

Characterizing and Approximating the Optimal Allocation for Top-*m* Arm Identification

Master Thesis

Kevin Klein, Johannes Kirschner, Mojmír Mutný, Prof. Dr. Andreas Krause

ETH zürich

Context

• Bandits, arms [k].

- Bandits, arms [k].
- Reward distributions: 1-dimensional exponential family.

- Bandits, arms [k].
- Reward distributions: 1-dimensional exponential family.
- Frequentist setting: true means θ^* and m true best arms $S^* \subset [k]$.

- Bandits, arms [k].
- Reward distributions: 1-dimensional exponential family.
- Frequentist setting: true means θ^* and m true best arms $S^* \subset [k]$.
- Top-*m* arm identification goal: identifying *S** with high confidence and few samples.

- Bandits, arms [k].
- Reward distributions: 1-dimensional exponential family.
- Frequentist setting: true means θ^* and m true best arms $S^* \subset [k]$.
- Top-m arm identification goal: identifying S* with high confidence and few samples.
- Confidence: $\max_{S} \Pr[S \text{ is top-} m | \mathcal{D}_n] \text{ with } S \subset [k] \text{ and } |S| = m.$

- Bandits, arms [k].
- Reward distributions: 1-dimensional exponential family.
- Frequentist setting: true means θ^* and m true best arms $S^* \subset [k]$.
- Top-m arm identification goal: identifying S* with high confidence and few samples.
- Confidence: $\max_{S} \Pr[S \text{ is top-} m | \mathcal{D}_n] \text{ with } S \subset [k] \text{ and } |S| = m.$
- Fixed vs adaptive.

- Bandits, arms [k].
- Reward distributions: 1-dimensional exponential family.
- Frequentist setting: true means θ^* and m true best arms $S^* \subset [k]$.
- Top-m arm identification goal: identifying S* with high confidence and few samples.
- Confidence: $\max_{S} \Pr[S \text{ is top-} m | \mathcal{D}_n] \text{ with } S \subset [k] \text{ and } |S| = m.$
- · Fixed vs adaptive.
- Allocation ψ with $\psi_{n,l} = \Pr[I_n = I]$.

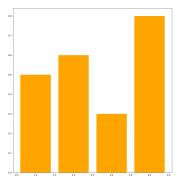


Figure: Arms and their true means θ^* . k = 4.

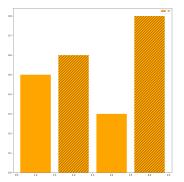


Figure: Arms, their true means θ^* and S^* . k = 4, m = 2.

ETH zürich

Credit

Most of the work is inspired by Daniel Russo's *Simple Bayesian algorithm for Best Arm Identification* ¹.

¹https://arxiv.org/abs/1602.08448

• $\Pr[S^* \text{ is top-}m|\mathcal{D}_n] \to 1 \text{ with } n \to \infty \text{ is not hard.}$

- $\Pr[S^* \text{ is top-}m|\mathcal{D}_n] \to 1 \text{ with } n \to \infty \text{ is not hard.}$
- What's hard: converge optimally fast.

- $\Pr[S^* \text{ is top-} m | \mathcal{D}_n] \to 1 \text{ with } n \to \infty \text{ is not hard.}$
- What's hard: converge optimally fast.
- Goal: Maximize rate at which $\Pr[S^* \text{ is top-} m | \mathcal{D}_n] \to 1$ with $n \to \infty$.

- $\Pr[S^* \text{ is top-} m | \mathcal{D}_n] \to 1 \text{ with } n \to \infty \text{ is not hard.}$
- What's hard: converge optimally fast.
- Goal: Maximize rate at which $\Pr[S^* \text{ is top-} m | \mathcal{D}_n] \to 1$ with $n \to \infty$.
- We prove that for any fixed allocation ψ :

$$\Pr[S^* \text{ is top-} m | \mathcal{D}_n] \tag{1}$$

$$\approx 1 - \exp\{-n \min_{i \notin S^*} \min_{j \in S^*} \min_{x \in \mathbb{R}} \psi_i d_{KL}(\theta_i^*||x) + \psi_j d_{KL}(\theta_j^*||x)\} \quad (2)$$

- $\Pr[S^* \text{ is top-} m | \mathcal{D}_n] \to 1 \text{ with } n \to \infty \text{ is not hard.}$
- What's hard: converge optimally fast.
- Goal: Maximize rate at which $\Pr[S^* \text{ is top-} m | \mathcal{D}_n] \to 1$ with $n \to \infty$.
- We prove that for any fixed allocation ψ :

$$\Pr[S^* \text{ is top-} m | \mathcal{D}_n] \tag{1}$$

$$\approx 1 - \exp\{-n \min_{i \notin S^*} \min_{j \in S^*} \min_{x \in \mathbb{R}} \psi_i d_{KL}(\theta_i^* || x) + \psi_j d_{KL}(\theta_j^* || x)\}$$
 (2)

As a consequence, the optimal minimizes the exponent.

$$\psi^* = \arg\max_{\psi} \min_{i \notin S^*} \min_{j \in S^*} \min_{x \in \mathbb{R}} \psi_i d_{KL}(\theta_i^*||x) + \psi_j d_{KL}(\theta_j^*||x)$$

- $\Pr[S^* \text{ is top-} m | \mathcal{D}_n] \to 1 \text{ with } n \to \infty \text{ is not hard.}$
- What's hard: converge optimally fast.
- Goal: Maximize rate at which $\Pr[S^* \text{ is top-} m | \mathcal{D}_n] \to 1$ with $n \to \infty$.
- We prove that for any fixed allocation ψ :

$$\Pr[S^* \text{ is top-} m | \mathcal{D}_n] \tag{1}$$

$$\approx 1 - \exp\{-n \min_{i \notin S^*} \min_{j \in S^*} \min_{x \in \mathbb{R}} \psi_i d_{KL}(\theta_i^* || x) + \psi_j d_{KL}(\theta_j^* || x)\}$$
 (2)

As a consequence, the optimal minimizes the exponent.

$$\psi^* = \arg\max_{\psi} \min_{i \notin S^*} \min_{j \in S^*} \min_{x \in \mathbb{R}} \psi_i d_{KL}(\theta_i^*||x) + \psi_j d_{KL}(\theta_j^*||x)$$

- $\Pr[S^* \text{ is top-} m | \mathcal{D}_n] \to 1 \text{ with } n \to \infty \text{ is not hard.}$
- What's hard: converge optimally fast.
- Goal: Maximize rate at which $\Pr[S^* \text{ is top-} m | \mathcal{D}_n] \to 1$ with $n \to \infty$.
- We prove that for any fixed allocation ψ :

$$\Pr[S^* \text{ is top-}m|\mathcal{D}_n] \tag{1}$$

$$\approx 1 - \exp\{-n \min_{\substack{i \notin S^* \ j \in S^* \\ \mathbf{x} \in \mathbb{R}}} \min_{\substack{k \in \mathbb{R} \\ \mathbf{x} \in \mathbb{R}}} \psi_i d_{KL}(\theta_i^* || \mathbf{x}) + \psi_j d_{KL}(\theta_j^* || \mathbf{x})\}$$
 (2)

As a consequence, the optimal minimizes the exponent.

$$\psi^* = \arg\max_{\psi} \min_{i \notin S^*} \min_{j \in S^*} \min_{x \in \mathbb{R}} \psi_i d_{KL}(\theta_i^*||x) + \psi_j d_{KL}(\theta_j^*||x)$$

Evidence for distinction

$$\bullet \ \ C_{j,i}(\psi_j,\psi_i) = \min\nolimits_{x \in \mathbb{R}} \psi_i d_{\mathit{KL}}(\theta_i^*||x) + \psi_j d_{\mathit{KL}}(\theta_j^*||x)$$

Evidence for distinction

- $C_{j,i}(\psi_j, \psi_i) = \min_{x \in \mathbb{R}} \psi_i d_{KL}(\theta_i^*||x) + \psi_j d_{KL}(\theta_i^*||x)$
- \bullet Distinction comprises both frequency ψ and distance of values, captured by KL divergence.

Characterization

Theorem (Characterization of optimal allocation)

There is a unique fixed allocation ψ^* maximizing the convergence rate of the posterior mass put on the true best arms. It enforces that:

$$\forall j_1, j_2 \in S^*, \forall i_1, i_2 \notin S^* : C_{j,i}(\psi_{j_1}^*, \psi_{i_1}^*) = C_{j,i}(\psi_{j_2}^*, \psi_{i_2}^*)$$

Characterization

Theorem (Characterization of optimal allocation)

There is a unique fixed allocation ψ^* maximizing the convergence rate of the posterior mass put on the true best arms. It enforces that:

$$\forall j_1, j_2 \in \mathcal{S}^*, \forall i_1, i_2 \notin \mathcal{S}^* : C_{j,i}(\psi_{j_1}^*, \psi_{i_1}^*) = C_{j,i}(\psi_{j_2}^*, \psi_{i_2}^*)$$

This leads to a slightly simpler convergence rate for the optimal allocation:

$$\Pr[S^* \text{ is top-} m | \mathcal{D}_n] \approx 1 - \exp\{-n \ C_{j,i}(\psi_j^*, \psi_i^*)\}$$

for any $j \in S^*$, $i \notin S^*$.

Example: Setup

• Top-4.

Example: Setup

- Top-4.
- Given true underlying means:

$$\theta^1 = [.1, .2, .3, .4, .5, \underbrace{.6, .7, .8, .9}_{S^*}]$$
 (3)

$$\theta^2 = [.4, .425, .45, .475, .5, .525, .55, .575, .6]$$
 (4)

Example: Setup

- Top-4.
- Given true underlying means:

$$\theta^1 = [.1, .2, .3, .4, .5, \underbrace{.6, .7, .8, .9}_{S^*}]$$
 (3)

$$\theta^2 = [.4, .425, .45, .475, .5, \underbrace{.525, .55, .575, .6}_{S^*}]$$
 (4)

• Overdetermined system of equations: Find ψ such that $\forall j_1, j_2 \in S^*, \forall i_1, i_2 \notin S^* : C_{j,i}(\psi_{j_1}, \psi_{i_1}) = C_{j,i}(\psi_{j_2}, \psi_{i_2}).$

Example: Resulting allocation

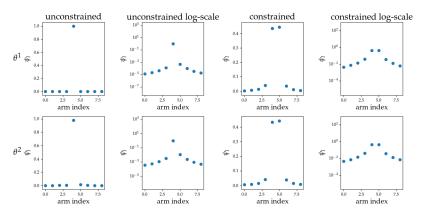


Figure: Unconstrained and constrained optimal allocation for θ^1 and θ^2 , top-4.

DINFK

Adaptive.



- · Adaptive.
- Simple.

- · Adaptive.
- Simple.
- Bayesian (remember: confidence).



- Adaptive.
- Simple.
- Bayesian (remember: confidence).
- Asymptotic consistency.

- Adaptive.
- Simple.
- Bayesian (remember: confidence).
- Asymptotic consistency.
- Based on Thompson sampling and another layer of randomization.

- Adaptive.
- Simple.
- Bayesian (remember: confidence).
- Asymptotic consistency.
- Based on Thompson sampling and another layer of randomization.
- Idea: Always sample two distinct candidates.

- · Adaptive.
- Simple.
- Bayesian (remember: confidence).
- Asymptotic consistency.
- Based on Thompson sampling and another layer of randomization.
- Idea: Always sample two distinct candidates.
- · Goal: Convergence towards optimal fixed allocation.

TXTS: Algorithm

Algorithm 1 TXTS: Given a posterior Π_{n-1} in step n.

$$\hat{\theta} \sim \Pi_{n-1}$$
 $S_1 = \text{top-}m(\hat{\theta})$

repeat
$$\hat{\theta} \sim \Pi_{n-1}$$
 $S_2 = \text{top-}m(\hat{\theta})$

until $S_1 \neq S_2$
 $I_n \sim \mathcal{U}(S_1 \oplus S_2)$

Play I_n , observe reward and update posterior.

DINFK

TXTS: Exemplary candidates

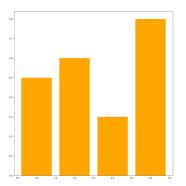


Figure: Arms and their true means θ^* . k = 4.

TXTS: Exemplary candidates

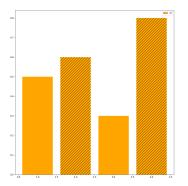


Figure: Arms, their true means θ^* and S_1 . k = 4, m = 2.

TXTS: Exemplary candidates

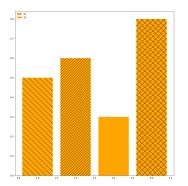


Figure: Arms, their true means θ^* , S_1 and S_2 . k = 4, m = 2.

• Bernoulli rewards.

- Bernoulli rewards.
- Beta posteriors, $\alpha = \beta = 1$.

- Bernoulli rewards.
- Beta posteriors, $\alpha = \beta = 1$.
- Top-4.

- · Bernoulli rewards.
- Beta posteriors, $\alpha = \beta = 1$.
- Top-4.
- $\theta^* = [.1, .2, .3, .4, .5, \underbrace{.6, .7, .8, .9}_{S^*}]$

TXTS: Evidence collection

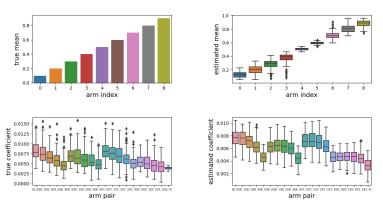


Figure: Top row: true and estimated θ . Bottom row: true and estimated coefficients $C_{j,i}$. 2000 steps, 150 seeds.

TXTS: Empricial average allocation comparison

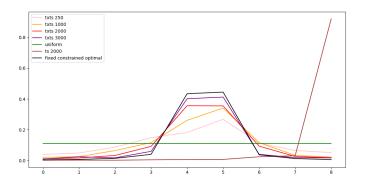


Figure: Comparison of allocations for different methods and numbers of samples. 50 seeds.

DINFK

• Allocation ψ hard to explicitly express in closed form.

DINFK

- Allocation ψ hard to explicitly express in closed form.
- Established bounds on ψ .

- Allocation ψ hard to explicitly express in closed form.
- Established bounds on ψ .
- Proven $\Pr[S^* \text{ is top-} m | \mathcal{D}_n] \to 1$.

- Allocation ψ hard to explicitly express in closed form.
- Established bounds on ψ .
- Proven $\Pr[S^* \text{ is top-} m | \mathcal{D}_n] \to 1$.
- Proven $\sum_{j \in S^*} \psi_{n,S^*} \to \frac{1}{2}$.

- Allocation ψ hard to explicitly express in closed form.
- Established bounds on ψ .
- Proven $\Pr[S^* \text{ is top-} m | \mathcal{D}_n] \to 1$.
- Proven $\sum_{j \in S^*} \psi_{n,S^*} \to \frac{1}{2}$.
- Proven that if converged on S^* , then convergence on S^{*c} and vice versa.

- Allocation ψ hard to explicitly express in closed form.
- Established bounds on ψ .
- Proven $\Pr[S^* \text{ is top-} m | \mathcal{D}_n] \to 1$.
- Proven $\sum_{j \in S^*} \psi_{n,S^*} \to \frac{1}{2}$.
- Proven that if converged on S*, then convergence on S*c and vice versa.
- Proven some more technical statements.

TXTS: Theoretical outlook

Prove overall convergence, i.e. $\frac{1}{N} \sum_{n \in [N]} \psi \to \psi^*$.

Thanks!

Appendix.

DINFK

1-d exponential family

- They have a scalar parameter θ .
- They come with the definition of functions T(x), $\nu(\theta)$, h(x) and $A(\theta)$. T corresponds to the sufficient statistic and A to the log-partition function.
- The probability density function is defined by:

$$f_X(x|\theta) = h(x) \exp(\nu(\theta)T(x) - A(\theta))$$

- They have conjugate priors.
- Bernoulli, binomial with known number of trials, Poisson, exponential, Pareto with known minimal value, chi-squared, normal distribution with known variance and more.

Logarithmic equivalence

Convergence is reasoned about in $a \doteq$ sense, with:

$$a_n = b_n \Leftrightarrow \lim_{n \to \infty} \frac{1}{n} \log \frac{a_n}{b_n} \to 0$$
 (5)

Computing evidence

The Bernoulli assumption allows us to solve the minimization over x analytically.

$$d(\theta_I||x) = \theta_I \log(\frac{\theta_I}{x}) + (1 - \theta_I) \log(\frac{1 - \theta_I}{1 - x})$$
 (6)

$$x_0 = \frac{\psi_j \theta_j + \psi_i \theta_i}{\psi_j + \psi_i} \tag{7}$$

TXTS: Increase in confidence

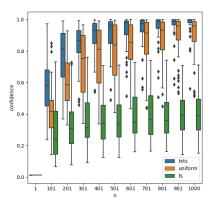


Figure: Confidence per steps for TXTS, uniform and Thompson sampling.

50 seeds.

TXTS: Empirical average allocation

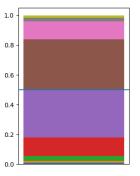


Figure: TXTS empirical average allocation after 1000 steps. Arms ordered by true mean. 50 seeds.

DINFK

Theorem (Sufficient condition for optimality)

lf

$$\forall I \in [k], \delta > 0: \sum_{n \in \mathbb{N}} \psi_{n,I} \mathbb{I}[\bar{\psi}_{n,I} \ge \psi_I^* + \delta] < \infty$$
 (8)

then $\bar{\psi}_n \to \psi^*$.