

# PAC-Bayesian Online Clustering

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# Notation

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- $(x_t)_{1:T}$  : online dataset, where  $x_t \in \mathbb{R}^d$
- $K_t$ : nb of clusters
- $\hat{c}_t = (\hat{c}_{t,1}, \hat{c}_{t,2}, \dots, \hat{c}_{t,K_t})$  : clusters location, depending on past information  $(x_s)_{1:(t-1)}$  and  $(\hat{c}_s)_{1:(t-1)}$
- When  $x_t$  is newly revealed, the instantaneous loss:

$$\ell(\hat{c}_t, x_t) = \min_{1 \leq k \leq K_t} |\hat{c}_{t,k} - x_t|^2$$

- $\mathcal{C} = \bigcup_{k=1}^p$
- $q$ : discrete probability distribution on the set  $[1,p] := 1, \dots, p$   
for any  $k \in [1,p]$ , let  $\pi_k$ , the probability distribution on  $\mathbb{R}^{dk}$
- For any  $c \in \mathcal{C}$ , we define  $\pi(c)$ , as
$$\pi(c) = \sum_{k \in [1,p]} q(k) \mathbb{1}_{\{c \in \mathbb{R}^{dk}\}} \pi_k(c)$$

- $c \in \mathcal{C}$  a partition of  $\mathbb{R}^d$ ,  $\pi \in \mathbb{P}(\mathcal{C})$  a quasi prior over this set
- $\lambda > 0$  : inverse temperature parameter
- At each time  $t$ , we observe  $x_t$  and a random partition  $\hat{c}_{t+1} \in \mathcal{C}$  is sampled from the quasi-posterior:  
$$d\hat{p}_{t+1} \propto \exp\{-\lambda S_t(c)\} d\pi(c)$$
- Cumulative loss:  
$$S_t(c) = S_{t-1}(c) + \ell(c, x_t) + \frac{\lambda}{2} \{\ell(c, x_t) - \ell(\hat{c}_t, x_t)\}^2$$

# Sparcity Regret Bounds

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## Algo 1: The PAC-Bayesian online Clustering algorithm

- 1: Input parameters:  $p > 0, \pi \in \mathcal{P}(\mathcal{C}), \lambda > 0$  and  $S_0 = 0$
- 2: Initialization: Draw  $\hat{c}_1 \sim \pi$
- 3: For  $t \in [1, T - 1]$  :
  - 4: Get the data  $x_t$
  - 5: Draw  $\hat{c}_{t+1} \sim \hat{\rho}_{t+1}(c)$  where  $d\hat{\rho}_{t+1} \propto \exp\{-\lambda S_t(c)\}d\pi(c)$ , and
$$S_t(c) = S_{t-1}(c) + \ell(c, x_t) + \frac{\lambda}{2}\{\ell(c, x_t) - \ell(\hat{c}_t, x_t)\}^2$$
- 6: End for



## Theorem 1:

For any  $(x_t)_{1:T} \in \mathcal{R}^{dT}$ , any quasi prior  $\pi \in \mathcal{P}(\mathcal{C})$ , any  $\lambda > 0$ ,

the procedure described in Algo 1 satisfies:

$$\sum_{t=1}^T \mathbb{E}_{(\hat{\rho}_1, \hat{\rho}_2, \dots, \hat{\rho}_t)} \ell(\hat{c}_t, x_t) \leq \inf_{\rho \in \mathcal{P}_\pi(\mathcal{C})} \left\{ \mathbb{E}_{c \sim \rho} [\sum_{t=1}^T \ell(c, x_t)] + \frac{\mathcal{K}(\rho, \pi)}{\lambda} + \frac{\lambda}{2} \mathbb{E}_{(\hat{\rho}_1, \hat{\rho}_2, \dots, \hat{\rho}_T)} \mathbb{E}_{c \sim \rho} \sum_{t=1}^T [\ell(c, x_t) - \ell(\hat{c}_t, x_t)] \right\}$$

# Sparsity Regret Bounds

The regret bound could be refined when :

- $q(k) = \frac{\exp -\eta k}{\sum_{i=1}^p \exp -\eta i}$ , with  $\eta > 0$ .
- $d\pi_k(c, R) = \left( \frac{\Gamma(\frac{d}{2}+1)}{\pi^{\frac{d}{2}}} \right) \frac{1}{(2R)^{dk}} \left\{ \prod_{j=1}^k \mathbb{1}_{\{\mathbb{B}_d(2R)\}}(c_j) \right\} dc$

## Corollary 1:

$$\sum_{t=1}^T \mathbb{E}_{(\hat{\rho}_1, \hat{\rho}_2, \dots, \hat{\rho}_t)} \ell(\hat{c}_t, x_t) \leq \inf_{k \in [1, p]} \left\{ \inf_{c \in \mathcal{C}(k, R)} \sum_{t=1}^T \ell(c, x_t) + \frac{dk}{2\lambda} \log \frac{8R^2 \lambda T}{d=2} + \frac{\eta}{\lambda} k \right\} + \left( \frac{\log p}{\lambda} + \frac{d}{2\lambda} + \frac{\lambda T C_1^2}{2} \right)$$

where  $C_1 = (2R + \max_{t=1..T} |x_t|_2)^2$

# Sparsity Regret Bounds

The below calibration yields a sublinear remainder term :

- $\lambda = \frac{d+2}{2\sqrt{T}R^2}$

## Corollary 2:

$$\sum_{t=1}^T \mathbb{E}_{(\hat{\rho}_1, \hat{\rho}_2, \dots, \hat{\rho}_t)} \ell(\hat{c}_t, x_t) \leq \inf_{k \in [1, p]} \left\{ \inf_{c \in \mathcal{C}(k, R)} \sum_{t=1}^T \ell(c, x_t) + k \frac{dR^2}{d+2} \sqrt{T} \log 4\sqrt{T} + k \frac{2R^2\eta}{d+2} \sqrt{T} \right\} + \left( \frac{2R^2 \log p}{d+2} + \frac{dR^2}{d+2} + \frac{(d+2)C_1^2}{4R^2} \right) \sqrt{T}$$

Hence, if there exist  $k^*$ , and  $c^* \in \mathcal{C}(k^*, R)$ , which achieve the infimum:

$$\sum_{t=1}^T \mathbb{E}_{(\hat{\rho}_1, \hat{\rho}_2, \dots, \hat{\rho}_t)} \ell(\hat{c}_t, x_t) - \sum_{t=1}^T \ell(c^*, x_t) \leq Jk^* \sqrt{T} \log T$$

$J$ : constant depending on  $d, R$ ,  $\log p$  and  $C_1^2$

Then the regret of the expected cumulative loss is sublinear in  $T$ .

# **Adaptative Sparsity Regret Bounds**

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$T$  is usually unknown, prompting us to choose  $\lambda = \lambda_t$

## **Algo 1: The adaptative PAC-Bayesian online Clustering algorithm**

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- 1: Input parameters:  $p > 0, \pi \in \mathcal{P}(\mathcal{C}), (\lambda_t)_{0:T} > 0$  and  $S_0 = 0$
- 2: Initialization: Draw  $\hat{c}_1 \sim \pi$
- 3: For  $t \in [1, T - 1]$  :
  - 4: Get the data  $x_t$
  - 5: Draw  $\hat{c}_{t+1} \sim \hat{p}_{t+1}(c)$  where  $d\hat{p}_{t+1} \propto \exp\{-\lambda_t S_t(c)\} d\pi(c)$ , and
$$S_t(c) = S_{t-1}(c) + \ell(c, x_t) + \frac{\lambda_{t-1}}{2} \{\ell(c, x_t) - \ell(\hat{c}_t, x_t)\}^2$$
- 6: End for

## Theorem 2:

For any  $(x_t)_{1:T} \in \mathcal{R}^{dT}$ , any quasi prior  $\pi \in \mathcal{P}(\mathcal{C})$ ,  
if  $(\lambda_t)_{0:T}$  a non-increasing sequence of positive numbers,

the procedure described in Algo 2 satisfies:

$$\sum_{t=1}^T \mathbb{E}_{(\hat{\rho}_1, \hat{\rho}_2, \dots, \hat{\rho}_t)} \ell(\hat{c}_t, x_t) \leq \inf_{\rho \in \mathcal{P}_\pi(\mathcal{C})} \left\{ \mathbb{E}_{c \sim \rho} [\sum_{t=1}^T \ell(c, x_t)] + \frac{\mathcal{K}(\rho, \pi)}{\lambda_T} + \mathbb{E}_{(\hat{\rho}_1, \hat{\rho}_2, \dots, \hat{\rho}_T)} \mathbb{E}_{c \sim \rho} \left[ \sum_{t=1}^T \frac{\lambda_{t-1}}{2} [\ell(c, x_t) - \right. \right.$$

# Adaptative Sparsity Regret Bounds

keeping previous setting for  $q$  and  $\pi_k$ , with  $\eta \geq 0$  and  $R \geq \max_{t=1..T} |x_t|_2$

The below adaptative calibration for any  $t \in [1, T]$  and  $\lambda_0 = 1$ :

- $\lambda_t = \frac{d+2}{2\sqrt{t}R^2}$

## Corollary 2:

Then the algorithm 2 satisfies:

$$\sum_{t=1}^T \mathbb{E}_{(\hat{\rho}_1, \hat{\rho}_2, \dots, \hat{\rho}_t)} \ell(\hat{c}_t, x_t) \leq \inf_{k \in [1, p]} \left\{ \inf_{c \in \mathcal{C}(k, R)} \sum_{t=1}^T \ell(c, x_t) + \frac{dkR^2}{d+2} \sqrt{T} \log 4\sqrt{T} + k \frac{2R^2\eta}{d+2} \sqrt{T} \right\} + \left( \frac{2R^2 \log p}{d+2} + \frac{dR^2}{d+2} + \frac{(d+2)C_1^2}{2R^2} \right) \sqrt{T}$$

The adaptative Algorithm 2 is supported by a sparsity regret bound with rate  $\sqrt{T} \log T$ .

# The PACO algorithm

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# The PACO algorithm

- Since direct sampling from the quasi-posterior  $\hat{p}_t$  is usually not possible, we will focus on a stochastic approximation, called PACO.
- Approximate  $\hat{p}_t$  through MCMC, favoring local move.
- States of interest of the MC  $(k^{(n)}, c^{(n)})_{0 \leq n \leq N}$ , where  $k^{(n)} \in [1, p]$  and  $c^{(n)} \in \mathbb{R}^{dk^{(n)}}$
- At each iteration, from  $(k^{(n)}, c^{(n)})$  to proposal state  $(k', c')$   
Hence  $c^{(n)} \in \mathbb{R}^{dk^{(n)}}$ , and  $c' \in \mathbb{R}^{dk'}$  may be of different dimensions  
( $k' \neq k^{(n)}$ )

We create auxiliary vectors  $\nu_1, \nu_2$  to compensate for dimensional difference ( $d_1, d_2$ ) s.t.  $dk^{(n)} + d_1 = dk' + d_2$

# The PACO algorithm

- Let  $\rho_{k'}(\cdot, c_{k'}, \tau_{k'})$  denote the multivariate Student distribution on  $\mathbb{R}^{dk'}$ :

$$\rho_{k'}(c, c_{k'}, \tau_{k'}) = \prod_{j=1}^{k'} \left\{ C_{\tau_{k'}}^{-1} \left( 1 + \frac{|c_j - c_{k',j}|_2^2}{6\tau_{k'}^2} \right)^{-\frac{3+d}{2}} \right\} dc,$$

where  $C_{\tau_{k'}}^{-1}$  is the normalizing constraint

- First a local move from  $k^{(n)}$  to  $k'$  is proposed by choosing  $k' \in [k^{(n)} - 1, k^{(n)} + 1]$  with probability  $q(k^{(n)}, \cdot)$
- Next, choosing  $d_1 = dk'$ ,  $d_2 = dk^{(n)}$ , we sample  $\nu_1$  from  $\rho_{k'}$
- Finally, the pair  $(\nu_2, c')$  is obtained by  $(\nu_2, c') = g(\nu_1, c^{(n)})$ , where  $g : (x, y) \in \mathbb{R}^{dk'} \times \mathbb{R}^{dk^{(n)}} \rightarrow (y, x) \in \mathbb{R}^{dk^{(n)}} \times \mathbb{R}^{dk'}$

# The PACO algorithm

## Algo 3: PACO

- 1: Initialization:  $(\lambda_t)$
- 2: For  $t \in [1, T - 1]$  :
- 3: Initialization:  $(k^{(0)}, c^{(0)}) \in [1, p] \times \mathbb{R}^{dk^{(0)}}$
- 4: For  $n \in [1, N - 1]$  :
- 5:   Sample  $k' \in [k^n - 1, kn + 1]$  from  $q(k^{(n)}, \cdot) = 1/3$
- 6:   Let  $c' \leftarrow$  standard k-means output.
- 7:   Let  $\tau' = 1/\sqrt{pt}$ .
- 8:   Sample  $\nu_1 \sim \rho_{k'}(\cdot, c_{k'}, \tau_{k'})$  .
- 9:   Let  $(\nu_2, c') = g((\nu_1, c^{(n)}))$ .
- 10:   Accept the move  $(k^{(n)}, c^{(n)}) = (k', c')$  with probability  
$$\alpha[(k^{(n)}, c^{(n)}), (k', c')] = \min \left\{ 1, \frac{\hat{\rho}_t(c')q(k', k^{(n)})\rho_{k^{(n)}}(c^{(n)}, c_{k^{(n)}}, \tau_{k^{(n)}})}{\hat{\rho}_t(c^{(n)})q(k^{(n)}, k')\rho'(c', c_{k'}, \tau_{k'})} \right\}$$
- 11:   Else  $(k^{n+1}, c^{n+1}) = (k^n, c^n)$
- 12: End for
- 13: Let  $\hat{c}_t = c^{(N)}$ .
- 14: End for

## Numerical studies

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