Missing Mass, and Optimal Discovery

based on a joint work with Sébastien Bubeck and Damien Ernst

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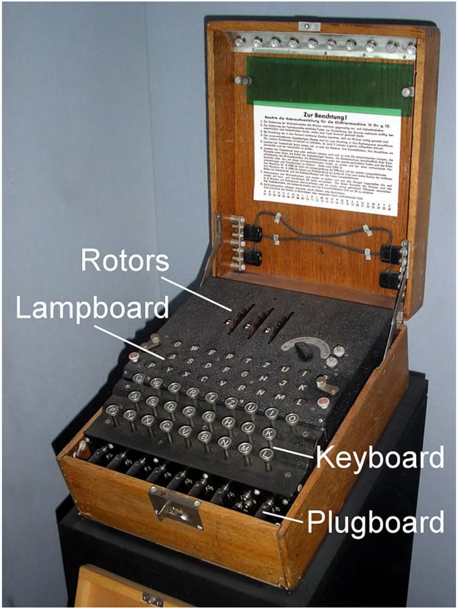
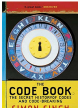
Estimating the Unseen

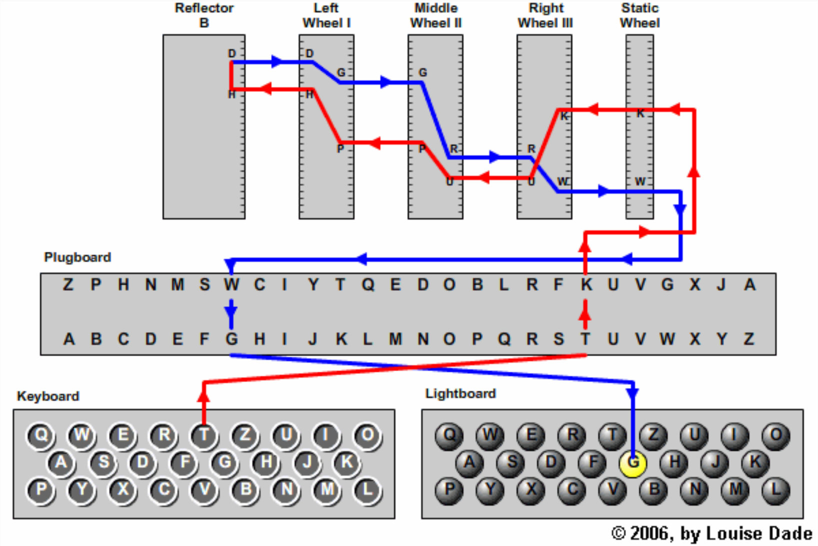
Enigma



- Electro-mechanical rotor cipher machines, 26 characters
- Invented at the end of WW1 by Arthur Scherbius
- Commercial use, then German Army during WW2
- First cracked by Marian Rejewski in the 1930s (Bomb), then improved to 3.10^{114} configurations
- Read Simon Singh, *The Code Book*

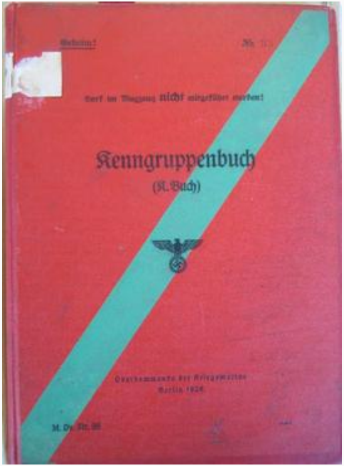


Enigma



Src: `http://enigma.louisedade.co.uk/`

Battle of the Atlantic



- Massively used by the German Kriegsmarine and Luftwaffe
- weakness: 3-letters setting to initiate communication, taken from the *Kenngruppenbuch*
- Government Code and Cypher School: Bletchley Park (on the train line between Cambridge and Oxford)
- Colossus (first programmable computers) in 1943

Estimating probabilities

- Discrete alphabet A.
- Unknown probability P on A
- Sample $X_1, \dots, X_n$ of independent draws of P.
- Goal : use the sample estimate $P(a)$ for all $a \in A$.

Natural idea:

$$\hat{P}(a) = \frac{N(a)}{n}, \quad \text{where } N(a) = \#\{i : X_i = a\}$$

Safari preparation

Observe animal sample

1 giraffe, 2 elephants, 3 zebras

Probability estimation?

Empirical frequency

Species	Probability
giraffes	1/6
elephants	2/6
zebras	3/6

Problem?

[Src: Alon Orlitsky, https://ic.epfl.ch/files/content/sites/ic/files/Inka/Orlitsky%20Talk%202016.pdf]

Bigram Model for NLP

[Src: https://nlp.stanford.edu/~wcmac]

Learning set:

john read moby dick

mary read a different book

she read a book by cher

$$P(w_i|w_{i-1}) = \frac{c(w_{i-1}w_i)}{\sum_w c(w_{i-1}w)}$$

$$P(s) = \prod_{i=1}^{l+1} p(w_i|w_{i-1})$$

$$\begin{array}{cccccc}
P(& john & read & a & book &) \\
= & P(john|\cdot) & P(read|john) & P(a|read) & P(book|a) & P(\cdot|book) \\
= & \frac{c(\cdot\ john)}{\sum_w c(\cdot\ w)} & \frac{c(john\ read)}{\sum_w c(john\ w)} & \frac{c(reada)}{\sum_w c(read\ w)} & \frac{c(a\ book)}{\sum_w c(a\ w)} & \frac{c(book\ \cdot)}{\sum_w c(book\ w)} \\
= & \frac{1}{3} & \frac{1}{1} & \frac{2}{3} & \frac{1}{2} & \frac{1}{2} \\
\approx & 0.06 & & & &
\end{array}$$

Bigram Model for NLP

[Src: `https://nlp.stanford.edu/~wcmac`]

Learning set:

john read moby dick

mary read a different book

she read a book by cher

$$P(w_i|w_{i-1}) = \frac{c(w_{i-1}w_i)}{\sum_w c(w_{i-1}w)}$$

$$P(s) = \prod_{i=1}^{l+1} p(w_i|w_{i-1})$$

$$\begin{array}{cccccc}
P(& cher & read & a & book &) \\
= & P(cher|\cdot) & P(read|john) & P(a|read) & P(book|a) & P(\cdot|book) \\
= & \frac{c(\cdot\ cher)}{\sum_w c(\cdot\ w)} & \frac{c(cher\ read)}{\sum_w c(cher\ w)} & \frac{c(reada)}{\sum_w c(read\ w)} & \frac{c(a\ book)}{\sum_w c(a\ w)} & \frac{c(book\ \cdot)}{\sum_w c(book\ w)} \\
= & \frac{0}{3} & \frac{0}{1} & \frac{2}{3} & \frac{1}{2} & \frac{1}{2} \\
= & 0 & & & &
\end{array}$$

$\Longrightarrow$ useless, the unseen **must** be treated correctly.

Bayesian Approach: Laplace Estimator

Pierre-Simon de Laplace (1749-1827), Thomas Bayes (1702-1761)

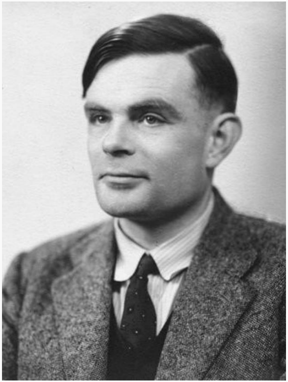
Will the sun rise tomorrow?

$$\hat{P}(a) = \frac{N(a) + 1}{n + |A|}$$

- good for small alphabets and many samples
- very bad when lots of items seen once (ex: DNA sequences)
- $|A|$ can be very large (or even infinite), but P concentrated on few items

$\Longrightarrow$ not a satisfying solution to the problem

Alan Turing



1912-1954

student of Godfrey Harold Hardy in Cambridge

PhD from Princeton with Alonzo Church

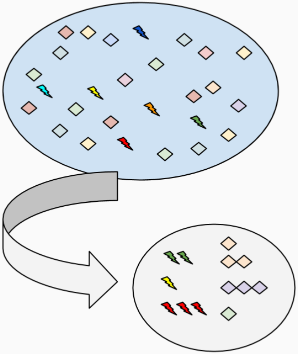
Irving John Good

1916-2009

Graduated in Cambridge

Academic carrer in Bayesian statistics in Manchester and then in the University of Virginia (USA)

Missing mass estimation



$X_1, \ldots, X_n$ independent draws of $P \in \mathfrak{M}_1(A)$.

$$O_n(x) = \sum_{m=1}^{n} \mathbb{1}\{X_m = x\}$$

How to 'estimate' the total mass of the *unseen* items

$$R_n = \sum_{x \in A} P(x)\, \mathbb{1}\{O_n(x) = 0\} \text{ ?}$$

The Good-Turing Estimator

See [I.J. Good, 1953], credits idea to A. Turing

Idea: in order to estimate the mass of the unseen

$$R_n = \sum_{x \in A} P(x) \, \mathbb{1}\{O_n(x) = 0\} ,$$

use the number of **hapaxes** = items seen only once (linguistic)

$$\hat{R}_n = \frac{U_n}{n}, \quad \text{where } U_n = \sum_{x \in A} \mathbb{1}\{O_n(x) = 1\}$$

Lemma [Good '53]: For *every* distribution P,

$$0 \leq \mathbb{E}\big[\hat{R}_n\big] - \mathbb{E}\big[R_n\big] \leq \frac{1}{n}$$

Completely non-parametric: no assumption on P

Bias of the Good-Turing Estimator

$$
\begin{aligned}
\mathbb{E}\big[\hat{R}_n\big] - \mathbb{E}\big[R_n\big] &= \frac{1}{n} \sum_{x \in A} \mathbb{P}\big(O_n(x) = 1\big) - \sum_{x \in A} P(x)\, \mathbb{P}\big(O_n(x) = 0\big) \\
&= \frac{1}{n} \sum_{x \in A} n\, P(x)\big(1 - P(x)\big)^{n-1} - \sum_{x \in A} P(x)\big(1 - P(x)\big)^{n} \\
&= \sum_{x \in A} P(x)\big(1 - P(x)\big)^{n-1} \Big(1 - \big(1 - P(x)\big)\Big) \\
&= \frac{1}{n} \sum_{x \in A} P(x) \times n\, P(x)\big(1 - P(x)\big)^{n-1} \\
&= \frac{1}{n} \sum_{x \in A} P(x)\, \mathbb{P}\big(O_n(x) = 1\big) \\
&= \frac{1}{n}\, \mathbb{E}\left[\sum_{x \in A} P(x) \mathbb{1}\{O_n(x) = 1\}\right] \quad \in \left[0, \frac{1}{n}\right]
\end{aligned}
$$

Jackknife interpretation

If we had additionnal samples, we would estimate R_n by the proportion of unseen elements in $X_{n+1}, X_{n+2}, \ldots$

We have no additionnal samples, **but** we keep every observation as a "test", pretending that the samples was made of everything else:

$$\begin{aligned}
\hat{R}_n &= \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}\left\{x_i \notin \{x_j : j \neq i\}\right\} \\
&= \frac{1}{n}\sum_{i=1} \mathbb{1}\left\{O_n(x_i) = 1\right\} \\
&= \frac{1}{n}\sum_{x\in A} \mathbb{1}\left\{O_n(x) = 1\right\}
\end{aligned}$$

Remark: jackknife is a **resampling method**, related to **bootstrap** and **crossvalidation** (of great use in Machine Learning).

Deviation Bounds

Proposition: With probability at least $1-\delta$ for *every* P,

$$\hat{R}_n - \frac{1}{n} - (1+\sqrt{2})\sqrt{\frac{\log(4/\delta)}{n}} \leq R_n \leq \hat{R}_n + (1+\sqrt{2})\sqrt{\frac{\log(4/\delta)}{n}}$$

See [McAllester and Schapire '00, McAllester and Ortiz '03]:

- deviations of $\hat{R}_n$: McDiarmid's inequality
- deviations of R_n: negative association

Other tool: Poissonization [see Optimal Probability Estimation with Applications to Prediction and Classification, by Acharya, Jafarpour, Orlitsky Suresh, Colt 2013]

Application to Classification: minimax optimality

[Optimal Probability Estimation with Applications to Prediction and Classification, by Acharya, Jafarpour, Orlitsky Suresh, Colt 2013]

- P_1, P_2 probability distributions on A
- Given: two samples $(X_1^1, \dots, X_n^1)$ of P_1 and $(X_1^2, \dots, X_n^2)$ of P_2
- Goal: if $I = 1, 2$ with probability $1/2$ and if $X \sim P_I$, build a classifier $\phi_n : A \to \{1, 2\}$ so that $P\big(\phi_n(X) = I\big)\big)$ is as large as possible
- Maximal risk :

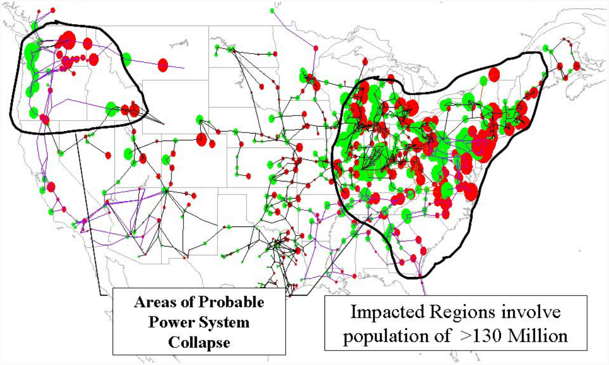
$$\bar{R}_n(\phi) = \max_{P_1, P_2} \mathbb{P}\big(\phi(X) \neq I\big)\big)$$

- **Prop**: if $\phi_n^{\mathrm{ML}}(x) = \arg\max_i \#\big\{j : X_j^i = x\big\}$ then there exists $c > 0$ such that for all $n \geq 1$, $\quad \bar{R}_n(\phi_n^{\mathrm{ML}}) \geq \min_\phi R_n(\phi) + c$.
- **Theorem**: there exists a Good-Turing based classifier ϕ_n^{GT} such that for all $n \geq 1$, $\quad \bar{R}_n(\phi_n^{\mathrm{GT}}) \leq \min_\phi R_n(\phi) + O\big(n^{-1/5}\big)$.

Discovering dangerous contigencies in electrical systems

The problem

Power system security assessment

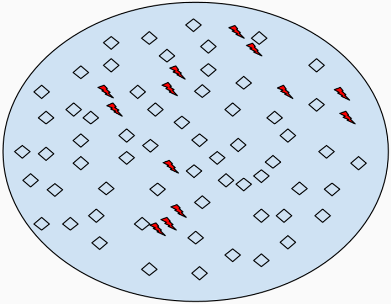


By Mark MacAlester, Federal Emergency Management Agency [Public domain], via Wikimedia Commons

Damien Ernst (Electrical Engineering, Liège): How to identify quickly contingencies/scenarios that could lead to unacceptable operating conditions (dangerous contingencies) if no preventive actions were taken?

The model

- Subset $A \subset \mathcal{X}$ of important items
- $|\mathcal{X}| \gg 1$, $|A| \ll |\mathcal{X}|$
- Access to $\mathcal{X}$ only by probabilistic experts $(P_i)_{1 \leq i \leq K}$: sequential independent draws



Goal: discover rapidly the elements of A

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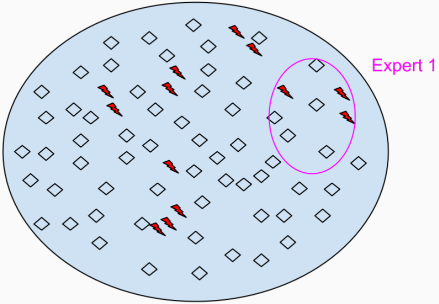

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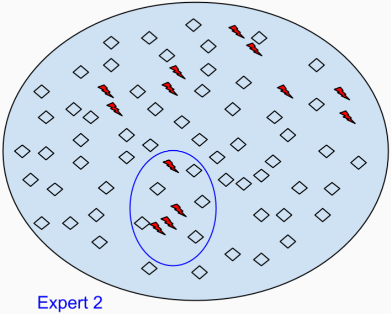

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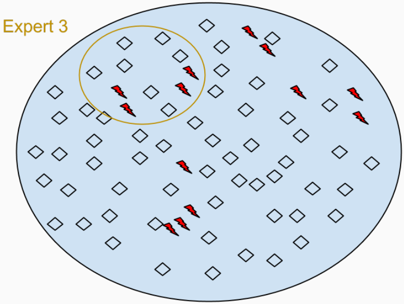

Goal: discover rapidly the elements of A

Goal

At each time step $t = 1, 2, \ldots$:

- pick an index $I_t = \pi_t\big(I_1, Y_1, \ldots, I_{s-1}, Y_{s-1}\big) \in \{1, \ldots, K\}$ according to past observations
- observe $Y_t = X_{I_t, n_{I_t,t}} \sim P_{I_t}$, where

$$n_{i,t} = \sum_{s \leq t} \mathbb{1}\{I_s = i\}$$

Goal: design the strategy $\pi = (\pi_t)_t$ so as to maximize the number of important items found after t requests

$$F^\pi(t) = \Big| A \cap \big\{ Y_1, \ldots, Y_t \big\} \Big|$$

Assumption: non-intersecting supports

$$A \cap \mathrm{supp}(P_i) \cap \mathrm{supp}(P_j) = \emptyset \text{ for } i \neq j$$

Is it a Bandit Problem ?

It looks like a bandit problem…

- sequential choices among K options
- want to maximize cumulative rewards
- exploration vs exploitation dilemma

… but it is **not a bandit problem** !

- rewards are not i.i.d.
- destructive rewards: no interest to observe twice the same important item
- all strategies eventually equivalent

The oracle strategy

Proposition: Under the non-intersecting support hypothesis, the greedy oracle strategy

$$I_t^* \in \arg\max_{1 \le i \le K} P_i \left(A \setminus \{ Y_1, \dots, Y_t \} \right)$$

is optimal: for every possible strategy π, $\mathbb{E}\big[F^\pi(t)\big] \le \mathbb{E}\big[F^*(t)\big]$.

Remark: the proposition is false if the supports may intersect

$\Longrightarrow$ estimate the "*missing mass* of important items"!

The Good-UCB algorithm

Our solution and analysis

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Optimal Discovery with Probabilistic Expert Advice: Finite Time Analysis and Macroscopic Optimality

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Abstract

We consider an original problem that arises from the issue of security analysis of a power system and that we name optimal discovery with probabilistic expert advice. We address it with an algorithm based on the optimistic paradigm and on the Good-Turing missing mass estimator. We prove two different regret bounds on the performance of this algorithm under weak assumptions on the probabilistic experts. Under more restrictive hypotheses, we also prove a macroscopic optimality result, comparing the algorithm both with an oracle strategy and with uniform sampling. Finally, we provide numerical experiments illustrating these theoretical findings.

Keywords: optimal discovery, probabilistic experts, optimistic algorithm, Good-Turing estimator, UCB

The Good-UCB algorithm

Estimator of the missing important mass for expert i:

$$\hat{R}_{i,n_{i,t-1}} = \frac{1}{n_{i,t-1}} \sum_{x \in A} \mathbb{1}\left\{ \sum_{s=1}^{n_{i,t-1}} \mathbb{1}\{X_{i,s} = x\} = 1 \text{ and } \sum_{j=1}^{K} \sum_{s=1}^{n_{j,t-1}} \mathbb{1}\{X_{j,s} = x\} = 1 \right\}$$

Good-UCB algorithm:

1: For $1 \le t \le K$ choose $I_t = t$.
2: **for** $t \ge K+1$ **do**
3: Choose $I_t = \arg\max_{1 \le i \le K} \left\{ \hat{R}_{i,n_{i,t-1}} + C\sqrt{\frac{\log(4t)}{n_{i,t-1}}} \right\}$
4: Observe Y_t distributed as P_{I_t}
5: Update the missing mass estimates accordingly
6: **end for**

Optimality results

Classical analysis

Theorem: For any $t \geq 1$, *under the non-intersecting support assumption*, Good-UCB (with constant $C = (1+\sqrt{2})\sqrt{3}$) satisfies

$$\mathbb{E}\left[F^*(t) - F^{UCB}(t)\right] \leq 17\sqrt{Kt\log(t)} + 20\sqrt{Kt} + K + K\log(t/K)$$

Remark: Usual result for bandit problem, but not-so-simple analysis

Sketch of proof

1. On a set $\tilde{\Omega}$ of probability at least $1-\sqrt{\frac{K}{t}}$, the "confidence intervals" hold true simultaneously all $u \geq \sqrt{Kt}$
2. Let $\bar{I}_u = \arg\max_{1\leq i\leq K} R_{i,n_{i,u-1}}$. On $\tilde{\Omega}$,

$$R_{I_u,n_{I_u,u-1}} \geq R_{\bar{I}_u,n_{\bar{I}_u,u-1}} - \frac{1}{n_{I_u,u-1}} - 2(1+\sqrt{2})\sqrt{\frac{3\log(4u)}{n_{I_u,u-1}}}$$

3. But one shows that $\mathbb{E}F^*(t) \leq \sum_{u=1}^{t} \mathbb{E}R_{\bar{I}_u,n^{\pi}_{\bar{I}_u,u-1}}$
4. Thus

$$\begin{aligned}
&\mathbb{E}\left[F^*(t) - F^{UCB}(t)\right] \\
&\leq \sqrt{Kt} + \mathbb{E}\left[\sum_{u=1}^{t} \frac{1}{n_{I_u,u-1}} + 2(1+\sqrt{2})\sqrt{\frac{3\log(4t)}{n_{I_u,u-1}}}\right] \\
&\leq \sqrt{Kt} + K + K\log(t/K) + 4(1+\sqrt{2})\sqrt{3Kt\log(4t)}
\end{aligned}$$

Experiment: restoring property

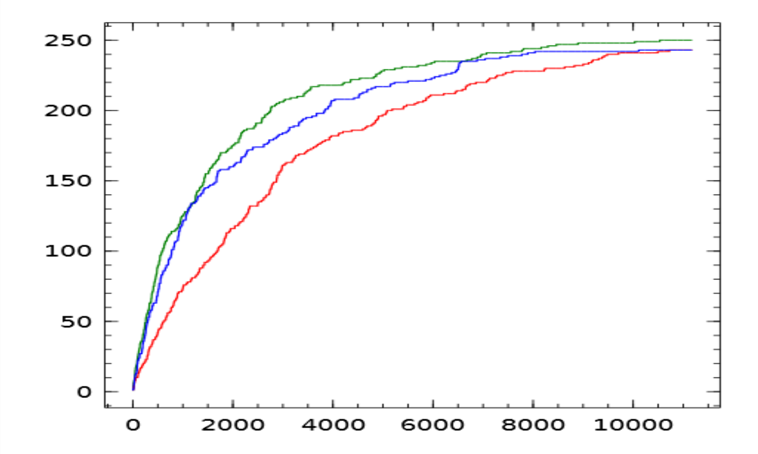


Figure 1: green: oracle, blue: Good-UCB, red: uniform sampling

Another analysis of Good-UCB

For $\lambda \in (0,1)$, $T(\lambda)$ = time at which missing mass of important items is smaller than λ on all experts:

$$T(\lambda) = \inf\left\{t : \forall i \in \{1,\ldots,K\}, P_i\big(A \setminus \{Y_1,\ldots,Y_t\}\big) \le \lambda\right\}$$

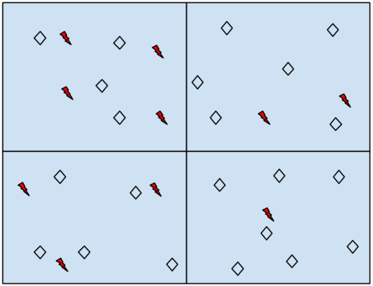
Theorem: Let $c > 0$ and $S \ge 1$. Under the non-intersecting support assumption, for Good-UCB with $C = (1+\sqrt{2})\sqrt{c+2}$, with probability at least $1 - \frac{K}{cS^c}$, for any $\lambda \in (0,1)$,

$$T_{UCB}(\lambda) \le T^* + KS\log\left(8T^* + 16KS\log(KS)\right),$$

$$\text{where} \quad T^* = T^*\left(\lambda - \frac{3}{S} - 2(1+\sqrt{2})\sqrt{\frac{c+2}{S}}\right)$$

The macroscopic limit

- Restricted framework: $P_i = \mathcal{U}\{1, \ldots, N\}$
- $N \to \infty$
- $|A \cap \mathrm{supp}(P_i)|/N \to q_i \in (0, 1)$, $q = \sum_i q_i$



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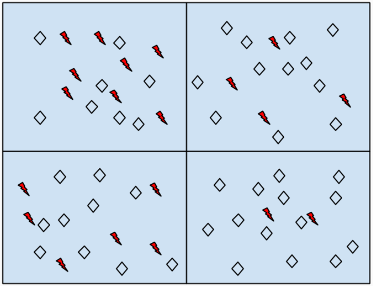

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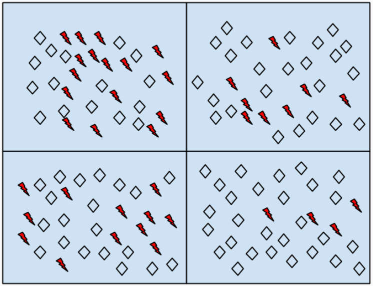


The Oracle behaviour

The limiting discovery process of the Oracle strategy is *deterministic*

Proposition: For every $\lambda \in (0, q_1)$, for every sequence $(\lambda^N)_N$ converging to λ as N goes to infinity, almost surely

$$\lim_{N \to \infty} \frac{T_*^N(\lambda^N)}{N} = \sum_i \left(\log \frac{q_i}{\lambda}\right)_+$$

Oracle vs. uniform sampling

Oracle: The proportion of important items not found after Nt draws tends to

$$q - F^*(t) = I(t)\underline{q}_{I(t)} \exp\left(-t/I(t)\right) \leq K\underline{q}_K \exp(-t/K)$$

with $\underline{q}_K = \left(\prod_{i=1}^K q_i\right)^{1/K}$ the geometric mean of the $(q_i)_i$.

Uniform: The proportion of important items not found after Nt draws tends to $K\bar{q}_K \exp(-t/K)$

$\implies$ Asymptotic ratio of efficiency

$$\rho(q) = \frac{\bar{q}_K}{\underline{q}_K} = \frac{\frac{1}{K}\sum_{i=1}^k q_i}{\left(\prod_{i=1}^k q_i\right)^{1/K}} \geq 1$$

larger if the $(q_i)_i$ are unbalanced

Macroscopic optimality

Theorem: Take $C = (1+\sqrt{2})\sqrt{c+2}$ with $c > 3/2$ in the Good-UCB algorithm.

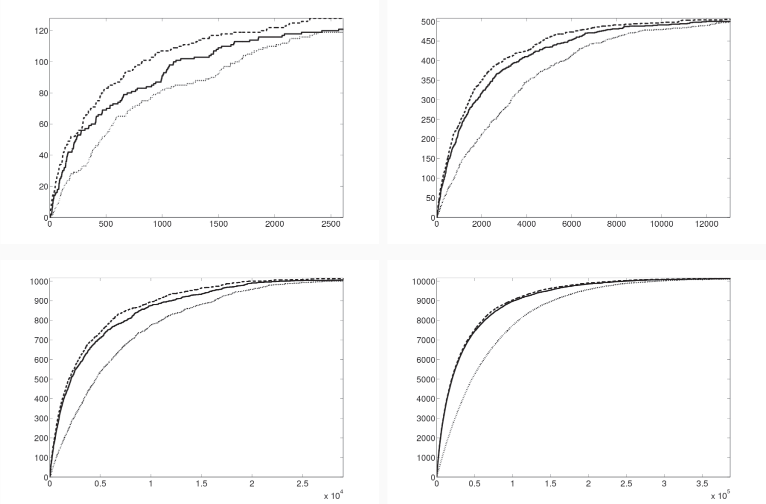
- For every sequence $(\lambda^N)_N$ converging to λ as N goes to infinity, almost surely

$$\limsup_{N\to+\infty} \frac{T^N_{UCB}(\lambda^N)}{N} \leq \sum_i \left(\log \frac{q_i}{\lambda}\right)_+$$

- The proportion of items found after Nt steps $F^{GUCB}(Nt)$ converges *uniformly* to $F^*(Nt)$ as N goes to infinity

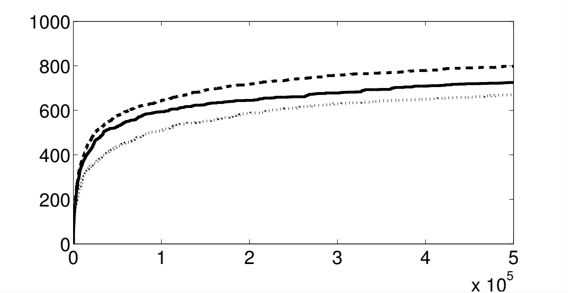
Experiment

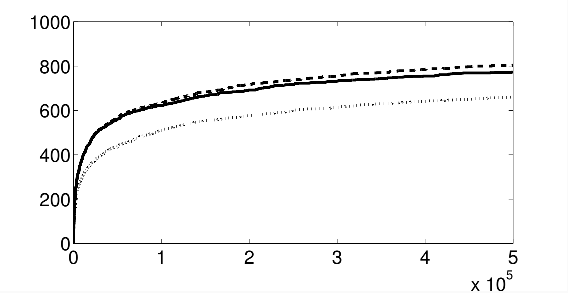
Number of items found by Good-UCB (solid), the OCL (dashed), and uniform sampling (dotted) as a function of time for sizes $N = 128$, $N = 500$, $N = 1000$ and $N = 10000$ in a 7-experts setting.



And when the assumptions are not satisfied?

Number of primes found by Good-UCB (solid), the oracle (dashed) and uniform sampling (dotted) using geometric experts with means 100, 300, 500, 700, 900, for $C = 0.1$ (top) and $C = 0.02$ (bottom).





Conclusion and perspectives

- We propose an algorithm for the optimal discovery with probabilistic expert advice
- We give a standard regret analysis under the only assumption that the supports of the experts are non-overlapping
- We propose a different optimality result, which permits a macroscopic analysis in the uniform case
- Another interesting limit to consider is when the number of important items to find is fixed, but the total number of items tends to infinity (Poisson regime)
- Then, the behavior of the algorithm is not very good: too large confidence bonus because no tight deviations bounds for the Good-Turing estimator when the proportion of important items tends to 0. Improvement by better deviation bounds?

Thank you for your attention!