# Fine-grained Analysis for the Phase Transition of Moment Matching, with Application in Infinite-Armed Bandit Problem

Devin Tang

Courant Institute of Mathematical Sciences

2024.10.11

## infinite bandits algorithm

- 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
- We consider a general class of distribution functionals $g(F)$. For the special case of median estimation, we identify a curious thresholding phenomenon

**Goal**

We aim to fine-grained analysis this thresholding behavior for median estimation.

## Indicator Based functionals

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

$$g(F) = \mathbb{E}[X \mid X \in S(F)]$$

for some set $S(F)$, where $X \sim F$. The set $S(F)$ is defined as follows:

$$S(F) = \left[F^{-1}(\alpha_1), F^{-1}(\alpha_2)\right], \quad 0 \leq \alpha_1 \leq \alpha_2 \leq 1.$$

### Functionals For Median

For median case, $\alpha_1 = \alpha_2 = \frac{1}{2}$

## Median Estimation

**Assumption1** There exist constants $c_2 > 0$ such that

- $|F''(x)| \leq c_2 \quad \text{for} \quad |x - \text{median}(F)| \lesssim \sqrt{\varepsilon}$.

**Comment:**

- The assumption precludes the distribution from being dumbbell-shaped.

## Median Estimation

### Le Cam's two-point lower bound

- Let $F_1$ and $F_2$ be two distributions with $|g(F_1) - g(F_2)| \geq 2\varepsilon$,
- Le Cam's two-point lower bound gives:

$$\inf_{\hat{g}} \sup_{F \in \{F_1, F_2\}} \mathbb{P}_F\left(|\hat{g} - g(F)| \geq \varepsilon\right) \geq \frac{1}{4} \exp\left(-\underbrace{D_{\mathrm{KL}}(p_{\pi,F_1} \parallel p_{\pi,F_2})}_{\text{Goal: Upper Bound}}\right).$$

where in the offline algorithm, $p_{\pi,F} = (F * \mathcal{N}(0, 1/m))^{\otimes n}$.

**Key quantity**

Let $\mathcal{F}$ denote the set of distributions satisfying Assumption 2

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

## How to characterize $\mathrm{KL}_\sigma(\varepsilon)$

- (Wang, Y., Baharav, T. Z., Han, Y., Jiao, J., Tse, D. (2022). Beyond the best: Estimating distribution functionals in infinite-armed bandits.) have proved:
  For $\varepsilon \in (0, 1/4)$, $\mathrm{KL}_\sigma(\varepsilon)$ can be characterized as follows:

$$\mathrm{KL}_\sigma(\varepsilon) \in \begin{cases} [C_1\varepsilon^2, C_2\varepsilon^2] & \text{if } \sigma \leq c\varepsilon^{1/2}, \\ \leq C(\theta,\kappa)\varepsilon^{\kappa} & \text{if } \sigma \geq \varepsilon^{1/2-\theta}, \end{cases}$$

  where $\theta \in (0, 1/4)$, $\kappa \in \mathbb{N}$ are arbitrary fixed parameters

## Thresholding Phenomenon

$$\mathrm{KL}_\sigma(\varepsilon) \in \begin{cases} [C_1\varepsilon^2, C_2\varepsilon^2] & \text{if } \sigma \le c\varepsilon^{1/2}, \\ \le C(\theta,\kappa)\varepsilon^\kappa & \text{if } \sigma \ge \varepsilon^{1/2-\theta}, \end{cases}$$

**Intuition behind the thresholding phenomenon:**

- When $\sigma = O(\varepsilon^{1/2})$, 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 Gaussian kernel (which preserves polynomials up to order 2) for smoothing $F_1 - F_2$ .
- 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 preserve polynomials up to any desired order) for smoothing $\mathcal{N}(0,\sigma^2)$.

## Main Result

### Finer characterization

In this project, we improved the result to be following

$$KL_\sigma(\varepsilon) \asymp \begin{cases} \Theta(\varepsilon^2) & \text{if } \varepsilon \geq \sigma^2, \\ \varepsilon^\kappa \exp[-\Theta(\frac{\sigma^2}{\varepsilon})] & \text{if } \sigma^4 < \varepsilon < \sigma^2 \\ \exp[-\Theta\left(\frac{1}{\sqrt{\varepsilon}} \log(\frac{\sigma^4}{\varepsilon})\right)] & \text{if } \varepsilon < \sigma^4 \end{cases}$$

### Note

For the second region, we have not achieved exact characterization.

## Upper Bound

### Characterize Upper bound

We could upper bound $\mathrm{KL}_\sigma(\varepsilon)$, by the its $\chi^2$ distance, similar strategy as (Yihong Wu and Pengkun Yang 2020):

$$KL(P, Q) \leq \chi^2(P, Q) \lesssim \sum_{j \geq 1} \frac{(\Delta_j)^2}{j! \sigma^{2j}}$$

where $P = \mu * N(0, \sigma^2)$, $Q = \nu * N(0, \sigma^2)$, $\mu, \nu$ are two probability measure supported on $[-1, 1]$, and $N(0, \sigma^2)$ is a centered gaussian with variance $\sigma^2$, $\Delta_j$ is the jth moment difference between P and Q

## Proof Sketch For Upper Bound

Proof.

- Write densities of two mixture distributions $\nu * N(0, \sigma^2)$ and $\nu' * N(0, \sigma^2)$ are
  $f(x) = \int \phi(x-u)d\nu(u) = \phi(x)\sum_{j\geq 1} H_j(\frac{x}{\sigma})\frac{m_j(\nu)}{j!}$,
  $g(x) = \int \phi(x-u)d\nu'(u) = \phi(x)\sum_{j\geq 1} H_j(\frac{x}{\sigma})\frac{m_j(\nu')}{j!}$,
- apply Jensen's Inequality and some simplification we have
  $$g(x) \geq \phi(x)\exp(-\sigma^2/2).$$
- $\chi^2(\nu * N(0,\sigma)\|\nu' * N(0,\sigma)) = \int \left(\frac{f(x)-g(x)}{g(x)}\right)^2 dx$
  $\leq e^{\frac{\sigma^2}{2}}\mathbb{E}\left[\left(\sum_{j\geq 1}\frac{H_j(Z)\Delta m_j}{j!\sigma^{2k}}\right)^2\right] = e^{\frac{\sigma^2}{2}}\sum_{j\geq 1}\frac{(\Delta m_j)^2}{j!\sigma^{2k}}$,
  where $Z(0,1)$ and the last step follows from the orthogonality of Hermite polynomials: $\mathbb{E}[H_i(Z)H_j(Z)] = j!\mathbf{1}_{\{i=j\}}$.

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## Proof Sketch For Upper Bound

With previous upper bound model, we now can upper bound $\mathrm{KL}_\sigma(\varepsilon)$ by following strategy:

$$\mathrm{KL}_\sigma(\varepsilon) \lesssim \sum_{j=1}^{\infty} \frac{(m_j(F_1) - m_j(F_2))^2}{\sigma^{2j} j!} \sim \frac{(m_k(F_1) - m_k(F_2))^2}{\sigma^{2k} k!}$$

where we set $m_1(F1) = m_1(F1)...m_{k-1}(F1) = m_{k-1}(F2)$, $supp(F1) = supp(F2) = [-1, 1]$

### Optimization Step

$Vk = \max_f \int_0^1 f(x)dx$

st: $\begin{cases} ||f'||_\infty \preceq 1 \\ \int_{-1}^{1} f(x)x^i dx = 0, \text{for } i = 1...k. \end{cases}$

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# Proof Sketch For Upper Bound

## Duality Step

By setting $g = f'$, optimization problem now becomes:

$Vk = \max_{g} \int_{-1}^{1} g(x)(x \vee 0)dx$

st: $\begin{cases} ||g||_\infty \preceq 1 \\ \int_{-1}^{1} g(x)x^i dx = 0, \text{for } i = 1...k. \end{cases}$

$$Vk = \max_{g} \inf_{a_1,a_2,\dots,a_k} \left[ \int_{-1}^{1} g(x) \left( x \vee 0 - \sum_{i=1}^{k} a_i x^i \right) dx : \|g\|_\infty \preceq 1, \int_{-1}^{1} g(x) x^l dx = 0 \right]$$

$$\leq \inf_{a_1,a_2,\dots,a_k} \max_{g} \left[ \int_{-1}^{1} g(x) \left( x \vee 0 - \sum_{i=1}^{k} a_i x^i \right) dx, \|g\|_\infty \preceq 1 \right]$$

$$\leq \inf_{a_1,a_2,\dots,a_k} \left\| x \vee 0 - \sum_{i=1}^{k} a_i x^i \right\|_{L^1[-1,1]} .$$

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## Proof Sketch For Upper Bound

**$L_1$ estimation step**

By approximation theory $\left\| x \vee 0 - \sum_{i=1}^{k} a_i x^i \right\|_{L^1[-1,1]} \begin{cases} \lesssim \frac{1}{k^{2-\delta}} \\ \gtrsim \frac{1}{k^2} \end{cases}$

By median difference assumption, we required
$t^2 V_k = \frac{t^2}{k^2} \sim V_k(t) \geq \varepsilon$, so we have $t_{\min} = k\sqrt{\varepsilon}$, then:
$\mathrm{KL}_\sigma(\varepsilon) \preceq \frac{(m_k(F1) - m_k(F2))^2}{\sigma^{2k} k!} \leq \frac{(k\sqrt{\varepsilon})^2}{\sigma^{2k} k!} \asymp (\frac{k\varepsilon}{\sigma^2})^k$
We know that $k^* \sim \frac{\sigma^2}{\varepsilon}$, $t^* = \frac{\sigma^2}{\sqrt{\varepsilon}}$, which divide this upper bound into two region for $t^* < 1$ or $t^* > 1$

## Lower Bound

We now construct a strategy for lower bound $\mathrm{KL}_\sigma(\varepsilon)$, by the its Hellinger distance.

$$KL(P,Q) \geq H^2(P,Q) \gtrsim \sum_{j=1}^{(\frac{t}{\sigma})^2} 2^{-j} \frac{\Delta_j^2}{\sigma^{2j} j! e^{\frac{t\sqrt{j}}{\sigma}}} + \sum_{j > \frac{t}{\sigma}^2} \frac{\Delta_j^2}{t^{2j}}$$

Here is proof sketch:

*Proof.*

- Observe $KL(P,Q) \geq H^2(P,Q) \asymp \int (\sqrt{p} - \sqrt{q})^2 \asymp \int \frac{(p-q)^2}{p+q} \geq \frac{(\int f(dp-dq))^2}{\int f^2(dp+dq)} = \sup_f \frac{(\mathbb{E}_p[f]-\mathbb{E}_q[f])^2}{\mathbb{E}_p[f^2]+E_q[f^2]}$
- Then we use Hermite polynomial approximate $(\mathbb{E}_p[f] - \mathbb{E}_q[f])^2$ and $\mathbb{E}_p[f^2]$, $\mathbb{E}_q[f^2]$

□

## Characterize Lower Bound

By Cauchy-Swartz inequality, $\exists\{w_j\}$, then the optimization problem becomes

$$
\begin{aligned}
Vk^* &\geq \max_{w_j} \left(\frac{1}{\sum_{j=0}^k w_j^2 j! \sigma^{2j} A_j(\sigma)}\right)\left(\int_{-t}^{t}\sum_{j=1}^{k} w_j f(x) x^j dx\right)^2 \\
&\geq \max_{w_j} \left(\frac{1}{\sum_{j=0}^k w_j^2 j! \sigma^{2j} A_j(\sigma)}\right)\left(\int_{-t}^{t}(x \vee 0) h(x) dx + (\sum_{j=1}^{k} w_j f(x) x^j dx - \int_{-t}^{t}(x \vee 0) h(x) dx)\right) \\
&\geq \underbrace{\max_{w_j} \left(\frac{1}{\sum_{j=0}^k w_j^2 j! \sigma^{2j} A_j(\sigma)}\right)}_{A}\underbrace{\left(\varepsilon - \|\sum_j w_j x^{j+1} - \max(x,0)\|_{L1[-t,t]}\right)^2}_{B}
\end{aligned}
$$

### $L_1$ estimation

$L_1$ estimation tells us $\|\sum_j w_j x^{j+1} - \max(x,0)\|_{L1[-1,1]} \preceq \frac{1}{k^{2-\delta}}$, and in order to make $B \asymp \varepsilon^2$, we then require $\frac{t^2}{k^2} \asymp \varepsilon$, which means $k \sim \frac{t}{\sqrt{\varepsilon}}$. Approximation theory itself gives us $w_j = O(t^{-j})$

## Characterize Lower Bound

$\varepsilon < \sigma^4$

Then we left with the characterization of A, for $\varepsilon < \sigma^4$:

$$A = \left( \frac{1}{\sum_{j=0}^{k} w_j^2 j! \sigma^{2j} A_j(\sigma)} \right) \geq \frac{1}{(k\sigma^2 t^2)^k} \geq \exp[-\frac{1}{\sqrt{\varepsilon}} \log(\frac{\sigma^4}{\varepsilon})]$$

Combined with upper bound, for this region, we have then proved

$$KL_\sigma(\varepsilon) \asymp \exp[-\Theta\left(\frac{1}{\sqrt{\varepsilon}} \log(\frac{\sigma^4}{\varepsilon})\right)]$$

$\sigma^4 < \varepsilon < \sigma^2$

We conjectured that $KL_\sigma(\varepsilon) \asymp \varepsilon^\kappa \exp[-\Theta(\frac{\sigma^2}{\varepsilon})]$

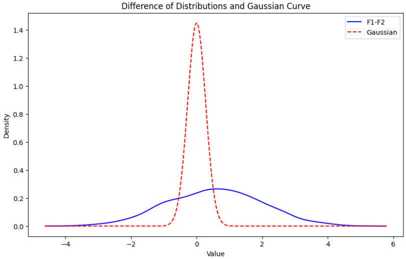
## Future Work

### Local Moment Matching

With small support t, the characterization is more delicate. We observe a following trade-off that ($t \sim \frac{\sigma^2}{\sqrt{\varepsilon}}$)

$$KL(1) \geq \max_t (KL(t) - \exp(-\frac{t^2}{\sigma^2}))$$

Goal: try to find the optimal $t^*$ that balance this trade-off



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