Beyond the Best: Distribution Functional Estimation in Infinite-Armed Bandits

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Abstract

In the infinite-armed bandit problem, each arm's average reward is sampled from an unknown distribution, and each arm can be sampled further to obtain noisy estimates of the average reward of that arm. Prior work focuses on the best arm, i.e. estimating the maximum of the average reward distribution. We consider a general class of distribution functionals beyond the maximum and obtain optimal sample complexities in both offline and online settings. We show that online estimation, where the learner can sequentially choose whether to sample a new or existing arm, offers no advantage over the offline setting for estimating the mean functional, but significantly reduces the sample complexity for other functionals such as the median, maximum, and trimmed mean. We propose unified meta algorithms for the online and offline settings and derive matching lower bounds using different Wasserstein distances. For the special case of median estimation, we identify a curious thresholding phenomenon on the indistinguishability between Gaussian convolutions with respect to the noise level, which may be of independent interest.

1 Introduction

In the infinite-armed bandit problem first formulated in (Berry et al., 1997), at each time the learner can either sample an arm that has been already observed in the past, or sample a new arm, whose average reward is sampled from an underlying distribution F. The learners objective is then to identify arms with large average rewards, with the objective being either achieving a small cumulative regret (Berry et al., 1997; Wang et al., 2008; Bonald and Proutiere, 2013), or small simple regret (Carpentier and Valko, 2015). This setting differs from the classical multi-armed bandit formulation as the number of observed arms is not fixed a priori and needs to be carefully chosen by the algorithm.

We consider the problem of estimating some functional $g(F)$ of an underlying distribution F. From this point of view, the classical infinite-armed bandit problem can be viewed as an *online* sampling algorithm to *estimate* the *maximum* of the distribution F. [1] Once we cast the infinite-armed bandit problem in this manner, it immediately suggests several additional questions. For example, what about *offline* sampling algorithms? Indeed, online sampling requires continual interactions with the environment which may be infeasible in certain applications, and recent work in online and offline reinforcement learning have demonstrated the significant value of both formulations (Rashidinejad et al., 2021; Zhang et al., 2021; Schrittwieser et al., 2021). Additionally, it is worth estimating functionals beyond the maximum: in many practical scenarios, including single-cell RNA-sequencing (Zhang et al., 2020), we are interested in the mean, median, or trimmed mean of the underlying distribution F. Since sampling is expensive, it is critical to identify the optimal method to collect

[1] To be precise, the objectives in infinite-armed bandit works (Berry et al., 1997; Wang et al., 2008; Bonald and Proutiere, 2013; Carpentier and Valko, 2015) are slightly different: achieving a small cumulative regret or identifying an arm whose expected reward is as close as possible to the maximum of the underlying distribution.

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samples. For example, do online methods offer significant gains over offline methods? Are the fundamental limits of estimating the median and trimmed mean different from that of the maximum?

In this paper we initiate the study of distribution functional estimation in both online and offline settings and obtain both information theoretic limits and efficient algorithms for estimating the mean, median, trimmed mean, and maximum. We propose unified meta algorithms for both offline and online settings, and provide matching upper and lower bounds for the sample complexity of estimating the aforementioned functionals in Table 1.

We also reveal new insights on the fundamental differences between offline and online algorithms, as well as the fundamental differences between different functionals. To determine the sharp statistical limits, we use the Wasserstein-2 distance to upper bound the KL divergence in the offline setting, while use the Wasserstein-∞ distance instead in the online setting. This approach leads to valid sample complexity lower bounds for general functionals g, which turn out to be tight for the estimation of mean and maximum. However, a curious thresholding phenomenon, which is not captured by the previous approach and does not occur for the *mean* and *maximum*, appears in the *median* and *trimmed mean* analyses: the KL divergence does not change smoothly with the noise level and enjoys a phase transition after the noise level exceeds some threshold. This phenomenon calls for different treatments under different estimation targets and could be of independent interest.

Functional	Offline complexity	Online complexity	Comments
Mean	$\Theta(\varepsilon^{-2})$	$\Theta(\varepsilon^{-2})$	No gain from online sampling
Median	$\Theta(\varepsilon^{-3})$	$\tilde{\Theta}(\varepsilon^{-2.5})$	Holds for any quantile not on boundary
Maximum	$\Theta(\varepsilon^{-(2+\beta)})$	$\tilde{\Theta}(\varepsilon^{-\max(\beta,2)})$	Depends on the tail regularity β
Trimmed mean	$\tilde{\Theta}(\varepsilon^{-3})$	$\tilde{\Theta}(\varepsilon^{-2.5})$	$g(F) = \mathbb{E}\{X \mid X \in [F^{-1}(\alpha), F^{-1}(1-\alpha)]\}$

Table 1: Sample complexity of estimating different functionals $g(F)$, where F is the cumulative distribution function (CDF) of the distribution to estimate. Here ε is the target accuracy and we use Θ to denote the matched upper and lower bounds. Additionally, we use the standard notation of $\tilde{O}, \tilde{\Theta}, \tilde{\Omega}, \gtrsim$ and $\lesssim$ to suppress constants and logarithmic factors in ε. If $h(\varepsilon) \lesssim f(\varepsilon)$ and $f(\varepsilon) \lesssim h(\varepsilon)$ then we denote this as $f(\varepsilon) \sim h(\varepsilon)$. For the maximum, the distribution satisfies $P(X \geq F^{-1}(1) - \varepsilon) \sim \varepsilon^{\beta}$. Other assumptions on F are detailed in Section 3.

The rest of this paper is structured as follows. In Section 1.1 we discuss the relevant infinite-armed bandit literature. We then formulate our distribution functional estimation problem in Section 2. Our unified meta algorithms for the offline and online settings are presented in Section 3, where we show the sample complexity upper bounds. We present lower bounds proofs via Wasserstein distance for the online and offline settings in Section 4, and a special thresholding phenomenon in Section 5. Section 6 concludes this work.

1.1 Related works

The field of multi-armed bandits has seen broad interest and utility since its formalization in 1985 (Lai et al., 1985). Across clinical trials, multi-agent learning, online recommendation systems, and beyond (Lattimore and Szepesvári, 2020), multi-armed bandits have proven to be an excellent framework for modeling and solving complex tasks regarding exploration in an unknown environment. In the classical multi-armed bandit setting we have a set of n distributions, where each distribution is associated with the rewards delivered by one of the arms. The gambler iteratively pulls one arm per round and observes a sample drawn from the associated reward distribution. In the setting of infinitely many-armed bandit (Berry et al., 1997), the average arm reward for each arm is sampled i.i.d. from an unknown distribution to draw from and the number of available arms is infinity. There are many possible objectives that can be formulated in this online learning problem, from regret minimization (maximizing the sum of arm pulls) (Wang et al., 2008; Bonald and Proutiere, 2013; Carpentier and Valko, 2015; Li and Xia, 2017) to identification tasks (for example identifying the distribution with the largest average reward) (Aziz et al., 2018; Chaudhuri and Kalyanakrishnan, 2017, 2019). Many works have studied best-arm identification, and we now have essentially matching instance dependent upper and lower bounds (Jamieson and Nowak, 2014; Kaufmann et al., 2016).

One could also use the average reward estimate of the identified best arm to estimate the maximum of the average reward distribution in the infinite-armed bandit setting (Carpentier and Valko, 2015; Aziz et al., 2018; Chaudhuri and Kalyanakrishnan, 2017, 2019).

2 Problem formulation

We are interested in estimating the distribution functional $g(F) \in \mathbb{R}$ of an underlying distribution with cumulative distribution function (CDF) F. We study a class of indicator-based functionals g defined as follows.

Definition 1 (Indicator-based functionals)**.** *The functional g can be represented as*

$$g(F) = \mathbb{E}\left[X | X \in S(F)\right] \tag{1}$$

for some set $S(F)$ (potentially unknown to the algorithm), where X is drawn from F. The set $S(F)$ is defined by $\alpha_1 \leq \alpha_2$, and takes the form:

$$S(F) = [F^{-1}(\alpha_1), F^{-1}(\alpha_2)]. \tag{2}$$

We denote $S(F)$ by S throughout this work, as S is clear from context. This class encompasses many natural functionals of interest, which we formulate in Table 2. In Appendix A, we discuss extending our results to more general functionals.

Functional	$g(F)$	α_1	α_2	Comment
Mean	$\int x \mathrm{d}F(x)$	0	1	
Quantile	$F^{-1}(\alpha)$	α	α	$\alpha \in (0,1)$, e.g. $\alpha = 1/2$ for median
Maximum	$F^{-1}(1)$	1	1	$\alpha_1 = \alpha_2 = 0$ for minimum
Trimmed mean	$\int_{x:\alpha_1 \leq F(x) \leq \alpha_2} x \mathrm{d}F(x)$	α	$1-\alpha$	$\alpha \in (0, 1/2)$

Table 2: Indicator-based functionals

As in the infinite-armed bandit setting, we only have access to noisy observations of samples drawn from the distribution with CDF F. At each round, we obtain an observation $Y = X + Z$. Here X is drawn from F and $Z \sim \mathcal{N}(0,1)$ is the noise. We can either choose X from a point which we already have some noisy observations or generate a new point X following F.

In this paper we characterize the online and offline sample complexities of these problems, and in the meantime propose online and offline sampling algorithms achieving them. For $\varepsilon > 0$ and $\delta \in (0,1)$, we call an estimator $\hat{G}$ an (ε, δ)-PAC approximation of $g(F)$ if $P(|\hat{G} - g(F)| \leq \varepsilon) \geq 1 - \delta$.

3 Offline and online algorithms

3.1 Offline estimation algorithms

We study a special class of offline algorithms, which uniformly obtain observations of the points following the underlying distribution. To be precise, based on prior information regarding the distribution in question, F, it will choose an appropriate number of points n and number of samples per point m to obtain an (ε, δ)-PAC approximation of $g(F)$. Specifically, the latent variables are $X_1, \ldots, X_n$ drawn from F, and our observations are $\{Y_{i,j}\}_{j=1}^m$ drawn i.i.d. from $\mathcal{N}(X_i, 1)$. For $i \in [n]$, denote $\hat{X}_i = m^{-1} \sum_{j=1}^m Y_{i,j}$ as the empirical mean of the observations. Then, we can write $\hat{X}_i = X_i + \hat{Z}_i$ where $\hat{Z}_i \sim \mathcal{N}(0, 1/m)$, independent across i. Define $S_n \triangleq \{i : X_{(\lfloor \alpha_1 n \rfloor)} \leq X_i \leq X_{(\lceil \alpha_2 n \rceil)}\}$ as the set of arms relevant for estimating the functional g, and define our n sample estimate of g as $g_n(\hat{X}_1, \ldots, \hat{X}_n) \triangleq |S_n|^{-1} \sum_{i \in S_n} \hat{X}_i$. Here $X_{(i)}$ is the i-th smallest entry in $X_1, \ldots, X_n$. Then, $G_{n,m} = g_n(\hat{X}_1, \ldots, \hat{X}_n)$ where each X_i has been sampled m times serves as a natural estimator for $g(F)$ from noisy observations. With this, we can state the following theorem:

Theorem 1 (Offline PAC sample complexity; informal)**.** *An (ε, δ)-PAC offline uniform-sampling-based algorithm for estimating $g(F)$ requires nm samples where n, m are chosen based on ε, δ, the functional g, and information about F, with orderwise dependence on ε detailed in Table 3.*

Functional	m	n
Mean	$\Theta(1)$	$\Theta(\varepsilon^{-2})$
Median	$\Theta(\varepsilon^{-1})$	$\Theta(\varepsilon^{-2})$
Maximum	$\Theta(\varepsilon^{-2})$	$\Theta(\varepsilon^{-\beta})$
Trimmed mean	$\Theta\left(\varepsilon^{-1}\log\left(\varepsilon^{-1}\right)\right)$	$\Theta(\varepsilon^{-2})$

Table 3: Choice of (m, n) for estimating different functionals to accuracy ε.

For the rest of this section, we discuss in greater detail our assumptions on the underlying distribution. We defer the proofs and calculations for n and m to Appendix C, as well as discussion regarding the trimmed mean to Appendix B.

3.1.1 Mean

In order to estimate the mean of a distribution in an offline manner, we need to know that the distribution does not spread out much. Thus, for mean estimation, we require the following assumption.

Assumption 1. *The distribution F satisfies $\mathrm{Var}_{X\sim F}[X] \leq c$.*

Assumption 1 ensures that estimation of the mean of the distribution can be accomplished with finite samples. The following proposition gives the sample complexity of the offline algorithm.

Proposition 1. *Suppose that Assumption 1 is satisfied. By choosing $m = 1$ and $n \geq \delta^{-1}(1+c)\varepsilon^{-2}$, the estimator $G_{n,m}$ is an (ε, δ)-PAC approximation of $g(F)$. Thus, the offline algorithm requires $O(\varepsilon^{-2})$ samples.*

3.1.2 Median

For median estimation we require different assumptions than the mean, as listed below.

Assumption 2. *There exist constants $c_1, c_2 > 0$ such that*

- $F'(x) \geq c_1$ *for* $|x - \mathrm{median}(F)| \lesssim \varepsilon$.
- $|F''(x)| \leq c_2$ *for* $|x - \mathrm{median}(F)| \lesssim \sqrt{\varepsilon}$.

The first assumption ensures that the median of F is unique. The second assumption precludes the distribution from being dumbbell-shaped (very little mass near the median), in which case estimating the true median is meaningless and can be arbitrarily difficult. The following proposition gives a suitable choice of (n, m) for providing an (ε, δ)-PAC approximation of $g(F)$.

Proposition 2. *Suppose that Assumption 2 holds. Then, by choosing $m \geq 4(c_2+1)/(c_1\varepsilon)$ and $n \geq 28\log(1/\delta)/(c_1\varepsilon)^2$, the estimator $G_{n,m}$ is an (ε, δ)-PAC approximation of $g(F)$. Thus, the offline algorithm requires $O(\varepsilon^{-3})$ samples.*

3.1.3 Maximum

For maximum estimation, we require an assumption on the tail of F as is common in the infinite-armed bandit literature.

Assumption 3. *Let $\eta = \max(F) = F^{-1}(1)$. There exist constants $0 < c_1 < c_2$ and $\beta > 0$ such that*

- $1 - F(\eta - t) \in [c_1 t^\beta, c_2 t^\beta]$, *for all* $0 \leq t \lesssim \varepsilon$.

This assumption is also known as the β-regularity of F around η, see (Wang et al., 2008). We present a suitable choice of (n, m) in the following proposition.

Proposition 3. *Suppose that Assumption 3 holds. By choosing $n \geq c_1^{-1}2^\beta\varepsilon^{-\beta}\log(2/\delta)$ and $m \geq 4\varepsilon^{-2}\log(2n\delta^{-1})$, the estimator $G_{n,m}$ is an (ε, δ)-PAC approximation of $g(F)$. Therefore, the offline algorithm requires $O(\varepsilon^{-\beta-2})$ samples.*

3.2 Online estimation algorithm

We now present our general algorithm (Algorithm 1), an elimination-based (ε, δ)-PAC algorithm that efficiently estimates $g(F)$, where g is a known input functional and F is an unknown distribution from which we are able to sample X_i independently, and observe noisy observations $Y_{i,j}$ of X_i.

In order to exploit the Bayesian nature of the problem, we analyze the algorithm in two parts. First, we use the fact that our arms are drawn from a common distribution to find some n, m as in Theorem 1 such that the plug-in estimator $G_{n,m}$ will be an $(\varepsilon/2, \delta/2)$-PAC estimator of $g(F)$. Second, we show that our adaptive algorithm is an $(\varepsilon/2, \delta/2)$-PAC estimator of $G_{n,m}$, but is able to accomplish this using significantly fewer samples.

Notationally, we denote by $\hat{\mu}(r)$ the estimated mean vector of all arms at round r. We have that with high probability each arm's mean estimate stays within its width $b_r = 2^{-r}$ confidence interval for each round r. To analyze our algorithm, we denote $\mu_1^{\text{uni}}, \ldots, \mu_n^{\text{uni}}$ as the estimates of $X_1, \ldots, X_n$ generated by the offline algorithm after sampling each arm m times. Then, we see that for the offline algorithm the arms relevant for the estimation task and the corresponding n sample estimator are

$$S_n = \left\{ i : \mu^{\text{uni}}_{(\lfloor \alpha_1 n \rfloor)} \leq \mu_i^{\text{uni}} \leq \mu^{\text{uni}}_{(\lfloor \alpha_2 n \rfloor)} \right\} \quad , \quad G_{n,m} = \frac{1}{|S_n|} \sum_{i \in S_n} \mu_i^{\text{uni}}. \tag{3}$$

Here S_n indicates the arms that the offline algorithm believes are in S. We show that our online algorithm is able to efficiently estimate the set S_n as $\hat{S}_n$, determining whether or not arms are in S_n, sampling these arms in S_n sufficiently, and returning a plug-in estimator. By construction each arm is only pulled by the adaptive algorithm at most m times, as we know from the analysis of the offline algorithm that for the utilized n, m, if each arm is pulled m times then the output is an $(\varepsilon/2, \delta/2)$-PAC estimate of $g(F)$. Thus, the online algorithm's objective is essentially emulating the output of the offline algorithm, for which it only needs to sample any arm at most m times.

Note that when $\alpha_1 \neq \alpha_2$, we have many samples X_i that are within S, with $|S_n| = n(\alpha_2 - \alpha_1)$. In order to avoid issues of dependence, we discard all previous samples (as arms in $\hat{S}_n$ will have been sampled different numbers of times), and see that since we have $\Theta(n)$ arms in $\hat{S}_n$ we can construct a sufficiently accurate estimate by sampling each arm in $\hat{S}_n$ once. Algorithmically, we denote this as obtaining one fresh observation and constructing $\hat{\mu}_i(0)$.

To upper bound the sample complexity of our algorithm, we see that each arm only needs to be sampled to determine whether it is in S_n or not. As we show in Appendix D, this requires for a point

Algorithm 1 `Meta Algorithm`

Input: target accuracy ε, error probability δ, functional g parameterized by (α_1, α_2)
Compute (n, m) for $(\varepsilon/2, \delta/2)$-PAC estimation of $g(F)$ based on Theorem 1
Construct active set $A_1 = [n]$, $r = 1$
Define $b_r = 2^{-r}$ and $t_r = \min(m, \lceil 16 b_r^{-2} \log(4n \log(m)/\delta) \rceil)$ for $r \in \mathbb{N}$
for $r = 1, 2, \ldots$ **do**
    Pull each arm in A_r for $t_r - t_{r-1}$ times
    Compute $\hat{\mu}(r)$
    Set $\hat{\eta}_1 = \hat{\mu}_{(\lfloor \alpha_1 n \rfloor)}(r), \hat{\eta}_2 = \hat{\mu}_{(\lfloor \alpha_2 n \rfloor)}(r)$
    Compute $A_{r+1} = \{i : |\hat{\mu}_i(r) - \hat{\eta}_1| \leq b_r \text{ or } |\hat{\mu}_i(r) - \hat{\eta}_2| \leq b_r\}$
    if $t_r \equiv m$ **then**
        Break, exit For loop
    end if
end for
Construct $\hat{S}_n = \{i : \hat{\eta}_1 \leq \hat{\mu}_i(r) \leq \hat{\eta}_2\}$
if $\alpha_1 \equiv \alpha_2$ **then**
    return $\frac{1}{|\hat{S}_n|} \sum_{i \in \hat{S}_n} \hat{\mu}_i(r)$
else
    Draw one observation from each $i \in \hat{S}_n$, construct $\hat{\mu}_i(0)$
    return $\frac{1}{|\hat{S}_n|} \sum_{i \in \hat{S}_n} \hat{\mu}_i(0)$
end if

X_i a number of samples scaling as

$$N(i) = O\left(\min\left(m, \frac{\log(1/\varepsilon)}{\text{dist}^2(X_i, \partial\hat{S}_n)}\right)\right). \tag{4}$$

where ∂A denotes the boundary of a set A. In the limit as $\varepsilon \to 0$ we show that $\mu^{\text{uni}}_{(\lfloor \alpha_1 n \rfloor)} \to F^{-1}(\alpha_1)$ (similarly with η_2). This allows us to state the following theorem.

Theorem 2 (Meta algorithm)**.** *For a functional g satisfying Definition 1, Algorithm 1 provides an (ε, δ)-PAC estimate of $g(F)$ when given the requisite inputs, requiring*

$$\mathbb{E}[M] = O\left(n\mathbb{E}\left[\min\left(m, \frac{\log(1/\varepsilon)}{\textit{dist}^2(X, \partial S)}\right)\right]\right) \tag{5}$$

samples on this success event, where m, n are calculated as in Theorem 1.

Evaluating this expression for the different functionals under their corresponding assumptions yields the stated sample complexity upper bounds.

4 Lower bounds via Wasserstein distance

In this section we derive general lower bounds on the sample complexity of functional estimation for both offline and online algorithms, where two different Wasserstein distances play important roles. These Wasserstein-based lower bounds yield tight results for mean and maximum estimation.

4.1 General lower bounds based on Wasserstein distance

A powerful classical technique for proving minimax lower bounds is Le Cam's two-point method (Le Cam et al., 2000): let F_1 and F_2 be two distributions with $|g(F_1) - g(F_2)| \geq 2\varepsilon$, and p_{π,F_1} and p_{π,F_2} be the probability distributions of all observations queried by policy π under the true population distributions F_1 and F_2, respectively. One version of Le Cam's two-point lower bound (Tsybakov, 2009, Theorem 2.2) gives

$$\inf_{\widehat{g}} \sup_{F \in \{F_1, F_2\}} \mathbb{P}_F(|\widehat{g} - g(F)| \geq \varepsilon) \geq \frac{1}{4}\exp\left(-D_{\text{KL}}(p_{\pi,F_1} \| p_{\pi,F_2})\right).$$

Consequently, to construct a lower bound on the PAC sample complexity of estimating $g(F)$, it suffices to find the largest ε such that there exist F_1, F_2 with $|g(F_1) - g(F_2)| \geq 2\varepsilon$ while $D_{\text{KL}}(p_{\pi,F_1} \| p_{\pi,F_2}) = O(1)$.

A key step in the above analysis is to upper bound the KL divergence $D_{\text{KL}}(p_{\pi,F_1} \| p_{\pi,F_2})$, which differ significantly for offline and online algorithms. For offline algorithms, the learner samples n arms i.i.d. from F with average rewards $X_1, \cdots, X_n \sim F$, and each arm is pulled m times with Gaussian observations. Consequently, $p_{\pi,F} = (\mathbb{E}_{X\sim F}[\mathcal{N}(X, 1/m)])^{\otimes n} = (F * \mathcal{N}(0, 1/m))^{\otimes n}$, where $p^{\otimes n}$ denotes the n-fold product distribution and $*$ denotes the convolution operation. The following lemma presents an upper bound on the KL divergence for offline algorithms.

Lemma 1. *For any offline algorithm π, it holds that*

$$D_{\text{KL}}(p_{\pi,F_1} \| p_{\pi,F_2}) \leq \frac{mn}{2}\mathcal{W}_2^2(F_1, F_2),$$

where $\mathcal{W}_2(P, Q)$ is the Wasserstein-2 distance defined as $\mathcal{W}_2^2(P, Q) = \inf_{\gamma\in\Gamma} \mathbb{E}_{(X,Y)\sim\Gamma}[(X - Y)^2]$, with Γ being the class of all couplings between P and Q.

For online algorithms the distribution $p_{\pi,F}$ is no longer a product distribution as actions can depend on past observations. As a result, the KL divergence becomes larger, but still enjoys an upper bound based on another Wasserstein distance.

Lemma 2. *For any online algorithm π which queries T samples, it holds that*

$$D_{\text{KL}}(p_{\pi,F_1} \| p_{\pi,F_2}) \leq \frac{T}{2}\mathcal{W}_\infty^2(F_1, F_2),$$

where $\mathcal{W}_\infty(P, Q)$ is the Wasserstein-∞ distance: $\mathcal{W}_\infty(P, Q) = \inf_{\gamma\in\Gamma} \operatorname{esssup}_{(X,Y)\sim\Gamma}|X - Y|$, with Γ being the class of all couplings between P and Q.

As $\mathcal{W}_2(P,Q) \le \mathcal{W}_\infty(P,Q)$, the upper bound of Lemma 2 is no smaller than that of Lemma 1, showing the stronger power of online algorithms. The following corollary is then immediate from Lemmas 1 and 2.

Corollary 2.1. *The sample complexity of $(\varepsilon, .1)$-PAC estimation of $g(F)$ is*

$$\Omega(1/\min\{\mathcal{W}_2^2(F_1,F_2) : F_1, F_2 \in \mathcal{F}, |g(F_1) - g(F_2)| \ge 2\varepsilon\})$$

for offline algorithms, and is

$$\Omega(1/\min\{\mathcal{W}_\infty^2(F_1,F_2) : F_1, F_2 \in \mathcal{F}, |g(F_1) - g(F_2)| \ge 2\varepsilon\})$$

for online algorithms.

In the remainder of this section, we show that Corollary 2.1 leads to tight lower bounds for the estimation of mean and maximum, under both offline and online algorithms.

4.2 Lower bounds for mean estimation

Consider two distributions F_1 and F_2 which are Dirac masses supported on $1/2 - \varepsilon$ and $1/2 + \varepsilon$, respectively. Clearly $\mathcal{W}_2(F_1,F_2) = \mathcal{W}_\infty(F_1,F_2) = 2\varepsilon$, which is the best possible as $\mathcal{W}_2(F_1,F_2) \ge |\mathrm{mean}(F_1) - \mathrm{mean}(F_2)| \ge 2\varepsilon$. Corollary 2.1 gives the following lower bounds.

Corollary 2.2. *The $(\varepsilon, .1)$-PAC sample complexity for mean estimation is $\Omega(\varepsilon^{-2})$ for both offline and online algorithms.*

4.3 Lower bounds for maximum estimation

For maximum estimation, the Wasserstein distances $\mathcal{W}_2$ and $\mathcal{W}_\infty$ behave differently, as summarized in the following lemma. Let $\mathcal{F}_\beta$ be the class of densities satisfying Assumption 3.

Lemma 3. *For $\varepsilon \in (0, 1/2)$, it holds that*

$$\begin{aligned}
\min\{\mathcal{W}_2(F_1,F_2) : F_1, F_2 \in \mathcal{F}_\beta, |\max(F_1) - \max(F_2)| \ge 2\varepsilon\} &= O(\varepsilon^{\beta/2+1});\\
\min\{\mathcal{W}_\infty(F_1,F_2) : F_1, F_2 \in \mathcal{F}_\beta, |\max(F_1) - \max(F_2)| \ge 2\varepsilon\} &= O(\varepsilon);\\
\min\{D_{\mathrm{KL}}(F_1 \| F_2) : F_1, F_2 \in \mathcal{F}_\beta, |\max(F_1) - \max(F_2)| \ge 2\varepsilon\} &= O(\varepsilon^{\beta}).
\end{aligned}$$

Note that we have included another term $D_{\mathrm{KL}}(F_1\|F_2)$ in Lemma 3 as it could provide a better lower bound than using $\mathcal{W}_\infty$ if $\beta \ge 2$, for $D_{\mathrm{KL}}(p_{\pi,F_1}\|p_{\pi,F_2}) \le T \cdot D_{\mathrm{KL}}(F_1\|F_2)$ always holds due to the data-processing inequality (i.e. assuming that all arm rewards are clean). Consequently, we have the following corollary on the sample complexity of maximum estimation.

Corollary 2.3. *The $(\varepsilon, .1)$-PAC sample complexity for maximum estimation over $\mathcal{F}_\beta$ is $\Omega(\varepsilon^{-(\beta+2)})$ for offline algorithms, and $\Omega(\varepsilon^{-\max\{\beta,2\}})$ for online algorithms.*

5 Lower bounds via thresholding phenomena

Although the Wasserstein distance based approach in Section 4 provides general lower bounds for both offline and online algorithms, and these lower bounds turn out to be tight for mean and maximum estimation, sometimes this approach can be loose. For example, Lemma 3 shows that using the $\mathcal{W}_\infty$ distance might be looser than using the original KL divergence for maximum estimation. This section provides tight lower bounds for median estimation, revealing a curious thresholding phenomenon.

5.1 Thresholding phenomenon for offline algorithms

To use Le Cam's two-point method to prove the lower bounds for offline algorithms for median estimation, the key quantity in the analysis is the following:

$$\mathrm{KL}_\sigma(\varepsilon) \triangleq \min\{D_{\mathrm{KL}}(F_1 * \mathcal{N}(0,\sigma^2)\|F_2 * \mathcal{N}(0,\sigma^2)) : F_1, F_2 \in \mathcal{F}, |F_1^{-1}(.5) - F_2^{-1}(.5)| \ge 2\varepsilon\}.$$

Its inverse $\mathrm{KL}_\sigma^{-1}(t)$ is often referred to as the modulus of smoothness of the median with respect to the KL divergence under Gaussian convolution. The Wasserstein-based approach to upper bound

$\mathrm{KL}_\sigma(\varepsilon)$ in Lemma 1 is the following: let $\mathcal{W}_{2,\sigma}(\varepsilon)$ be the counterpart of the above quantity with the KL divergence replaced by the Wasserstein-2 distance, Lemma 1 shows that

$$\mathrm{KL}_\sigma(\varepsilon) \le \frac{\mathcal{W}_{2,\sigma}(\varepsilon)^2}{2\sigma^2} = \Theta\left(\frac{\varepsilon^{2.5}}{\sigma^2}\right),$$

an upper bound decreasing continuously with σ, where the proof of the last identity is presented in the appendix. However, this upper bound is not tight, as shown in the following lemma.

Lemma 4. *For $\varepsilon \in (0, 1/4)$, the following characterization of $\mathrm{KL}_\sigma(\varepsilon)$ holds as a function of σ:*

$$\mathrm{KL}_\sigma(\varepsilon) \begin{cases} \in [c_1\varepsilon^2, c_2\varepsilon^2] & \text{if } \sigma \le c\varepsilon^{1/2}, \\ \le C(\theta,\kappa)\varepsilon^\kappa & \text{if } \sigma \ge \varepsilon^{1/2-\theta}, \end{cases}$$

where $\theta \in (0, 1/4), \kappa \in \mathbb{N}$ are arbitrary parameters, and $c, c_1, c_2, C(\theta, \kappa)$ are absolute constants with the last one depending only on (θ, κ).

Lemma 4 shows a thresholding phenomenon as follows: when σ increases from 0 to 1, the quantity $\mathrm{KL}_\sigma(\varepsilon)$ stabilizes at $\Theta(\varepsilon^2)$ whenever $\sigma \lesssim \varepsilon^{1/2}$; however, when σ exceeds this threshold slightly (i.e. $\sigma \gtrsim \varepsilon^{1/2-\theta}$ for any constant $\theta > 0$), this quantity immediately drops to $o(\varepsilon^\kappa)$ for every possible κ. The main intuition behind this thresholding phenomenon is that, if $\sigma = O(\varepsilon^{1/2})$, the "bandwidth" of $F_1 - F_2$ exceeds that of $\mathcal{N}(0, \sigma^2)$, and the convolution is effectively using $\mathcal{N}(0, \sigma^2)$ as a kernel (which keeps polynomials up to order 2) for smoothing $F_1 - F_2$ (which is second-order differentiable). In contrast, when $\sigma \gg \varepsilon^{1/2}$, the "bandwidth" of $F_1 - F_2$ could be smaller than $\mathcal{N}(0, \sigma^2)$, and the convolution is effectively using $F_1 - F_2$ as a kernel (which could keep polynomials up to any desired order) for smoothing $\mathcal{N}(0, 1)$ (which is infinitely-order differentiable). Approximation theory tells us that the latter approximation error could be much smaller than the former, leading to the thresholding phenomenon. We remark that this phenomenon is not captured by using the $\mathcal{W}_2$ distance.

This thresholding phenomenon has an important consequence on the median estimation. By Lemma 4, PAC learning requires that $m = \Omega(\varepsilon^{2\theta-1})$ for any offline algorithm, as otherwise the KL divergence could be made arbitrarily small. When m is large enough, the first line of Lemma 4 then requires $n = \Omega(\varepsilon^{-2})$ to result in a large KL divergence for PAC learning. Consequently, we have the following corollary for median estimation under offline algorithms.

Corollary 2.4. *Fix any $\theta > 0$. The $(\varepsilon, .1)$-PAC sample complexity for median estimation is $\Omega(\varepsilon^{-3+\theta})$ for any offline algorithm.*

5.2 Thresholding phenomenon for online algorithms

To prove the PAC lower bound for online algorithms, one first wonders if the same observation in Lemma 4 could still work. However, a close inspection of the proof reveals an issue: the optimizers (F_1, F_2) in the definition of $\mathrm{KL}_\sigma(\varepsilon)$ are different under the regimes $\sigma = O(\varepsilon^{1/2})$ and $\sigma = \Omega(\varepsilon^{1/2-\theta})$. An online learning algorithm could first identify the right scenario and then choose a proper sample size to tackle the problem, and thus the above lower bound arguments break down.

To resolve this issue, we aim to choose a proper pair of distributions (F_1, F_2) with $|\mathrm{median}(F_1) - \mathrm{median}(F_2)| \ge 2\varepsilon$, and investigate the behavior of $D_{\mathrm{KL}}(F_1 * \mathcal{N}(0, \sigma^2) \| F_2 * \mathcal{N}(0, \sigma^2))$ as a function of σ *with (F_1, F_2) fixed along the line*. The following lemma shows that, even for some fixed pair (F_1, F_2), a similar thresholding phenomenon still holds for the KL divergence.

Lemma 5. *Fix any $\varepsilon, \theta \in (0, 1/4)$, and $\kappa \in \mathbb{N}$. There exists two distributions $F_1, F_2 \in \mathcal{F}$ with $|\mathrm{median}(F_1) - \mathrm{median}(F_2)| \ge 2\varepsilon$, and*

$$D_{\mathrm{KL}}(F_1 * \mathcal{N}(0, \sigma^2) \| F_2 * \mathcal{N}(0, \sigma^2)) \begin{cases} \in [c_1\varepsilon^{3/2}, c_2\varepsilon^{3/2-\theta}] & \text{if } \sigma \le c\varepsilon^{1/2}, \\ \le C(\theta,\kappa)\varepsilon^\kappa & \text{if } \sigma \ge \varepsilon^{1/2-\theta}, \end{cases}$$

where $c, c_1, c_2, C(\theta, \kappa)$ are absolute constants with the last one depending only on (θ, κ).

Compared with Lemma 4, Lemma 5 still shows a similar thresholding phenomenon for the KL divergence when $\sigma \gg \varepsilon^{1/2}$, but the KL divergence becomes larger for small σ due to the additional constraint that (F_1, F_2) is held fixed. Under the choice of (F_1, F_2) in Lemma 5, each arm should be pulled at least $\Omega(\varepsilon^{2\theta-1})$ times, while $\Omega(\varepsilon^{-3/2})$ arms need to be pulled in view of the first line. The following theorem makes the above intuition formal.

Theorem 3. *The $(\varepsilon, .1)$-PAC sample complexity for median estimation is $\Omega(\varepsilon^{-5/2+\theta})$ for any fixed $\theta > 0$ and any online algorithm.*

The formal proof of Theorem 3 is more complicated and requires an explicit computation of the KL divergence $D_{\mathrm{KL}}(p_{\pi,F_1} \| p_{\pi,F_2})$. We relegate the full proof to Appendix F.

6 Conclusion

In this work we studied offline and online algorithms for estimating functionals of distributions, problems arising at the intersection of density estimation and infinite-armed bandits. We developed unified algorithms for estimating the mean, median, maximum, and trimmed mean, providing sample complexity upper bounds. We additionally provide information theoretic lower bounds in these settings, which show that our algorithms are optimal up to logarithmic factors. We emphasize that our lower bound analyses for the cases of median and trimmed mean are fundamentally different from existing approaches for analyzing mean and maximum estimation. This analysis elucidates an interesting thresholding phenomenon of the noise level to distinguish two distributions after Gaussian convolution.

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Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes] Results are stated and properly qualified.
   (b) Did you describe the limitations of your work? [Yes]
   (c) Did you discuss any potential negative societal impacts of your work? [N/A]
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes] All theorem's have clearly stated assumptions
   (b) Did you include complete proofs of all theoretical results? [Yes] All proofs are detailed in the Appendix
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [N/A]
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [N/A]
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