Improving the Knowledge Gradient Algorithm

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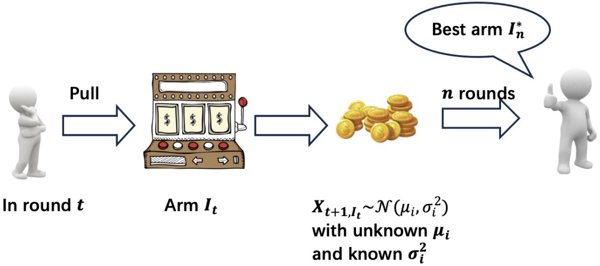
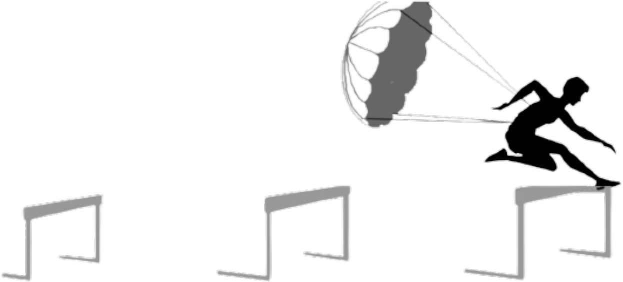
Best Arm Identification (BAI) Problem



Goal: Identify the best arm I^* (unique), i.e., the arm with the largest mean reward.

Contributions

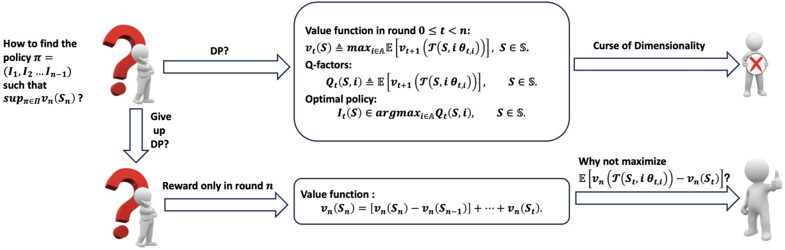


Propose iKG algorithm, which pulls the arm that yields the greatest one-step improvement in the probability of selecting the best arm.

iKG algorithm is asymptotically optimal.

iKG is more general and can be more easily extended to variant problems of BAI, such as ϵ-good arm identification and feasible arm identification

One-step Look Ahead Algorithm



Motivation

Our goal is identifying the best arm $I^* = argmax_{i \in \mathbb{A}} \mu_i$, and designing an algorithm with the fastest posterior convergence rate of $1 - \mathbb{P}(I_n^* = I^*)$ the probability that the best arm is falsely selected.

How to define $v_n(S_n)$?

KG algorithm: $v_n(S_n) = \mu_{I_n^*}$.

one-step Improvement:

$$KG_{t,i} = \mathbb{E}[max\{\mathcal{T}(\mu_{t,i}, i\ \theta_{t,i}), max_{i' \neq i}\mu_{t,i'}\} - max_{i \in \mathbb{A}}\mu_{t,i}]$$

convergence rate?

Proposition 1. *Let* $c_{\langle i\rangle} = \frac{(\mu_{\langle 1\rangle} - \mu_{\langle i\rangle})/\sigma_{\langle i\rangle}}{(\mu_{\langle 1\rangle} - \mu_{\langle 2\rangle})/\sigma_{\langle 2\rangle}}$, $i = 2, \ldots, k$. *For the KG algorithm,*

$$\lim_{n\to\infty} -\frac{1}{n}\log(1 - \mathbb{P}\{I_n^* = I^*\}) = \Gamma^{KG},$$

where

$$\Gamma^{KG} = \min_{i\neq 1}\left(\frac{(\mu_{\langle i\rangle} - \mu_{\langle 1\rangle})^2}{2((\sum_{i\neq 1}\sigma_{\langle 2\rangle}/c_{\langle i\rangle} + \sigma_{\langle 1\rangle})\sigma_{\langle 1\rangle} + c_{\langle i\rangle}\sigma_{\langle i\rangle}^2(\sum_{i\neq 1} 1/c_{\langle i\rangle} + \sigma_{\langle 1\rangle}/\sigma_{\langle 2\rangle}))}\right).$$

Is Γ^{KG} optimal?

Proposition 2. *For the TTEI algorithm (Qin et al. 2017), the rate of posterior convergence of* $1 - \mathbb{P}\{I_n^* = I^*\}$ *exists and is denoted as* Γ^{TTEI}. *Let its probability of sampling the best arm* $\beta = (\sigma_{\langle 2\rangle}/\sigma_{\langle 1\rangle}\sum_{i\neq 1} 1/c_{\langle i\rangle} + 1)^{-1}$. *We have* $\Gamma^{KG} \leq \Gamma^{TTEI}$.

Γ^{KG} is not optimal.

Why not define $v_n(S_n) = \mathbb{I}(I_n^* = I^*)$? Then $\mathbb{E}[v_n(S_n)] = \mathbb{P}(I_n^* = I^*)$ directly.

Derivation of Improved Knowledge Gradient Algorithm

Introduction of the Improved Knowledge Gradient Algorithm (iKG)

How to analyze $\mathbb{P}(I_n^* = I^*)$?

$$\mathbb{P}\{I_n^* = I^*\} = \mathbb{P}\left\{ \bigcap_{i \neq I_n^*} (\theta_{I_n^*} > \theta_i) \right\} = 1 - \mathbb{P}\left\{ \bigcup_{i \neq I_n^*} (\theta_i > \theta_{I_n^*}) \right\}.$$

By Bonferroni inequality

$$\mathbb{P}\left\{ \bigcup_{i \neq I_n^*} (\theta_i > \theta_{I_n^*}) \right\} \leq \sum_{i \neq I_n^*} \mathbb{P}(\theta_i > \theta_{I_n^*}),$$

Asymptotic analytic expression

$$\mathbb{E}[v_n(S_n)] \approx 1 - \sum_{i \neq I_n^*} \mathbb{P}(\theta_i > \theta_{I_n^*}) = 1 - \sum_{i \neq I_n^*} \exp\left(\frac{(\mu_{n,i} - \mu_{n,I_n^*})^2}{2(\sigma_{n,i}^2 + \sigma_{n,I_n^*}^2)} \right)$$

one-step Improvement:

$$iKG_{t,i} = \begin{cases} \exp\left(-\frac{(\mu_{t,i} - \mu_{t,I_t^*})^2}{2(\sigma_{t,i}^2 + \sigma_{t,I_t^*}^2)}\right) - \exp\left(-\frac{(\mu_{t,i} - \mu_{t,I_t^*})^2}{2(\sigma_{t+1,i}^2 + \sigma_{t,I_t^*}^2 + \sigma_i^2(\sigma_{t+1,i}^2/\sigma_i^2)^2)}\right), & if\ i \neq I_t^*, \\ \sum_{i' \neq I_t^*} \exp\left(-\frac{(\mu_{t,i'} - \mu_{t,I_t^*})^2}{2(\sigma_{t,i'}^2 + \sigma_{t,I_t^*}^2)}\right) - \sum_{i' \neq I_t^*} \exp\left(-\frac{(\mu_{t,i'} - \mu_{t,I_t^*})^2}{2(\sigma_{t,i'}^2 + \sigma_{t+1,I_t^*}^2 + \sigma_{I_t^*}^2(\sigma_{t+1,I_t^*}^2/\sigma_{I_t^*}^2)^2)}\right), & if\ i = I_t^*. \end{cases}$$

Pull arm $I_t = argmax_{i \in \mathbb{A}} iKG_{t,i}$, In round t

Algorithm Description:

Algorithm 1 iKG Algorithm

Input: $k \geq 2$, n.
Collect n_0 samples for each arm i.
for $t = 0$ **to** $n - 1$ **do**
  Compute $\text{iKG}_{t,i}$ and set $I_t = \text{argmax}_{i \in \mathbb{A}} \text{iKG}_{t,i}$.
  Play I_t.
  Update $\mu_{t+1,i}$, $\sigma_{t+1,i}$ and I^*_{t+1}
  $t \leftarrow t + 1$.
end for
Output: I^*_n.

Theorem

For the iKG algorithm, $\lim_{n\to\infty} -\frac{1}{n}\log(1-\mathbb{P}\{I_n^* = I^*\}) = \Gamma^{iKG}$, *where*

$$\Gamma^{iKG} = \frac{(\mu_{\langle i\rangle} - \mu_{\langle 1\rangle})^2}{2(\sigma^2_{\langle i\rangle}/w_{\langle i\rangle} + \sigma^2_{\langle 1\rangle}/w_{\langle 1\rangle})},$$

and w_i *is the sampling rate of arm* i *satisfying*

$$\sum_{i=1}^{k} w_i = 1, \qquad \frac{w^2_{\langle 1\rangle}}{\sigma^2_{\langle 1\rangle}} = \sum_{i=2}^{k} \frac{w^2_{\langle i\rangle}}{\sigma^2_{\langle i\rangle}}, \quad \text{and}$$

$$\frac{(\mu_{\langle i\rangle} - \mu_{\langle 1\rangle})^2}{2(\sigma^2_{\langle i\rangle}/w_{\langle i\rangle} + \sigma^2_{\langle 1\rangle}/w_{\langle 1\rangle})} = \frac{(\mu_{\langle i'\rangle} - \mu_{\langle 1\rangle})^2}{2(\sigma^2_{\langle i'\rangle}/w_{\langle i'\rangle} + \sigma^2_{\langle 1\rangle}/w_{\langle 1\rangle})}, \quad i \neq i' \neq 1.$$

In addition, for any BAI algorithms,

$$\limsup_{n\to\infty} -\frac{1}{n}\log(1-\mathbb{P}\{I_n^* = I^*\}) \leq \Gamma^{iKG}.$$

Numerical Results

Table: Probabilities of false selection for the tested algorithms in best arm identification problem.

Example		Example 1		Example 2		Example 3		Dose-finding		Drug Selection		Caption 853		Caption 854	
Algorithms \ Sample size		1000	5000	4400	18000	400	1000	1200	13000	2400	98000	1600	3000	12000	18000
BAI	Equal Allocation	0.38	0.22	0.44	0.31	0.25	0.13	0.35	0.05	0.43	0.27	0.17	0.11	0.26	0.18
	EI	0.36	0.21	0.40	0.28	0.28	0.22	0.46	0.21	0.46	0.37	0.14	0.12	0.26	0.23
	TTEI	0.25	0.07	0.32	0.09	0.13	0.02	0.31	0.03	0.55	0.28	0.04	0.01	0.10	0.06
	KG	0.29	0.14	0.32	0.13	0.14	0.03	0.40	0.03	0.44	0.28	0.04	0.01	0.11	0.05
	iKG	0.21	0.03	0.23	0.03	0.09	0.01	0.29	0.01	0.38	0.23	0.02	0.00	0.07	0.04

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