Machine Learning Theory 2025
Lecture 13

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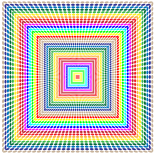
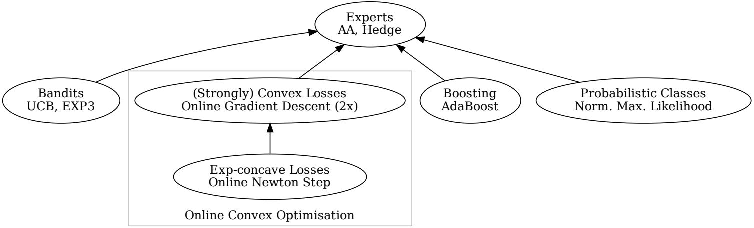
- Prediction with log-loss:
  - NML/Shtarkov
  - Bayes Uniform Prior/Jeffreys Prior
  - Finite Θ/Parametric Θ

  Application:
  - Markov and CTW prediction



Recap

Overview of Second Half of Course



Material: course notes on MLT website.

Background Material: Chapter 9 from *Prediction, Learning and Games* by Cesa-Bianchi and Lugosi.

Outlook

Today: **adversarial online learning** with **statistical models** as our hypotheses

Main points:

- Minimax analyis tractable, elegant, insightful
- Bayesian methods can get very close
- Foundation for practical methods

Log-loss prediction

Log Loss Prediction Setup

Start with a class Θ of *simulatable* predictors for outcomes $y_1, y_2, \ldots$.

After seeing past y^{n-1}, each $\theta \in \Theta$ assigns a probability p_θ to the next outcome y_n denoted by

$$p_\theta(y_n|y^{n-1})$$

Interesting examples:

- Finite class
- Bernoulli
- Mixtures (categorical distributions)
- Markov chains
- Logistic regression

Conditional vs Joint Equivalence

A sequential one-step-ahead forecaster (aka conditional distribution)

$$p(y_t|y^{t-1})$$

induces a distribution on length-T sequences (aka joint distribution)

$$p(y^T) \;:=\; \prod_{t=1}^{T} p(y_t|y^{t-1})$$

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Conversely, any distribution over full T-length outcome sequences

$$p(y^T)$$

induces a one-step forecaster (by integrating out the future)

$$p(y_t|y^{t-1}) \;:=\; \frac{\sum_{y_{t+1}^T} p(y^{t-1}, y_t, y_{t+1}^T)}{\sum_{y_t^T} p(y^{t-1}, y_t^T)}$$

So: two **equivalent representations** of the same object

Log Loss Prediction Notation

A predictor θ assigns to sequence y^T probability

$$p_\theta(y^T) = \prod_{t=1}^{T} p_\theta(y_t | y^{t-1})$$

Definition

The **maximum likelihood estimator** (MLE) for data y^T is

$$\hat{\theta}(y^T) \ = \ \arg\max_{\theta \in \Theta} p_\theta(y^T),$$

and the **maximum likelihood** is

$$p_{\hat{\theta}(y^T)}(y^T) \ = \ \max_{\theta \in \Theta} p_\theta(y^T).$$

NB: $\sum_{y^T} p_{\hat{\theta}(y^T)}(y^T) \gg 1$.

Log-loss Prediction Game

Fix a class Θ of simulatable predictors

Protocol

- For $t = 1, 2, \ldots, T$
  1. The learner assigns probability $\tilde{p}_t \in \triangle_{\mathcal{Y}}$ to the next outcome.
  2. The next outcome $y_t \in \mathcal{Y}$ is revealed
  3. Learner incurs **log loss** $-\ln \tilde{p}_t(y_t)$.

NB: $\tilde{p}_t$ typically improper (not itself in Θ)

Definition (Regret)

After T rounds, the regret is

$$\underbrace{\sum_{t=1}^{T} -\ln \tilde{p}_t(y_t)}_{\text{Learner's log loss}} - \underbrace{\min_{\theta \in \Theta} \sum_{t=1}^{T} -\ln p_\theta(y_t | y^{t-1})}_{\text{log loss of MLE: } -\ln p_{\hat{\theta}(y^T)}(y^T)}$$

Data compression connection

Intuition

#bits $\approx$ log-loss

Key words:

- Shannon-Fano code : code lengths are $-\log(p)$ rounded-up
- Kraft Inequality : $2^{-\text{bit length}}$ sums to ≤ 1 for any code
- arithmetic coding: bits $\approx -\log(p^T)$ *sequentially*

What we already know: Experts

Theorem

For finite $|\Theta| < \infty$, there is an algorithm for the log loss game with regret at most $\ln|\Theta|$.

Proof.

By reduction to the mix loss game. Consider running the Agregating Algorithm from Lecture 8 on experts Θ with losses

$$\ell_t^\theta \;=\; -\ln p_\theta(y_t|y^{t-1})$$

and using $\boldsymbol{w}_t$ to form the predictions

$$\tilde{p}_t(y) \;=\; \sum_{\theta\in\Theta} w_t^\theta p_\theta(y|y^{t-1}).$$

Then log loss equals mix loss

$$-\ln \tilde{p}_t(y_t) \;=\; -\ln \sum_{\theta\in\Theta} w_t^\theta e^{-\ell_t^\theta}$$

and the $\ln|\Theta|$ regret bound follows. □

What we already know: Experts

AA-based strategy takes a particularly simple form

$$
\begin{aligned}
\tilde{p}_t(y) &= \sum_{\theta\in\Theta} w_t^\theta p_\theta(y|y^{t-1}) \\
&= \frac{\sum_{\theta\in\Theta} e^{-\sum_{s=1}^{t-1}\ell_s^\theta} p_\theta(y|y^{t-1})}{\sum_{\theta\in\Theta} e^{-\sum_{s=1}^{t-1}\ell_s^\theta}} \\
&= \frac{\sum_{\theta\in\Theta} e^{-\sum_{s=1}^{t-1} -\ln p_\theta(y_s|y^{s-1})} p_\theta(y|y^{t-1})}{\sum_{\theta\in\Theta} e^{-\sum_{s=1}^{t-1} -\ln p_\theta(y_s|y^{s-1})}} \\
&= \frac{\sum_{\theta\in\Theta} \prod_{s=1}^{t-1} p_\theta(y_s|y^{s-1}) p_\theta(y|y^{t-1})}{\sum_{\theta\in\Theta} \prod_{s=1}^{t-1} p_\theta(y_s|y^{s-1})} \\
&= \frac{\sum_{\theta\in\Theta} p_\theta(y^{t-1}) p_\theta(y|y^{t-1})}{\sum_{\theta\in\Theta} p_\theta(y^{t-1})}
\end{aligned}
$$

Average of predictions $p_\theta(y|y^{t-1})$ with weights $\propto p_\theta(y^{t-1})$.

Bayes rule (uniform prior on Θ).

What we already know: Exp-concavity

Log loss is a **1-exp concave** function of the prediction $\tilde{p}_t \in \triangle_{\mathcal{Y}}$.

With $f_t(\tilde{p}_t) = -\ln \tilde{p}_t(y_t)$, we have gradient

$$\nabla f_t(\tilde{p}_t) \;=\; \nabla - \ln \tilde{p}_t(y_t) \;=\; -\frac{\boldsymbol{e}_{y_t}}{\tilde{p}_t(y_t)}.$$

Potentially **unbounded** gradient (as we saw in Homework 11.2). Online Newton Step may need additional assumptions.

Questions for Today

- Is regret $\leq \ln|\Theta|$ good for this problem?
- And what if $|\Theta| = \infty$?

Minimax Regret for Log Loss

Log Loss Prediction Minimax Regret

Fix a model Θ.

Definition

The minimax regret of the T-round log-loss game on Θ is

$$\mathcal{V}_T(\Theta) \; := \; \min_{\tilde{p}_1} \max_{y_1} \min_{\tilde{p}_2} \max_{y_2} \ldots \min_{\tilde{p}_T} \max_{y_T} \; \text{Regret}$$

Note: can be linear if Θ is too large.

Normalised Maximum Likelihood

Easier to solve the problem in whole-sequence-at-once form:

$$\begin{aligned}\mathcal{V}_T(\Theta) &= \min_{\tilde{p}_1} \max_{y_1} \min_{\tilde{p}_2} \max_{y_2} \ldots \min_{\tilde{p}_T} \max_{y_T} \text{ Regret} \\ &= \min_{\tilde{p}(y^T)} \max_{y^T} -\ln \tilde{p}(y^T) + \ln p_{\hat{\theta}(y^T)}(y^T)\end{aligned}$$

Normalised Maximum Likelihood

Theorem (Shtarkov)

The minimax predictor is **Normalised Maximum Likelihood**

$$p_{NML}(y^T) \;=\; \frac{\max_{\theta \in \Theta} p_\theta(y^T)}{\sum_{y^T} \max_{\theta \in \Theta} p_\theta(y^T)}$$

and the minimax regret is

$$\mathcal{V}_T(\Theta) \;=\; \ln \left(\sum_{y^T} \max_{\theta \in \Theta} p_\theta(y^T) \right)$$

Game-theoretic measure of capacity of Θ called **Stochastic Complexity**

Counts number of parameters $\theta \in \Theta$ that are "essentially different" at horizon T.

Rate at which you need to grow cardinality when using finite discretisation.

Proof

See Theorem 9.1 in the material.

Minimax regret

Consider again the finite Θ case. Then

$$\begin{aligned}\mathcal{V}_T(\Theta) &= \ln\left(\sum_{y^T} \max_{\theta\in\Theta} p_\theta(y^T)\right) \\ &\leq \ln\left(\sum_{y^T} \sum_{\theta\in\Theta} p_\theta(y^T)\right) \\ &= \ln|\Theta|\end{aligned}$$

Can be much smaller in practise.

Asymptotic Expansion for Minimax Regret I

Now consider the i.i.d. Bernoulli model $\Theta = [0,1]$ where $p_\theta(1|y^{t-1}) = \theta$.

Theorem

$$\mathcal{V}_T(\Theta) \;=\; \frac{1}{2}\ln\frac{T\pi}{2} + o(1)$$

Asymptotic Expansion for Minimax Regret II

Proof.

$$\begin{aligned}\mathcal{V}_T(\Theta) &= \ln\left(\sum_{y^T}\max_{\theta\in\Theta} p_\theta(y^T)\right)\\ &= \ln\left(\sum_{i=0}^{T}\binom{T}{i}\left(\frac{i}{T}\right)^{i}\left(\frac{T-i}{T}\right)^{T-i}\right)\\ &\overset{\text{Stirling}}{\approx} \ln\left(\sum_{i=0}^{T}\sqrt{\frac{T}{2\pi i(T-i)}}\right) \overset{\text{Integral}}{\approx} \ln\left(\sqrt{\frac{T\pi}{2}}\right)\end{aligned}$$

Where the approximation is Stirling's $n! \approx \sqrt{2\pi n}\left(\frac{n}{e}\right)^n$. So that

$$\binom{T}{i} \approx \frac{\sqrt{2\pi T}\left(\frac{T}{e}\right)^T}{\sqrt{2\pi i}\left(\frac{i}{e}\right)^i\sqrt{2\pi(T-i)}\left(\frac{T-i}{e}\right)^{T-i}} = \sqrt{\frac{T}{2\pi i(T-i)}}\left(\frac{T}{i}\right)^i\left(\frac{T}{T-i}\right)^{T-i}$$

□

Asymptotic Expansion for Categorical

Consider the k-outcome categorical model $\Theta = \triangle_k$ with $p_\theta = \theta$.
Bernoulli is the case $k = 2$

Theorem

$$\mathcal{V}_T(\Theta) \;=\; \frac{k-1}{2} \ln \frac{T}{2\pi} + \ln \frac{\Gamma(1/2)^k}{\Gamma(k/2)} + o(1)$$

Proof.
See reading material □

Asymptotic Expansion for i.i.d. Classes

NB: This is **just for context**

Theorem

Consider any "suitably regular" model $\Theta \subseteq \mathbb{R}^k$ of i.i.d. predictors. Then

$$\mathcal{V}_T(\Theta) \;=\; \frac{k}{2} \ln \frac{T}{2\pi} + \log \int \sqrt{\det I(\theta)}\, \mathrm{d}\theta + o(1)$$

where $I(\theta)$ is the Fisher information matrix (Hessian of negative entropy)

$$I(\theta) \;=\; \mathop{\mathbb{E}}_{Y \sim p_\theta} \left[\nabla_\theta^2 \ln p_\theta(Y) \right].$$

Bayesian Predictors

Idea

For finite classes Θ, we saw that AA reduces to a Bayesian mixture.

Do Bayesian mixtures also control the regret for infinite Θ?

For example, what about Bernoulli? How good is e.g. the uniform average

$$p(y^T) = \int_0^1 p_\theta(y^T)\, \mathrm{d}\theta$$

Uniform Average aka Laplace Mixture

Theorem

The uniform average predictor has predictions

$$p_t(1|y^{t-1}) \;=\; \frac{n_1(y^{t-1})+1}{t+1}$$

and worst-case regret equal to

$$\max_{y^T} \mathit{Regret} \;=\; \ln(T+1)$$

About twice $\mathcal{V}_T(\Theta)$ ...

Jeffreys' Average

Jeffreys proposed (based on invariance considerations) the prior

$$p(\theta) \;=\; \frac{1}{\pi\sqrt{\theta(1-\theta)}}$$

Theorem

The Jeffreys predictor is equivalent to the Krichevsky-Trofimoff predictor

$$p_t(1|y^{t-1}) \;=\; \frac{n_1(y^{t-1}) + 1/2}{t}$$

and has worst-case regret equal to

$$\max_{y^T} Regret \;\leq\; \frac{1}{2}\ln(T) + \ln 2$$

Matches $\mathcal{V}_T(\Theta)$ up to lower-order constant.

General Bayesian Mixures

NB: **this is just for context**

For a general model, Jeffreys' prior is

$$p(\theta) = \frac{\sqrt{\det I(\theta)}}{\int \sqrt{\det I(\theta)}\, \mathrm{d}\theta}$$

Where $I(\theta)$ is the Fisher Information matrix.

Theorem

Consider a suitably regular i.i.d. $\Theta \subseteq \mathbb{R}^k$. The worst-case regret of Bayesian model averaging with Jeffreys' prior is

$$\max_{y^T} Regret = \frac{k}{2} \ln \frac{T}{2\pi} + \log \int \sqrt{\det I(\theta)}\, \mathrm{d}\theta + o(1)$$

Equal to minimax regret $\mathcal{V}(\Theta)$ up to $o(1)$.

Practice: Bayesian methods easier to interpret/compute than minimax.

Applications

Markov Models

kth order Markov model can be summarised by a table

context	prediction
00	θ_{00}
01	θ_{01}
10	θ_{10}
11	θ_{11}

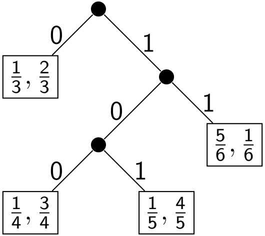
In context x, assign probability θ_x to seeing outcome 1 next.

$$0\ 1\ 0\ 1\ 0\ 0\ 1\ 0\ 1\ 0\ 1\ 0\ 1\ \underbrace{0\ 1}_{\text{context}}\ ?$$

2^k parameters.

Bayesian average can be maintained efficiently. Regret is about $2^{k-1} \ln T$.

Application: Context Tree Weighting (CTW)



To predict next symbol: look up context right-to-left from root, use leaf dist.

$$\overbrace{0\ 1\ 1\ 0\ 1\ \underbrace{0\ 0\ 1}_{\text{used}}}^{\text{context}}\ ? \qquad \Rightarrow \qquad \underbrace{\tfrac{1}{4}, \tfrac{3}{4}}_{\text{prediction}}$$

- 2^{k+1} parameters for maximum context length k.
- $O(k)$ per round implementation of Bayesian model average over all context tree predictors
- Excellent data compression performance.

Conclusion

- Prediction with log loss has elegant exact minimax solution: **normalized maximum likelihood**
- **Bayesian mixtures** (version of AA) with carefully selected priors can often match the minimax regret
- Can tackle complex models with (hierarchical) Bayesian mixtures