \mathcal{H}$
for $t = 1, 2...n$ do
    Nature reveals unlabeled data point $x_t$
    if $x_t \in DIS(V_t)$ then
        Query $y_t$, and set $Z_t = Z_{t-1} \cup (x_t, y_t)$
    else
        $Z_t = Z_{t-1}$
    end if
    if $\log_2(t) \in \mathbb{N}$ then
        $\widehat{L}_t(h) = \frac{1}{t}\sum_{(x_s,y_s)\in Z_t}\mathbf{1}\{h(x_s) \neq y_s\}$ for all $h \in \mathcal{H}$, $\widehat{h}_t = \arg\min_{h\in V_t}\widehat{L}_t(h)$
        $\widehat{\rho}_t(h,h') = \frac{1}{t}\sum_{s=1}^{t}\mathbf{1}\{h(x_s) \neq h'(x_s)\}$, $\beta_t = \sqrt{\frac{2\log(2\log_2(t)^2|\mathcal{H}|^2/\delta)}{t}}$
        $V_{t+1} = \{h \in V_t : \widehat{L}_t(h) - \widehat{L}_t(\widehat{h}_t) \leq \beta_t\sqrt{\widehat{\rho}_t(h,\widehat{h}_t)} + \beta_t^2/2\}$
    else
        $V_{t+1} = V_t$, $\beta_{t+1} = \beta_t$, $\widehat{h}_{t+1} = \widehat{h}_t$
    end if
end for
return any $h \in V$
```

Define the empirical risk of all the data up to time t as $\widehat{R}_t(h) = \frac{1}{t}\sum_{s=1}^t \mathbf{1}\{h(x_s) \neq y_s\}$. The first thing to note about this algorithm is that for any $h, h' \in V_t$ we have

$$\begin{aligned}
\widehat{R}_t(h) - \widehat{R}_t(h') &= \frac{1}{t}\sum_{s=1}^{t}(\mathbf{1}\{h(x_s) \neq y_s\} - \mathbf{1}\{h'(x_s) \neq y_s\}) \\
&= \underbrace{\frac{1}{t}\sum_{(x_s,y_s)\in Z_t}(\mathbf{1}\{h(x_s) \neq y_s\} - \mathbf{1}\{h'(x_s) \neq y_s\})}_{=L_t(h)-L_t(h')} + \underbrace{\frac{1}{t}\sum_{(x_s,y_s)\notin Z_t}(\mathbf{1}\{h(x_s) \neq y_s\} - \mathbf{1}\{h'(x_s) \neq y_s\})}_{=0}
\end{aligned}$$

because if for some $s \leq t$ we have $(x_s, y_s) \notin Z_t$, then $x_s \notin DIS(V_s)$, and thus all $h, h' \in V_s$ satisfy $(\mathbf{1}\{h(x_s) \neq y_s\} - \mathbf{1}\{h'(x_s) \neq y_s\}) = 0$. Since $V_t \subset V_{t-1} \subset \ldots V_s$ we also have that all $h, h' \in V_t$ have this difference equal to 0. However, it is important to note that while $\widehat{R}_t(h) - \widehat{R}_t(h') = \widehat{L}_t(h) - \widehat{L}_t(h')$, we can only guarantee that $\widehat{L}_t(h) \leq \widehat{R}_t(h)$.

Define the events

$$\begin{aligned}
\mathcal{E}_0 &:= \bigcap_{\ell=1}^{\infty}\bigcap_{h\in\mathcal{H}}\{|\widehat{R}_{2^\ell}(h) - R(h)| \leq \beta_{2^\ell}\sqrt{R(h)} + \beta_{2^\ell}^2/2\}, \\
\mathcal{E}_1 &:= \bigcap_{\ell=1}^{\infty}\bigcap_{h\in\mathcal{H}}\{\widehat{R}_{2^\ell}(h) - \widehat{R}_{2^\ell}(h') \leq R(h) - R(h') + \beta_{2^\ell}\sqrt{\widehat{\rho}_{2^\ell}(h,h')} + \beta_{2^\ell}^2/2\}.
\end{aligned}$$

To show $\mathbb{P}(\mathcal{E}_0) \geq 1 - \delta/2$ one simply applies Bernstein's inequality and a union bound, exploiting the fact that Variance$(\mathbf{1}\{h(X) \neq Y\}) \leq \mathbb{E}[(\mathbf{1}\{h(X) \neq Y\})^2] = R(h)$ (note: the chosen value of β_t is chosen to be larger than necessary for convenience). To show $\mathbb{P}(\mathcal{E}_1) \geq 1 - \delta/2$ we apply empirical Bernstein's inequality [Maurer and Pontil, 2009] similar to as in Section 13.3.1 plus a union bound. This implies that with probability at least $1 - \delta/2$ for any t that is a power of 2 and any $h, h' \in \mathcal{H}$ we have

$$\begin{aligned}
\widehat{R}_t(h) - \widehat{R}_t(h') &\leq R(h) - R(h') + \sqrt{\frac{2\widehat{\rho}_t(h,h)\log(2\log_2(t)^2|\mathcal{H}|/\delta)}{t}} + \frac{\log(2\log_2(t)^2|\mathcal{H}|/\delta)}{t} \\
&= R(h) - R(h') + \beta_t\sqrt{\widehat{\rho}_t(h,h')} + \beta_t^2/2
\end{aligned}$$

In particular, using the observations above, this implies that

$$\begin{aligned}
\widehat{L}_t(h^*) - \widehat{L}_t(\widehat{h}_t) &= \widehat{R}_t(h^*) - \widehat{R}_t(\widehat{h}_t) \\
&\leq R(h^*) - R(\widehat{h}_t) + \beta_t\sqrt{\widehat{\rho}_t(h^*,\widehat{h}_t)} + \beta_t^2/2 \\
&\leq \beta_t\sqrt{\widehat{\rho}_t(h^*,\widehat{h}_t)} + \beta_t^2/2
\end{aligned}$$

which implies $h^* \in V_t$ for all t. This proves correctness, we next prove the sample complexity.

Sample complexity analysis For any $h \in V_{t+1}$ we have

$$
\begin{aligned}
\widehat{R}_t(h) - \widehat{R}_t(h^*) &= \widehat{L}_t(h) - \widehat{L}_t(\widehat{h}_t) \\
&\leq \sqrt{\widehat{\rho}_t(h, \widehat{h}_t)}\beta_t + \beta_t^2/2 \\
&= \sqrt{\widehat{L}_t(h)}\beta_t + \sqrt{\widehat{L}_t(\widehat{h}_t)}\beta_t + \beta_t^2/2 \\
&\leq \sqrt{\widehat{L}_t(h)}\beta_t + \sqrt{\widehat{L}_t(h^*)}\beta_t + \beta_t^2/2 \\
&\leq \sqrt{\widehat{R}_t(h)}\beta_t + \sqrt{\widehat{R}_t(h^*)}\beta_t + \beta_t^2/2.
\end{aligned}
$$

where we have exploited that for any $h, h' \in V_t$

$$
\begin{aligned}
\widehat{\rho}_t(h, h') &= \frac{1}{t}\sum_{s=1}^{t} \mathbf{1}\{h(x_s) \neq h'(x_s)\} \\
&= \frac{1}{t}\sum_{(x_s,y_s)\in Z_t} \mathbf{1}\{h(x_s) \neq h'(x_s)\} \\
&\leq \frac{1}{t}\sum_{s=1}^{t} \mathbf{1}\{h(x_s) \neq y_s\} + \mathbf{1}\{h'(x_s) \neq y_s\} \leq \widehat{L}_t(h) + \widehat{L}_t(h')
\end{aligned}
$$

and the facts that (i) $\widehat{R}_t(h) - \widehat{R}_t(h') = \widehat{L}_t(h) - \widehat{L}_t(h')$ for all $h, h' \in V_t$, (ii) $\widehat{L}_t(\widehat{h}_t) \leq \widehat{L}_t(h^*)$, and (iii) $\widehat{L}_t(h) \leq \widehat{R}_t(h)$ for all $h \in V_t$. We now use the crazy useful fact that $A \leq B + C\sqrt{A} \implies A \leq B + C^2 + C\sqrt{B}$ for $A, B, C \geq 0$ we have

$$
\begin{aligned}
R(h) - \beta_t\sqrt{R(h)} - \beta_t^2/2 \leq& \widehat{R}_t(h) \\
\leq& \widehat{R}_t(h^*) + \sqrt{\widehat{R}_t(h)}\beta_t + \sqrt{\widehat{R}_t(h^*)}\beta_t + \beta_t^2/2 \\
\leq& \widehat{R}_t(h^*) + \sqrt{\widehat{R}_t(h^*)}\beta_t + \beta_t^2/2 + \beta_t^2 + \beta_t\sqrt{\widehat{R}_t(h^*) + \sqrt{\widehat{R}_t(h^*)}\beta_t + \beta_t^2/2} \\
\leq& R(h^*) + \beta_t\sqrt{R(h^*)} + \beta_t^2 + \beta_t\sqrt{R(h^*) + \beta_t\sqrt{R(h^*)} + \beta_t^2} + (3/2)\beta_t^2 \\
&+ \beta_t\sqrt{R(h^*) + \beta_t\sqrt{R(h^*)} + \beta_t^2 + \beta_t\sqrt{R(h^*) + \beta_t\sqrt{R(h^*)} + \beta_t^2} + \beta_t^2/2} \\
\leq& R(h^*) + c_1'\beta_t\sqrt{R(h^*)} + c_2'\beta_t^2
\end{aligned}
$$

for some constants c_1, c_2'. Applying the crazy useful fact again to $A = R(h)$ we get that

$$
R(h) \leq c_0 R(h^*) + c_1\beta_t\sqrt{R(h^*)} + c_2\beta_t^2
$$

for some constants c_0, c_1, c_2. Noting that $\rho_\nu(h, h^*) = \mathbb{E}_{X\sim\nu}[\mathbf{1}\{h(x) \neq h^*(X)\}] \leq R(h) + R(h^*)$ we have that

$$
\begin{aligned}
\mathbb{P}(x_{t+1} \in DIS(V_{t+1})) &= \mathbb{P}(\exists h, h' \in V_{t+1} : h(x_t) \neq h'(x_t)) \\
&= \mathbb{P}(\exists h \in V_{t+1} : h(x_t) \neq h^*(x_t)) \\
&\leq \mathbb{P}(\exists h \in \mathcal{H} : h(x_t) \neq h^*(x_t),\ R(h) \leq c_0 R(h^*) + c_1\beta_t\sqrt{R(h^*)} + c_2\beta_t^2) \\
&\leq \mathbb{P}(\exists h \in \mathcal{H} : h(x_t) \neq h^*(x_t),\ \rho(h, h^*) \leq (1 + c_0)R(h^*) + c_1\beta_t\sqrt{R(h^*)} + c_2\beta_t^2) \\
&\leq \theta^*(R(h^*) + c_1\beta_t\sqrt{R(h^*)} + c_2\beta_t^2)\big((1 + c_0)R(h^*) + c_1\beta_t\sqrt{R(h^*)} + c_2\beta_t^2\big)
\end{aligned}
$$

where we have used the definition of the disagreement coefficient. We summarize our findings in the following theorem.

Theorem 29. *Fix $\epsilon > 0$ and $\delta \in (0,1)$. With probability at least $1-\delta$ if $t \gtrsim (\frac{R(h^*)}{\epsilon^2}+\frac{1}{\epsilon}) \log(|\mathcal{H}| \log(1/\epsilon)/\delta)$ then $R(\widehat{h}_t) - R(h^*) \leq \epsilon$ and*

$$\begin{aligned}\#\ \textit{labels requested} &\lesssim \theta^*(\nu+\epsilon)\Big(R(h^*)t + \sqrt{t\log(|\mathcal{H}|\log(t)/\delta)} + \log(t)\log(|\mathcal{H}|\log(t)/\delta)\Big) \\ &\lesssim \theta^*(\nu+\epsilon)\Big(\frac{R(h^*)^2}{\epsilon^2} + \log(\frac{1}{\epsilon})\Big)\log(|\mathcal{H}|\log(1/\epsilon)/\delta)\end{aligned}$$

Note that we always have $\theta^*(\nu+\epsilon) \leq 1/(\nu+\epsilon)$. If $\theta^*(\nu+\epsilon)$ is a constant independent of ϵ then this theorem says that it requires just $O(\log(1/\epsilon))$ labels to obtain an ϵ-good classifier when $\epsilon \geq R(h^*)$. On the other hand, if $\epsilon \ll R(h^*)$ then one requires $O(R(h^*)^2/\epsilon^2)$ labels. Note, this is not much better than the passive guarantee of $O(R(h^*)/\epsilon^2)$! While this ladder observation is somewhat discouraging, note that under favorable noise distributions such as Massart noise (separable, but each label is flipped with a constant probability bounded away from 1/2) or Tsybakov noise then the number of labels required by active and passive can be quite large.

13.3.3 Computationally efficient algorithms

Researchers approach computationally efficiency in different ways. The first approach simply assumes access to an empirical risk oracle that returns a classifier from $\mathcal{H}$ that minimizes the (weighted) empirical 0/1-loss on any set of examples. The second replaces the objective of 0/1-loss with a convex loss and performs active learning to minimizes this convex loss (c.f., [Beygelzimer et al., 2009]). The third approach uses a convex surrogate loss in place of a empirical 0/1-loss but still remains the objective of 0/1-loss (c.f., [Hanneke et al., 2014]). This third approach relies on the function class being sufficiently rich and the loss function being *classification calibrated* which allows one to relate the quality of the solution of the convex loss to the 0/1-loss [Bartlett et al., 2006]. [Hanneke et al., 2014] argues against the second approach as there are examples where the second approach requires exponentially more labels than the first or third. The third approach requires unverifiable assumptions, such as the Bayes classifier being in $\mathcal{H}$. The first approach rests on naive hope that the minimizer of the convex loss will be close to the minimizer of 0/1-loss without justification. But it is also the most practical solution, and tends to work well if not too much is demanded from the oracle (e.g., oracle is constrained in some way).

Just like with CAL, we can derive an exactly equivalent version of Robust CAL that does not explicitly maintain a version space. However, this reduction requires a minimization oracle that minimizes empirical risk on one set of examples subject to making no mistakes on a different set of examples. In practice constructing such an oracle is very awkward so we do not discuss it further, see the original paper [Dasgupta et al., 2008] for details. [Beygelzimer et al., 2010] requires far less from its procedure by requiring the oracle to minimize a weighted empirical subject to classifying just a single data point as a specific label, so a single constraint. There are natural hypothesis classes like halfspaces and trees where this is easy satisfy, and in any case, one can simply take the Lagrange multiplier approach and place a large weight on this one loss to satisfy a constraint. Ideally, we would like our method to rely on performing empirical risk minimization on a set of examples, without any constraints. [Huang et al., 2015] is one of the first algorithms to achieve this feat.

13.3.4 Minimax lower bounds

To the best of my knowledge, only *minimax* lower bounds are known for active learning outside of a few specific settings [Kääriäinen, 2006, Castro and Nowak, 2008, Raginsky and Rakhlin, 2011, Hanneke and Yang, 2015]. An instance is defined as a joint probability distribution $\mathcal{D}$ defined over $\mathcal{X} \times \{0,1\}$. That is, if we interpreted $\mathcal{D}$ as a density then $\mathcal{D}(x,y) = \nu(x)(\eta(x)\mathbf{1}\{y=1\} + (1-\eta(x))\mathbf{1}\{y=0\})$. Fix a collection of instances $\mathbb{D}$. For any $\epsilon \in (0,\epsilon_0)$ and $\delta \in (0,\delta_0)$, let $(S)(\mathcal{D},\mathcal{H},\epsilon,\delta,\mathcal{A})$ denote the number of queries taken by algorithm $\mathcal{A}$ on instance $\mathcal{D}$ with hypothesis class $\mathcal{D}$ to output a ϵ-good classifier with probability at least $1-\delta$. Minimax lower bounds are stated as follows: for any $\epsilon \in (0,\epsilon_0)$ and $\delta \in (0,\delta_0)$ we have that $\min_{\mathcal{A}} \max_{\mathcal{D}\in\mathbb{D}} \mathfrak{S}(\mathcal{D},\mathcal{H},\epsilon,\delta,\mathcal{A}) \geq \Lambda(\mathbb{D},\mathcal{H},\epsilon,\delta)$. We say an algorithm $\mathcal{A}$ is minimax optimal if $\mathfrak{S}(\mathcal{D},\mathcal{H},\epsilon,\delta,\mathcal{A}) \lesssim \Lambda(\mathbb{D},\mathcal{H},\epsilon,\delta)$, but typically we will allow the upper and lower bounds to differ by small amounts. An excellent survey of known minimax lower bounds is available in [Hanneke and Yang, 2015] for a variety of classes $\mathbb{D}$ with assumed access to a sampling oracle with no cost attributed to sampling unbounded amounts of unlabeled data. Some important classes of $\mathbb{D}$ include:

- **Realizable/separable**: There exists an $h^* \in \mathcal{H}$ such that $h^*(x) = 2\eta(x) - 1 \in \{0,1\}$ for all $x \in \mathcal{X}$. ν is arbitrary.

- **Massart noise**: There exists an $h^* \in \mathcal{H}$ such that $h^*(x) = \text{sign}(2\eta(x)-1)$, and there exists a constant $\alpha > 0$ such that $|\eta(x) - 1/2| \geq \alpha$. ν is arbitrary.

- **Tsybakov noise**: There exists an $h^* \in \mathcal{H}$ such that $h^*(x) = \text{sign}(2\eta(x)-1)$, and there exists constants $a \geq 1$ and $\alpha \in (0,1)$ such that for all $\gamma > 0$ we have $\mathbb{P}_{X\sim\nu}(|\eta(X) - 1/2| \leq \gamma) \leq a'\gamma^{a/(1-a)}$ where $a' = (1-\alpha)(2\alpha)^{\alpha/(1-\alpha)}a^{1/(1-\alpha)}$.

- **Agnostic noise**: For $\alpha \geq 0$ there exists an $h^* \in \mathcal{H}$ such that $R(h^*) \leq \alpha$. ν is arbitrary.

Note that each of the above classes is a subset of the class that follows it. Algorithms are typically designed for either the realizable setting or agnostic setting, and then only algorithms for the ladder are analyzed under the easier settings.

Minimax lower bounds are sometimes **very weak** and can even be misleading. For example, consider the "hard instance" $\mathcal{D}$ of Section 13.2.3. The splitting index algorithm can identify an ϵ-good classifier with just $\log(1/\epsilon)$ queries using binary search on Γ'. On the other hand, CAL will essentially only sample from Γ if τ is very small, and require $1/\epsilon$ labels to obtain an ϵ-good classifier. Thus, the splitting algorithm requires exponentially fewer samples than CAL on this instance, but nevertheless, CAL is nearly minimax optimal for the realizable case [Hanneke and Yang, 2015]. This is because the hard instance is a particular choice of ν, not the worst-case distribution ν.

Ideally we would want instance-dependent lower bounds. That is, how many labels does an algorithm require for the *particular* instance $\mathcal{D}$ you care about? We will expand on this discussion and describe what is known for this case in the next section.

13.4 Agnostic, pool-based setting

We are again in the agnostic setting and therefore, when we request the label of some $x \in \mathcal{X}$ we observe a Bernoulli random variable $Y \in \{0,1\}$ with $\mathbb{P}(Y=1|X=x) = \eta(x)$ where $\eta : \mathcal{X} \to [0,1]$ is arbitrary. In this pool-based setting we are going to assume that $\mathcal{X}$ is finite with $|\mathcal{X}| = n$ and that there exists a *known* probability density ν defined over $\mathcal{X}$ that we wish to evaluate risk with respect to. Define the risk of any $h \in \mathcal{H}$ as $R(h) := \mathbb{E}_{X\sim\nu, Y\sim\eta(X)}[\mathbf{1}\{Y \neq h(X)\}]$. For any $\epsilon > 0$ and $\delta \in (0,1)$ we want an algorithm that identifies an $\widehat{h} \in \mathcal{H}$ such that $R(\widehat{h}) - \min_{h\in\mathcal{H}} R(h) \leq \epsilon$ with probability at least $1-\delta$ using as few total requested labels as possible. While we could apply a disagreement-based algorithm from the streaming setting to accomplish this, instead we will reduce the problem to an instance of linear bandits. We will see that this algorithm obtains a sample complexity that is provably superior to disagreement-based learning, sometimes requiring exponentially fewer labels.

13.4.1 Reduction to linear bandits

Note that

$$\begin{aligned} R(h) := \mathbb{E}_{X\sim\nu, Y\sim\eta(X)}[\mathbf{1}\{Y \neq h(X)\}] &= \sum_{x\in\mathcal{X}} \nu(x)(\eta(x)\mathbf{1}\{h(x)\neq 1\} + (1-\eta(x))\mathbf{1}\{h(x)\neq 0\}) \\ &= \sum_{x\in\mathcal{X}} \nu(x)\eta(x) + \sum_{x\in\mathcal{X}} \nu(x)(1-2\eta(x))h(x). \end{aligned}$$

Binary classification is intimately related with transductive linear bandits as we now show. Define $\theta^* = [(2\eta(x)-1)]_{x\in\mathcal{X}} \in \mathbb{R}^n$ and for each $h \in \mathcal{H}$ we define a vector $z_h = [\nu(x)h(x)]_{x\in\mathcal{X}} \in \mathbb{R}^n$ and set $\mathcal{Z} = \{z_h : h \in \mathcal{H}\}$. When requesting the label of example $x \in \mathcal{X}$, we observe $Y \in \{0,1\}$ and convert this into a "pull" of arm $\mathbf{e}_x \in \{0,1\}^n$ by feeding the bandit algorithm $2Y-1$ so that $\mathbb{E}[2Y-1|X=x] = 2\eta(x)-1 = \langle \mathbf{e}_x, \theta* \rangle$. Thus, identifying a $\widehat{h}$ such that $R(\widehat{h}) - \min_{h\in\mathcal{H}} R(h) \leq \epsilon$ is equivalent to identifying a $\widehat{z} \in \mathcal{Z}$ such that $\max_{z\in\mathcal{Z}}\langle z, \theta^*\rangle - \langle \widehat{z}, \theta^*\rangle \leq \epsilon$. We can now apply the pure-exploration algorithm for linear bandits! Note that in that algorithm, at each stage we solved $\arg\min_{\lambda\in\triangle_{\mathcal{X}}} \max_{z,z'\in\mathcal{Z}_\ell} \|z-z'\|^2_{A(\lambda)^{-1}}$. We observe that

$$\|z-z'\|^2_{A(\lambda)^{-1}} = \sum_{x\in\mathcal{X}} \frac{|h(x)-h'(x)|^2\nu(x)^2}{\lambda(x)} = \sum_{x\in\mathcal{X}} \nu(x)\frac{\mathbf{1}\{h(x)\neq h'(x)\}}{\lambda(x)/\nu(x)} = \mathbb{E}_{X\sim\nu}\left[\frac{\mathbf{1}\{h(X)\neq h'(X)\}}{\lambda(X)/\nu(X)}\right].$$

It appears we can run the linear bandit algorithm precisely as before. But there is a problem: that algorithm used the least squares estimator for θ^*, which assumes the number of samples exceeds that dimension, which is $|\mathcal{X}| = n$ here–this is equivalent to labeling every example, trivial. Fortunately, we can solve this problem by using a regularized estimator.

13.4.2 Regularized empirical risk minimization

First, we need a deviation result. Define $\rho_\lambda(h,h') = \mathbb{E}_{X\sim\nu}[\frac{\mathbf{1}\{h(X)\neq h'(X)\}}{\lambda(X)/\nu(X)}]$.

Lemma 24. *Let λ and ν be two probability densities defined over $\mathcal{X}$ with $\lambda \ll \nu$*[2]*. Consider a dataset $\{(x_t, y_t, w_t)\}_{t=1}^{\tau}$ where $x_t \sim \lambda$, $y_t \sim$ Bernoulli$(\eta(x_t))$, and $w_t = \frac{\lambda(x_t)}{\nu(x_t)}$. For any $\gamma > 0$ define*

$$\widetilde{R}^\gamma(h) = \frac{1}{\tau}\sum_{t=1}^{\tau} \frac{1}{w_t+\gamma}\mathbf{1}\{h(x_t)\neq y_t\}.$$

Then for any $h, h' \in \mathcal{H}$ we have with probability at least $1-\delta$

$$\widetilde{R}^\gamma(h) - \widetilde{R}^\gamma(h') \leq R(h) - R(h') + \gamma\rho_\lambda(h,h') + \sqrt{\rho_\lambda(h,h')\ \frac{2\log(1/\delta)}{\tau}} + \frac{\log(1/\delta)}{\tau(\gamma + \min_{x\in\mathcal{X}}\lambda(x)/\nu(x))}.$$

[2] We say density p dominates q, or $p \gg q$, if support$(q) \subseteq$ support(p)

Proof. Since γ is fixed, to simplify notation in the remainder of this proof let $\widetilde{R}(h) = \widetilde{R}^\gamma(h)$. First note that for any $h, h' \in \mathcal{H}_\ell$ we have $\mathbb{E}[\frac{1}{\tau}\sum_{t=1}^\tau \frac{1}{w_t}(\mathbf{1}\{h(x_t) \neq y_t\} - \mathbf{1}\{h'(x_t) \neq y_t\})] = R(h) - R(h')$. Thus,

$$\begin{aligned}
\mathbb{E}[\widetilde{R}(h) - \widetilde{R}(h')] - [R(h) - R(h')] &= \mathbb{E}\left[\frac{1}{\tau}\sum_{t=1}^{\tau}(\frac{1}{w_t+\gamma} - \frac{1}{w_t})(\mathbf{1}\{h(x_t) \neq y_t\} - \mathbf{1}\{h'(x_t) \neq y_t\})\right] \\
&= \mathbb{E}\left[\frac{1}{\tau}\sum_{t=1}^{\tau}\frac{-\gamma}{w_t(w_t+\gamma)}(\mathbf{1}\{h(x_t) \neq y_t\} - \mathbf{1}\{h'(x_t) \neq y_t\})\right] \\
&\leq \mathbb{E}\left[\frac{1}{\tau}\sum_{t=1}^{\tau}\frac{\gamma}{w_t(w_t+\gamma)}\mathbf{1}\{h(x_t) \neq h'(x_t)\}\right] \\
&= \gamma\mathbb{E}_{X\sim\nu}\left[\frac{\mathbf{1}\{h(X) \neq h'(X)\}}{\lambda(X)/\nu(X)+\gamma}\right] \\
&\leq \gamma\mathbb{E}_{X\sim\nu}\left[\frac{\mathbf{1}\{h(X) \neq h'(X)\}}{\lambda(X)/\nu(X)}\right] = \gamma\rho_\lambda(h,h')
\end{aligned}$$

If $\alpha_t := \frac{1}{w_t+\gamma}(\mathbf{1}\{h(x_t) \neq y_t\} - \mathbf{1}\{h'(x_t) \neq y_t\}$ then $\widetilde{R}(h) - \widetilde{R}(h') = \frac{1}{\tau}\sum_{t=1}^\tau \alpha_t$ where each α_t is IID. Note that $\alpha_t \leq 1/(\gamma + \min_{x\in\mathcal{X}} \lambda(x)/\nu(x))$ and

$$\begin{aligned}
\mathbb{E}[\alpha_t^2] &\leq \mathbb{E}[\left(\frac{1}{w_t+\gamma}(\mathbf{1}\{h(x_t) \neq y_t\} - \mathbf{1}\{h'(x_t) \neq y_t\}\right)^2] \\
&\leq \mathbb{E}[\left(\frac{1}{w_t+\gamma}\right)^2\mathbf{1}\{h(x_t) \neq h'(x_t)\}] \\
&= \mathbb{E}_{X\sim\nu}\left[\frac{\lambda(X)/\nu(X)}{(\lambda(X)/\nu(X)+\gamma)^2}\mathbf{1}\{h(X) \neq h'(X)\}\right] \\
&= \mathbb{E}_{X\sim\nu}\left[\frac{\mathbf{1}\{h(X) \neq h'(X)\}}{\lambda(X)/\nu(X)}\right] = \rho_\lambda(h,h').
\end{aligned}$$

By Bernstein's inequality we have with probability at least $1-\delta$

$$\begin{aligned}
\widetilde{R}(h) - \widetilde{R}(h') &\leq \mathbb{E}[\widetilde{R}(h) - \widetilde{R}(h')] + \sqrt{\rho_\lambda(h,h')\ \frac{2\log(1/\delta)}{\tau}} + \frac{\log(1/\delta)}{\gamma\tau} \\
&\leq R(h) - R(h') + \gamma\rho_\lambda(h,h') + \sqrt{\rho_\lambda(h,h')\ \frac{2\log(1/\delta)}{\tau}} + \frac{\log(1/\delta)}{\gamma\tau}.
\end{aligned}$$

□

Note that the regularized estimator $\widetilde{R}^\gamma(h)$ is only an unbiased estimator of $R(h)$ when $\gamma = 0$. Also, because $a + \sqrt{2ab} + b \leq (\sqrt{a} + \sqrt{b})^2 \leq 2(a+b)$ we always have that for each $h, h' \in \mathcal{H}$

$$\widetilde{R}^\gamma(h) - \widetilde{R}^\gamma(h') \leq R(h) - R(h') + 2\gamma\rho_\lambda(h,h') + \frac{2\log(1/\delta)}{\tau\gamma}$$

with probability $1-\delta$ which may be more convenient.

Algorithm 4 An efficient estimator with importance-sampled data

```
**Input**: $\gamma_0 > 0$, $\epsilon > 0$, $\{(x_t, y_t, w_t)\}_{t=1}^{\tau}$ s.t. $w_t = \lambda(x_t)/\nu(x_t)$, $\mathcal{H}$, $\delta \in (0,1)$
Pick $h_0 \in \mathcal{H}$ arbitrarily, set $\Gamma = \{\gamma' : 1/\epsilon > \gamma' > \gamma_0 : \log_2(\gamma) \in \mathbb{Z}\}$
**for** $k = 0, 1, 2, \dots$ **do**
    For every $\gamma \in \Gamma$ let $h_{k+1}^{\gamma} = \arg\min_{h \in \mathcal{H}} f(h, h_k; \gamma)$ where
        $$f(h, h'; \gamma) = \widetilde{R}^{\gamma}(h) - \widetilde{R}^{\gamma}(h') + 2\gamma\rho_{\lambda}(h, h') + \frac{2\log(|\mathcal{H}|^2 \log_2(8/\gamma_0\epsilon)/\delta)}{\tau\gamma}$$
    **if** $\min_{\gamma \in \Gamma} f(h_{k+1}^{\gamma}, h_k; \gamma) \geq -\epsilon$ **then**
        **Terminate** and **output** $h_k$
    **else**
        Set $h_{k+1} = h_{k+1}^{\gamma_{k+1}}$ where $\gamma_{k+1} = \arg\min_{\gamma \in \Gamma} f(h_{k+1}^{\gamma}, h_k; \gamma)$
    **end if**
**end for**
```

Lemma 25. *Consider the setting of Lemma 24. If one runs Algorithm 4 with $\gamma_0 > 0$ and $\epsilon > 0$ then after $k \leq 1/\gamma_0\epsilon$ iterations the procedure returns an $h_k \in \mathcal{H}$ such that with probability at least $1 - \delta$*

$$R(h_k) - R(h^*) \leq \epsilon + \sqrt{\frac{\rho_{\lambda}(h^*, h_k)\ 256\log(|\mathcal{H}|^2 \log_2(8/\gamma_0\epsilon)/\delta)}{\tau}}.$$

Moreover, without loss of generality one can take $\gamma_0 = 1/\tau$.

Proof. Fix a finite subset $\Gamma \subset \{2^k : k \in \mathbb{Z}\}$ that will be determined later. By Lemma 24 we have with probability at least $1 - \delta$ that

$$|\widetilde{R}^{\gamma}(h) - \widetilde{R}^{\gamma}(h') - R(h) + R(h')| \leq 2\gamma\rho_{\lambda}(h, h') + \frac{2\log(|\mathcal{H}|^2|\Gamma|/\delta)}{\tau\gamma}$$

for all $\gamma \in \Gamma$ and $h, h' \in \mathcal{H}$.

Note that since $R(h) \leq 1$ and we want a non-trivial guarantee, without loss of generality we can take $\gamma_0 \geq \frac{1}{\tau}$. This means the number of iterations before the stopping criteria is met is at most $1/\gamma_0\epsilon$ since before the stopping criteria is met, the objective is reduced by at least ϵ each iteration, and $0 \leq \widetilde{R}^{\gamma}(h) \leq \tau$. We also would never need $\gamma \geq 1/\epsilon$. Thus, it suffices to take $\Gamma = \{2^k : -\lceil \log_2(1/\gamma_0) \rceil k \leq \lceil \log_2(1/\epsilon) \rceil$ which means $|\Gamma| \leq \log_2(8/\gamma_0\epsilon)$.

To see the performance guarantee, at the final iterate,

$$\begin{aligned}
-\epsilon &\leq \widetilde{R}^{\gamma_{k+1}}(h_{k+1}) - \widetilde{R}^{\gamma_{k+1}}(h_k) + 2\gamma_{k+1}\rho_\lambda(h_{k+1}, h_k) + \frac{2\log(|\mathcal{H}|^2|\Gamma|/\delta)}{\tau\gamma_{k+1}} \\
&= \min_{\gamma\in\Gamma}\min_{h\in\mathcal{H}} \widetilde{R}^{\gamma}(h) - \widetilde{R}^{\gamma}(h_k) + 2\gamma\rho_\lambda(h, h_k) + \frac{2\log(|\mathcal{H}|^2|\Gamma|/\delta)}{\tau\gamma} \\
&\leq \min_{\gamma\in\Gamma}\min_{h\in\mathcal{H}} R(h) - R(h_k) + 4\gamma\rho_\lambda(h, h_k) + \frac{4\log(|\mathcal{H}|^2|\Gamma|/\delta)}{\tau\gamma} \\
&\leq \min_{\gamma\in\Gamma} R(h^*) - R(h_k) + 4\gamma\rho_\lambda(h^*, h_k) + \frac{4\log(|\mathcal{H}|^2|\Gamma|/\delta)}{\tau\gamma} \\
&\leq \min_{\gamma\geq 0} R(h^*) - R(h_k) + 8\gamma\rho_\lambda(h^*, h_k) + \frac{8\log(|\mathcal{H}|^2|\Gamma|/\delta)}{\tau\gamma} \\
&= R(h^*) - R(h_k) + \sqrt{\frac{\rho_\lambda(h^*, h_k)\ 256\log(|\mathcal{H}|^2|\Gamma|/\delta)}{\tau}}.
\end{aligned}$$

Thus, if we output h_k then $R(h_k) - R(h^*) \leq \epsilon + \sqrt{\frac{\rho_\lambda(h^*,h_k)\ 256\log(|\mathcal{H}|^2|\Gamma|/\delta)}{\tau}}$. □

13.4.3 A Version-space Elimination Algorithm

Consider Algorithm 5. It leverages the estimator of the previous section.

Algorithm 5 An Elimination-style algorithm for Binary Classification

```
Input: Policy set $\mathcal{H}$ such that $h : \mathcal{X} \to \{0,1\}$ for all $h \in \mathcal{H}$, confidence level $\delta \in (0,1)$.
Let $\widehat{\mathcal{H}}_1 \leftarrow \mathcal{H}$
for $\ell = 1, 2, \ldots$ do
    Let $\rho_\ell = \min_{\lambda\in\triangle_{\mathcal{X}}} \max_{h,h'\in\widehat{\mathcal{H}}_\ell} \mathbb{E}_{X\sim\nu}\left[\frac{\mathbf{1}\{h(X)\neq h'(X)\}}{\lambda(X)/\nu(X)}\right]$ and $\lambda_\ell$ be its minimizer
    Set $\epsilon_\ell = 2^{-\ell}$, $\tau_\ell = \lceil 12\rho_\ell\epsilon_\ell^{-2}\log(2\ell^2|\mathcal{H}|/\delta)\rceil$, $\gamma_\ell = \sqrt{\frac{\log(2\ell^2|\mathcal{H}|/\delta)}{\tau_\ell\rho_\ell}}$
    Draw $x_1, \ldots, x_{\tau_\ell} \sim \lambda_\ell$, let $w_t = \lambda(x_t)/\nu(x_t)$, and request their labels to obtain $\{(x_t, y_t, w_t)\}_{t=1}^{\tau_\ell}$

    Set $\widetilde{R}_\ell(h) = \frac{1}{\tau_\ell}\sum_{t=1}^{\tau_\ell}\frac{1}{w_t+\gamma_\ell}\mathbf{1}\{h(x_t)\neq y_t\}$ for all $h \in \mathcal{H}_\ell$
    $\widehat{\mathcal{H}}_{\ell+1} \leftarrow \widehat{\mathcal{H}}_\ell \setminus \left\{h \in \widehat{\mathcal{H}}_\ell | \widetilde{R}_\ell(h) - \min_{h'\in\widehat{\mathcal{H}}_\ell}\widetilde{R}_\ell(h') \geq \epsilon_\ell\right\}$
    $\ell \leftarrow \ell + 1$
end for
Output:
```

For some $h^* \in \arg\min_{h\in\mathcal{H}}$ define the event

$$\mathcal{E} := \bigcap_{\ell=1}^{\infty}\bigcap_{h\in\mathcal{H}}\{\widetilde{R}_\ell(h^*) - \widetilde{R}_\ell(h) \leq R(h^*) - R(h) \leq \epsilon_\ell\}$$

Noting that

$$\begin{aligned}\gamma_\ell \rho_\ell + \sqrt{\frac{2\rho_\ell \log(2\ell^2|\mathcal{H}|/\delta)}{\tau_\ell}} + \frac{\log(2\ell^2|\mathcal{H}|/\delta)}{\gamma_\ell \tau_\ell} &= (1+\sqrt{2})\sqrt{\frac{2\rho_\ell \log(2\ell^2|\mathcal{H}|/\delta)}{\tau_\ell}} \\ &< \sqrt{\frac{12\rho_\ell \log(2\ell^2|\mathcal{H}|/\delta)}{\tau_\ell}} \leq \epsilon_\ell\end{aligned}$$

showing that $\mathbb{P}(\mathcal{E}) \geq 1-\delta$ is nearly identical to the linear bandit case. Thus, in what follows assume $\mathcal{E}$ holds.

If $h^* \in \widehat{\mathcal{H}}_\ell$ then for *any* $h' \in \mathcal{H}$ we have

$$\widetilde{R}_\ell(h^*) - \widetilde{R}_\ell(h') \leq R(h^*) - R(h') + \epsilon_\ell \leq \epsilon_\ell.$$

Since $h^* \in \widehat{\mathcal{H}}_1$, we have by induction that $h^* \in \widehat{\mathcal{H}}_\ell$ for all ℓ, showing correctness. Now suppose for some $h \in \mathcal{H}$ we have that $R(h) - R(h^*) > 2\epsilon_\ell$. Then

$$\begin{aligned}\widetilde{R}_\ell(h) - \min_{h' \in \widehat{\mathcal{H}}_\ell} \widetilde{R}_\ell(h') &\geq \widetilde{R}_\ell(h) - \widetilde{R}_\ell(h^*) \\ &\geq R(h) - R(h^*) - \epsilon_\ell \\ &> \epsilon_\ell\end{aligned}$$

which implies $h \notin \widehat{\mathcal{H}}_\ell$. Moreover, it implies that $\max_{h \in \widehat{\mathcal{H}}_{\ell+1}} R(h) - R(h^*) \leq 2\epsilon_\ell$ for all ℓ, or equivalently $\max_{h \in \widehat{\mathcal{H}}_\ell} R(h) - R(h^*) \leq 4\epsilon_\ell$ for all ℓ. Thus, the number of samples taken before some round ℓ satisfies $\max_{h \in \widehat{\mathcal{H}}_\ell} R(h) - R(h^*) \leq \epsilon$ is bounded by

$$\begin{aligned}\sum_{\ell=1}^{\lceil \log_2(4/\epsilon) \rceil} \tau_\ell &= \sum_{\ell=1}^{\lceil \log_2(4/\epsilon) \rceil} \lceil 12\rho_\ell \epsilon_\ell^{-2} \log(2\ell^2|\mathcal{H}|/\delta) \rceil \\ &\lesssim \log(\log(1/\epsilon)|\mathcal{H}|/\delta) \sum_{\ell=1}^{\lceil \log_2(4/\epsilon) \rceil} \rho_\ell \epsilon_\ell^{-2} \\ &= \log(\log(1/\epsilon)|\mathcal{H}|/\delta) \sum_{\ell=1}^{\lceil \log_2(4/\epsilon) \rceil} \epsilon_\ell^{-2} \min_{\lambda \in \triangle_{\mathcal{X}}} \max_{h,h' \in \widehat{\mathcal{H}}_\ell} \mathbb{E}_{X \sim \nu}\left[\frac{\mathbf{1}\{h(X) \neq h'(X)\}}{\lambda(X)/\nu(X)}\right] \\ &\lesssim \log(\log(1/\epsilon)|\mathcal{H}|/\delta) \sum_{\ell=1}^{\lceil \log_2(4/\epsilon) \rceil} \epsilon_\ell^{-2} \min_{\lambda \in \triangle_{\mathcal{X}}} \max_{h \in \widehat{\mathcal{H}}_\ell} \mathbb{E}_{X \sim \nu}\left[\frac{\mathbf{1}\{h(X) \neq h^*(X)\}}{\lambda(X)/\nu(X)}\right] \\ &\lesssim \log(\log(1/\epsilon)|\mathcal{H}|/\delta) \sum_{\ell=1}^{\lceil \log_2(4/\epsilon) \rceil} \min_{\lambda \in \triangle_{\mathcal{X}}} \max_{h \in \mathcal{H}: R(h)-R(h^*) \leq 4\epsilon_\ell} \frac{\mathbb{E}_{X \sim \nu}\left[\frac{\mathbf{1}\{h(X) \neq h^*(X)\}}{\lambda(X)/\nu(X)}\right]}{4\epsilon_\ell^2} \\ &\lesssim \log(\log(1/\epsilon)|\mathcal{H}|/\delta) \lceil \log_2(4/\epsilon) \rceil \max_{\ell=1,\dots,\lceil \log_2(4/\epsilon) \rceil} \min_{\lambda \in \triangle_{\mathcal{X}}} \max_{h \in \mathcal{H}: R(h)-R(h^*) \leq 4\epsilon_\ell} \frac{\mathbb{E}_{X \sim \nu}\left[\frac{\mathbf{1}\{h(X) \neq h^*(X)\}}{\lambda(X)/\nu(X)}\right]}{4\epsilon_\ell^2} \\ &\lesssim \log(\log(1/\epsilon)|\mathcal{H}|/\delta) \log(1/\epsilon) \max_{\xi \geq \epsilon} \min_{\lambda \in \triangle_{\mathcal{X}}} \max_{h \in \mathcal{H}: R(h)-R(h^*) \leq \xi} \frac{\mathbb{E}_{X \sim \nu}\left[\frac{\mathbf{1}\{h(X) \neq h^*(X)\}}{\lambda(X)/\nu(X)}\right]}{\xi^2}\end{aligned}$$

where we have upper bounded the sum over ℓ by the max. We immediately obtain the following theorem.

Theorem 30. *Fix any $\epsilon > 0$ and $\delta \in (0,1)$. Define*

$$\rho^*(\epsilon) := \sup_{\xi \geq \epsilon} \min_{\lambda \in \triangle_{\mathcal{X}}} \max_{h \in \mathcal{H}: R(h)-R(h^*) \leq \xi} \frac{\mathbb{E}_{X\sim\nu}\left[\frac{\mathbf{1}\{h(X)\neq h^*(X)\}}{\lambda(X)/\nu(X)}\right]}{\xi^2} \leq \min_{\lambda \in \triangle_{\mathcal{X}}} \max_{h \in \mathcal{H}} \frac{\mathbb{E}_{X\sim\nu}\left[\frac{\mathbf{1}\{h(X)\neq h^*(X)\}}{\lambda(X)/\nu(X)}\right]}{\epsilon^2 \vee (R(h)-R(h^*))^2}$$

Any $\widehat{h}$ in the version space of Algorithm 5 satisfies $R(\widehat{h})-R(h^*) \leq \epsilon$ once $\gtrsim \rho^*(\epsilon)\log(\log(1/\epsilon)|\mathcal{H}|/\delta)\log(1/\epsilon)$ labels have been requested.

Note that $\rho^*(\epsilon)$ is balancing the variance (numerator) with the sub-optimality gap squared (denominator) for every $h \in \mathcal{H}$. By inspecting the proof of the following proposition, disagreement based learning corresponds to a very particular choice of λ_ℓ at each round, namely, uniform distribution over the disagreement region. Our optimized choice of λ is never worse than this particular choice.

Proposition 10. *Define the disagreement coefficient as*

$$\theta^*(u) = \sup_{\xi \geq u} \frac{\mathbb{E}_{X\sim\nu}[\mathbf{1}\{\exists h \in \mathcal{H} : h(X) \neq h^*(X), \rho_\nu(h,h^*) \leq \xi\}]}{\xi}.$$

Then $\rho^*(\epsilon) \leq 4(\frac{R(h^*)^2}{\epsilon^2}+1)\theta^*(R(h^*)+\epsilon)$.

Proof. Now, for any each ξ, if we take $\lambda^\xi(x) = \frac{\nu(x)\mathbf{1}\{\exists h\in\mathcal{H}:h(x)\neq h^*(x),R(h)-R(h^*)\leq\xi\}}{\mathbb{E}_{X\sim\nu}[\mathbf{1}\{\exists h\in\mathcal{H}:h(X)\neq h^*(X),R(h)-R(h^*)\leq\xi\}]}$ then

$$\begin{aligned}
\min_{\lambda \in \triangle_{\mathcal{X}}} \max_{h \in \mathcal{H}: R(h)-R(h^*) \leq \xi} \frac{\mathbb{E}_{X\sim\nu}\left[\frac{\mathbf{1}\{h(X)\neq h^*(X)\}}{\lambda(X)/\nu(X)}\right]}{\xi^2} &\leq \max_{h \in \mathcal{H}: R(h)-R(h^*) \leq \xi} \frac{\mathbb{E}_{X\sim\nu}\left[\frac{\mathbf{1}\{h(X)\neq h^*(X)\}}{\lambda^\xi(X)/\nu(X)}\right]}{\xi^2} \\
&= \max_{h \in \mathcal{H}: R(h)-R(h^*) \leq \xi} \frac{\mathbb{E}_{X\sim\nu}\left[\mathbf{1}\{h(X)\neq h^*(X)\}\right]\mathbb{E}_{X\sim\nu}[\mathbf{1}\{\exists h \in \mathcal{H} : h(X)\neq h^*(X), R(h)-R(h^*)\leq \xi\}]}{\xi^2} \\
&= \max_{h \in \mathcal{H}: R(h)-R(h^*) \leq \xi} \frac{\rho_\nu(h,h^*)\mathbb{E}_{X\sim\nu}[\mathbf{1}\{\exists h \in \mathcal{H} : h(X)\neq h^*(X), R(h)-R(h^*)\leq \xi\}]}{\xi^2} \\
&\leq \max_{h \in \mathcal{H}: R(h)-R(h^*) \leq \xi} \frac{\rho_\nu(h,h^*)\mathbb{E}_{X\sim\nu}[\mathbf{1}\{\exists h \in \mathcal{H} : h(X)\neq h^*(X), \rho_\nu(h,h^*)\leq 2R(h^*)+\xi\}]}{\xi^2} \\
&\leq \frac{(2R(h^*)+\xi)\mathbb{E}_{X\sim\nu}[\mathbf{1}\{\exists h \in \mathcal{H} : h(X)\neq h^*(X), \rho_\nu(h,h^*)\leq 2R(h^*)+\xi\}]}{\xi^2} \\
&\leq \begin{cases} \frac{9R(h^*)^2}{\xi^2}\frac{\mathbb{E}_{X\sim\nu}[\mathbf{1}\{\exists h\in\mathcal{H}:h(X)\neq h^*(X),\rho_\nu(h,h^*)\leq 2R(h^*)+\xi\}]}{2R(h^*)+\xi} & \text{if } \xi \leq R(h^*) \\ \frac{9\mathbb{E}_{X\sim\nu}[\mathbf{1}\{\exists h\in\mathcal{H}:h(X)\neq h^*(X),\rho_\nu(h,h^*)\leq 2R(h^*)+\xi\}]}{2R(h^*)+\xi} & \text{if } \xi > R(h^*) \end{cases} \\
&\leq 9(\tfrac{R(h^*)^2}{\xi^2}+1)\theta^*(2R(h^*)+\xi)
\end{aligned}$$

where we have used the fact that

$$\rho_\nu(h,h^*) = \mathbb{E}_{X\sim\nu}\left[\mathbf{1}\{h(X)\neq h^*(X)\}\right] \leq \mathbb{E}_{X\sim\nu}\left[\mathbf{1}\{h(X)\neq Y\} + \mathbf{1}\{Y \neq h^*(X)\}\right] = R(h)+R(h^*)$$

so that $\rho_\nu(h,h^*) \leq \xi + 2R(h^*)$ whenever $R(h)-R(h^*) \leq \xi$. □

13.4.4 A Computationally efficient Algorithm

Consider Algorithm 6.

Algorithm 6 Computationally efficient Algorithm for Binary Classification

```
Input: Policy set $\mathcal{H}$ such that $h : \mathcal{X} \to \{0,1\}$ for all $h \in \mathcal{H}$, confidence level $\delta \in (0,1)$.
Choose $\widehat{h}_{-1} \in \mathcal{H}$ arbitrarily, set $\lambda_0 = \arg\min_{\lambda \in \triangle_{\mathcal{X}}} \max_{h \in \mathcal{H}} \rho_\lambda(h, \widehat{h}_{-1})$ and $\tau_0 \approx \epsilon_0^{-2} \max_{h \in \mathcal{H}} \rho_\lambda(h, \widehat{h}_0) \log(|\mathcal{H}|/\delta)$.
Draw $x_1, \dots, x_{\tau_0} \sim \lambda_0$, set $w_t = \lambda_\ell(x_t)/\nu(x_t)$, and request their labels to obtain $\{(x_t, y_t, w_t)\}_{t=1}^{\tau_0}$. Set $\widetilde{R}_0^\gamma(h) = \frac{1}{\tau_\ell} \sum_{t=1}^{\tau_0} \frac{1}{w_t + \gamma} \mathbf{1}\{h(x_t) \neq y_t\}$ for all $h \in \mathcal{H}$ and $\gamma > 0$. Find $\widetilde{h}_0$
for $\ell = 1, 2, \dots$ do
    Let $\tau_\ell$ be a minimal value of $\tau$ such that the objective, achieved by $\lambda_\ell$, is no greater than $\epsilon_\ell$:
        $\min_{\lambda \in \triangle_{\mathcal{X}}} \max_{h \in \mathcal{H}} \min_{\gamma' \in \Gamma} -\frac{8}{9} \widetilde{\Delta}_{\ell-1}(h) + 384\gamma' \rho_\lambda(h, \widehat{h}_{\ell-1}) + \frac{192 \log(2\ell^2 |\mathcal{H}|^2/\delta)}{\gamma' \tau}$
    Draw $x_1, \dots, x_{\tau_\ell} \sim \lambda_\ell$, set $w_t = \lambda_\ell(x_t)/\nu(x_t)$, and request their labels to obtain $\{(x_t, y_t, w_t)\}_{t=1}^{\tau_\ell}$. Set $\widetilde{R}_\ell^\gamma(h) = \frac{1}{\tau_\ell} \sum_{t=1}^{\tau_\ell} \frac{1}{w_t + \gamma} \mathbf{1}\{h(x_t) \neq y_t\}$ for all $h \in \mathcal{H}$ and $\gamma > 0$.
    Set
        $\widehat{h}_\ell = \arg\min_{h \in \mathcal{H}} \min_{\gamma} \widetilde{R}_\ell^\gamma(h) - \widetilde{R}_\ell^\gamma(\widehat{h}_{\ell-1}) + 6\gamma \rho_{\lambda_\ell}(h, \widehat{h}_{\ell-1}) + \frac{6 \log(2\ell^2 |\mathcal{H}|^2/\delta)}{\gamma \tau_\ell}$
    Set
        $\widetilde{\Delta}_\ell(h) = \min_{\gamma} \widetilde{R}_\ell^\gamma(h) - \widetilde{R}_\ell^\gamma(\widetilde{h}_\ell) + 2\gamma \rho_{\lambda_\ell}(h, \widetilde{h}_\ell) + \frac{4 \log(2\ell^2 |\mathcal{H}|^2/\delta)}{\gamma \tau_\ell}$
end for
Output:
```

Let $\epsilon_\ell = 2^{-\ell}$ and $S_\ell = \{h \in \mathcal{H} : R(h) - R(h^*) \leq \epsilon_\ell\}$ for all $\ell \in \mathbb{N}$. Define the events

$$\mathcal{E}_\ell = \bigcap_{h,h' \in \mathcal{H}} \{\widetilde{R}_\ell^\gamma(h) - \widetilde{R}_\ell^\gamma(h') - R(h) + R(h') \leq 2\gamma \rho_{\lambda_\ell}(h, h') + \frac{2 \log(2\ell^2 |\mathcal{H}|^2/\delta)}{\gamma \tau_\ell}\}$$

and $\mathcal{E} = \cap_{\ell=0}^\infty \mathcal{E}_\ell$. Define $\Delta(h, h') = R(h) - R(h')$ and for each ℓ define

$$\widetilde{\Delta}_\ell(h, h') = \min_{\gamma} \widetilde{R}_\ell^\gamma(h) - \widetilde{R}_\ell^\gamma(h') + 2\gamma \rho_{\lambda_\ell}(h, \widetilde{h}_\ell) + 2\gamma \rho_{\lambda_\ell}(h', \widetilde{h}_\ell) + \frac{4 \log(2\ell^2 |\mathcal{H}|^2/\delta)}{\gamma \tau_\ell}$$

Note that $\widetilde{\Delta}_\ell(h, h')$ is a *pessimistic* estimate of the true gap $\Delta(h, h')$ in the sense that on $\mathcal{E}$ we have $\widetilde{\Delta}_\ell(h, h') \geq \Delta(h, h')$ for all h, h'.

We need to show that we are estimating the gaps well. We will prove a helper lemma first.

Lemma 26. *Fix $\ell \in \mathbb{N}$. Then, on the event $\{\widetilde{\Delta}_{\ell-1}(h^*) \leq \epsilon_{\ell-1}/8\} \cap \mathcal{E}$ we have that $R(\widehat{h}_\ell) - R(h^*) \leq \epsilon_\ell/8$.*

Proof. On $\mathcal{E}$ and the event that $\widetilde{\Delta}_{\ell-1}(h^*) \leq \epsilon_{\ell-1}/8 = \epsilon_\ell/4$

$$\begin{aligned}
\epsilon_\ell &\geq \max_{h\in\mathcal{H}} \min_{\gamma'\in\Gamma} -\frac{8}{9}\widetilde{\Delta}_{\ell-1}(h) + 384\gamma'\rho_{\lambda_\ell}(h,\widehat{h}_{\ell-1}) + \frac{192\log(2\ell^2|\mathcal{H}|/\delta)}{\gamma'\tau_\ell} \\
&\geq \min_{\gamma'\in\Gamma} -\frac{8}{9}\widetilde{\Delta}_{\ell-1}(h^*) + 384\gamma'\rho_{\lambda_\ell}(h^*,\widehat{h}_{\ell-1}) + \frac{192\log(2\ell^2|\mathcal{H}|/\delta)}{\gamma'\tau_\ell} \\
&\geq \min_{\gamma'\in\Gamma} -\frac{2}{9}\epsilon_\ell + 384\gamma'\rho_{\lambda_\ell}(h^*,\widehat{h}_{\ell-1}) + \frac{192\log(2\ell^2|\mathcal{H}|/\delta)}{\gamma'\tau_\ell} \\
&\geq 64\sqrt{\frac{\rho_{\lambda_\ell}(h^*,\widehat{h}_{\ell-1})\log(2\ell^2|\mathcal{H}|/\delta)}{\tau_\ell}}.
\end{aligned}$$

Now,

$$\begin{aligned}
R(\widehat{h}_\ell) - R(\widehat{h}_{\ell-1}) &\leq \min_{\gamma} \widetilde{R}_\ell^\gamma(\widehat{h}_\ell) - \widetilde{R}_\ell^\gamma(\widehat{h}_{\ell-1}) + 2\gamma\rho_{\lambda_\ell}(\widehat{h}_\ell,\widehat{h}_{\ell-1}) + \frac{2\log(2\ell^2|\mathcal{H}|/\delta)}{\gamma\tau_\ell} \\
&= \min_{h\in\mathcal{H}} \min_{\gamma} \widetilde{R}_\ell^\gamma(h) - \widetilde{R}_\ell^\gamma(\widehat{h}_{\ell-1}) + 2\gamma\rho_{\lambda_\ell}(h,\widehat{h}_{\ell-1}) + \frac{2\log(2\ell^2|\mathcal{H}|/\delta)}{\gamma\tau_\ell} \\
&\leq \min_{\gamma} \widetilde{R}_\ell^\gamma(h^*) - \widetilde{R}_\ell^\gamma(\widehat{h}_{\ell-1}) + 2\gamma\rho_{\lambda_\ell}(h^*,\widehat{h}_{\ell-1}) + \frac{2\log(2\ell^2|\mathcal{H}|/\delta)}{\gamma\tau_\ell} \\
&\leq \min_{\gamma} R(h^*) - R(\widehat{h}_{\ell-1}) + 4\gamma\rho_{\lambda_\ell}(h^*,\widehat{h}_{\ell-1}) + \frac{4\log(2\ell^2|\mathcal{H}|/\delta)}{\gamma\tau_\ell} \\
&= R(h^*) - R(\widehat{h}_{\ell-1}) + 8\sqrt{\frac{\rho_{\lambda_\ell}(h^*,\widehat{h}_{\ell-1})\log(2\ell^2|\mathcal{H}|/\delta)}{\tau_\ell}} \\
&= R(h^*) - R(\widehat{h}_{\ell-1}) + \epsilon_\ell/8
\end{aligned}$$

where the last line follows from the above display. Rearranging, we conclude the proof. □

Lemma 27. *On event $\mathcal{E}$ we have for all $\ell \in \mathbb{N}$*

$$0 \leq \widetilde{\Delta}_\ell(h,h^*) - \Delta(h,h^*) \leq \begin{cases} \frac{\Delta(h,h^*)}{8} & \text{if } h \notin S_\ell \\ \epsilon_\ell/8 & \text{if } h \in S_\ell, \end{cases}$$

.

Proof. We will proceed inductively assuming it holds for $\ell-1$ and then show this implies the result for round ℓ. Note that for $\ell = 0$ we have for any $h \in S_0 = \mathcal{H}$

$$\begin{aligned}
&\max_{h \in S_0} \widetilde{\Delta}_\ell(h, h^*) - \Delta(h, h^*) \\
&= \max_{h \in S_0} \min_{\gamma} \widetilde{R}_0^\gamma(h) - \widetilde{R}_0^\gamma(h^*) + 2\gamma\rho_{\lambda_\ell}(h, \widetilde{h}_0) + 2\gamma\rho_{\lambda_\ell}(h^*, \widetilde{h}_0) + \frac{4\log(2\ell^2|\mathcal{H}|^2/\delta)}{\gamma\tau_0} - R(h) + R(h^*) \\
&\le \max_{h, h' \in S_0} \min_{\gamma} \widetilde{R}_0^\gamma(h) - \widetilde{R}_0^\gamma(h') + 2\gamma\rho_{\lambda_\ell}(h, \widetilde{h}_0) + 2\gamma\rho_{\lambda_\ell}(h', \widetilde{h}_0) + \frac{4\log(2\ell^2|\mathcal{H}|^2/\delta)}{\gamma\tau_0} - R(h) + R(h') \\
&\le \max_{h, h' \in S_0} \min_{\gamma} 4\gamma\rho_{\lambda_\ell}(h, \widetilde{h}_0) + 4\gamma\rho_{\lambda_\ell}(h', \widetilde{h}_0) + \frac{8\log(2\ell^2|\mathcal{H}|^2/\delta)}{\gamma\tau_0} \\
&\le \max_{h \in S_0} \min_{\gamma} 8\gamma\rho_{\lambda_\ell}(h, \widetilde{h}_0) + \frac{8\log(2\ell^2|\mathcal{H}|^2/\delta)}{\gamma\tau_0} \\
&= 16\sqrt{\frac{\max_{h \in \mathcal{H}} \rho_{\lambda_0}(h, \widetilde{h}_0) \log(2\ell^2|\mathcal{H}|^2/\delta)}{\tau_0}} \\
&\le \epsilon_0/8
\end{aligned}$$

by choosing τ_0 sufficiently large. Thus $\widetilde{\Delta}_0(h, h^*) - \Delta(h, h^*) \le \epsilon_0/8$ for all $h \in S_0 = \mathcal{H}$. Now we use induction to prove the rest. For any $\widetilde{h} \in \mathcal{H}$ we have

$$\begin{aligned}
&\widetilde{\Delta}_\ell(\widetilde{h}, h^*) - \Delta(\widetilde{h}, h^*) \\
&= \min_{\gamma} \widetilde{R}_\ell^\gamma(\widetilde{h}) - \widetilde{R}_\ell^\gamma(h^*) + 2\gamma\rho_{\lambda_\ell}(\widetilde{h}, \widetilde{h}_\ell) + 2\gamma\rho_{\lambda_\ell}(h^*, \widetilde{h}_\ell) + \frac{4\log(2\ell^2|\mathcal{H}|^2/\delta)}{\gamma\tau_\ell} - R(\widetilde{h}) + R(h^*) \\
&\le \min_{\gamma} 4\gamma\rho_{\lambda_\ell}(\widetilde{h}, \widetilde{h}_\ell) + 4\gamma\rho_{\lambda_\ell}(h^*, \widetilde{h}_\ell) + \frac{8\log(2\ell^2|\mathcal{H}|^2/\delta)}{\gamma\tau_\ell} \\
&\le \min_{\gamma} 4\gamma\rho_{\lambda_\ell}(\widetilde{h}, \widetilde{h}_{\ell-1}) + 4\gamma\rho_{\lambda_\ell}(\widetilde{h}_{\ell-1}, h^*) + 8\gamma\rho_{\lambda_\ell}(\widetilde{h}_\ell, \widetilde{h}_{\ell-1}) + \frac{8\log(2\ell^2|\mathcal{H}|^2/\delta)}{\gamma\tau_\ell}.
\end{aligned}$$

This last line will be used as the starting point for the two cases.

Case 1: $\widetilde{h} \in S_\ell$

Now, on the base case and Lemma 26 we have that $\widetilde{h}_{\ell-1} \in S_{\ell+2} \subset S_\ell$ and $\widetilde{h}_\ell \in S_{\ell+3} \subset S_\ell$. Thus, for any $\widetilde{h} \in S_\ell$ we have

$$\begin{aligned}
&\widetilde{\Delta}_\ell(\widetilde{h}, h^*) - \Delta(\widetilde{h}, h^*) \leq \min_\gamma 4\gamma\rho_{\lambda_\ell}(\widetilde{h}, \widetilde{h}_{\ell-1}) + 4\gamma\rho_{\lambda_\ell}(\widetilde{h}_{\ell-1}, h^*) + 8\gamma\rho_{\lambda_\ell}(\widetilde{h}_\ell, \widetilde{h}_{\ell-1}) + \frac{8\log(2\ell^2|\mathcal{H}|^2/\delta)}{\gamma\tau_\ell} \\
&\leq \max_{h\in S_\ell} \min_\gamma 16\gamma\rho_{\lambda_\ell}(h, \widetilde{h}_{\ell-1}) + \frac{8\log(2\ell^2|\mathcal{H}|^2/\delta)}{\gamma\tau_\ell} \\
&\leq \frac{1}{20} \max_{h\in S_\ell} \min_\gamma -\frac{8}{9}\widetilde{\Delta}_{\ell-1}(h, \widetilde{h}_{\ell-1}) + \frac{8}{9}\widetilde{\Delta}_{\ell-1}(h, \widetilde{h}_{\ell-1}) + 382\gamma\rho_{\lambda_\ell}(h, \widehat{h}_{\ell-1}) + \frac{190\log(2\ell^2|\mathcal{H}|^2/\delta)}{\gamma\tau_\ell} \\
&\leq \frac{1}{20} \max_{h\in S_\ell} \min_\gamma -\frac{8}{9}\widetilde{\Delta}_{\ell-1}(h, \widetilde{h}_{\ell-1}) + \frac{8}{9}\Delta(h, \widetilde{h}_{\ell-1}) + 384\gamma\rho_{\lambda_\ell}(h, \widehat{h}_{\ell-1}) + \frac{192\log(2\ell^2|\mathcal{H}|^2/\delta)}{\gamma\tau_\ell} \\
&\leq \frac{1}{20} \max_{h\in S_\ell} \min_\gamma -\frac{8}{9}\widetilde{\Delta}_{\ell-1}(h, \widetilde{h}_{\ell-1}) + \frac{8}{9}\Delta(h, \widetilde{h}_{\ell-1}) + 384\gamma\rho_{\lambda_\ell}(h, \widehat{h}_{\ell-1}) + \frac{192\log(2\ell^2|\mathcal{H}|^2/\delta)}{\gamma\tau_\ell} \\
&\leq \frac{1}{20} \max_{h\in S_\ell} \min_\gamma -\frac{8}{9}\widetilde{\Delta}_{\ell-1}(h, \widetilde{h}_{\ell-1}) + \frac{8}{9}\Delta(h, h^*) + 384\gamma\rho_{\lambda_\ell}(h, \widehat{h}_{\ell-1}) + \frac{192\log(2\ell^2|\mathcal{H}|^2/\delta)}{\gamma\tau_\ell} \\
&\leq \frac{1}{20}(\epsilon_\ell + \max_{h\in\mathcal{H}} \min_\gamma -\frac{8}{9}\widetilde{\Delta}_{\ell-1}(h, \widetilde{h}_{\ell-1}) + 384\gamma\rho_{\lambda_\ell}(h, \widehat{h}_{\ell-1}) + \frac{192\log(2\ell^2|\mathcal{H}|^2/\delta)}{\gamma\tau_\ell}) \\
&\leq \epsilon_\ell/8
\end{aligned}$$

using the facts that $\Delta(h, \widetilde{h}_{\ell-1}) = R(h) - R(\widetilde{h}_{\ell-1}) \leq R(h) - R(h^*) = \Delta(h, h^*) \leq \epsilon_\ell$ for $h \in S_\ell$, and plugging in the condition of the optimization problem. This completes the first case.

Case 2: $\widetilde{h} \notin S_\ell$

If $\widetilde{h} \notin S_\ell$ then there exists some $j \leq \ell$ such that $2^{-j} < R(h) - R(h^*) \leq 2^{-j+1}$. On Lemma 27, we have again that on the inductive hypothesis, $\widetilde{h}_\ell \in S_{\ell+3} \subset S_j$ so

$$\begin{aligned}
\frac{\widetilde{\Delta}_\ell(\widetilde{h}, h^*) - \Delta(\widetilde{h}, h^*)}{\Delta(\widetilde{h}, h^*)} &\leq \frac{\min_\gamma 4\gamma\rho_{\lambda_\ell}(\widetilde{h}, \widetilde{h}_{\ell-1}) + 4\gamma\rho_{\lambda_\ell}(\widetilde{h}_{\ell-1}, h^*) + 8\gamma\rho_{\lambda_\ell}(\widetilde{h}_\ell, \widetilde{h}_{\ell-1}) + \frac{8\log(2\ell^2|\mathcal{H}|^2/\delta)}{\gamma\tau_\ell}}{\Delta(\widetilde{h}, h^*)} \\
&\leq \max_{h\in S_j} \frac{\min_\gamma 16\gamma\rho_{\lambda_\ell}(h, \widetilde{h}_{\ell-1}) + \frac{8\log(2\ell^2|\mathcal{H}|^2/\delta)}{\gamma\tau_\ell}}{R(\widetilde{h}) - R(h^*)} \\
&\leq 3\max_{h\in S_j} \frac{\min_\gamma 16\gamma\rho_{\lambda_\ell}(h, \widetilde{h}_{\ell-1}) + \frac{8\log(2\ell^2|\mathcal{H}|^2/\delta)}{\gamma\tau_\ell}}{2^{-\ell} + 2[R(\widetilde{h}) - R(h^*)]} \\
&\leq 3\max_{h\in\mathcal{H}} \frac{\min_\gamma 16\gamma\rho_{\lambda_\ell}(h, \widetilde{h}_{\ell-1}) + \frac{8\log(2\ell^2|\mathcal{H}|^2/\delta)}{\gamma\tau_\ell}}{2^{-\ell} + R(h) - R(h^*)} \\
&= \max_{h\in\mathcal{H}} \frac{\min_\gamma 48\gamma\rho_{\lambda_\ell}(h, \widetilde{h}_{\ell-1}) + \frac{24\log(2\ell^2|\mathcal{H}|^2/\delta)}{\gamma\tau_\ell}}{\epsilon_\ell + \Delta(h)}
\end{aligned}$$

Now, on the inductive hypothesis we have for any $h \in \mathcal{H}$ that

$$\widetilde{\Delta}_{\ell-1}(h, h^*) - \Delta(h) \leq \max\{\epsilon_{\ell-1}, \Delta(h)\}/8 \leq \epsilon_\ell/4 + \Delta(h)/8.$$

Rearranging, we have that

$$
\begin{aligned}
&\frac{9}{8}\Delta(h) + \epsilon_\ell/4 \geq \widetilde{\Delta}_{\ell-1}(h, h^*) \\
&= \min_\gamma \widetilde{R}^\gamma_{\ell-1}(h) - \widetilde{R}^\gamma_{\ell-1}(h^*) + 2\gamma\rho_{\lambda_{\ell-1}}(h, \widetilde{h}_{\ell-1}) + 2\gamma\rho_{\lambda_{\ell-1}}(\widetilde{h}_{\ell-1}, h^*) + \frac{4\log(\ell^2|\mathcal{H}|^2/\delta)}{\gamma\tau_{\ell-1}} \\
&\geq \min_\gamma \widetilde{R}^\gamma_{\ell-1}(h) - \widetilde{R}^\gamma_{\ell-1}(\widetilde{h}_{\ell-1}) + \widetilde{R}^\gamma_{\ell-1}(\widetilde{h}_{\ell-1}) - \widetilde{R}^\gamma_{\ell-1}(h^*) + 2\gamma\rho_{\lambda_{\ell-1}}(h, \widetilde{h}_{\ell-1}) + 2\gamma\rho_{\lambda_{\ell-1}}(\widetilde{h}_{\ell-1}, h^*) + \frac{4\log(2\ell^2|\mathcal{H}|^2/\delta)}{\gamma\tau_{\ell-1}} \\
&\geq \min_\gamma \widetilde{R}^\gamma_{\ell-1}(h) - \widetilde{R}^\gamma_{\ell-1}(\widetilde{h}_{\ell-1}) + 2\gamma\rho_{\lambda_{\ell-1}}(h, \widetilde{h}_{\ell-1}) + \frac{2\log(2\ell^2|\mathcal{H}|^2/\delta)}{\gamma\tau_{\ell-1}} + R(\widetilde{h}_{\ell-1}) - R(h^*) \\
&\geq \widetilde{\Delta}_{\ell-1}(h, \widetilde{h}_{\ell-1})/2 = \widetilde{\Delta}_{\ell-1}(h)/2.
\end{aligned}
$$

Thus, rearranging once more we have $\Delta(h) \geq \frac{4}{9}\widetilde{\Delta}_{\ell-1}(h) - \epsilon_\ell/4$ and

$$
\begin{aligned}
\frac{\widetilde{\Delta}_\ell(\widetilde{h}, h^*) - \Delta(\widetilde{h}, h^*)}{\Delta(\widetilde{h}, h^*)} &\leq \max_{h\in\mathcal{H}} \frac{\min_\gamma 48\gamma\rho_{\lambda_\ell}(h, \widetilde{h}_{\ell-1}) + \frac{24\log(2\ell^2|\mathcal{H}|^2/\delta)}{\gamma\tau_\ell}}{\epsilon_\ell + \Delta(h)} \\
&\leq \max_{h\in\mathcal{H}} \frac{\min_\gamma 48\gamma\rho_{\lambda_\ell}(h, \widetilde{h}_{\ell-1}) + \frac{24\log(2\ell^2|\mathcal{H}|^2/\delta)}{\gamma\tau_\ell}}{\epsilon_\ell/2 + \frac{4}{9}\widetilde{\Delta}_{\ell-1}(h)} \leq 1/8
\end{aligned}
$$

where the last inequality follows from the solution of the optimization problem. □

The above lemmas imply that

$$
\begin{aligned}
\Delta(h) &= \Delta(h, h^*) \\
&= \Delta(h, \widetilde{h}_{\ell-1}) + \Delta(\widetilde{h}_{\ell-1}, h^*) \\
&\leq \widetilde{\Delta}_{\ell-1}(h, \widetilde{h}_{\ell-1}) + \epsilon_{\ell-1}/8 \\
&= \widetilde{\Delta}_{\ell-1}(h) + \epsilon_{\ell-1}/8.
\end{aligned}
$$

We leverage this to compute the sample complexity as follows:

$$
\begin{aligned}
&\min_{\lambda\in\triangle_\mathcal{X}} \max_{h\in\mathcal{H}} \min_{\gamma'\in\Gamma} -\frac{8}{9}\widetilde{\Delta}_{\ell-1}(h) + 384\gamma'\rho_\lambda(h, \widehat{h}_{\ell-1}) + \frac{192\log(2\ell^2|\mathcal{H}|/\delta)}{\gamma'\tau} \\
&\leq \min_{\lambda\in\triangle_\mathcal{X}} \max_{h\in\mathcal{H}} \min_{\gamma'\in\Gamma} -\frac{8}{9}\Delta(h) + \epsilon_\ell/8 + 384\gamma'\rho_\lambda(h, \widehat{h}_{\ell-1}) + \frac{192\log(2\ell^2|\mathcal{H}|/\delta)}{\gamma'\tau} \\
&\leq \min_{\lambda\in\triangle_\mathcal{X}} \max_{h\in\mathcal{H}} -\frac{8}{9}\Delta(h) + \epsilon_\ell/8 + 544\sqrt{\rho_\lambda(h, \widehat{h}_{\ell-1})\frac{\log(2\ell^2|\mathcal{H}|/\delta)}{\gamma'\tau}} \\
&\leq \min_{\lambda\in\triangle_\mathcal{X}} \max_{h\in\mathcal{H}} -\frac{8}{9}\Delta(h) + \epsilon_\ell/8 + 544\sqrt{\rho_\lambda(h, h^*)\frac{\log(2\ell^2|\mathcal{H}|/\delta)}{\tau}} + 544\sqrt{\rho_\lambda(h^*, \widehat{h}_{\ell-1})\frac{\log(2\ell^2|\mathcal{H}|/\delta)}{\tau}} \\
&\leq \min_{\lambda\in\triangle_\mathcal{X}} \max_{h\in\mathcal{H}} -\frac{8}{9}\Delta(h) + \epsilon_\ell/8 + 544\sqrt{\rho_\lambda(h, h^*)\frac{\log(2\ell^2|\mathcal{H}|/\delta)}{\tau}} + 544\sqrt{\max_{h'\in S_\ell}\rho_\lambda(h^*, h')\frac{\log(2\ell^2|\mathcal{H}|/\delta)}{\tau}}
\end{aligned}
$$

which is less than ϵ_ℓ whenever

$$
\tau \gtrsim \min_{\lambda\in\triangle_\mathcal{X}} \max_{h\in\mathcal{H}} \frac{\rho_\lambda(h, h^*)}{\epsilon_\ell^2 + \Delta(h)^2} \log(|\mathcal{H}|/\delta).
$$

We summarize the conclusions in the following theorem.

Theorem 31. *Fix $\delta \in (0,1)$. Then on the ℓth round, $R(\widetilde{h}_\ell) - R(h^*) \leq \epsilon_\ell/8$ and the total number of samples is bounded by $\min_{\lambda \in \triangle_{\mathcal{X}}} \max_{h \in \mathcal{H}} \frac{\rho_\lambda(h,h^*)}{\epsilon_\ell^2 + \Delta(h)^2} \log(|\mathcal{H}|/\delta) \log(1/\epsilon_\ell)$.*

13.4.5 Instance-dependent Lower bounds

Combinatorial bandits sheds some light on instance-dependent lower-bounds for the pool-based setting.

13.5 Heuristics of note

13.5.1 Uncertainty sampling

13.5.2 Covering algorithms

13.5.3 Hypothesis-class agnostic algorithms

Part V

Markov Decision Processes

Chapter 14

Finite Horizon Markov Decision Processes

14.1 Tabular MDPs

This presentation closely follows the monograph of [Agarwal et al., 2019] with slight notation and presentation changes.

A finite horizon Markov Decision Process (MDP) is defined as the tuple $(\mathcal{S}, \mathcal{A}, \{P_h\}_h, \{r_h\}_h, H, \nu)$ where

- State space $\mathcal{S}$ is finite with $S = |\mathcal{S}|$
- Action space $\mathcal{A}$ is finite with $A = |\mathcal{A}|$, all actions are available in all states
- Transition function $P_h : \mathcal{S} \times \mathcal{A} \to \triangle_{\mathcal{S}}$ for all $h \in [H]$ dictates next state probabilities. If action a_h is taken in state s_{h+1} at time h, then $P_h(s'|s,a)$ is the probability that $s_{h+1} = s'$.
- Reward function $r_h : \mathcal{S} \times \mathcal{A} \to [0,1]$ for all $h \in [H]$. If action a_h is taken in state s_{h+1} at time h, then the agent receives reward $r_h(s_h, a_h)$.
- Horizon length $H \in \mathbb{N}$
- Initial state distribution $\mu \in \triangle_{\mathcal{S}}$ from which s_1 is drawn

For a policy π, a state s, and $h \in [H]$, define the value function $V_h^\pi : \mathcal{S} \to \mathbb{R}$ as

$$V_h^\pi(s) = \mathbb{E}\left[\sum_{t=h}^{H} r_h(s_h, a_h)|\pi, s_h = h\right]$$

where the expectation is with respect to both the random transitions and potentially stochastic policy. It is understood in the above equation that $\pi = \{\pi_h\}_h$ and $a_t = \pi_t(s_t)$ for all t. The state-action value $Q_h^\pi : \mathcal{S} \times \mathcal{A} \to \mathbb{R}$ is defined as

$$Q_h^\pi(s,a) = \mathbb{E}\left[\sum_{t=h}^{H} r_h(s_h, a_h)|\pi, s_h = h, a_h = a\right].$$

Note that $V_h^\pi(s) \in [0, H-h+1]$ and $Q_h^\pi(s) \in [0, H-h+1]$ for any policy π. We will define $V_0^\pi = \mathbb{E}_{s_1 \sim \nu}[V_1^\pi(s_1)]$. The objective is to optimize $\max_\pi V_0^\pi$.

Theorem 32 (Bellman Optimality Equations). *For all $(s, a, h) \in \mathcal{S} \times \mathcal{A} \times [H]$ define*

$$Q_h^\star(s,a) = \sup_\pi Q_h^\pi(s,a)$$

where the sup *is taken over all non-stationary and stochastic policies. For some function $Q_h : \mathcal{S} \times \mathcal{A} \to \mathbb{R}$, we have that $Q_h = Q_h^\star$ for all $h \in [H]$ if and only if for all $h \in [H]$,*

$$Q_h(s,a) = r_h(s,a) + \mathbb{E}_{s' \sim P(\cdot|s,a)} \left[\max_{a' \in \mathcal{A}} Q_{h+1}(s', a') \right]$$

where $Q_{H+1} = 0$. Furthermore, the deterministic policy $\pi_h(s) = \arg\max_{a \in \mathcal{A}} Q_h(s,a)$ is an optimal policy.

14.1.1 Value iteration

We will leverage the above Bellman optimality equations to derive the optimal policy. The following procedure is known as *value iteration.*

- Set $Q_H(s,a) = r_H(s,a)$.
- For $h = H-1, \dots, 1$ set:

$$Q_h(s,a) = r_h(s,a) + \mathbb{E}_{s' \sim P(\cdot|s,a)} \left[\max_{a' \in \mathcal{A}} Q_{h+1}(s', a') \right]$$

By Theorem 32, we have that $Q_h(s,a) = Q_h^{\pi_*}(s,a)$ and consequently, $\pi_h(s) = \arg\max_a Q_h(s,a)$ is an optimal policy.

14.1.2 Reinforcement learning

The value iteration algorithm is optimal if the rewards and transition functions are *known.* But what if they are unknown, how hard is it to learn the optimal policy? Consider an episodic setting where before the start of each episode k, an agent defines a policy $\{\pi_h^k\}_{h=1}^H$ and applies it in the environment so that $s_1^k \sim \nu$, $\pi_h(s_h^k) = a_h^k$, and $s_{h+1}^k \sim P(\cdot|s_h^k, a_h^k)$. This results in a *trajectory* $\tau^k = \{s_h^k, a_h^k\}_{h=1}^H$. We care about regret:

$$\text{Regret} := \mathbb{E}\left[K V_1^{\pi_*}(s_1) - \sum_{k=1}^K \sum_{h=1}^H r_h(s_h^k, a_h^k) \right]$$

Ideally, we would like an algorithm that satisfies $O(\sqrt{K})$ regret.

Why is this problem hard? Consider the combination lock instance (TODO). Its very clear that a policy that just uniform exploration will only reach the reward state with probability A^{-H}.

14.1.3 UCB Value Iteration Algorithm

This section presents the UCB-VI algorithm of [Azar et al., 2017] and closely follows the analysis of [Agarwal et al., 2019].

```
UCB-VI for Reinforcement Learning
Input: deterministic reward functions $r_h : \mathcal{S} \times \mathcal{A} \to [0,1]$ for all $h \in [H]$, $\delta \in (0,1)$
Initialize: For all $\ell \in \mathbb{N}$ let  $n^\ell_h(s,a,s') = \sum_{i=1}^{\ell-1} \mathbf{1}\{(s^i_h, a^i_h, s^i_{h+1}) = (s,a,s')\}$,
                                  $n^\ell_h(s,a) = \sum_{i=1}^{\ell-1} \mathbf{1}\{(s^i_h, a^i_h) = (s,a)\}$,
                                  $\widehat{P}^\ell_h(s'|s,a) = n^\ell_h(s,a,s')/n^\ell_h(s,a)$

for $k = 1, 2, \ldots, K$
    $\widehat{V}^k_{H+1} = \mathbf{0}$
    for $h = H, H-1, \ldots, 1$
        $\widehat{Q}^k_h(s,a) = \min\left\{H, H\sqrt{\frac{\log(2KHSA/\delta)}{2n^k_h(s,a)}} + r_h(s,a) + \widehat{P}^k_h \cdot V^k_{h+1}\right\}$
        $\widehat{V}^k_h(s) = \max_a \widehat{Q}^k_h(s,a)$ and $\pi^k_h(s) \arg\max_a \widehat{Q}^k_h(s,a)$
    Roll-out $\{\pi^k_h\}$ such that $s_1 \sim \nu$ and $a^k_h = \pi^k_h(s_h)$ and $s_{h+1} \sim P_h(\cdot|s^k_h, a^k_h)$ for all $h \in [H]$
```

The intuition for this algorithm is that $\widehat{V}^k_h$ and $\widehat{Q}^k_h$ are *optimistic* in the sense that with high probability, we have that $\widehat{V}^k_h(s) \geq V^{\pi_*}_h(s)$ and $\widehat{Q}^k_h(s,a) \geq Q^{\pi_*}_h(s,a)$ for all s, a, h. Thus, just like UCB for bandits, at least intuitively, taking an action either results in a high reward, or information against taking that action in the future.

Theorem 33. *For any $K \in \mathbb{N}$ we have that UCB-VI satsifies*

$$\sum_{k=1}^K V_0^{\pi_*} - V_0^{\pi_k} \leq H^2 S\sqrt{8AK\log(2KHSA/\delta)}$$

with probability at least $1 - 2\delta$.

Define the event

$$\mathcal{E}_{optimism} := \bigcap_{k=1}^K \bigcap_{h=1}^H \bigcap_{s,a} \left\{ \left| \sum_{s'} (P_h(s'|s,a) - \widehat{P}^k_h(s'|s,a)) V^{\pi_*}_{h+1}(s') \right| \leq H\sqrt{\frac{\log(2KHSA/\delta)}{2n^k_h(s,a)}} \right\}$$

We have that $\mathbb{P}(\mathcal{E}_{optimism}) \geq 1 - \delta$ as a corollary of the following lemma.

Lemma 28. *Fix any $V : \mathcal{S} \to [0, H]$. Then for any $(s,a,h,k) \in \mathcal{S} \times \mathcal{A} \times [H] \times \mathbb{N}$*

$$\mathbb{P}\left(\left| \sum_{s'} (P_h(s'|s,a) - \widehat{P}^k_h(s'|s,a)) V(s') \right| \leq H\sqrt{\frac{\log(2/\delta)}{2n^k_h(s,a)}} \right) \geq 1 - \delta.$$

Proof. If $X_\ell = \mathbf{1}\{s = s^\ell_h, a = a^\ell_h\} \sum_{s'} (P_h(s'|s,a) - \mathbf{1}\{s^\ell_{h+1} = s'\}) V(s')$ then $\mathbb{E}[X_\ell | \mathcal{F}^\ell_h] = 0$. Note that $\mathbf{1}\{s = s^\ell_h, a = a^\ell_h\}$ is a predictable sequence and $\mathcal{F}^\ell_h$-measurable. Thus, by Hoeffding's inequality we have $\mathbb{E}[\exp(\lambda X_\ell) | \mathcal{F}^\ell_h] \leq \exp(\lambda^2 H^2 \mathbf{1}\{s = s^\ell_h, a = a^\ell_h\}/8)$. It follows from Azuma-Hoeffding that

$$\begin{aligned} \left| n^k_h(s,a) \sum_{s'} (P_h(s'|s,a) - \widehat{P}_h(s'|s,a)) V(s') \right| &= \left| \sum_{\ell=1}^{k-1} X_\ell \right| \\ &\leq H\sqrt{n^k_h(s,a)\log(2/\delta)/2} \end{aligned}$$

where we have used the fact that $\sum_{\ell=1}^{k-1} H^2 \mathbf{1}\{s = s^\ell_h, a = a^\ell_h\} = n^k_h(s,a)$. Union bounding over all S, A, K, H completes the proof. □

Lemma 29. *On event $\mathcal{E}_{optimism}$ we have that $\widehat{V}_h^k(s) \geq V_h^{\pi_*}(s)$ and $\widehat{Q}_h^k(s,a) \geq Q_h^{\pi_*}(s,a)$ for all s, a, h.*

Proof. First note that if $\widehat{Q}_h^k(s,a) = H$ for any (s,a,h,k) then we trivially have that $\widehat{Q}_h^k(s,a) = H \geq Q_h^{\pi_*}(s,a)$. Thus, assume otherwise. Note that trivially we have that $\widehat{Q}_H^k(s,a) \geq Q_H^{\pi_*}(s,a) = r_H(s,a)$ for all s, a. We will prove the result by induction using the base case of

$$\widehat{V}_H^k(s) = \max_a \widehat{Q}_H^k(s,a) \geq \widehat{Q}_H^k(s, \pi_*(s)) \geq Q_H^{\pi_*}(s, \pi_*(s)) = V_H^{\pi_*}(s).$$

Thus, assume $\widehat{V}_{h+1}^k(s') \geq V_{h+1}^{\pi_*}(s')$ for all $s' \in \mathcal{S}$ and observe that for all s, a

$$\begin{aligned}
Q_h^{\pi_*}(s,a) &= r_h(s,a) + \sum_{s'} P_h(s'|s,a) V_{h+1}^{\pi_*}(s') \\
&= r_h(s,a) + \sum_{s'} \widehat{P}_h^k(s'|s,a) V_{h+1}^{\pi_*}(s') + \sum_{s'} (P_h(s'|s,a) - \widehat{P}_h^k(s'|s,a)) V_{h+1}^{\pi_*}(s') \\
&\leq r_h(s,a) + \sum_{s'} \widehat{P}_h(s'|s,a) \widehat{V}_{h+1}^k(s') + H\sqrt{\frac{\log(2KHSA/\delta)}{n_h^k(s,a)}} \\
&= \widehat{Q}_h^k(s,a).
\end{aligned}$$

Using the same logic as for H, we conclude that $\widehat{V}_h^k(s) \geq V_h^k(s)$ for all $h \in [H]$. □

$$\begin{aligned}
&V_0^{\pi_*} - V_0^{\pi_k} = \mathbb{E}_{s_1}\left[V_1^{\pi_*}(s_1) - V_1^{\pi_k}(s_1)\right] \\
&\leq \mathbb{E}_{s_1}\left[\widehat{V}_1^k(s_1) - V_1^{\pi_k}(s_1)\right] \\
&= \mathbb{E}_{s_1}\left[\widehat{V}_1^k(s_1) - r(s_1, \pi_k(s_1)) - \sum_{s'} P_1(s'|s_1, \pi_k(s_1)) V_2^{\pi_k}(s')\right] \\
&= \mathbb{E}_{s_1}\left[\widehat{Q}_1^k(s_1, \pi_k(s_1)) - r(s_1, \pi_k(s_1)) - \sum_{s'} P_1(s'|s_1, \pi_k(s_1)) V_2^{\pi_k}(s')\right] \\
&= \mathbb{E}_{s_1}\left[H\sqrt{\frac{\log(2KHSA/\delta)}{2n_1^k(s_1,a_1)}} + \sum_{s'} \widehat{P}_1^k(s'|s_1, \pi_k(s_1)) \widehat{V}_2^k(s') - \sum_{s'} P_1(s'|s_1, \pi_k(s_1)) V_2^{\pi_k}(s')\right] \\
&= \mathbb{E}_{s_1}\Bigg[H\sqrt{\frac{\log(2KHSA/\delta)}{2n_1^k(s_1,a_1)}} + \sum_{s'} [\widehat{P}_1^k(s'|s_1, \pi_k(s_1)) - P_1(s'|s_1, \pi_k(s_1))] \widehat{V}_2^k(s') + \sum_{s'} P_1(s'|s_1, \pi_k(s_1)) [\widehat{V}_2^k(s') - V_2^{\pi_k} \\
&= \mathbb{E}_{s_1, a_1 \sim \pi^k}\left[H\sqrt{\frac{\log(2KHSA/\delta)}{2n_1^k(s_1,a_1)}} + \sum_{s'} [\widehat{P}_1^k(s'|s_1, a_1) - P_1(s'|s_1, a_1)] \widehat{V}_2^k(s')\right] + \mathbb{E}_{s_2 \sim \pi^k}[\widehat{V}_2^k(s_2) - V_2^{\pi_k}(s_2)] \\
&= \sum_{h=1}^H \mathbb{E}_{s_h, a_h \sim \pi^k}\left[H\sqrt{\frac{\log(2KHSA/\delta)}{2n_1^k(s_h,a_h)}} + \sum_{s'} [\widehat{P}_h^k(s'|s_h, a_h) - P_h(s'|s_h, a_h)] \widehat{V}_h^k(s')\right]
\end{aligned}$$

Now define the event

$$\mathcal{E}_{complexity} := \bigcap_{k=1}^K \bigcap_{h=1}^H \bigcap_{s,a} \left\{ \sup_{V \in [0,H]^S} \left| \sum_{s'} [\widehat{P}_h^k(s'|s,a) - P_h(s'|s,a)] V(s') \right| \leq H\sqrt{\frac{S \log(2KHSA/\delta)}{2n_h^k(s,a)}} \right\}.$$

Lemma 30. *For any $K \in \mathbb{N}$, we have that $\mathbb{P}(\mathcal{E}_{complexity}) \geq 1 - \delta$.*

Proof. Fix any $(s,a) \in \mathcal{S} \times \mathcal{A}$ and $h \in [H]$. Observe that

$$\begin{aligned}
\sup_{V \in [0,H]^S} \left| \sum_{s'} (P_h(s'|s,a) - \widehat{P}_h^k(s'|s,a)) V(s') \right| &= \max_{V \in \{0,H\}^S} \left| \sum_{s'} (P_h(s'|s,a) - \widehat{P}_h^k(s'|s,a)) V(s') \right| \\
&\leq H \sqrt{\frac{\log(2 \cdot 2^S/\delta)}{2 n_h^k(s,a)}} \\
&\leq H \sqrt{\frac{S \log(2/\delta)}{2 n_h^k(s,a)}}
\end{aligned}$$

where the second-to-last line holds with probability at least $1-\delta$ by applying Lemma 28 with a union bound over all $V \in \{0,1\}^S$. The final result follows from a union bound over all $\mathcal{S} \times \mathcal{A} \times [H]$. □

If $\mathcal{E}_{optimism} \cap \mathcal{E}_{complexity}$ holds then

$$\begin{aligned}
\sum_{k=1}^{K} V_0^{\pi_*} - V_0^{\pi_k} &\leq \sum_{k=1}^{K} \sum_{h=1}^{H} \mathbb{E}\left[H \sqrt{\frac{\log(2KHSA/\delta)}{2 n_1^k(s_h, a_h)}} + \sum_{s'} [\widehat{P}_h^k(s'|s_h, a_h) - P_h(s'|s_h, a_h)] \widehat{V}_h^k(s') \right] \\
&\leq \sum_{k=1}^{K} \sum_{h=1}^{H} \mathbb{E}\left[H \sqrt{\frac{2S \log(2KHSA/\delta)}{n_h^k(s_h^k, a_h^k)}} \right] \\
&= H \sqrt{2S \log(2KHSA/\delta)} \sum_{h=1}^{H} \mathbb{E}\left[\sum_{k=1}^{K} \frac{1}{\sqrt{n_h^k(s_h^k, a_h^k)}} \right] \\
&= H \sqrt{2S \log(2KHSA/\delta)} \sum_{h=1}^{H} \mathbb{E}\left[\sum_{s,a} \sum_{k=1}^{K} \mathbf{1}\{(s,a) = (s_h^k, a_h^k)\} \frac{1}{\sqrt{n_h^k(s_h^k, a_h^k)}} \right] \\
&= H \sqrt{2S \log(2KHSA/\delta)} \sum_{h=1}^{H} \mathbb{E}\left[\sum_{s,a} \sum_{i=1}^{n_h^K(s,a)} \frac{1}{\sqrt{i}} \right] \\
&\leq H \sqrt{8S \log(2KHSA/\delta)} \sum_{h=1}^{H} \mathbb{E}\left[\sum_{s,a} \sqrt{n_h^K(s,a)} \right] \\
&\leq H \sqrt{8S \log(2KHSA/\delta)} \sum_{h=1}^{H} \sqrt{SAK} \\
&= H^2 S \sqrt{8AK \log(2KHSA/\delta)}
\end{aligned}$$

where the second-to-last inequality follows from $\sum_{i=1}^{k} 1/\sqrt{i} \leq 2\sqrt{k}$, and the last inequality is Cauchy-Schwartz.

14.1.4 An improved regret bound for UCB-VI

With a more sophisticated argument, this section shows that the same algorithm achieves a regret of $\widetilde{O}\left(H^2\sqrt{SAK} + H^2 S^2 A \log(K)\right)$.

With probability at least $1-\delta$ we have for any $f:\mathcal{S}\to[-H,H]$ that

$$\begin{aligned}
\left|\sum_{s'}(P_h(s'|s,a)-\widehat{P}_h^k(s'|s,a))f(s')\right| &\leq \sum_{s'}\left|P_h(s'|s,a)-\widehat{P}_h^k(s'|s,a))\right|f(s')\\
&\leq \sum_{s'} f(s')\left(\sqrt{\frac{2P_h(s'|s,a)\log(2S/\delta)}{n_h^k(s,a)}}+\frac{2\log(2S/\delta)}{3n_h^k(s,a)}\right)\\
&\leq \frac{2HS\log(2S/\delta)}{3n_h^k(s,a)}+\sum_{s'}\sqrt{\frac{f^2(s')P_h(s'|s,a)\ 2\log(2S/\delta)}{n_h^k(s,a)}}\\
&\leq \frac{2HS\log(2S/\delta)}{3n_h^k(s,a)}+\sqrt{\frac{\sum_{s'}f^2(s')P_h(s'|s,a)\ 2S\log(2S/\delta)}{n_h^k(s,a)}}\\
&\leq \frac{2HS\log(2S/\delta)}{3n_h^k(s,a)}+\sqrt{\frac{\sum_{s'}f(s')P_h(s'|s,a)\ 2HS\log(2S/\delta)}{n_h^k(s,a)}}\\
&\leq \frac{2HS\log(2S/\delta)}{3n_h^k(s,a)}+\frac{1}{H}\sum_{s'}f(s')P_h(s'|s,a)+\frac{H^2S\log(2S/\delta)}{2n_h^k(s,a)}\\
&= \frac{2HS\log(2S/\delta)}{n_h^k(s,a)}+\frac{1}{H}\mathbb{E}_{s'\sim P_h(s'|s,a)}[f(s')]
\end{aligned}$$

where the second inequality applies Azume-Bernstein, the fourth inequality applies Cauchy-Schwartz, and the last inequality follows from for positive a,b we have $ab\leq(a^2+b^2)/2$ since $0\leq(a-b)^2/2$.

Picking up where we left off above in the regret bound, we have

$$\begin{aligned}
&\sum_{k=1}^K V_0^{\pi_*}-V_0^{\pi_k}\\
&\leq \sum_{k=1}^K \mathbb{E}_{s_1,a_1\sim\pi^k}\left[H\sqrt{\frac{\log(2KHSA/\delta)}{2n_1^k(s_1,a_1)}}+\sum_{s'}[\widehat{P}_1^k(s'|s_1,a_1)-P_1(s'|s_1,a_1)]\widehat{V}_2^k(s')\right]+\mathbb{E}_{s_2\sim\pi^k}[\widehat{V}_2^k(s_2)-V_2^{\pi_k}(s_2)]\\
&\leq \sum_{k=1}^K \mathbb{E}_{s_1,a_1\sim\pi^k}\left[H\sqrt{\frac{2\log(2KHSA/\delta)}{n_1^k(s_1,a_1)}}+\sum_{s'}[\widehat{P}_1^k(s'|s_1,a_1)-P_1(s'|s_1,a_1)](\widehat{V}_2^k(s')-V_2^{\pi_*}(s')\right]+\mathbb{E}_{s_2\sim\pi^k}[\widehat{V}_2^k(s_2)-V\\
&\leq \sum_{k=1}^K \mathbb{E}_{s_1,a_1\sim\pi^k}\left[H\sqrt{\frac{2\log(2KHSA/\delta)}{n_1^k(s_1,a_1)}}+\frac{2H^2S\log(2KHS^2A/\delta)}{n_1^k(s_1,a_1)}\right]+(1+1/H)\mathbb{E}_{s_2\sim\pi^k}[\widehat{V}_2^k(s_2)-V_2^{\pi_k}(s_2)]\\
&\leq \sum_{k=1}^K\sum_{h=1}^H(1+1/H)^{h-1}\mathbb{E}\left[H\sqrt{\frac{2\log(2KHSA/\delta)}{n_1^k(s_h,a_h)}}+\frac{2H^2S\log(2KHS^2A/\delta)}{n_h^k(s_h,a_h)}\right]\\
&\leq e\sum_{k=1}^K\sum_{h=1}^H\mathbb{E}\left[H\sqrt{\frac{2\log(2KHSA/\delta)}{n_h^k(s_h,a_h)}}+\frac{2H^2S\log(2KHS^2A/\delta)}{n_h^k(s_h,a_h)}\right]
\end{aligned}$$

where the last line follows from $(1+1/H)^{h-1}\leq(1+1/H)^H\leq e$. By the same sequence of steps as above, $\sum_{k=1}^K\sum_{h=1}^H\frac{1}{\sqrt{n_h^k(s_h,a_h)}}\leq 2H\sqrt{SAK}$. Analogously, using the fact that $\sum_{i=1}^n\frac{1}{i}\leq 2\log(n)$ we have

$$\mathbb{E}\left[\sum_{k=1}^K\sum_{h=1}^H\frac{1}{n_h^k(s_h,a_h)}\right]\leq\mathbb{E}\left[\sum_{h=1}^H\sum_{s,a}\log(n_h^K(s,a))\right]\leq 2SAH\log(K).$$

Putting it all together we have a final regret bound of

$$\begin{aligned}
\sum_{k=1}^{K} V_0^{\pi_*} - V_0^{\pi_k} \leq & e \sum_{k=1}^{K} \sum_{h=1}^{H} \mathbb{E}\left[H \sqrt{\frac{2\log(2KHSA/\delta)}{n_h^k(s_h, a_h)}} + \frac{2HS\log(2KHS^2A/\delta)}{n_h^k(s_h, a_h)} \right] \\
= & eH\sqrt{2\log(2KHSA/\delta)} \sum_{k=1}^{K} \sum_{h=1}^{H} \mathbb{E}\left[\frac{1}{\sqrt{n_h^k(s_h, a_h)}} \right] \\
& + 2eH^2S\log(2KHS^2A/\delta) \sum_{k=1}^{K} \sum_{h=1}^{H} \mathbb{E}\left[\frac{1}{n_h^k(s_h, a_h)} \right] \\
\leq & H^2\sqrt{8e^2SAK\log(2KHSA/\delta)} + 4eH^3S^2A\log(K)\log(2KHS^2A/\delta).
\end{aligned}$$

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