

Online Learning under Logarithmic Loss

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October 21, 2024



- ▶ **Sequential Probability Assignment**
 - Weather forecasting, proper scoring, logarithmic loss
 - Bayesian algorithm
- ▶ **Minimax Regret under Log-loss**
 - Fixed design, Shtarkov sum
 - Truncated Bayesian Algorithm
 - Contextual Shtarkov sum
- ▶ **Application of Prediction with Log-loss**
 - Portfolio optimization
 - Converting prediction to investment strategy

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Formally, we aim to find a **loss** function $\ell : \Delta(\{0, 1\}) \times \{0, 1\} \rightarrow \mathbb{R}$ that satisfies the following **minimal** criteria:

1. It should penalize the **true** distribution **minimally**, i.e.,

$$\forall \mathbf{p}, \mathbf{q} \in \Delta(\{0, 1\}), \mathbb{E}_{y \sim \mathbf{p}}[\ell(\mathbf{p}, y)] \leq \mathbb{E}_{y \sim \mathbf{p}}[\ell(\mathbf{q}, y)].$$

2. Ideally, the function ℓ should have a natural **interpretation**.

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Key properties of log-loss:

- ▶ It relates naturally to **Shannon entropy** and **KL-divergence** as: (**verify it!**)

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- ▶ **Equality** is achieved when $p = q$.

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For $t = 1, \dots, T$

- ▶ Nature selects an instance $\mathbf{x}_t \in \mathcal{X}$;
- ▶ Learner predicts **distribution** $\hat{p}_t \in \hat{\mathcal{Y}}$;
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Goal of Learner: Find predictor Φ that minimizes the **worst-case** regret:

$$\text{reg}_T(\mathcal{H}, \Phi) = \sup_{\mathbf{x}^T, \mathbf{y}^T} \left[\sum_{t=1}^T \ell^{\log}(\hat{p}_t, y_t) - \inf_{h \in \mathcal{H}} \sum_{t=1}^T \ell^{\log}(h(\mathbf{x}_t), y_t) \right].$$

Regret Bound for Finite Class: the Bayesian Algorithm

Recall from **Lecture 2** that for a **finite** class \mathcal{H} , the **EWA** algorithm Φ enjoys the **worst-case** regret for **bounded convex**:

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Let $\mathcal{H} = \{h_1, \dots, h_K\}$.

The Bayesian Algorithm:

1. Maintain a weight vector $\mathbf{w}^{(t)} \in \mathbb{R}^K$, initially $\mathbf{w}^{(0)} = (1, \dots, 1)$.
2. At each step t , predict $\hat{p}_t := \sum_{k=1}^K \tilde{p}_t[k] \cdot h_k(\mathbf{x}_t)$, where

$$\forall k \in [K], \tilde{p}_t[k] = \frac{\mathbf{w}_k^{(t-1)}}{\sum_{k=1}^K \mathbf{w}_k^{(t-1)}}.$$

3. Let y_t be the true label, and update $\mathbf{w}_k^{(t)} = \mathbf{w}_k^{(t-1)} \cdot h_k(\mathbf{x}_t)[y_t]$.

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Observe that $h_k(\mathbf{x}_t)[y_t] = e^{-\ell^{\log}(h_k(\mathbf{x}_t), y_t)}$, i.e., the **Bayesian algorithm** is simply the **EWA** algorithm with a learning rate of $\eta = 1$.

Regret Bound for Bayesian Algorithm

Theorem 1: Let \mathcal{H} be a finite class. The Bayesian algorithm Φ enjoys the worst-case regret under logarithmic loss:

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- ▶ Although our predictions are **probabilities**, we do not assume any probabilistic mechanism for generating the **data**.
- ▶ The regret bound holds for any **individual** sequences \mathbf{x}^T, y^T .

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Therefore,

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Problem 2: What **algorithm** achieves the **minimax regret**?

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For any **given** \mathbf{x}^T , we define the **fixed design minimax regret** as:

$$\text{reg}_T^{\text{fix}}(\mathcal{H} \mid \mathbf{x}^T) = \inf_{\Phi} \sup_{\mathbf{y}^T} \left[\sum_{t=1}^T \ell^{\log}(\hat{\mathbf{p}}_t, \mathbf{y}_t) - \inf_{h \in \mathcal{H}} \sum_{t=1}^T \ell^{\log}(h(\mathbf{x}_t), \mathbf{y}_t) \right].$$

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It is easy to observe that: **(Why?)**

$$\sup_{\mathbf{x}^T} \text{reg}_T^{\text{fix}}(\mathcal{H} \mid \mathbf{x}^T) \leq \text{reg}_T(\mathcal{H}).$$

Characterizing Fixed-Design Minimax Regret: Shtarkov Sum

Shtarkov Sum: Let $\mathcal{H} \subset \Delta(\mathcal{Y})^{\mathcal{X}}$ be a hypothesis class and \mathbf{x}^T be any given instances. The *Shtarkov sum* of \mathcal{H} conditioning on \mathbf{x}^T is defined as

$$\text{Sht}(\mathcal{H} \mid \mathbf{x}^T) = \sum_{\mathbf{y}^T \in \mathcal{Y}^T} \sup_{h \in \mathcal{H}} \prod_{t=1}^T h(\mathbf{x}_t)[y_t].$$

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Example 1: Let \mathcal{H} be a **finite** class, we have for any \mathbf{x}^T that

$$\begin{aligned} \text{Sht}(\mathcal{H} \mid \mathbf{x}^T) &= \sum_{\mathbf{y}^T \in \mathcal{Y}^T} \sup_{h \in \mathcal{H}} \prod_{t=1}^T h(\mathbf{x}_t)[y_t] \\ &\leq \sum_{\mathbf{y}^T \in \mathcal{Y}^T} \sum_{h \in \mathcal{H}} \prod_{t=1}^T h(\mathbf{x}_t)[y_t] \\ &= \sum_{h \in \mathcal{H}} \sum_{\mathbf{y}^T \in \mathcal{Y}^T} \prod_{t=1}^T h(\mathbf{x}_t)[y_t] \stackrel{(*)}{\leq} \sum_{h \in \mathcal{H}} 1 = |\mathcal{H}|. \end{aligned}$$

Characterizing Fixed-Design Minimax Regret: Shtarkov Sum

Theorem 2: Let $\mathcal{H} \subset \Delta(\mathcal{Y})^{\mathcal{X}}$ be any hypothesis class, and let \mathbf{x}^T be any given instances. Then

$$\text{reg}_T^{\text{fix}}(\mathcal{H} \mid \mathbf{x}^T) = \log \text{Sht}(\mathcal{H} \mid \mathbf{x}^T).$$

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- ▶ These two quantities are **exactly equal**.
- ▶ For a **finite** class \mathcal{H} , we immediately have

$$\text{reg}_T^{\text{fix}}(\mathcal{H} \mid \mathbf{x}^T) = \log \text{Sht}(\mathcal{H} \mid \mathbf{x}^T) \leq \log |\mathcal{H}|.$$

- ▶ The Shtarkov sum forms a **lower bound** for the (sequential) **minimax regret**:

$$\text{reg}_T(\mathcal{H}) \geq \sup_{\mathbf{x}^T} \text{reg}_T^{\text{fix}}(\mathcal{H} \mid \mathbf{x}^T) \geq \sup_{\mathbf{x}^T} \log \text{Sht}(\mathcal{H} \mid \mathbf{x}^T).$$

Proof of Theorem 2

We introduce the **short-hand** notations

$$P_h(y^T | \mathbf{x}^T) = \prod_{t=1}^T h(\mathbf{x}_t)[y_t], \quad \hat{Q}(y^T) = \prod_{t=1}^T \hat{p}_t[y_t].$$

Observe, by definition of log-loss, that

$$\begin{aligned} \text{reg}_T^{\text{fix}}(\mathcal{H} | \mathbf{x}^T) &= \inf_{\hat{Q}} \sup_{y^T} \left[-\log \hat{Q}(y^T) + \log \sup_h P_h(y^T | \mathbf{x}^T) \right] \\ &= \inf_{\hat{Q}} \sup_{y^T} \left[-\log \hat{Q}(y^T) + \log P^*(y^T | \mathbf{x}^T) \right] + \log \sum_{y^T} \sup_h P_h(y^T | \mathbf{x}^T) \\ &\stackrel{(*)}{=} \log \sum_{y^T} \sup_h P_h(y^T | \mathbf{x}^T) = \log \text{Sht}(\mathcal{H} | \mathbf{x}^T), \end{aligned}$$

where $P^*(y^T | \mathbf{x}^T) := \frac{\sup_h P_h(y^T | \mathbf{x}^T)}{\sum \sup_h P_h(y^T | \mathbf{x}^T)}$ and $(*)$ attains when $\hat{Q}(\cdot) \equiv P^*(\cdot | \mathbf{x}^T)$.

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A by-product of our previous proof shows that the **minimax optimal** predictor satisfies **equality**

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To satisfy the **equality**, we can define (**Why?**)

$$\hat{p}_t[y] = \frac{\sum_{y^{T-t}} P^*(y^{t-1} y y^{T-t} | \mathbf{x}^T)}{\sum_{y^{T-t+1}} P^*(y^{t-1} y^{T-t+1} | \mathbf{x}^T)}$$

Minimax Optimal Predictor: Normalized Maximum Likelihood

A by-product of our previous proof shows that the **minimax optimal** predictor satisfies **equality**

$$\hat{Q}(\cdot) \equiv P^*(\cdot | \mathbf{x}^T),$$

where $P^*(y^T | \mathbf{x}^T) := \frac{\sup_h P_h(y^T | \mathbf{x}^T)}{\sum_{y^T} \sup_h P_h(y^T | \mathbf{x}^T)}$ and $\hat{Q}(y^T) = \prod_{t=1}^T \hat{p}_t[y_t]$.

To satisfy the **equality**, we can define (**Why?**)

$$\hat{p}_t[y] = \frac{\sum_{y^{T-t}} P^*(y^{t-1} y y^{T-t} | \mathbf{x}^T)}{\sum_{y^{T-t+1}} P^*(y^{t-1} y^{T-t+1} | \mathbf{x}^T)}$$

This predictor is known as the **Normalized Maximum Likelihood** (NML) predictor.

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$$\forall t \leq T, \|g(\mathbf{x}^t) - h(\mathbf{x}_t)\|_\infty \leq \alpha,$$

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- Note that a crucial property when we apply the sequential cover for a **Lipschitz** loss ℓ is that: $\ell(\hat{y}_1, y) - \ell(\hat{y}_2, y) \leq L|\hat{y}_1 - \hat{y}_2|$.

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- ▶ Therefore, small regret on the cover \mathcal{G}_α automatically implies small regret on \mathcal{H} , offset by αLT .
- ▶ This, unfortunately, is **not true** for log-loss, e.g., $\ell^{\log}(0, y) - \ell^{\log}(\alpha, y) = \infty$.

From Covering to Dominance: The Smooth Truncation

Lemma 1: Let \mathcal{G} be a sequential α -cover of \mathcal{H} . Then, for any $h \in \mathcal{H}$ and $\mathbf{x}^T, \mathbf{y}^T$, there exists $g \in \mathcal{G}$ such that

$$\frac{\prod_{t=1}^T h(\mathbf{x}_t)[y_t]}{\prod_{t=1}^T g^{(\alpha)}(\mathbf{x}_t)[y_t]} \leq (1 + \alpha|\mathcal{Y}|)^T,$$

where $g^{(\alpha)} = \frac{g + \alpha}{1 + \alpha|\mathcal{Y}|}$ is the **smooth truncation** of g .

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Proof: For any $h \in \mathcal{H}$ and \mathbf{x}^T, y^T , we choose $g \in \mathcal{G}$ as the sequential α -cover of h on \mathbf{x}^T . This implies that, for all $t \leq T$ and $y \in \mathcal{Y}$,

$$h(\mathbf{x}_t)[y] \leq g(\mathbf{x}^t)[y] + \alpha.$$

Therefore, for any $t \leq T$, we have

$$\frac{h[y_t]}{g^{(\alpha)}[y_t]} = \frac{h[y_t]}{(g[y_t] + \alpha)/(1 + \alpha|\mathcal{Y}|)} \leq (1 + \alpha|\mathcal{Y}|).$$

Bounding sequential Minimax Regret via Sequential Cover

Theorem 2: Let $\mathcal{H} \subset \Delta(\mathcal{Y})^{\mathcal{X}}$ be a hypothesis class that admits a sequential α -cover \mathcal{G}_α for all $\alpha \geq 0$. Then

$$\text{reg}_T(\mathcal{H}) \leq \inf_{\alpha \geq 0} \{\alpha |\mathcal{Y}| T + \log |\mathcal{G}_\alpha|\}.$$

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Example 2: Let $\mathcal{Y} := \{0, 1\}$, $\mathcal{X} := B_2$ and

$$\mathcal{H}^{\text{lin}} := \{h_{\mathbf{w}}(\mathbf{x}) := |\langle \mathbf{w}, \mathbf{x} \rangle| : \mathbf{w} \in B_2\} \subset [0, 1]^{\mathcal{X}}.$$

Here we interpret $h(\mathbf{x}) \in [0, 1]$ as Bernoulli distribution with parameter $h(\mathbf{x})$.

From **lecture 3**, we know that $|\log \mathcal{G}_\alpha| \leq \tilde{O}(\alpha^{-2})$. This leads to the regret bound (verify it!)

$$\text{reg}_T(\mathcal{H}^{\text{lin}}) \leq \tilde{O}(T^{2/3}).$$

Proof of Theorem 2

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We have for any \mathbf{x}^T, y^T that

$$\sum_{t=1}^T \ell^{\log}(\hat{p}_t, y_t) - \inf_{g \in \mathcal{G}_\alpha^{(\alpha)}} \sum_{t=1}^T \ell^{\log}(g(\mathbf{x}^t), y_t) \leq \log |\mathcal{G}_\alpha^{(\alpha)}| = \log |\mathcal{G}_\alpha|.$$

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Invoking **Lemma 1**, we have (**verify it!**)

$$- \inf_{h \in \mathcal{H}} \sum_{t=1}^T \ell^{\log}(h(\mathbf{x}_t), y_t) \leq - \inf_{g \in \mathcal{G}_\alpha^{(\alpha)}} \sum_{t=1}^T \ell^{\log}(g(\mathbf{x}^t), y_t) + T \log(1 + \alpha|\mathcal{Y}|). \quad (1)$$

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Note: The use of $\mathcal{G}_\alpha^{(\alpha)}$ instead of \mathcal{G}_α is crucial for (1) to work.

Sub-optimality of Covering-Based Bounds

We now mention the following theorem without proof.

Theorem 3: Let $\mathcal{Y} := \{0, 1\}$, and assume $\hat{\mathcal{Y}} := [0, 1]$, interpreted as Bernoulli distributions. Then for any class $\mathcal{H} \subset \hat{\mathcal{Y}}^{\mathcal{X}}$ with a sequential α -cover \mathcal{G}_α of size $\log |\mathcal{G}_\alpha| \leq \tilde{O}(\alpha^{-p})$ for all $\alpha \geq 0$, we have

$$\text{reg}_T(\mathcal{H}) \leq \tilde{O}(T^{\frac{p}{p+1}}).$$

Moreover, for any $p \geq 2$, there exists a class that satisfies the above condition and

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- ▶ We need a new complexity measure...

The Contextual Shtarkov Sum

Very recently, Liu, Attias, and Roy (to appear in NeurIPS 2024) demonstrated that a variant of the **Shtarkov sum with context** **completely** characterizes the (sequential) minimax regret...

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Contextual Shtarkov Sum: Let $\tau : \bigcup_{t=1}^T \mathcal{Y}^t \rightarrow \mathcal{X}$ be an \mathcal{X} -valued $|\mathcal{Y}|$ -ary tree of depth T . The contextual Shtarkov sum w.r.t. τ is defined as

$$\text{Sht}(\mathcal{H} \mid \tau) = \sum_{y^T} \sup_{h \in \mathcal{H}} \prod_{t=1}^T h(\tau(y^{t-1})) [y_t].$$

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- ▶ This result can be used to recover **Theorem 2** using (smaller) **local** covers.
- ▶ It remains **largely open** how the **contextual Shtarkov sum** can be estimated for any non-trivial classes beyond covering methods...

Proof of Theorem 4

We provide only the high-level idea.

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Step One: Using the **minimax switching** trick (see **lecture 3**) to obtain the following **Bayesian representation**:

$$\sup_{\mathbf{x}_1, p_1} \mathbb{E}_{y_1 \sim p_1} \cdots \sup_{\mathbf{x}_T, p_T} \mathbb{E}_{y_T \sim p_T} \left[\sum_{t=1}^T \inf_{\hat{p}_t} \mathbb{E}_{y_t \sim p_t} \left[\ell^{\log}(\hat{p}_t, y_t) \right] - \inf_{h \in \mathcal{H}} \sum_{t=1}^T \ell^{\log}(h(\mathbf{x}_t), y_t) \right].$$

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Step Two: Show that (recall from our previous slides):

$$\inf_{\hat{p}_t} \mathbb{E}_{y_t \sim p_t} \left[\ell^{\log}(\hat{p}_t, y_t) \right] = H(p_t),$$

where $H(p_t)$ is the **Shannon entropy**.

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Step Three: Show that via **Skolemization** the expression reduces to:

$$\sup_{\tau} \sup_P \mathbb{E}_{y^T \sim P} \left[H(P) - \inf_{h \in \mathcal{H}} \sum_{t=1}^T \ell^{\log}(h(\tau(y^{t-1})), y_t) \right],$$

where τ runs over trees $\tau : \bigcup_{t=1}^T \mathcal{Y}^t \rightarrow \mathcal{X}$ and $P \in \Delta(\mathcal{Y}^T)$.

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Step Four: Denote $\mathbf{x}_t = \tau(y^{t-1})$, and let $P_h(y^T | \mathbf{x}^T) = \prod_{t=1}^T h(\mathbf{x}_t)[y_t]$.

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Step Four: Denote $\mathbf{x}_t = \tau(y^{t-1})$, and let $P_h(y^T | \mathbf{x}^T) = \prod_{t=1}^T h(\mathbf{x}_t)[y_t]$. We have

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Therefore, we are reduced to

$$\begin{aligned} \sup_P \mathbb{E}_{y^T \sim P} \left[H(P) + \log \sup P_h(y^T | \mathbf{x}^T) \right] &= \sup_P \mathbb{E} \left[-\log P(y^T) + \log \sup P_h(y^T | \mathbf{x}^T) \right] \\ &= \sup_P \mathbb{E} \left[-\log P(y^T) + \log P^*(y^T | \mathbf{x}^T) \right] + \log \sum_{y^T} \sup_h \prod_{t=1}^T h(\mathbf{x}_t)[y_t] \\ &= \underbrace{\sup_P -\text{KL}(P, P^*)}_{=0} + \log \sum_{y^T} \sup_h \prod_{t=1}^T h(\mathbf{x}_t)[y_t]. \end{aligned}$$

Here, $P^*(y^T | \mathbf{x}^T) = \frac{\sup_h P_h(y^T | \mathbf{x}^T)}{\sum_{y^T} \sup_h P_h(y^T | \mathbf{x}^T)}$, and equality is attained at $P = P^*$.

Proof of Theorem 4

Step Four: Denote $\mathbf{x}_t = \tau(y^{t-1})$, and let $P_h(y^T | \mathbf{x}^T) = \prod_{t=1}^T h(\mathbf{x}_t)[y_t]$. We have

$$\inf_{h \in \mathcal{H}} \sum_{t=1}^T \ell^{\log}(h(\tau(y^{t-1})), y_t) = \inf_h -\log P_h(y^T | \mathbf{x}^T) = -\sup_h \log P_h(y^T | \mathbf{x}^T).$$

Therefore, we are reduced to

$$\begin{aligned} \sup_P \mathbb{E}_{y^T \sim P} \left[H(P) + \log \sup P_h(y^T | \mathbf{x}^T) \right] &= \sup_P \mathbb{E} \left[-\log P(y^T) + \log \sup P_h(y^T | \mathbf{x}^T) \right] \\ &= \sup_P \mathbb{E} \left[-\log P(y^T) + \log P^*(y^T | \mathbf{x}^T) \right] + \log \sum_{y^T} \sup_h \prod_{t=1}^T h(\mathbf{x}_t)[y_t] \\ &= \underbrace{\sup_P -\text{KL}(P, P^*)}_{=0} + \log \sum_{y^T} \sup_h \prod_{t=1}^T h(\mathbf{x}_t)[y_t]. \end{aligned}$$

Here, $P^*(y^T | \mathbf{x}^T) = \frac{\sup_h P_h(y^T | \mathbf{x}^T)}{\sum_{y^T} \sup_h P_h(y^T | \mathbf{x}^T)}$, and equality is attained at $P = P^*$.

Note: The distribution P^* is **not** a minimax optimal strategy; achieving this would require using the **relaxation-based** approach (c.f. **lecture 3**)...

- ▶ **Sequential Probability Assignment**
 - Weather forecasting, proper scoring, logarithmic loss
 - Bayesian algorithm
- ▶ **Minimax Regret under Log-loss**
 - Fixed design, Shtarkov sum
 - Truncated Bayesian Algorithm
 - Contextual Shtarkov sum
- ▶ **Application of Prediction with Log-loss**
 - Portfolio optimization
 - Converting prediction to investment strategy

Portfolio Optimization

Consider a (simplified) **stock market** that operates in discrete time steps.

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Goal: Find an investment strategy \hat{p}^T that maximizes total wealth.

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Here, we assume that $\mathbf{v}^{t-1} \subset \mathbf{x}_t$, i.e., the side information contains all the past market vectors, so that our investment strategy could rely solely on \mathbf{x}^T .

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Recall that an **online predictor** is a function $\Phi : (\mathcal{X} \times \mathcal{Y})^* \times \mathcal{Y} \rightarrow \Delta(\mathcal{Y})$.

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Theorem 5: Let Φ be an **online predictor** and Ψ be the **induced investment strategy**. Then, for **any market vectors** \mathbf{v}^T , **side information** \mathbf{x}^T , and **hypothesis class** \mathcal{H} , we have

$$\sup_{h \in \mathcal{H}} \log \frac{S_T(\mathbf{v}^T, \mathbf{x}^T, h)}{S_T(\mathbf{v}^T, \mathbf{x}^T, \Psi)} \leq \sup_{\mathbf{y}^T} \sup_{h \in \mathcal{H}} \log \frac{\prod_{t=1}^T h(\mathbf{x}_t)[y_t]}{\prod_{t=1}^T \hat{p}_t[y_t]} \leq \text{reg}_T(\mathcal{H}, \Phi),$$

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- ▶ Any **online predictor** with **low worst-case regret** can be **converted** into an **investment strategy** that achieves a **low logarithmic wealth ratio**.

Proof of Theorem 5

Observe that

$$\begin{aligned} S_T(\mathbf{v}^T, \mathbf{x}^T, h) &= \prod_{t=1}^T \left(\sum_y \mathbf{v}_t[y] \cdot h(\mathbf{x}_t)[y] \right) \\ &= \sum_{\mathbf{y}^T} \left(\prod_{t=1}^T \mathbf{v}_t[y_t] \right) \left(\prod_{t=1}^T h(\mathbf{x}_t)[y_t] \right). \end{aligned}$$

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Moreover, by the definition of Ψ , we have

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The theorem now follows from the inequality $\log \frac{\sum_i a_i}{\sum_i b_i} \leq \sup_i \log \frac{a_i}{b_i}$. (Why?)

Concluding Remarks

- ▶ In this lecture, we introduced online learning under **logarithmic loss**.
- ▶ We provided several approaches, such as **sequential covering** and the **Shtarkov sum**, for characterizing the **minimax regret** under log-loss.
- ▶ We also introduced an application of prediction under log-loss in the context of **portfolio optimization**.
- ▶ There are also many other applications of log-loss across various domains, such as **universal compression**, **interactive decision-making**, and **online distribution estimation**, which we unfortunately could not cover.
 - We refer interested readers to "*Prediction, Learning, and Games*" by N. Cesa-Bianchi and G. Lugosi.