Offline to Online Conversion

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Abstract

I consider the problem of converting offline estimators into an online predictor or estimator with small extra regret. Formally this is the problem of merging a collection of probability measures over strings of length 1,2,3,... into a single probability measure over infinite sequences. I describe various approaches and their pros and cons on various examples. As a side-result I give an elementary non-heuristic purely combinatoric derivation of Turing's famous estimator. My main technical contribution is to determine the computational complexity of online estimators with good guarantees in general.

Keywords: offline, online, batch, sequential, probability, estimation, prediction, time-consistency, tractable, regret, combinatorics, Bayes, Laplace, Ristad, Good-Turing.

Contents

- Introduce and discuss the problem of converting offline estimators (q_n) to an online predictor q̃.
- Define the worst-case extra regret R_n of online \tilde{q} over offline (q_n) estimator, measuring the conversion quality.
- Compare and discuss the pros and cons of four offline-to-online conversion proposals (rat,n1,lim,mix).
- Illustrate their behavior for various classical estimators (Bayes, MDL, Laplace, Good-Turing, Ristad)
- Computational complexity of online estimators with good guarantee.
- Open problems regarding efficient low-regret online estimators.
- Simple and non-heuristic derivation of the famous Good-Turing estimator.

PROBLEM FORMULATION

Problem Formulation (Online=TC=Norm)

Notation: $x_{t:n} := x_t...x_n \in \mathcal{X}^{n-t+1}$, $x_{< n} := x_1...x_{n-1}$, $x_{1:0} = x_{<1} = \epsilon$. Formulation 1 (measures)

- Given: Probability measures Q_n on \mathcal{X}^n for n = 1, 2, 3, ...

Formulation 2 (probability mass function for finite \mathcal{X})

- Given: Prob. mass functions $q_n : \mathcal{X}^n \to [0; 1]$, i.e. $\sum_{x_{1:n}} q_n(x_{1:n}) = 1$.
- Seeked: Time-consistent (TC) fct. $\tilde{q} : \mathcal{X}^* \to [0; 1]$ with $\sum_{x_n} \tilde{q}(x_{1:n}) = \tilde{q}(x_{< n}) \ \forall n, x_{< n} \text{ and } \tilde{q}(\epsilon) = 1$ close to q_n i.e. $\tilde{q}(x_{1:n}) \approx q_n(x_{1:n})$ for all n and $x_{1:n}$.

Formulation 3 (predictors)

• Seeked: Normalized (Norm) predictor $\tilde{q} : \mathcal{X} \times \mathcal{X}^* \to [0; 1]$ with

 $\sum_{x_n} \tilde{q}(x_n | x_{< n}) = 1 \quad \forall n, x_{< n} \text{ such that its joint probability} \\ \tilde{q}(x_{1:n}) := \prod_{t=1}^n \tilde{q}(x_t | x_{< t}) \text{ is close to } q_n \text{ as before.}$

Discussion: $\tilde{q}(x_{1:n})$ is prob. that an (infinite) sequence starts with $x_{1:n}$. $\tilde{q}(x_n|x_{< n}) \equiv \tilde{q}(x_{1:n})/\tilde{q}(x_{< n})$ is the probability that x_n follows given $x_{< n}$.

Example Applications

- (i) To use an offline estimator (q_n) to make stochastic predictions we need to expand and normalize it.
- (ii) Maximum likelihood estimation $\hat{\theta}_n$ of parameter $\theta \in \Theta$ leads to offline estimator $(q_n) := (q^{\hat{\theta}_n})$ even if q^{θ} was online for all θ .
- (iii) Arithmetic coding requires an online estimator, but is often based on a class of distributions as described in (ii).
- (iv) Computing the cumulative distribution function $\sum_{y_{1:n} \le x_{1:n}} q_n(y_{1:n})$ can be hard for an offline estimator, but fast=O(n) if (q_n) is (converted to) online.

Performance/Distance Measure

Natural measure of distance of \tilde{q} from q_n : Worst-case log-loss regret:

$$R_n \equiv R_n(\tilde{q}) \equiv R_n(\tilde{q}||q_n) := \max_{x_{1:n}} \ln \frac{q_n(x_{1:n})}{\tilde{q}(x_{1:n})}$$

Properties:

- Quantifies $\tilde{q} \approx q_n$.
- $R_n \ge 0$, and $R_n = 0$ iff $\tilde{q}_{|\mathcal{X}^n} = q_n$.
- Online arithmetic code of x_{1:n} w.r.t. q̃ has length |log₂ q̃(x_{1:n})|.
 Offline Huffman code for x_{1:n} w.r.t. q_n has code length |log₂ q_n(x_{1:n})|.

$$\implies$$
 $CL^{online}(x_{1:n}) - CL^{offline}(x_{1:n}) \leq R_n \ln 2$

Plenty of alternatives: E.g. $KL(q_n||\tilde{q}) \leq R_n \geq KL(\tilde{q}||q_n)$ not considered.

Extending q_s from \mathcal{X}^s to \mathcal{X}^∞

It is always possible to choose $\tilde{q} := \bar{q}_s$ such that $R_s = 0$ for some $s \in \mathbb{N}_0$

(but $R_n > 0$ for $n \neq s \implies$ naive minimization of R_n w.r.t. \tilde{q} fails)

$$ar{q}_s(x_{1:n}) := \left\{egin{array}{ccc} q_s(x_{1:s}) & ext{if} & n=s, \ \sum_{x_{n+1:s}} q_s(x_{1:s}) & ext{if} & ns \end{array}
ight.$$

Q can be an arbitrary measure on \mathcal{X}^{∞} , e.g. uniform $Q(x_{s+1:n}|x_{1:s}) = |\mathcal{X}|^{n-s}$

I now consider four methods of converting offline estimators to online predictors ...

CONVERSION METHODS

Naive Ratio \tilde{q}^{rat}

The simplest way to define a predictor \tilde{q} from q_n is via Ratio

$$ilde{q}^{\mathsf{rat}}(x_t|x_{< t}) \ := \ rac{q_t(x_{1:t})}{q_{t-1}(x_{< t})} \quad ext{or equivalently} \quad ilde{q}^{\mathsf{rat}}(x_{1:n}) \ := \ q_n(x_{1:n})$$

Tractable but obviously only works when q_n already is Online.

Otherwise \tilde{q}^{rat} violates TC.

Degree of violation = Normalizer:

$$\mathcal{N}(x_{\le t}) \; := \; \sum_{x_t} ilde{q}^{\mathsf{rat}}(x_t | x_{\le t}) \; \equiv \; rac{\sum_{x_t} q_t(x_{1:t})}{q_{t-1}(x_{\le t})}$$

Naive Normalization \tilde{q}^{n1}

Correct failure of $\tilde{q}^{rat}(x_t|x_{< t})$ to satisfy Norm by Normalization: [Sol78]

$$egin{array}{rll} ilde{q}^{n1}(x_t|x_{< t}) & := & rac{q_t(x_{1:t})}{\sum_{x_t} q_t(x_{1:t})} & \equiv & rac{ ilde{q}^{\operatorname{rat}}(x_t|x_{< t})}{\mathcal{N}(x_{< t})} & ext{and} \ ilde{q}^{n1}(x_{1:n}) & := & \prod_{t=1}^n ilde{q}^{n1}(x_t|x_{< t}) & \equiv & rac{q_n(x_{1:n})}{\prod_{t=1}^n \mathcal{N}(x_{< t})} \end{array}$$

For small \mathcal{X} is still tractable but can result in very large regret $R_n \propto n$.

Express and upper bound regret R_n in terms of Normalizer \mathcal{N} :

$$R_n(\tilde{q}^{n1}) = \max_{x_{1:n}} \sum_{t=1}^n \ln \mathcal{N}(x_{< t}) \leq \sum_{t=1}^n \ln \max_{x_{< t}} \mathcal{N}(x_{< t})$$

If q_n is TC, then $\mathcal{N} \equiv 1$, hence R_n as well as the upper bound are $\equiv 0$.

Limit \tilde{q}^{lim}

Since $R_s(\bar{q}_s) = 0$ for any fixed s, a natural idea is taking the Limit

$$\tilde{q}^{\lim}(x_{1:n}) := \lim_{s \to \infty} \bar{q}_s(x_{1:n}) = \lim_{s \to \infty} \sum_{x_{n+1:s}} q_s(x_{1:s})$$

in the hope to make $\lim_{s\to\infty} R_s = 0$.

Effectively what \tilde{q}^{lim} does is to use q_s for very large s also for short strings of length n by marginalization.

Problems are plenty:

- The limit may not exist,
- may exist but be incomputable,
- R_n may be hard to impossible to compute or upper bound,
- and even if the limit exists, \tilde{q}^{lim} may perform badly.

Mixture \tilde{q}^{mix}

Take Bayesian Mixture over the class $\{\bar{q}_1, \bar{q}_2, ...\}$ of all \bar{q}_s [San06]

$$ilde{q}^{\mathsf{mix}}(x_{1:n}) := \sum_{s=0}^{\infty} \overline{q}_s(x_{1:n}) w_s$$
 with prior $w_s > 0$, $\sum_{s=0}^{\infty} w_s = 1$.

 \tilde{q}^{mix} is TC and its regret can easily be upper bounded:

$$R_n(\tilde{q}^{\min}) = \max_{x_{1:n}} \ln \frac{q_n(x_{1:n})}{\sum_{s=0}^{\infty} \bar{q}_s(x_{1:n}) w_s} \le \max_{x_{1:n}} \ln \frac{q_n(x_{1:n})}{\bar{q}_n(x_{1:n}) w_n} = \ln w_n^{-1}$$

For e.g. $w_n := \frac{1}{(n+1)(n+2)}$ we have $\ln w_n^{-1} \le 2 \ln(n+2) =$ small.

Conclusion: **Any** offline estimator can be converted into an online predictor with very small extra regret.

Problem: How convert this heavy construction into an efficient algorithm?

Variations: $Q \equiv 0$ -or- sparser w_n .

[San06]

EXAMPLES

Examples by Category

Class of Probabilities (ML/MAP/MDL/NML/Bayes):

Start with a class *M* of probability measures ν on *X*[∞] in the hope one of them is good.

Combinatorial (Uniform,Laplace,Good-Turing,Ristad):

• Assigns uniform probabilities over subsets of \mathcal{X}^n .

Exponentiated Code Length:

not further discussed

Bayes

The Bayesian mixture over \mathcal{M} w.r.t. some prior (density) w() is

$$q_n(x_{1:n}) := \int_{\mathcal{M}} \nu(x_{1:n}) w(\nu) d\nu$$

 $q_n \text{ is TC} \implies (q_n^{\mathsf{rat}}) \equiv (q_n^{\mathsf{n1}}) \equiv (q_n^{\mathsf{lim}}) \equiv \tilde{q} \implies R_n = 0.$

 $\tilde{q}^{\rm rat}$ is tractable if the Bayes mixture is.

Assume the true sampling distribution μ is in \mathcal{M} :

For countable \mathcal{M} and counting measure $d\nu$, we have $q_n(x_{1:n}) \geq \mu(x_{1:n})w(\mu)$, hence $R_n^{\text{online}} = R_n^{\text{offline}} \leq \ln w(\mu)^{-1}$.

For continuous classes \mathcal{M} under mild conditions: $R_n^{\text{online}} = R_n^{\text{offline}} \lesssim \ln w(\mu)^{-1} + O(\ln n).$ [BC91, Hut03, ?, RH07]

16 / 30

ML/MAP/MDL/NML/MML

$$\begin{aligned} \mathsf{MAP}=\mathsf{MDL} \text{ estimator:} \quad \hat{q}_n(x_{1:n}) &:= \sup_{\nu \in \mathcal{M}} \{\nu(x_{1:n}) w(\nu)\} \\ \mathsf{NML} \text{ estimator:} \quad q_n(x_{1:n}) &:= \frac{\hat{q}_n(x_{1:n})}{\sum_{x_{1:n}} \hat{q}_n(x_{1:n})} \end{aligned}$$

Since \hat{q}_n is not even a probability on \mathcal{X}^n , we have to normalize it to q_n (ML/NML).

Unlike Bayes, q_n is not TC, causing various complications. [Grü07, Hut09]

Crude MDL: $q_n := \arg \max_{\nu \in \mathcal{M}} \{\nu(x_{1:n}) w(\nu)\}$ is a probability measure on \mathcal{X}^{∞} for each *n*, but also not TC. [PH05]

Uniform

• The uniform probability $q_n(x_{1:n}) := |\mathcal{X}|^{-n}$ is TC

 \implies all four \tilde{q} coincide and $R_n = 0 \forall n$.

- Lousy estimator, since predictor $\tilde{q}(x_t|x_{< t}) = 1/|\mathcal{X}|$ is indifferent and ignores all evidence $x_{< t}$ to the contrary.
- Improvement: Partition the sample space (here \mathcal{X}^n) and assign uniform probabilities to and within each partition.
- The Laplace rule can be derived that way, and the Good-Turing and Ristad estimators by further sub-partitioning.

Laplace (Double Uniform)

- $n_i := |\{t : x_t = i\}|$ is number of times, symbol $i \in \mathcal{X} = \{1, ..., d\}$ appears in $x_{1:n}$.
- Assign uniform probability to all sequences $x_{1:n}$ with the same counts $\mathbf{n} := (n_1, ..., n_d)$, therefore $q_n(x_{1:n}|\mathbf{n}) = {n \choose n_1...n_d}^{-1}$.
- Assign uniform probability to the counts **n** themselves, therefore $q_n(\mathbf{n}) = |\{\mathbf{n} : n_1 + ... + n_d = n\}|^{-1} = \binom{n+d-1}{d-1}^{-1}$.
- Together

$$q_n(x_{1:n}) = {\binom{n}{n_1 \dots n_d}}^{-1} {\binom{n+d-1}{d-1}}^{-1} = {\binom{n+d-1}{n_1 \dots n_d \ d-1}}^{-1}$$

$$\implies \tilde{q}^{rat}(x_{n+1} = i | x_{1:n}) = \frac{q_{n+1}(x_{1:n}i)}{q_n(x_{1:n})} = \frac{n_i + 1}{n+d}$$

- Is properly normalized (Norm), so \tilde{q}^{rat} is TC.
- $(q_n^{\text{rat}}) \equiv (q_n^{\text{n1}}) \equiv (q_n^{\text{lim}})$ coincide with \tilde{q} and $R_n = 0$.
- \tilde{q}^{rat} is nothing but Laplace's famous rule.

Good-Turing (Triple Uniform)

- $M_r := \{i : n_i = r\}$ = symbols that appear exactly $r \in \mathbb{N}_0$ times in $x_{1:n}$, and $m_r := |M_r|$ is their number.
- Assign 3× uniform probabilities: (i) $q_n(x_{1:n}|\mathbf{n}) := {\binom{n}{n_1...n_d}}^{-1}$ (as for Laplace) (ii) $q_n(\mathbf{n}|\mathbf{m}) := {\binom{d}{m_0...m_n}}^{-1}$, where $\mathbf{m} := (m_0, ..., m_n)$ (iii) $q_n(\mathbf{m}) := \operatorname{Part}(n)^{-1} = (\# \text{integer partitions of } n)^{-1}$
- Together: $q_n(x_{1:n}) = {n \choose n_1 \dots n_d}^{-1} {d \choose m_0 \dots m_n}^{-1} \operatorname{Part}(n)^{-1}$ is not TC.
- Normalization: $\tilde{q}^{n1}(x_{n+1} = i | x_{1:n}) = \frac{1}{N_n} \cdot \frac{r+1}{n+1} \cdot \frac{m_{r+1}+1}{m_r}$ $[r = n_i]$ $\mathcal{N}_n := \frac{1}{n+1} \sum_{r=0, m_r \neq 0}^n (r+1)(m_{r+1}+1)$
- Is very interesting predictor: $\frac{r+1}{n+1}$ is Laplace is estimate. $\frac{m_{r+1}+1}{m_r}$ is close to the Good-Turing (GT) correction $\frac{m_{r+1}}{m_r}$. [Goo53]

Good-Turing (Triple Uniform)

Worst-case regret of GT is very large: $R_n(\tilde{q}^{n1}||q_n) = n \ln 2 \pm O(\sqrt{n})$

 \implies Naive norm. severely harms the offline triple uniform estimator q_n

- Heuristic smoothing of the function m₍₎ leads to excellent estimators in practice, [Goo53]
 e.g. Kneser-Ney smoothing for text data. [CG99]
- \tilde{q}^{mix} may be regarded as an (unusual) kind of smoothing with the strong guarantee $R_n \leq 2\ln(n+2)$

[San06]

Ristad (Quadrupel Uniform)

- Motivation: If X is the set of English words and x_{1:n} some typical English text, then most symbols=words will not appear.
- \implies Laplace assigns not enough probability $\left(\frac{n_i+1}{n+d} \ll \frac{n_i}{n}\right)$ to observed words.
 - Rectification: Treat symbols A := {i : n_i > 0} that do appear different from symbols X \ A that don't:

(i) $x_{1:n}$ may contain *m* different symbols, so $q_n(m) := 1/\min\{n, d\}$ (ii) Choose uniformly which $m \equiv |\mathcal{A}|$ symbols appear: $q_n(\mathcal{A}|m) := {\binom{d}{m}}^{-1}$ (iii) Choose counts \mathbf{n} $(n_i > 0 \Leftrightarrow i \in \mathcal{A})$ uniformly: $q_n(\mathbf{n}|\mathcal{A}) = {\binom{n-1}{m-1}}^{-1}$ (iv) Finally, $q_n(x_{1:n}|\mathbf{n}) = {\binom{n}{n_1...n_d}}^{-1}$ as for Laplace.

• Together: $q_n(x_{1:n}) = {n \choose n_1 \dots n_d}^{-1} {n-1 \choose m-1}^{-1} {d \choose m}^{-1} \frac{1}{\min\{n,d\}}$ is not TC

22 / 30

Ristad (Quadrupel Uniform)

Normalization:

$$\tilde{q}^{n1}(x_{n+1} = i | x_{1:n}) = \begin{cases} \frac{(n_i+1)(n-m+1)}{n(n+1)+2m} & \text{if } n_i > 0 \text{ and } m < d \\ \frac{m(m+1)}{n(n+1)+2m} \cdot \frac{1}{d-m} & \text{if } n_i = 0 \\ \frac{n_i+1}{n+m} & \text{if } m = d \quad [\Rightarrow n_i > 0] \end{cases}$$

Regret of Ristad estimator: $R_n(\tilde{q}^{n1}||q_n) \le 2 \ln n$

- This shows that simple normalization does not ruin performance.
- Indeed, the regret bound is as excellent as that for \tilde{q}^{mix}

COMPUTATIONAL COMPLEXITY

Computability and Complexity of \tilde{q}^{mix}

- From the four discussed online estimators only q̃^{mix} guarantees small extra regret over offline (q_n),
- Problem: The definition of \tilde{q}^{mix} is quite heavy.
- At least: \tilde{q}^{mix} can be computed in double-exponential time:

Theorem (Computational Complexity of \tilde{q}^{mix})

There is an algorithm A that computes \tilde{q}^{mix} (with uniform choice for Q) to accuracy $|A(x_{1:n},\varepsilon)/\tilde{q}^{mix}(x_{1:n})-1| < \varepsilon$ in time $O(|\mathcal{X}|^{\frac{4}{\varepsilon}|\mathcal{X}|^n})$ for all $\varepsilon > 0$.

Allows us to:

- compute the predictive distribution $\tilde{q}^{\min}(x_t|x_{< t})$ to accuracy ε ,
- ensures that $A(x_{1:n},\varepsilon) > (1-\varepsilon)\tilde{q}_n^{\min}(x_{1:n})$,
- hence $R_n(A(x_{1:n},\varepsilon)||q_n) \leq R_n(\tilde{q}_n^{\min}(x_{1:n})||q_n) + \frac{\varepsilon}{1-\varepsilon}$, and
- approximate normalization $|1 \sum_{x_{1:n}} A(x_{1:n}, \varepsilon)| < \varepsilon$.

Computational Complexity: Definitions

- TIME(g(n)) := all algs that run in time O(g(n)) on inputs of length n
- Algorithms in $E^c := TIME(2^{cn})$ run in exponential time.
- $P := \bigcup_{k=1}^{\infty} \text{TIME}(n^k)$ is the classical class of all algorithms that run in polynomial time (strictly speaking Function-P or FP). [AB09]
- Theorems are stated for binary alphabet $\mathcal{X} = \mathbb{B} = \{0, 1\}$. The generalization to arbitrary finite alphabet is trivial.
- 'For all large *n*' shall mean 'for all but finitely many *n*', denoted $\forall' n$.

Computational Complexity of General \tilde{q}

Theorem (Sub-optimal fast online for fast offline)

$\begin{array}{ll} \textit{For all } r > 0 \textit{ and } c > 0 \textit{ and } \varepsilon > 0 \\ (ii) \quad \exists (q_s) \in P \; \forall \tilde{q} \in E^c : R_n \geq r \ln n \; \forall' n \qquad [e.g. \; large \; c \; and \; r] \\ (iii) \quad \exists (q_s) \in TIME(s^{r+1+\varepsilon}) \; \forall \tilde{q} \in P : R_n \geq r \ln n \; \forall' n \qquad [e.g. \; small \; c, \varepsilon] \\ (iv) \quad \exists (q_s) \in P : \tilde{q}^{mix} \notin E^c \qquad [from \; (ii) \; and \; R_n(\tilde{q}^{mix}) < 3 \ln n] \end{array}$

- (iii) implies that there is an offline estimator (q_s) computable in quartic time s^4 on a RAM for which no polynomial-time online estimator \tilde{q} is as good as \tilde{q}^{mix} .
- The slower (q_s) we admit (larger r), the higher the lower bound gets.
- (ii) says that even algorithms for *q̃* running in exponential time 2^{cn} cannot achieve logarithmic regret for all (*q_s*) ∈ P.
- In particular this implies that (iv) any algorithm for q̃^{mix} requires super-exponential time for some (q_s) ∈ P on some arguments.

Marcus Hutter

Computational Complexity of General \tilde{q}

- TIME^o(g(n)) := all algs with oracle access that run in time O(g(n))
- Each oracle call is counted only as one step. Similarly P^o and $E^{c,o}$.

Theorem (Very poor fast online using offline oracle)

 $\forall \varepsilon > 0 \ \exists o \equiv (q_s) \in E^1 \ \forall \tilde{q}^o \in E^{\varepsilon/2,o} : R_n(\tilde{q}^o || q_n) \ge (1-\varepsilon)n \ln 2 \ \forall' n$ Or cruder: $\forall \varepsilon > 0 \ \exists o \equiv (q_s) \ \forall \tilde{q}^o \in P^o : R_n(\tilde{q}^o || q_n) \ge (1-\varepsilon)n \ln 2 \ \forall' n$

- Strength: It rules out even very modest demands on R_n: Trivial R_n ≤ n ln 2 unimprovable by a fast q̃^o with (only) oracle access.
- Weakness: Only applies to online q̃ using (q_s) as a black box oracle. That is, q̃^o(x_{1:n}) can call q_s(z_{1:s}) for any s and z_{1:s} and receives the correct answer.

Open Problems

Open Problem (Fast online from offline with small extra regret)

Can every polynomial-time offline estimator (q_n) be converted to a polynomial-time online estimator \tilde{q} with small regret $R_n(\tilde{q}||q_n) \le \sqrt{n} \forall' n$? Or weaker: $\forall (q_n) \in P \exists \tilde{q} \in P : R_n = o(n)$? Or stronger: $R_n = O(logn)^2$?

- Would reduce finding good online estimators to the apparently easier problem of finding good offline estimators.
- For specific offline (q_n) , does there exist efficient \tilde{q} with small R_n ?
- A tractable smoothing of the GT estimator with $R_n = O(\ln n)$.
- Are there offline estimators of practical relevance (such as GT) for which no fast online estimator can achieve logarithmic regret?
- Weaken notion of regret to e.g. expected regret $\mathbb{E}[\ln(q_n/\tilde{q})]$.
- Is $R_n = O(\ln n)$ the best one can achieve in general.
- Devise general techniques to upper bound $R_n(\tilde{q}^{n1}||q_n)$.

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