

A chaining algorithm for online nonparametric regression

Sébastien Gerchinovitz

Institut de Mathématiques de Toulouse, Université Toulouse III – Paul Sabatier

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We consider the problem of **online nonparametric regression** with **individual sequences**. We present a hierarchical algorithm based on the chaining technique.

Outline of the talk:

- 1 Setting: online regression with individual sequences
- 2 A classical algorithm for the finite case
- 3 Large (nonparametric) function sets
- 4 An algorithm based on the chaining technique

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Setting: online regression with individual sequences

Prediction task: at each time $t \in \mathbb{N}^*$, predict the observation $y_t \in \mathbb{R}$ from the input $x_t \in \mathcal{X}$, on the basis of the past data $(x_1, y_1), \dots, (x_{t-1}, y_{t-1})$.

Initial step: the environment chooses **arbitrary deterministic sequences** $(y_t)_{t \geq 1}$ in \mathbb{R} and $(x_t)_{t \geq 1}$ in \mathcal{X} but the forecaster has not access to them.

At each time round $t \in \mathbb{N}^*$,

- 1 The environment reveals the input $x_t \in \mathcal{X}$.
- 2 The forecaster chooses a prediction $\hat{y}_t \in \mathbb{R}$.
- 3 The environment reveals the observation $y_t \in \mathbb{R}$ and the forecaster incurs the loss $(y_t - \hat{y}_t)^2$.

Goal: minimizing regret

Let $\mathcal{F} \subseteq \mathbb{R}^{\mathcal{X}}$ be a set of functions.

Goal of the forecaster: on the long run, to predict almost as well as the best function $f \in \mathcal{F}$ in hindsight, that is, to minimize the **regret**:

$$\text{Reg}_T(\mathcal{F}) \triangleq \sum_{t=1}^T (y_t - \hat{y}_t)^2 - \inf_{f \in \mathcal{F}} \sum_{t=1}^T (y_t - f(x_t))^2 .$$

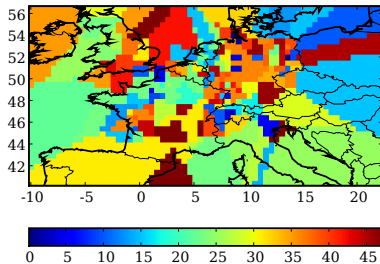
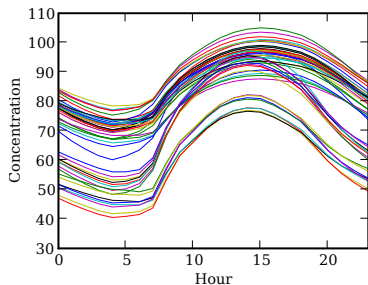
Individual sequence setting: our goal is to minimize the regret $\text{Reg}_T(\mathcal{F})$ **uniformly** over all sequences $(y_t)_{t \geq 1}$ in $[-B, B]$ and $(x_t)_{t \geq 1}$ in \mathcal{X} ; typically:

$$\sup_{\substack{|y_t| \leq B \\ x_t \in \mathcal{X}}} \left\{ \frac{1}{T} \sum_{t=1}^T (y_t - \hat{y}_t)^2 - \inf_{f \in \mathcal{F}} \frac{1}{T} \sum_{t=1}^T (y_t - f(x_t))^2 \right\} \leq o(1) \quad \text{when } T \rightarrow +\infty .$$

Example: ozone daily peaks forecasting

Work initiated by Vivien Mallet (INRIA CLIME) and Gilles Stoltz (HEC Paris).

Goal : daily forecasting of ozone peaks over Europe from 48 simultaneous numerical simulations (different physicochemical models, different numerical schemes, etc).



Left: ozone concentration average profile ($\mu\text{g}/\text{m}^3$).

Right: color of best local predictor.

Example: ozone daily peaks forecasting (2)

Setting: online linear régression (the goal is to minimize RMSE).

Benefits from using online aggregation techniques:

RMSE over 1 year ($\mu\text{g}/\text{m}^3$):

uniform average of 48 predictors	24.41
best of 48 predictors	22.43
<hr/>	
Exponentiated Gradient algorithm	21.47
Ridge algorithm (with discount factor)	19.45

See paper by Mallet, Mauricette, and Stoltz (2009).

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Particular case: finite \mathcal{F}

Assume that $\mathcal{F} = \{f_1, f_2, \dots, f_N\} \subseteq \mathbb{R}^X$ is **finite**. We can use a well-known algorithm studied, e.g., by Kivinen and Warmuth (1999) and Vovk (2001):

Algorithm (Exponentially Weighted Average forecaster (EWA))

Parameter: $\eta > 0$

At each round $t \geq 1$,

- *Using past data, compute the weight vector* $\hat{\mathbf{w}}_t = (\hat{w}_{t,1}, \dots, \hat{w}_{t,N})$ *as*

$$\hat{w}_{t,j} \triangleq \frac{\exp\left(-\eta \sum_{s=1}^{t-1} (y_s - f_j(x_s))^2\right)}{\sum_{j'=1}^N \exp\left(-\eta \sum_{s=1}^{t-1} (y_s - f_{j'}(x_s))^2\right)}, \quad 1 \leq j \leq N;$$

- *Compute the convex combination (convex aggregate):*

$$\hat{y}_t \triangleq \sum_{j=1}^N \hat{w}_{t,j} f_j(x_t).$$

Regret guarantee when \mathcal{F} is finite

If \mathcal{F} contains N functions, then we have a $\mathcal{O}(\log N)$ upper bound on the regret under the boundedness assumption:

$$|y_1|, \dots, |y_T| \leq B \quad \text{and} \quad \|f_1\|_\infty, \dots, \|f_N\|_\infty \leq B .$$

Theorem (Kivinen and Warmuth 1999)

Assume that $\mathcal{F} = \{f_1, f_2, \dots, f_N\} \subseteq [-B, B]^{\mathcal{X}}$.

Then, the EWA algorithm tuned with $\eta = 1/(8B^2)$ satisfies: for all sequences $(y_t)_{t \geq 1}$ in $[-B, B]$ and $(x_t)_{t \geq 1}$ in \mathcal{X} , for all $T \geq 1$,

$$\sum_{t=1}^T (y_t - \hat{y}_t)^2 - \min_{1 \leq j \leq N} \sum_{t=1}^T (y_t - f_j(x_t))^2 \leq 8B^2 \log N .$$

Remark 1: the requirement $\forall j, \|f_j\|_\infty \leq B$ can be removed via clipping.

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Remark 1: the requirement $\forall j, \|f_j\|_\infty \leq B$ can be removed via clipping.

Remark 2: we can obtain a similar bound if $B = \max_{1 \leq t \leq T} |y_t|$ is **unknown**.

Main reference

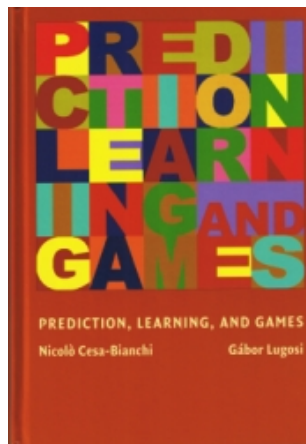
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Prediction, learning, and games, Cesa-Bianchi and Lugosi (2006).

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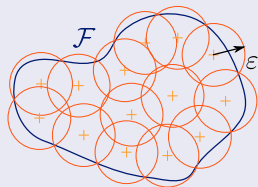
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Large function sets \mathcal{F} : finite approximation

Definition (metric entropy for sup norm)

- Let $\mathcal{F} \subseteq \mathbb{R}^{\mathcal{X}}$ be a set of bounded functions endowed with the sup norm $\|f\|_{\infty} \triangleq \sup_{x \in \mathcal{X}} |f(x)|$.
- ε -net: any subset $\mathcal{G} \subseteq \mathcal{F}$ such that

$$\forall f \in \mathcal{F}, \exists g \in \mathcal{G} : \|f - g\|_{\infty} \leq \varepsilon .$$



- $\mathcal{N}_{\infty}(\mathcal{F}, \varepsilon)$: smallest cardinality of an ε -net.
- metric entropy of \mathcal{F} at scale ε : $\log \mathcal{N}_{\infty}(\mathcal{F}, \varepsilon)$.

Large function sets \mathcal{F} : finite approximation (2)

Assume that \mathcal{F} is infinite (the EWA algorithm cannot be used). Small regret is still achievable if \mathcal{F} can be well approximated by a finite set.

Discretizing \mathcal{F} (Vovk, 2006): approximate \mathcal{F} with a minimal ε -net and run the EWA algorithm on this finite subset:

$$\begin{aligned} \sum_{t=1}^T (y_t - \hat{y}_t)^2 &\leq \min_{1 \leq j \leq \mathcal{N}_\infty(\mathcal{F}, \varepsilon)} \sum_{t=1}^T (y_t - f_j(x_t))^2 + 8B^2 \log \mathcal{N}_\infty(\mathcal{F}, \varepsilon) \\ &\leq \inf_{f \in \mathcal{F}} \sum_{t=1}^T (y_t - f(x_t))^2 + T\varepsilon^2 + 4TB\varepsilon + 8B^2 \log \mathcal{N}_\infty(\mathcal{F}, \varepsilon) \end{aligned}$$

Finite-dimensional case: given $\varphi_j : \mathcal{X} \rightarrow [-B, B]$ and a compact set $\Theta \subseteq \mathbb{R}^d$, define

$$\mathcal{F} = \left\{ \sum_{j=1}^d \theta_j \varphi_j : \theta \in \Theta \right\} \subseteq \mathbb{R}^{\mathcal{X}}.$$

Note that $\mathcal{N}_\infty(\mathcal{F}, \varepsilon) \lesssim (1/\varepsilon)^d$. Choosing $\varepsilon \approx 1/T$ yields a regret at most of the order of $d \log(T)$, which is optimal (**parametric** rate).

What if \mathcal{F} is very large (nonparametric)?

Nonparametric set: assume that \mathcal{F} is much larger than in the finite-dimensional case:

$$\log \mathcal{N}_\infty(\mathcal{F}, \varepsilon) \approx (1/\varepsilon)^p \quad \text{as} \quad \varepsilon \rightarrow 0 .$$

Example: Hölder class $\mathcal{F} \subseteq \mathbb{R}^{[0,1]}$ of regularity $\beta = q + \alpha$:

$$|f^{(q)}(x) - f^{(q)}(y)| \leq \lambda |x - y|^\alpha \quad \text{and} \quad \forall k \leq q, \|f^{(k)}\|_\infty \leq B$$

In this case, $\log \mathcal{N}_\infty(\mathcal{F}, \varepsilon) \approx \varepsilon^{-1/\beta}$ so that $p = 1/\beta$.

EWA is suboptimal: the regret bound $T\varepsilon^2 + 4TB\varepsilon + 8B^2 \log \mathcal{N}_\infty(\mathcal{F}, \varepsilon)$ becomes roughly $T\varepsilon + (1/\varepsilon)^p$. Optimizing in ε only yields:

$$\sum_{t=1}^T (y_t - \hat{y}_t)^2 \leq \inf_{f \in \mathcal{F}} \sum_{t=1}^T (y_t - f(x_t))^2 + \mathcal{O}(T^{p/(p+1)}) ,$$

which is worse than the optimal rate $\mathcal{O}(T^{p/(p+2)})$.

Optimal rates by Rakhlin and Sridharan (2014)

We still assume that $\log \mathcal{N}_\infty(\mathcal{F}, \varepsilon) \approx (1/\varepsilon)^p$ as $\varepsilon \rightarrow 0$.

Optimal regret: through a **non-constructive approach** (reduction to a stochastic problem via von Neumann minimax theorem), Rakhlin and Sridharan (2014) proved that, if $p \in (0, 2)$, then

$$\begin{aligned} \text{Reg}_T(\mathcal{F}) &\leq c_1 B^2 (1 + \log \mathcal{N}_\infty(\mathcal{F}, \gamma)) + c_2 B \sqrt{T} \int_0^\gamma \sqrt{\log \mathcal{N}_\infty(\mathcal{F}, \varepsilon)} d\varepsilon \\ &\lesssim \gamma^{-p} + \sqrt{T} \int_0^\gamma \varepsilon^{-p/2} d\varepsilon \\ &\lesssim T^{p/(p+2)} \quad \text{for } \gamma = T^{-1/(p+2)}. \end{aligned}$$

The rate $T^{p/(p+2)}$ is better than $T^{p/(p+1)}$ obtained previously with EWA, and it is (in a sense) **optimal**.

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Example (Hölder class with regularity β):

Since $p = 1/\beta$, we get $\text{Reg}_T(\mathcal{F})/T = \mathcal{O}(T^{-2\beta/(2\beta+1)})$ if $\beta > 1/2$.

Therefore, same rate as in the statistical setting (for $\beta > 1/2$).

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The above integral is a **Dudley entropy integral**.

- In statistical learning with i.i.d. data, useful to derive risk bounds for empirical risk minimizers (e.g., Massart 2007; Rakhlin et al. 2013).
- Also appears in online learning with individual sequences. Earlier appearances: Opper and Haussler (1997); Cesa-Bianchi and Lugosi (1999, 2001).

Our contributions

- 1 We provide an **explicit algorithm** that achieves the Dudley-type regret bound (when $p \in (0, 2)$):

$$\text{Reg}_T(\mathcal{F}) \leq c_1 B^2 (1 + \log \mathcal{N}_\infty(\mathcal{F}, \gamma)) + c_2 B \sqrt{T} \int_0^\gamma \sqrt{\log \mathcal{N}_\infty(\mathcal{F}, \varepsilon)} d\varepsilon.$$

Nota: contrary to Rakhlin and Sridharan (2014), our bounds are not in terms of the stronger notion of *sequential entropy*.

- 2 This algorithm uses ideas from the **chaining technique**, and relies on a new subroutine (Multi-variable Exponentiated Gradient algorithm) to perform optimization at different scales simultaneously.
- 3 We address computational issues by showing how to construct **more efficient** and quasi-optimal **ε -nets** (for Hölder classes).

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Linearizing the square loss can help locally (1)

Suppose we play with loss functions $\mathbf{u} \mapsto \ell_t(\mathbf{u})$, $t \geq 1$, that are convex and differentiable over the simplex $\Delta_N = \{\mathbf{u} \in \mathbb{R}_+^N : \sum_{i=1}^N u_i = 1\}$.

Algorithm (Exponentiated Gradient—EG)

Parameter: $\eta > 0$

At each round $t \geq 1$, compute the weight vector $\hat{\mathbf{u}}_t \in \Delta_N$ by

$$\hat{u}_{t,j} \triangleq \frac{1}{Z_t} \exp\left(-\eta \sum_{s=1}^{t-1} \partial_{\hat{u}_{s,j}} \ell_s(\hat{\mathbf{u}}_s)\right), \quad 1 \leq j \leq N.$$

Theorem (Kivinen and Warmuth 1999 and Cesa-Bianchi 1999)

Assume ℓ_t convex, diff, and $\|\nabla \ell_t\|_\infty \leq G$. For $\eta = G^{-1} \sqrt{2 \log(N)/T}$,

$$\sum_{t=1}^T \ell_t(\hat{\mathbf{u}}_t) \leq \min_{\mathbf{u} \in \Delta_N} \sum_{t=1}^T \ell_t(\mathbf{u}) + G \sqrt{2T \log N}.$$

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Linearizing the square loss can help locally (2)

Application: we want to predict almost as well as the best function in $\mathcal{F} = \{f_0 + g_j : j = 1, \dots, N\}$ with $\|g_j\|_\infty$ small (neighbors of f_0).

We use EG with $\ell_t(\mathbf{u}) = \left(y_t - f_0(x_t) - \sum_{j=1}^N u_j g_j(x_t)\right)^2$, $\mathbf{u} \in \Delta_N$.

Since $\|\nabla \ell_t\|_\infty \lesssim B \max_j \|g_j\|_\infty$, the EG algorithm satisfies:

$$\sum_{t=1}^T \underbrace{\left(y_t - f_0(x_t) - \sum_{j=1}^N \hat{u}_{t,j} g_j(x_t)\right)^2}_{= \hat{y}_t} \leq \min_{1 \leq j \leq N} \sum_{t=1}^T (y_t - f_0(x_t) - g_j(x_t))^2 + \square B \max_{1 \leq j \leq N} \|g_j\|_\infty \sqrt{T \log N}$$

Advantage: the above regret bound $B \max_j \|g_j\|_\infty \sqrt{T \log N}$ improves on $B^2 \log N$ (obtained by EWA) when $\max_j \|g_j\|_\infty \ll B \sqrt{\log(N)/T}$.

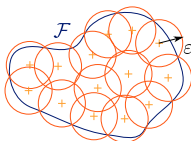
Thus, **linearizing the square loss** can help if the functions in \mathcal{F} are **close**.

Turning the chaining technique into an online algorithm

We still assume that $\log \mathcal{N}_\infty(\mathcal{F}, \varepsilon) \approx (1/\varepsilon)^p$ as $\varepsilon \rightarrow 0$. Recall that we want to prove a bound of the form:

$$\sum_{t=1}^T (y_t - \hat{y}_t)^2 \leq \inf_{f \in \mathcal{F}} \sum_{t=1}^T (y_t - f(x_t))^2 + [\text{small term}]$$

Chaining principle: we discretize \mathcal{F} and use projections $\pi_k(f)$ such that $\sup_f \|\pi_k(f) - f\|_\infty \leq \gamma/2^k$ for all $k \geq 0$.



$$\inf_{f \in \mathcal{F}} \sum_{t=1}^T (y_t - f(x_t))^2 = \inf_{f \in \mathcal{F}} \sum_{t=1}^T \left(y_t - \pi_0(f)(x_t) - \underbrace{\sum_{k=1}^{\infty} [\pi_k(f) - \pi_{k-1}(f)](x_t)}_{|\text{small increments}| \leq 3\gamma/2^k} \right)^2$$

Aggregation at two different levels

$$\inf_{f \in \mathcal{F}} \sum_{t=1}^T (y_t - f(x_t))^2 = \inf_{f \in \mathcal{F}} \sum_{t=1}^T \left(y_t - \underbrace{\pi_0(f)}_{\in \mathcal{F}^{(0)}}(x_t) - \sum_{k=1}^{\infty} \underbrace{[\pi_k(f) - \pi_{k-1}(f)]}_{\in \mathcal{G}^{(k)}}(x_t) \right)^2$$

Sufficient goal:

$$\sum_{t=1}^T (y_t - \hat{y}_t)^2 \leq \inf_{f_0, g_1, \dots, g_K} \sum_{t=1}^T (y_t - (f_0 + g_1 + \dots + g_K)(x_t))^2 + [\text{small term}]$$

Two aggregation levels:

$$\left. \begin{array}{l} f_{0,1} \xrightarrow{\text{low scale multi-variable EG}} \hat{f}_{t,1} \\ f_{0,2} \xrightarrow{\quad \quad \quad \quad \quad \quad \quad} \hat{f}_{t,2} \\ \vdots \\ f_{0,N_0} \xrightarrow{\quad \quad \quad \quad \quad \quad \quad} \hat{f}_{t,N_0} \end{array} \right\} \xrightarrow{\text{high scale EWA}} \hat{y}_t = \sum_{j=1}^{N_0} \hat{w}_{t,j} \hat{f}_{t,j}(x_t)$$

Combining two regret guarantees

High-scale aggregation Using an Exponentially Weighted Average (EWA) forecaster $\hat{f}_t = \sum_{j=1}^{N_0} \hat{w}_{t,j} \hat{f}_{t,j}$ yields

$$\sum_{t=1}^T (y_t - \hat{y}_t)^2 \leq \min_{1 \leq j \leq N_0} \sum_{t=1}^T \left(y_t - \hat{f}_{t,j}(x_t) \right)^2 + \square B^2 \log N_0$$

Low-scale aggregation Recall that $\mathcal{G}^{(k)} = \{ \pi_k(f) - \pi_{k-1}(f) : f \in \mathcal{F} \}$. Denote $\mathcal{G}^{(k)} = \{ g_1^{(k)}, \dots, g_{N_k}^{(k)} \}$.

We designed a multi-variable extension of the Exponentiated Gradient algorithm:

$$\hat{f}_{t,j} \triangleq f_{0,j} + \sum_{k=1}^K \sum_{i=1}^{N_k} \hat{u}_{t,i}^{(j,k)} g_i^{(k)}$$

which yields, for all $j = 1, \dots, N_0$,

$$\begin{aligned} \sum_{t=1}^T \left(y_t - \hat{f}_{t,j}(x_t) \right)^2 &\leq \min_{g_1, \dots, g_K} \sum_{t=1}^T \left(y_t - (f_{0,j} + g_1 + \dots + g_K)(x_t) \right)^2 \\ &\quad + 120B\sqrt{T} \int_0^{\gamma/2} \sqrt{\log \mathcal{N}_\infty(\mathcal{F}, \varepsilon)} d\varepsilon. \end{aligned}$$

Main result

The next theorem indicates that the Chaining Exponentially Weighted Average forecaster satisfies a **Dudley-type regret bound**.

Theorem (Gaillard and G., 2015)

Let $B > 0$, $T \geq 1$, and $\gamma \in (\frac{B}{T}, B)$.

- Assume that $\max_{1 \leq t \leq T} |y_t| \leq B$ and that $\sup_{f \in \mathcal{F}} \|f\|_\infty \leq B$.
- Assume that $(\mathcal{F}, \|\cdot\|_\infty)$ is totally bounded and define $\mathcal{F}^{(0)}$ and $\mathcal{G}^{(k)}$ as above.

Then, the Chaining Exponentially Weighted Average forecaster (tuned with appropriate parameters) satisfies:

$$\text{Reg}_T(\mathcal{F}) \leq B^2(5 + 50 \log \mathcal{N}_\infty(\mathcal{F}, \gamma)) + 120B\sqrt{T} \int_0^{\gamma/2} \sqrt{\log \mathcal{N}_\infty(\mathcal{F}, \varepsilon)} d\varepsilon.$$

Computational issues: dyadic discretization

We assume that $\mathcal{F} = \{f : [0, 1] \rightarrow [-B, B] : f \text{ is 1-Lipschitz}\}$.

Regret bound:

We know that $\log \mathcal{N}_\infty(\mathcal{F}, \varepsilon) = \mathcal{O}(\varepsilon^{-1})$.

Therefore, our algorithm obtains $\text{Reg}_T(\mathcal{F}) = \mathcal{O}(T^{1/3})$, which is optimal.

Computational issue:

Our algorithm updates $\exp(\mathcal{O}(T))$ weights at every round t .

Hence **very poor time and space computational complexities**.

Solution:

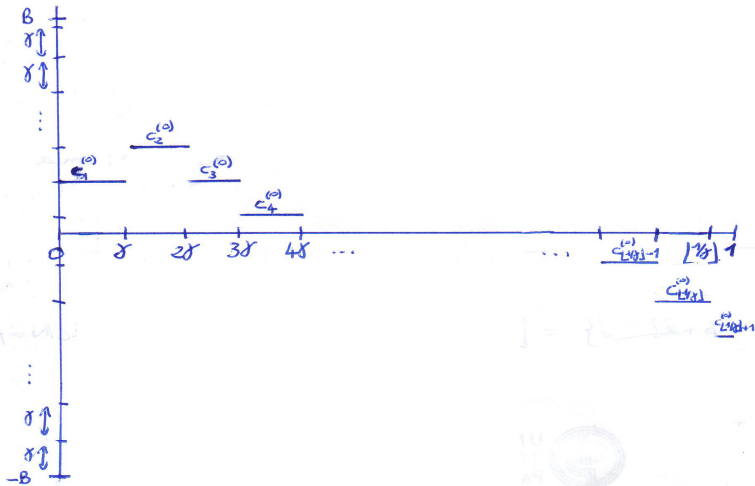
\mathcal{F} has a sufficiently nice structure that can be exploited to construct **computationally manageable ε -nets** with quasi-optimal cardinality.

For example: piecewise-constant approximations on a dyadic discretization lead to $\mathcal{O}(T^{1/3} \log T)$ regret and per-round time complexity.

High-level discretization (piecewise-constant approximation)

- Partition the x -axis $[0, 1]$: $I_a \triangleq [(a-1)\gamma, a\gamma)$, $a = 1, \dots, \frac{1}{\gamma}$.
- Discretize the y -axis $[-B, B]$: $\mathcal{C}^{(0)} = \{-B + j\gamma : j = 0, \dots, \frac{2B}{\gamma}\}$.

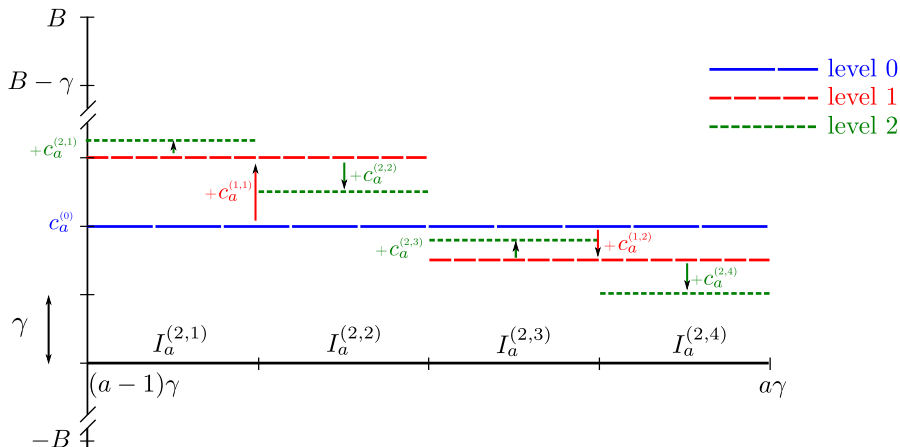
$\mathcal{F}^{(0)}$: set of piecewise-constant functions $f^{(0)}(x) = \sum_{a=1}^{1/\gamma} c_a^{(0)} \mathbb{I}_{x \in I_a}$, $c_a^{(0)} \in \mathcal{C}^{(0)}$.



Low-level discretization (dyadic approximation)

$\mathcal{F}^{(M)}$: set of all functions $f_c : [0, 1] \rightarrow \mathbb{R}$ of the form

$$f_c(x) = \underbrace{\sum_{a=1}^{1/\gamma} c_a^{(0)} \mathbb{I}_{x \in I_a}}_{f^{(0)}(x)} + \sum_{m=1}^M \underbrace{\sum_{a=1}^{1/\gamma} \sum_{n=1}^{2^m} c_a^{(m,n)} \mathbb{I}_{x \in I_a^{(m,n)}}}_{g^{(m)}(x)} .$$



Theorem (Gaillard and G., 2015)

Let $B > 0$, $T \geq 2$, and \mathcal{F} be the set of all 1-Lipschitz functions from $[0, 1]$ to $[-B, B]$. Assume that $\max_{1 \leq t \leq T} |y_t| \leq B$.

Then, the Dyadic Chaining Algorithm (see paper) satisfies, for some absolute constant $c > 0$,

$$\text{Reg}_T(\mathcal{F}) \leq c \max\{B, B^2\} T^{1/3} \log T .$$

Remark: additional log factor, but computationally **tractable**:

- per-round time complexity: $\mathcal{O}(T^{1/3} \log T)$;
- space complexity: $\mathcal{O}(T^{4/3} \log T)$.

Conclusion

- Online aggregation techniques are a robust way to combine several predictions (without any assumptions on the model).
- In the online nonparametric setting, we designed an explicit algorithm with (quasi-optimal) regret guarantees and an efficient implementation for Hölder classes.

Thank you for your attention!

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