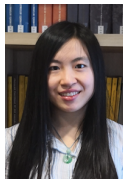


Optimal Clustering with Bandit Feedback

<https://arxiv.org/abs/2202.04294>

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Stanford RL Seminar

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Outline

- 1 Motivation
- 2 Problem Setup and Preliminaries
- 3 Lower Bound
- 4 Algorithm: Bandit Online Clustering
- 5 Numerical Experiments

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- The task of partitioning a set of items into smaller clusters
- One of the most fundamental tasks in machine learning
- Numerous algorithms proposed (e.g., K -means and spectral clustering)

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Challenges

- Measurement noise
- Sequential and adaptive data collection

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- An online variant of the classical offline clustering problem

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High-Level Description of our Problem

- An online variant of the classical offline clustering problem
- Bandit feedback: at each time step, the agent only observes a noisy measurement on the selected arm (or item)
- Pull arms adaptively, so as to minimize the expected number of total arm pulls it takes to correctly partition the given arm set with a given high probability

Applications in Digital Marketing

Sequential Collection of Customer Feedback

Customer feedback on certain products are collected in an online manner and always accompanied by random or systematic noise.

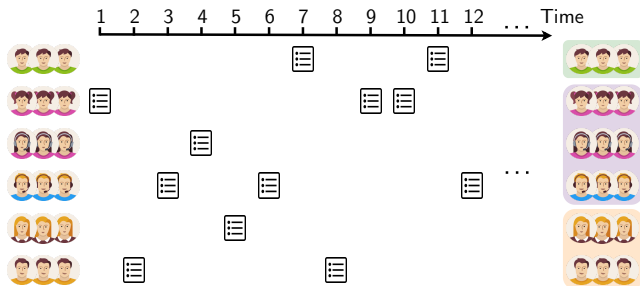


Figure: Example involving partitioning 6 sub-groups of customers into 3 market segments with bandit feedback.

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A Bandit Feedback Model with Cluster Structure

Mathematical Model I

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- An instance of cluster bandits can be fully characterized by a pair (c, \mathcal{U}) , where $c = [c_1, c_2, \dots, c_M] \in [K]^M$ consists of the cluster indices of the arms and $\mathcal{U} = [\mu(1), \mu(2), \dots, \mu(K)] \in \mathbb{R}^{d \times K}$ represents the K centers of the clusters.

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- Only consider partitioning the instances in which the mean vectors for different clusters are **distinct**.

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- The K centers of the clusters: $\mathcal{U} = [\mu(1), \mu(2), \dots, \mu(K)] \in \mathbb{R}^{d \times K}$
- At each time t , the agent selects an arm A_t from the arm set \mathcal{A} , and then observes a noisy measurement on the mean vector of A_t , i.e.,

$$X_t = \mu(c_{A_t}) + \eta_t$$

where $\eta_t \in \mathbb{R}^d$ is independent noise, following the standard d -dimensional Gaussian distribution $\mathcal{N}(0, \mathbf{I}_d)$.

A Bandit Feedback Model with Cluster Structure

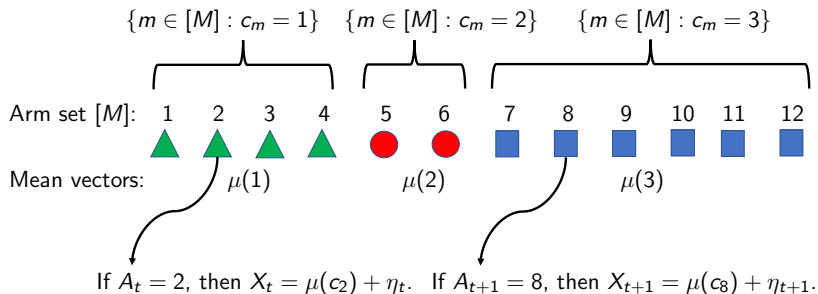


Figure: Online clustering with bandit feedback with $K = 3$ and $M = 12$.

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- For two partitions c and c' , if there exists a permutation σ on $[K]$ such that $c = \sigma(c')$, then we write $c \sim c'$.
- For two instances (c, \mathcal{U}) and (c', \mathcal{U}') , if $\mu(c_m) = \mu'(c'_m)$ for all $m \in [M]$, then we write $(c, \mathcal{U}) \sim (c', \mathcal{U}')$.

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- and to recommend a *correct* partition c^{out} of the arm set $[M]$ (i.e., $c^{\text{out}} \sim c$) with a probability of at least $1 - \delta$ (*recommendation rule*)

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Performance Metric

$$\min_{\pi} \mathbb{E}[\tau_\delta] \quad \text{s.t.} \quad \underbrace{\Pr(\tau_\delta < \infty) = 1 \text{ and } \Pr(c^{\text{out}} \not\sim c) \leq \delta}_{\delta\text{-PAC}}$$

Other Notations

- $\mathcal{P}_N := \{x \in [0, 1]^N : \|x\|_1 = 1\}$ denotes the probability simplex in \mathbb{R}^N while $\mathcal{P}_N^+ := \{x \in (0, 1)^N : \|x\|_1 = 1\}$ denotes the open simplex.

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- For any $a, b \in (0, 1)$, the binary relative entropy between Bernoulli distributions with means a and b , is denoted as

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- $i^* = \arg \min_{i \in A} f(i)$ refers to the **minimum** index in the set $\{i \in A : f(i) = \min_{j \in A} f(j)\}$.

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$$\mathbb{P}(A) + \mathbb{Q}(A^c) \geq \frac{1}{2} \exp(-D(\mathbb{P} \parallel \mathbb{Q})) \quad D(\mathbb{P} \parallel \mathbb{Q}) := \int_{\Omega} d\mathbb{P} \log \frac{d\mathbb{P}}{d\mathbb{Q}}.$$

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- For any fixed instance (c, \mathcal{U}) , we define

$$\text{Alt}(c) := \{(c', \mathcal{U}') : c'' \neq c \text{ for any } (c'', \mathcal{U}'') \sim (c', \mathcal{U}')\},$$

the set of alternative instances where c is **not** a correct partition.

Lower Bound

Theorem 1

For a fixed confidence level $\delta \in (0, 1)$ and instance (c, \mathcal{U}) , any δ -PAC online clustering algorithm satisfies

$$\mathbb{E}[\tau_\delta] \geq d_{\text{KL}}(\delta, 1 - \delta) D^*(c, \mathcal{U})$$

where

$$D^*(c, \mathcal{U}) := \left(\frac{1}{2} \sup_{\lambda \in \mathcal{P}_M} \inf_{(c', \mathcal{U}') \in \text{Alt}(c)} \sum_{m=1}^M \lambda_m \|\mu(c_m) - \mu'(c'_m)\|^2 \right)^{-1}.$$

Furthermore,

$$\liminf_{\delta \rightarrow 0} \frac{\mathbb{E}[\tau_\delta]}{\log(1/\delta)} \geq D^*(c, \mathcal{U}).$$

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- Wish to find the optimal proportion of arm pulls to distinguish the instance c from the **most confusing** alternative instances in $\text{Alt}(c)$.
- With the knowledge of the instance (c, \mathcal{U}) , the optimization problem naturally reveals the optimal sampling rule, which will be the basic idea behind the design of our sampling rule.

Two Optimization Problems

Key Optimization Problems

Problem (SupInf):
$$\sup_{\lambda \in \mathcal{P}_M} \inf_{(c', \mathcal{U}') \in \text{Alt}(c)} \sum_{m=1}^M \lambda_m \|\mu(c_m) - \mu'(c'_m)\|^2$$

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- These optimization problems in their original form appear to be intractable.
- The definition of $\text{Alt}(c)$ is combinatorial and the number of instances in it is obviously infinite.
- For a fixed number of clusters K , the total number of possible partitions grows asymptotically as $K^M/K!$

A Combinatorial Property of Problem (InnerInf)

Lemma 2

For any $\lambda \in \mathcal{P}_M$ and (c, \mathcal{U}) ,

$$\inf_{(c', \mathcal{U}') \in \text{Alt}(c)} \sum_{m=1}^M \lambda_m \|\mu(c_m) - \mu'(c'_m)\|^2 = \inf_{\substack{(c', \mathcal{U}') \in \text{Alt}(c): \\ d_H(c', c) = 1}} \sum_{m=1}^M \lambda_m \|\mu(c_m) - \mu'(c'_m)\|^2.$$

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- Instead of considering all the alternative instances in $\text{Alt}(c)$, Lemma 2 shows it suffices to consider the instances whose partitions have a **Hamming distance of 1** from the given partition c .
- **Sketch of the proof:** for any instance $(c^\dagger, \mathcal{U}^\dagger) \in \text{Alt}(c)$ such that $d_H(c^\dagger, c) > 1$, there exists another instance $(c^*, \mathcal{U}^*) \in \text{Alt}(c)$ such that $d_H(c^*, c) = 1$ and the objective function under (c^*, \mathcal{U}^*) is not larger than that under $(c^\dagger, \mathcal{U}^\dagger)$.

Solution to Problem (InnerInf)

Proposition 1

For any $\lambda \in \mathcal{P}_M$ and (c, \mathcal{U}) ,

$$\inf_{(c', \mathcal{U}') \in \text{Alt}(c)} \sum_{m=1}^M \lambda_m \|\mu(c_m) - \mu'(c'_m)\|^2$$

$$= \begin{cases} \min_{\substack{k, k' \in [K]: \\ n(k) > 1, k' \neq k}} \frac{\bar{w}(k)w(k')}{\bar{w}(k)+w(k')} \|\mu(k) - \mu(k')\|^2 & \text{if } \lambda \in \mathcal{P}_M^+ \\ 0 & \text{otherwise} \end{cases}$$

where $w(k) := \sum_{m=1}^M \lambda_m \mathbb{1}\{c_m = k\}$, $n(k) := \sum_{m=1}^M \mathbb{1}\{c_m = k\}$ and $\bar{w}(k) := \min_{m \in [M]: c_m = k} \lambda_m$.

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InnerInf becomes a **finite minimization problem**.

Continuity of Problem (InnerInf)

Proposition 2

For any fixed c , define $g : \mathcal{P}_M \times \mathbb{R}^{d \times K} \rightarrow \mathbb{R}^+$ as

$$g(\lambda, \mathcal{U}) := \inf_{(c', \mathcal{U}') \in \text{Alt}(c)} \sum_{m=1}^M \lambda_m \|\mu(c_m) - \mu'(c'_m)\|^2.$$

Then g is continuous on $\mathcal{P}_M \times \mathcal{U}$.

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Then g is continuous on $\mathcal{P}_M \times \mathcal{U}$.

- Helps to assert that the stopping rule in our algorithm BOC is asymptotically optimal.

Solution to Problem (SupInf)

Recall that Problem (SupInf) is

$$D^*(c, \mathcal{U}) := \left(\frac{1}{2} \sup_{\lambda \in \mathcal{P}_M} \inf_{(c', \mathcal{U}') \in \text{Alt}(c)} \sum_{m=1}^M \lambda_m \|\mu(c_m) - \mu'(c'_m)\|^2 \right)^{-1}$$

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Proposition 3

For any (c, \mathcal{U}) , $D^*(c, \mathcal{U})$ can be *simplified* as

$$D^*(c, \mathcal{U}) = 2 \min_{w \in \mathcal{P}_K^+} \max_{\substack{k, k' \in [K]: \\ n(k) > 1, k' \neq k}} \left(\frac{n(k)}{w(k)} + \frac{1}{w(k')} \right) \|\mu(k) - \mu(k')\|^{-2}.$$

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- Outer supremum in Problem (SupInf) is **attained**.

Solution to Problem (SupInf)

Proposition 4

For any (c, \mathcal{U}) , the solution to $D^*(c, \mathcal{U})$

$$\arg \max_{\lambda \in \mathcal{P}_M} \inf_{(c', \mathcal{U}') \in \text{Alt}(c)} \sum_{m=1}^M \lambda_m \|\mu(c_m) - \mu'(c'_m)\|^2 \quad (1)$$

is unique. If λ^* denotes the solution to (1) and w^* denotes the *solution* to

$$\arg \min_{w \in \mathcal{P}_K^+} \max_{\substack{k, k' \in [K]: \\ n(k) > 1, k' \neq k}} \left(\frac{n(k)}{w(k)} + \frac{1}{w(k')} \right) \|\mu(k) - \mu(k')\|^{-2},$$

then λ^* can be expressed in terms of w^* as (*bijection between λ^* and w^**)

$$\lambda_m^* = \frac{w^*(c_m)}{n(c_m)} \text{ for all } m \in [M].$$

Continuity of Problem (SupInf)

Proposition 5

For any fixed c , define $\Lambda : \mathbb{R}^{d \times K} \rightarrow \mathcal{P}_M$ as

$$\Lambda(\mathcal{U}) := \arg \max_{\lambda \in \mathcal{P}_M} \inf_{(c', \mathcal{U}') \in \text{Alt}(c)} \sum_{m=1}^M \lambda_m \|\mu(c_m) - \mu'(c'_m)\|^2$$

where $\mathcal{U} = [\mu(1), \mu(2), \dots, \mu(K)] \in \mathbb{R}^{d \times K}$. Then Λ is *continuous* on \mathcal{U} .

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where $\mathcal{U} = [\mu(1), \mu(2), \dots, \mu(K)] \in \mathbb{R}^{d \times K}$. Then Λ is *continuous* on \mathcal{U} .

- The correspondence $\Lambda(\mathcal{U})$ is single-valued and upper hemicontinuous.
- A single-valued correspondence that is hemicontinuous is continuous (Sundaram, 1996).
- Guarantees *computationally efficiency* and *asymptotic optimality* of our sampling rule.

Two Optimization Problems

Simplifications of InnerInf and SupInf

- Problem (InnerInf) \Leftrightarrow A finite minimization problem
- Problem (SupInf) \Leftrightarrow A finite convex minimax problem (Gigola and Gomez, 1990; Herrmann, 1999; Gaudioso et al., 2006)

Implications of simplifications

- Problem (InnerInf) plays an essential role in the computation of the **stopping rule** of our method.
- Problem (SupInf) guarantees the computationally efficiency and the asymptotic optimality of our **sampling rule**.

Outline

- 1 Motivation
- 2 Problem Setup and Preliminaries
- 3 Lower Bound
- 4 Algorithm: Bandit Online Clustering**
- 5 Numerical Experiments

Weighted K -means with Maximin Initialization

Our Goal at Each Step

- Although we only aim at producing a correct partition in the final recommendation rule, learning the K unknown mean vectors of the clusters is essential in the sampling rule as well as the stopping rule.

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Our Goal at Each Step

- Although we only aim at producing a correct partition in the final recommendation rule, learning the K unknown mean vectors of the clusters is essential in the sampling rule as well as the stopping rule.
- **Question:** Given some past measurements on the arm set, how to produce an estimate of the pair (c, \mathcal{U}) ?

Weighted K -means with Maximin Initialization

- Given the past arm pulls and observations up to time t , the **log-likelihood function** that the instance is (c', \mathcal{U}') is

$$\ell(c', \mathcal{U}' \mid A_1, X_1, \dots, A_t, X_t) := -\frac{1}{2} \sum_{\bar{t}=1}^t \|X_{\bar{t}} - \mu'(c'_{A_{\bar{t}}})\|^2 - \frac{td}{2} \log(2\pi).$$

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- For any arm $m \in [M]$, let $N_m(t)$ and $\hat{\mu}_m(t)$ denote the number of pulls and the empirical estimate up to time t , respectively.

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- For any arm $m \in [M]$, let $N_m(t)$ and $\hat{\mu}_m(t)$ denote the number of pulls and the empirical estimate up to time t , respectively.
- The **maximum likelihood estimate** of the unknown pair (c, \mathcal{U}) is

$$\arg \min_{(c', \mathcal{U}')} \sum_{m=1}^M N_m(t) \|\hat{\mu}_m(t) - \mu'(c'_m)\|^2$$

which involves minimizing a weighted sum of squared distances between the empirical estimate of each arm and its associated center.

Weighted K -means with Maximin Initialization

Weighted K -means problem

$$\arg \min_{(c', \mathcal{U}')} \sum_{m=1}^M N_m(t) \|\hat{\mu}_m(t) - \mu'(c'_m)\|^2$$

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Remarks

- MLE \Leftrightarrow The classical offline **weighted K -means clustering** problem

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- Any algorithm designed for the weighted K -means clustering problem is applicable to obtain an approximate (**not exact**) solution to the MLE problem.
- No theoretical guarantees for finding a global minimum of this problem in general.
- **Weighted K -means with Maximin Initialization** (Gonzalez, 1985) possesses useful properties!

Weighted K -means with Maximin Initialization

Algorithm 1 Weighted K -means with Maximin Initialization (K-MEANS-MAXIMIN)

Input: Number of clusters K , empirical estimate $\hat{\mu}_m$ and weighting N_m for all $m \in [M]$

- 1: Choose the empirical estimate of an arbitrary arm as the first cluster center $\hat{\mu}(1)$
- 2: **for** $k = 2$ **to** K **do** ▷ Maximin Initialization
- 3: Choose the empirical estimate of the arm that has the **greatest Euclidean distance** to the nearest existing center as the k -th center $\hat{\mu}(k)$:

$$\hat{\mu}(k) = \arg \max_{m \in [M]} \min_{1 \leq k' \leq k-1} \|\hat{\mu}_m - \hat{\mu}(k')\|$$

4: **end for**

Weighted K -means with Maximin Initialization

5: **repeat**

▷ Weighted K -means

6: Assign each arm to its closest cluster center:

$$\hat{c}_m = \arg \min_{k \in [K]} \|\hat{\mu}_m - \hat{\mu}(k)\|$$

7: Update each cluster center as the weighted mean of the empirical estimates of the arms in it:

$$\hat{\mu}(k) = \frac{\sum_{m \in [M]} N_m \hat{\mu}_m \mathbb{1}\{\hat{c}_m = k\}}{\sum_{m \in [M]} N_m \mathbb{1}\{\hat{c}_m = k\}}$$

8: **until** Clustering \hat{c} no longer changes

9: Set $\mu^{\text{out}}(k) = \hat{\mu}(k)$ for all $k \in [K]$

Output: $c^{\text{out}} = \hat{c}$ and $\mathcal{U}^{\text{out}} = [\mu^{\text{out}}(1), \mu^{\text{out}}(2), \dots, \mu^{\text{out}}(K)]$

Stopping Rule

Usual Strategy

- As the arm sampling proceeds, the algorithm needs to determine when to stop the sampling and then to recommend a partition with an error probability of at most δ .

Stopping Rule

Usual Strategy

- As the arm sampling proceeds, the algorithm needs to determine when to stop the sampling and then to recommend a partition with an error probability of at most δ .
- Most existing algorithms for pure exploration in the fixed-confidence setting (e.g., Garivier and Kaufmann (2016), Jedra and Proutiere (2020), Feng et al. (2021), Réda et al. (2021)) consider the **Generalized Likelihood Ratio** (GLR) statistic and find suitable task-specific threshold functions.

Stopping Rule: Problems with the GLR

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- The logarithm of the GLR statistic for testing $(c^{t*}, \mathcal{U}^{t*})$ against its alternative instances can be written as

$$\begin{aligned} \log -\text{GLR}(c^{t*}, \mathcal{U}^{t*}) = & \frac{1}{2} \left(- \sum_{m=1}^M N_m(t) \|\hat{\mu}_m(t) - \mu^{t*}(c_m^{t*})\|^2 \right. \\ & \left. + \min_{(c', \mathcal{U}') \in \text{Alt}(c^{t*})} \sum_{m=1}^M N_m(t) \|\hat{\mu}_m(t) - \mu'(c'_m)\|^2 \right). \end{aligned}$$

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- Problem 1: Requires **exact** global minimizer in the log-GLR statistic.

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- Problem 1: Requires **exact** global minimizer in the log-GLR statistic.
- Problem 2: Similar Hamming distance 1 nice property (Lemma 2) does not hold when $\mu(c_m)$ is replaced by $\hat{\mu}_m(t) \implies$ **Mismatch!**

Stopping Rule: Our Remedy

- Let $(c^{t-1}, \mathcal{U}^{t-1})$ be the estimate of the true pair (c, \mathcal{U}) produced by the K-MEANS-MAXIMIN based on the past measurements up to time $t - 1$.

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- Consider the statistic

$$Z(t) := \frac{1}{2} \left(\left(-\sqrt{Z_1(t)} + \sqrt{Z_2(t)} \right)_+ \right)^2$$

with

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which is analogous to

$$\text{Problem (InnerInf): } \inf_{(c', \mathcal{U}') \in \text{Alt}(c)} \sum_{m=1}^M \lambda_m \|\mu(c_m) - \mu'(c'_m)\|^2$$

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Stopping Rule

Stopping Time

The stopping time is defined as

$$\tau_\delta := \inf\{t \in \mathbb{N} : Z(t) \geq \beta(\delta, t)\}$$

where $\beta(\delta, t)$ is a threshold function inspired by the concentration results for univariate Gaussian distributions (Kaufmann and Koolen, 2021).

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Proposition 6

The stopping time satisfies that

$$\Pr(\tau_\delta < \infty, c^{\text{out}} \neq c) \leq \delta.$$

Algorithm: Bandit Online Clustering (BOC)

Algorithm 2 Bandit Online Clustering (BOC)

Input: Number of clusters K , confidence level δ and arm set $[M]$

1: Sample each arm once, set $t = M$ and initialize $\hat{\mu}_m(t)$ and $N_m(t) = 1$ for all $m \in [M]$.

2: **repeat**

3: **if** $\min_{m \in [M]} N_m(t) \leq \max(\sqrt{t} - M/2, 0)$ **then** ▷ Forced exploration

4: Sample $A_{t+1} = \arg \min_{m \in [M]} N_m(t)$ and $(c^t, \mathcal{U}^t) \leftarrow (c^{t-1}, \mathcal{U}^{t-1})$

5: **else**

6: $(c^t, \mathcal{U}^t) \leftarrow \text{K-MEANS-MAXIMIN}(K, \{\hat{\mu}_m(t)\}_{m \in [M]}, \{N_m(t)\}_{m \in [M]})$

7: Solve ▷ Problem (SupInf)

$$\lambda^*(t) = \arg \max_{\lambda \in \mathcal{P}_M} \inf_{(c', \mathcal{U}') \in \text{Alt}(c^t)} \sum_{m=1}^M \lambda_m \|\mu^t(c_m^t) - \mu'(c_m')\|^2$$

8: Sample $A_{t+1} = \arg \max_{m \in [M]} (t\lambda_m^*(t) - N_m(t))$

9: **end if**

10: $t \leftarrow t + 1$, update $\hat{\mu}_m(t)$ and $N_m(t)$ for all $m \in [M]$

Algorithm

11: Compute

$$Z_1(t) = \sum_{m=1}^M N_m(t) \|\hat{\mu}_m(t) - \mu^{t-1}(c_m^{t-1})\|^2$$

and solve

▷ Problem (InnerInf)

$$Z_2(t) = \min_{(c', \mu') \in \text{Alt}(c^{t-1})} \sum_{m=1}^M N_m(t) \|\mu^{t-1}(c_m^{t-1}) - \mu'(c'_m)\|^2$$

12: Set

$$Z(t) = \frac{1}{2} \left(\left(-\sqrt{Z_1(t)} + \sqrt{Z_2(t)} \right)_+ \right)^2$$

13: **until** $Z(t) \geq \beta(\delta, t)$

Output: $\tau_\delta = t$ and $c^{\text{out}} = c^{t-1}$

Sample Complexity

Theorem 3

For any instance (c, \mathcal{U}) , Bandit Online Clustering ensures that $\Pr(\tau_\delta < \infty) = 1$ and

$$\limsup_{\delta \rightarrow 0} \frac{\mathbb{E}[\tau_\delta]}{\log(1/\delta)} \leq D^*(c, \mathcal{U}).$$

Hence, combining this with the lower bound,

$$\lim_{\delta \rightarrow 0} \frac{\mathbb{E}[\tau_\delta^*]}{\log(1/\delta)} = D^*(c, \mathcal{U}).$$

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- The expected sample complexity of BOC **asymptotically matches the instance-dependent lower bound** as the confidence level $\delta \rightarrow 0$.
- It is also **computationally efficient** in terms of its sampling, stopping and recommendation rules.

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Synthetic Dataset: Verifying the Asymptotic Behavior

- Three synthetic instances with varying difficulty levels, where $K = 4$, $M = 11$ and $d = 3$.
- The partitions and the first three cluster centers of all the three instances are the same, while their fourth cluster centers vary.

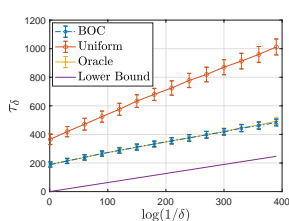
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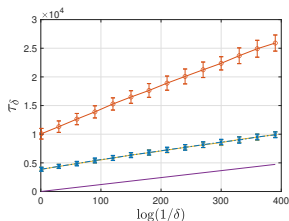
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$$\left\{ \begin{array}{l} c = [1, 1, 2, 2, 2, 2, 3, 3, 3, 4, 4] \\ \mu(1) = [0, 0, 0]^\top \\ \mu(2) = [0, 10, 0]^\top \\ \mu(3) = [0, 0, 10]^\top \\ \mu(4) = \begin{cases} [5, 0, 0]^\top & \text{for the } \textit{easy} \text{ instance,} \\ [1, 0, 0]^\top & \text{for the } \textit{moderate} \text{ instance,} \\ [0.5, 0, 0]^\top & \text{for the } \textit{challenging} \text{ instance} \end{cases} \end{array} \right.$$

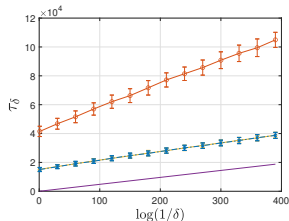
Synthetic Dataset: Verifying the Asymptotic Behavior



(a) Easy



(b) Moderate



(c) Challenging

Figure: The empirical averaged sample complexities of the different methods (BOC, Uniform, Oracle) with respect to $\log(1/\delta)$.

Thanks for listening!

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