A Tale of Top Two Algorithms

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Ínnía -

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The stochastic Multi Armed Bandit (MAB) model

- *K* unknown distributions ν_1, \ldots, ν_K called arms
- a time t, select an arm A_t and collect an observation $X_t \sim
 u_{A_t}$



Sequential strategy / algorithm : A_{t+1} can depend on:

- previous observation $A_1, X_1, \ldots, A_t, X_t$
- some external randomization $U_t \sim \mathcal{U}([0,1])$
- some knowledge about the possible distributions: ν_a ∈ D
 [Thompson, 1933, Robbins, 1952, Lattimore and Szepesvari, 2019]

Two classical bandit problems

Example: A/B/n testing



 p_a : probability that a visitor seeing version *a* buys a product

 p_2

For the *t*-th visitor:

• choose a version A_t to display

 p_1

• observe $X_t = 1$ if a product is bought, 0 otherwise

Objective 1: observation = reward \rightarrow maximize rewards

- maximize $\mathbb{E}[\sum_{t=1}^{T} X_t]$ for some (possibly unknown) T
- maximize profit

a reinforcement learning problem

*p*_K

Two classical bandit problems

Example: A/B/n testing



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For the *t*-th visitor:

• choose a version A_t to display

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• observe $X_t = 1$ if a product is bought, 0 otherwise

Objective 2: best arm identification

- identify quickly $a_{\star} = \arg \max_{a} p_{a}$
- find the best version (in order to keep displaying it)

an *adaptive testing* problem

*p*_K

Other applications

• clinical trials \rightarrow observation: success/failure (Bernoulli)



• movie recommendation \rightarrow observation: rating (multinomial)



• website optimization \rightarrow observation: amount of money spent (Gaussian distribution?)

Other applications

• recommendation in agriculture \rightarrow reward: yield (complex bounded distribution)



Distribution of the yield of a maize field for different planting dates obtained using the OSSAT crop-yield simulator

1 Thompson Sampling for Rewards Maximization

2 Thompson Sampling for Best Arm Identification?

3 Top Two Algorithms Beyond Thompson Sampling

Performance measure

$$\boldsymbol{\nu} = (\nu_1, \dots, \nu_K) \quad \mu_{\boldsymbol{a}} = \mathbb{E}_{\boldsymbol{X} \sim \nu_{\boldsymbol{a}}}[\boldsymbol{X}]$$

$$\mu_{\star} = \max_{a \in \{1, \dots, K\}} \mu_a \qquad a_{\star} = \underset{a \in \{1, \dots, K\}}{\arg \max} \mu_a.$$

 $\begin{array}{rcl} \text{Maximizing rewards} & \leftrightarrow & \text{selecting } a_{\star} \text{ as much as possible} \\ & \leftrightarrow & \text{minimizing the regret [Robbins, 52]} \end{array}$

$$\mathcal{R}_{\nu}(\mathcal{A}, T) = \underbrace{\mathcal{T}\mu_{\star}}_{\substack{\text{sum of rewards of} \\ \text{an oracle strategy} \\ \text{always selecting } a_{\star}} - \underbrace{\mathbb{E}_{\nu}\left[\sum_{t=1}^{T} X_{t}\right]}_{\substack{\text{sum of rewards of} \\ \text{the strategy } A}}$$

Regret decomposition

$$\mathcal{R}_{oldsymbol{
u}}(\mathcal{A},\mathcal{T}) = \mathbb{E}_{oldsymbol{
u}}\left[\sum_{t=1}^{\mathcal{T}}(\mu_{\star}-\mu_{A_t})
ight]$$

 $N_a(T)$: number of selections of arm a up to round T.

Performance measure

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Regret decomposition

$$\mathcal{R}_{\nu}(\mathcal{A},T) = \sum_{a=1}^{K} \mathbb{E}_{\nu}[N_{a}(T)](\mu_{\star} - \mu_{a})$$

 $N_a(T)$: number of selections of arm *a* up to round *T*.

Under an algorithm achieving small regret for any bandit model $\nu\in\mathcal{D}^{K},$ it holds that

$$\forall a \neq a_{\star}(\boldsymbol{\nu}), \quad \liminf_{T \to \infty} \frac{\mathbb{E}_{\boldsymbol{\nu}}[N_{a}(T)]}{\log(T)} \geq \frac{1}{\mathcal{K}_{\inf}^{\mathcal{D}}(\nu_{a}; \mu_{\star})}$$

where

$$\mathcal{K}^{\mathcal{D}}_{\mathsf{inf}}(\nu;\mu) = \mathsf{inf}\left\{ \left. \mathrm{KL}(\nu,\nu') \right| \nu' \in \mathcal{D} : \mathbb{E}_{X \sim \nu'}[X] \geq \mu \right\}$$

with $KL(\nu, \nu')$ the Kullback-Leibler divergence.

Gaussian bandits

$$egin{aligned} \mathcal{D} &= ig\{\mathcal{N}(\mu,\sigma^2),\mu\in\mathbb{R}ig\} \ \mathcal{K}^{\mathcal{D}}_{\mathsf{inf}}(\mathcal{N}(\mu,\sigma^2);\mu') &= rac{(\mu-\mu')^2}{2\sigma^2} \end{aligned}$$

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Bernoulli bandits $\mathcal{D} = \{\mathcal{B}(\mu), \mu \in [0, 1]\}$ $\mathcal{K}_{\mathsf{inf}}^{\mathcal{D}}(\mathcal{B}(\mu); \mu') = \mu \log \frac{\mu}{\mu'} + (1 - \mu) \log \frac{1 - \mu}{1 - \mu'}$

Under an algorithm achieving small regret for any bandit model $\nu \in \mathcal{D}^{K},$ it holds that

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Single Parameter Exponential Family (SPEF)

$$\mathcal{D} = \{\nu_{\mu}, \mu \in \mathcal{I}\}$$
$$\mathcal{K}_{\mathsf{inf}}^{\mathcal{D}}(\nu_{\mu}; \mu') = \mathrm{KL}\left(\nu_{\mu}, \nu_{\mu'}\right)$$

Under an algorithm achieving small regret for any bandit model $\nu \in \mathcal{D}^{K},$ it holds that

$$\forall a \neq a_{\star}(\boldsymbol{\nu}), \quad \liminf_{T \to \infty} \frac{\mathbb{E}_{\boldsymbol{\nu}}[N_{a}(T)]}{\log(T)} \geq \frac{1}{\mathcal{K}_{\inf}^{\mathcal{D}}(\nu_{a}; \mu_{\star})}$$

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with $KL(\nu, \nu')$ the Kullback-Leibler divergence.

Bounded distributions $\mathcal{D}_B = \{\nu, \nu \text{ supported in } [0, B]\}$

 $\mathcal{K}_{\mathsf{inf}}^{\mathcal{D}_{\mathcal{B}}}(
u;\mu')=$ non explicit, but computable

Select each arm once, then exploit the current knowledge:

```
A_{t+1} = \underset{a \in [K]}{\operatorname{arg max}} \hat{\mu}_a(t)
```

where

N_a(t) = ∑^t_{s=1} 1(A_s = a) is the number of selections of arm a
 μ̂_a(t) = 1/N_a(t) ∑^t_{s=1} X_s1(A_s = a) is the empirical mean of the rewards collected from arm a

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Follow the leader can fail! $\nu_1 = \mathcal{B}(\mu_1), \nu_2 = \mathcal{B}(\mu_2), \ \mu_1 > \mu_2$

$$\mathbb{E}[N_2(T)] \ge (1-\mu_1)\mu_2 \times (T-1)$$

→ Exploitation is not enough, we need to add some exploration

A Bayesian algorithm: Thompson Sampling

 $\pi_a(0)$: prior distribution on μ_a $\pi_a(t) = \mathcal{L}(\mu_a | Y_{a,1}, \dots, Y_{a,N_a(t)})$: posterior distribution on μ_a



Two equivalent interpretations:

- [Thompson, 1933]: "randomize the arms according to their posterior probability of being optimal"
- modern view: "draw a possible bandit model from the posterior distribution and act optimally in this sampled model"

Russo et al. 2018, A Tutorial on Thompson Sampling

A Bayesian algorithm: Thompson Sampling

Input: a prior distribution $\pi(0)$

$$\begin{cases} \forall a \in \{1..K\}, \quad \widetilde{\theta}_{a}(t) \sim \pi_{a}(t) \\ A_{t+1} = \operatorname*{argmax}_{a=1..K} \widetilde{\theta}_{a}(t). \end{cases}$$

Thompson Sampling for Bernoulli distributions

$$u_{\mathsf{a}} = \mathcal{B}(\mu_{\mathsf{a}})$$

•
$$\pi_a(0) = \mathcal{U}([0,1])$$

•
$$\pi_a(t) = \text{Beta}(S_a(t) + 1; N_a(t) - S_a(t) + 1)$$



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Thompson Sampling for Gaussian distributions $\nu_a = \mathcal{N}(\mu_a, \sigma^2)$

•
$$\pi_a(0) \propto 1$$

• $\pi_a(t) = \mathcal{N}\left(\hat{\mu}_a(t); \frac{\sigma^2}{N_a(t)}\right)$

For different Single Parameter Exponential Families, TS with a conjugate prior satisfy the following:

Upper bound on sub-optimal selections

$$\forall a \neq a_{\star}, \ \mathbb{E}_{\mu}[N_{a}(T)] \leq rac{\log(T)}{\operatorname{KL}(
u_{\mu_{a}},
u_{\mu_{\star}})} + o_{\mu}(\log(T)).$$

→ matching the lower bound! TS is asymptotically optimal

[Kaufmann et al., 2012, Agrawal and Goyal, 2013, Korda et al., 2013]

the best arm (arm 1) has to be drawn a lot
probability of selecting a sub-optimal arm a:

$$\begin{split} \mathbb{P}(A_t = a | \mathcal{F}_{t-1}) &= \mathbb{P}\left(\widetilde{\theta}_a(t) = \max_i \widetilde{\theta}_i(t) | \mathcal{F}_{t-1}\right) \\ &\simeq \mathbb{P}\left(\widetilde{\theta}_a(t) \ge \widetilde{\theta}_1(t) | \mathcal{F}_{t-1}\right) \\ &\simeq \mathbb{P}\left(\widetilde{\theta}_a(t) \ge \mu_1 | \mathcal{F}_{t-1}\right) \end{split}$$

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For Gaussian bandits $\tilde{\theta}_{a}(t)|\mathcal{F}_{t-1} = \mathcal{N}(\hat{\mu}_{a}(t), \sigma^{2}/N_{a}(t))$, thus

$$\begin{split} \mathbb{P}(A_t = a | \mathcal{F}_{t-1}) &\simeq & \mathbb{P}\left(X \geq \frac{\sqrt{N_a(t)}(\mu_1 - \hat{\mu}_a(t))}{\sigma}\right) \\ &\leq & \exp\left(-\frac{N_a(t)(\hat{\mu}_a(t) - \mu_1)^2}{2\sigma^2}\right) \end{split}$$

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$$\mathbb{P}(A_t = a | \mathcal{F}_{t-1}) \leq rac{1}{T} \;\; \Rightarrow \;\; N_a(t) \simeq rac{\log(T)}{\operatorname{KL}(\hat{\mu}_a(t), \mu_1)}$$

Beyond Parametric Distributions

[Riou and Honda, 2020] : NPTS for Bounded distributions $\mathcal{D}_B = \{\nu: \nu \text{ is support in } [0, B]\}$

Non Parametric Thompson Sampling

$$A_{t+1} = \mathop{\mathrm{arg\,max}}_{a \in [K]} \widetilde{ heta}_a(t)$$

where

$$\widetilde{\theta}_{a}(t) = \frac{1}{N_{a}(t)+1} \left(\sum_{i=1}^{N_{a}(t)} w_{i}^{(a)} Y_{a,i} + w_{N_{a}(t)+1}^{(a)} B \right)$$

with

(Y_{a,1},...,Y_{a,Na(t)}, B) is the augmented history of observations gathered from arm a

•
$$w^{(a)} \sim \operatorname{Dir}(\underbrace{1, \ldots, 1}_{N_a(t)+1})$$
 a random probability vector

→ TS is asymptotically optimal for bounded distributions!

Thompson Sampling for Rewards Maximization

2 Thompson Sampling for Best Arm Identification?

3 Top Two Algorithms Beyond Thompson Sampling

Algorithm: made of three components:

- \rightarrow sampling rule: A_t (arm to explore)
- → recommendation rule: \hat{a}_t (current guess for the best arm)
- → (optional) stopping rule τ (when do we stop exploring?)

• Settings studied in the literature:

Fixed-confidence	Fixed-budget	Anytime		
input: error bound δ	input: budget T			
min. $\mathbb{E}[\tau]$	au = T	$orall t \in \mathbb{N}$,		
$\mathbb{P}(\hat{\pmb{a}}_ au eq \pmb{a}_{\star}) \leq \delta$	min. $\mathbb{P}(\hat{a}_T eq a_\star)$	min. $\mathbb{P}(\hat{a}_t eq a_\star)$		
[Even-Dar et al., 2006]	[Audibert et al., 2010]	[Bubeck et al., 2011]		

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Can Thompson Sampling find the best arm?

 \hat{a}_T : guess for the best arm after T samples.

Thompson Sampling selects a lot the best arm...

- idea (1): $\hat{a}_T = \arg \max_a N_a(T)$
- idea (2) : $\mathbb{P}(\hat{a}_T = a | \mathcal{F}_T) = \frac{N_a(T)}{T}$

Thompson Sampling + (2):

$$\mathbb{E}[\mu_{\star} - \mu_{\hat{a}_{\tau}}] = \mathbb{E}\left[\sum_{a=1}^{K} (\mu_{\star} - \mu_{a}) \frac{N_{a}(T)}{T}\right]$$

$$= \frac{\mathcal{R}(\text{TS}, T)}{T} = O\left(\frac{K \log(T)}{\Delta T}\right)$$

 \odot the estimation error decays with T

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Uniform Sampling + Empirical Best Arm:

$$\mathbb{E}[\mu_{\star} - \mu_{\hat{a}_{\tau}}] = O\left(K \exp\left(-\frac{T}{K}\Delta^{2}\right)\right)$$

but not as fast as with uniform sampling...

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$$\Delta \mathbb{P}(\hat{a}_{T} \neq a_{\star}) \simeq \mathbb{E}\left[\sum_{a=1}^{K} (\mu_{\star} - \mu_{a}) \frac{N_{a}(T)}{T}\right]$$

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 $\Pi_t = (\pi_1(t), \dots, \pi_K(t))$ posterior distribution on (μ_1, \dots, μ_K)

Top-Two Thompson Sampling (TTTS) [Russo, 2016]

Input: parameter $\beta \in (0, 1)$. In round t + 1:

- draw a posterior sample $\theta \sim \Pi_t$, $a_{\star}(\theta) = \arg \max_a \theta_a$
- with probability eta, select $A_{t+1} = a_\star(m{ heta})$
- with probability 1β , re-sample the posterior $\theta' \sim \prod_t$ until $a_{\star}(\theta') \neq a_{\star}(\theta)$, select $A_{t+1} = a_{\star}(\theta')$

[Russo, 2016] Bayesian analysis of TTTS (for exp. families):

$$\Pi_t\left(\{\boldsymbol{\theta}: a_\star(\boldsymbol{\theta}) \neq a_\star\}\right) \lesssim C \exp\left(-t/\mathcal{T}^\star_\beta(\boldsymbol{\mu})\right) \quad \text{a.s.}$$

where the rate is proved to be optimal.

The optimal exponent

 connected with the optimal sample complexity of fixed-confidence best arm identification

Lower bound [Garivier and Kaufmann, 2016]

For any strategy such that $\mathbb{P}_{\boldsymbol{\nu}} (B_{\tau} \neq a_{\star}(\boldsymbol{\nu})) \leq \delta$ for all $\boldsymbol{\nu} = (\nu_1, \dots, \nu_K) \in \mathcal{D}^K$,

$$orall oldsymbol{
u} \in \mathcal{D}^{\mathcal{K}}, \ \ \mathbb{E}_{oldsymbol{
u}}[au_{\delta}] \geq T^{\star}(oldsymbol{
u}) \ln\left(rac{1}{3\delta}
ight),$$

where $T^{\star}(\nu) = \min_{\beta \in (0,1)} T^{\star}_{\beta}(\nu)$.

General expression:

$$T^{\star}_{\beta}(\boldsymbol{\nu})^{-1} = \sup_{\substack{\boldsymbol{w} \in \triangle_{K} \\ w_{a_{\star}} = \beta}} \min_{\substack{a \neq a^{\star} \\ \lambda_{a} \geq \lambda_{a_{\star}}}} \left[w_{a_{\star}} \mathcal{K}^{-}_{\inf}(\nu_{a_{\star}}, \lambda_{a_{\star}}) + w_{a} \mathcal{K}^{+}_{\inf}(\nu_{a}, \lambda_{a}) \right]$$

"transportation cost"

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Back to the parametric case: Gaussian bandits

$$T^{\star}_{\beta}(\boldsymbol{\mu})^{-1} = \sup_{\substack{\boldsymbol{w} \in \triangle_{K} \\ w_{i^{\star}} = \beta}} \min_{\substack{a \neq a^{\star}}} \frac{(\mu_{a_{\star}} - \mu_{a})^{2}}{2\sigma^{2} \left(\frac{1}{w_{a_{\star}}} + \frac{1}{w_{a}}\right)}$$

Sample complexity of TTTS

For Gaussian bandits, one can analyze TTTS with the posterior

$$\pi_{a}(t) = \mathcal{N}\left(\hat{\mu}_{a}(t), rac{\sigma^{2}}{N_{a}(t)}
ight)$$

coupled with the (Generalized Likelihood Ratio) stopping rule

$$au_{\delta} = \inf \left\{ t \in \mathbb{N} : \min_{oldsymbol{a}
eq \hat{a}_t^\star} rac{(\hat{\mu}_{\hat{a}_t^\star} - \hat{\mu}_{oldsymbol{a}}(t))^2}{2\sigma^2 \left(rac{1}{N_{oldsymbol{a}_t^\star}(t)} + rac{1}{N_{oldsymbol{a}}(t)}
ight)} > c(t,\delta)
ight\}$$

with threshold $c(t,\delta) \simeq \log(1/\delta) + K \log \log(t)$.

$$T^{\star}_{\beta}(\boldsymbol{\mu})^{-1} = \min_{\boldsymbol{a}\neq\boldsymbol{a}^{\star}} \frac{(\mu_{\boldsymbol{a}_{\star}}-\mu_{\boldsymbol{a}})^2}{2\sigma^2 \left(\frac{1}{w^{\star}_{\boldsymbol{a}_{\star}}}+\frac{1}{w^{\star}_{\boldsymbol{a}}}\right)}$$

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with threshold $c(t, \delta) \simeq \log(1/\delta) + K \log \log(t)$.

Theorem [Shang et al., 2020]

 $TTTS(\beta)$ is δ -correct and

$$orall m{\mu}, \;\; \lim_{\delta o 0} rac{\mathbb{E}_{m{\mu}}[au_{\delta}]}{\log(1/\delta)} \leq T^{\star}_{m{eta}}(m{\mu})$$

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$$\pi_{a}(t) = \mathcal{N}\left(\hat{\mu}_{a}(t), \frac{\sigma^{2}}{N_{a}(t)}\right)$$

coupled with the (Generalized Likelihood Ratio) stopping rule

$$au_{\delta} = \inf \left\{ t \in \mathbb{N} : \min_{oldsymbol{a}
eq \hat{a}_t^\star} rac{(\hat{\mu}_{\hat{a}_t^\star} - \hat{\mu}_{oldsymbol{a}}(t))^2}{2\sigma^2 \left(rac{1}{N_{\hat{a}_t^\star}(t)} + rac{1}{N_{oldsymbol{a}}(t)}
ight)} > c(t,\delta)
ight\}$$

with threshold $c(t, \delta) \simeq \log(1/\delta) + K \log \log(t)$.

Theorem [Shang et al., 2020]

TTTS(1/2) is δ -correct and

$$orall oldsymbol{\mu}, \ \ \lim_{\delta o 0} rac{\mathbb{E}_{oldsymbol{\mu}}[au_{\delta}]}{\log(1/\delta)} \leq 2 \, \mathcal{T}^{\star}(oldsymbol{\mu})$$

Thompson Sampling for Rewards Maximization

2 Thompson Sampling for Best Arm Identification?

3 Top Two Algorithms Beyond Thompson Sampling

The Top Two structure

Top Two algorithm

Given a parameter $\beta \in (0, 1)$, in round *t*:

- define a leader $B_t \in [K]$
- define a challenger $C_t \neq B_t$
- select arm $A_t \in \{B_t, C_t\}$ at random:

$$\mathbb{P}(A_t = B_t) = \beta$$
 $\mathbb{P}(A_t = C_t) = 1 - \beta$

In Top Two Thompson Sampling,

- TS leader: $B_t^{\mathsf{TS}} = a_{\star}(\theta)$ with $\theta \sim \Pi_{t-1}$
- Re-Sampling (RS) challenger: $C_t^{\mathsf{RS}} = a_\star(\theta')$ where

$$oldsymbol{ heta}' \sim \mathsf{\Pi}_{t-1} | \left(\mathsf{a}_{\star}(oldsymbol{ heta}')
eq \mathsf{B}_t
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In Top Two Thompson Sampling,

- TS leader: $B_t^{\mathsf{TS}} = a_{\star}(\theta)$ with $\theta \sim \prod_{t=1}^{t} \theta_{t}$
- Re-Sampling (RS) challenger: $C_t^{\mathsf{RS}} = a_\star(\theta')$ where

$$oldsymbol{ heta}' \sim \mathsf{\Pi}_{t-1} | \left(oldsymbol{a}_{\star}(oldsymbol{ heta}')
eq oldsymbol{B}_t
ight)$$

Liminations:

- → re-sampling can be numerically costly
- → do we need a posterior distribution?

Approximating Re-Sampling

Under the RS challenger,

$$\mathbb{P}\left(C_t^{\mathsf{RS}} = a | B_t = b\right) = \frac{p_{t,a}}{\sum_{i \neq b} p_{t,i}}$$

where $p_{t,a} = \prod_t (\theta_a = \max_j \theta_j) \simeq \prod_t (\theta_a > \theta_b)$.

For Gaussian bandits when $\hat{\mu}_b(t) > \hat{\mu}_a(t)$,

$$\Pi_t \left(\theta_a > \theta_b \right) \simeq \exp \left(-t \frac{(\hat{\mu}_b(t) - \hat{\mu}_a(t))^2}{2\sigma^2 \left(\frac{1}{N_b(t)} + \frac{1}{N_a(t)} \right)} \right)$$

Idea: select the mode from this distribution instead of sampling!

$$C_t^{\mathsf{TC}} = \arg\min_{\mathbf{a} \neq B_t} \frac{(\hat{\mu}_{B_t}(t) - \hat{\mu}_{\mathbf{a}}(t))^2}{2\sigma^2 \left(\frac{1}{N_{B_t}(t)} + \frac{1}{N_{\mathbf{a}}(t)}\right)} \mathbb{1}(\hat{\mu}_{B_t}(t) \ge \hat{\mu}_{\mathbf{a}}(t))$$

[Shang et al., 2020]

Recall that TTTS was analyzed with

$$\tau_{\delta} = \inf \left\{ t \in \mathbb{N} : \min_{\substack{a \neq \hat{a}_{t}^{\star}}} \frac{(\hat{\mu}_{\hat{a}_{t}^{\star}} - \hat{\mu}_{a}(t))^{2}}{2\sigma^{2} \left(\frac{1}{N_{\hat{a}_{t}^{\star}}(t)} + \frac{1}{N_{a}(t)}\right)} > c(t, \delta) \right\}$$

→ another interpretation: C_t^{TC} minimizes the Empirical Transportation Cost (TC) featured in the stopping rule Recall that TTTS was analyzed with

$$\tau_{\delta} = \inf \left\{ t \in \mathbb{N} : \min_{\substack{a \neq \hat{a}_{t}^{\star}}} \frac{(\hat{\mu}_{\hat{a}_{t}^{\star}} - \hat{\mu}_{a}(t))^{2}}{2\sigma^{2} \left(\frac{1}{N_{\hat{a}_{t}^{\star}}(t)} + \frac{1}{N_{a}(t)}\right)} > c(t, \delta) \right\}$$

 → another interpretation: C_t^{TC} minimizes the Empirical Transportation Cost (TC) featured in the stopping rule
 → could we use B_T^{EB} = â_t^{*}, i.e. Empirical Best leader?

Theorem

Given a calibrated GLR stopping rule, instantiating the Top Two sampling rule with any pair of leader/challenger satisfying some properties yields a δ -correct algorithm satisfying for all $\nu \in \mathcal{D}^K$ with distincts means

$$\limsup_{\delta o 0} rac{\mathbb{E}_{oldsymbol{
u}}[au_{\delta}]}{\log(1/\delta)} \leq T^{\star}_{eta}(oldsymbol{
u})\,.$$

Distributions	ΤS	EB	RS	ТС	TCI
Gaussian KV	1	1	1	1	1
Bernoulli	1	1	1	1	1
sub-Exp SPEF	?	1	?	1	1
Gaussian UV	?	1	?	1	1
Bounded	1	 Image: A second s	1	 Image: A second s	1

[Jourdan et al., 2022, Jourdan et al., 2023a]

But exploration is nice for finite-time performance

TS-TC

$$B_t \sim \arg \max_{a \in [K]} \widetilde{\theta}_a(t) \quad \widetilde{\theta}(t) \sim \Pi_t$$
$$C_t = \arg \min_{a \neq B_t} \frac{(\hat{\mu}_{B_t}(t) - \hat{\mu}_a(t))_+^2}{2\sigma^2 \left(\frac{1}{N_{B_t}(t)} + \frac{1}{N_a(t)}\right)}$$

EB-TCI

$$B_t = \underset{a \in [K]}{\operatorname{arg max}} \hat{\mu}_a(t)$$

$$C_t = \underset{a \neq B_t}{\operatorname{arg min}} \left[\frac{(\hat{\mu}_{B_t}(t) - \hat{\mu}_a(t))_+^2}{2\sigma^2 \left(\frac{1}{N_{B_t}(t)} + \frac{1}{N_a(t)}\right)} + \log N_a(t) \right]$$

Numerical experiments

Moderate regime, $\delta = 0.1$. Top Two algorithms with $\beta = 1/2$.



Figure: Empirical sample complexity averaged over 5000 random (Bernoulli) instances with K = 8 and $\Delta_{\min} \ge 0.01$.

arm = planting date / observation = yield Moderate regime, $\delta = 0.01$. Top Two algorithms with $\beta = 1/2$.



Figure: Empirical stopping time (a) on scaled DSSAT instances with their density and mean (b). Lower bound is $T^*(\nu) \ln(1/\delta)$.

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Figure: Empirical stopping time (a) on scaled DSSAT instances with their density and mean (b). Lower bound is $T^*(\nu) \ln(1/\delta)$.

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Figure: Empirical stopping time (a) on scaled DSSAT instances with their density and mean (b). Lower bound is $T^*(\nu) \ln(1/\delta)$.

Top Two algorithms beyond Fixed Confidence

$$B_{t} = \arg \max_{a \in [K]} \hat{\mu}_{a}(t)$$

$$C_{t} = \arg \min_{a \neq B_{t}} \left[\frac{\hat{\mu}_{B_{t}}(t) - \hat{\mu}_{a}(t) + \varepsilon_{0}}{\sqrt{\frac{1}{N_{B_{t}}(t)} + \frac{1}{N_{a}(t)}}} \right]$$

[Jourdan et al., 2023b]

- motivated by the lower bound for (ε_0, δ) -PAC identification
- can be used for (ε, δ) -PAC identification¹ for $\varepsilon \neq \epsilon_0$
- first guarantees in the anytime setting...

¹
$$\mathbb{P}\Big(\mu_{\hat{a}_{\tau}} > \mu_{\star} - \varepsilon\Big) \ge 1 - \delta$$

Top Two algorithms Beyond Fixed Confidence



Figure: Simple regret as a function of time on an instance $\mu \in \{0.4, 0.6\}^{10}$ with 2 best arms

(... but the theory is just saying that the algorithm is not too much worse than uniform sampling...)

Thompson Sampling for maximizing rewards:

- is asymptotically optimal for simple parametric distributions
- can be extended to some non-parametric settings

Top Two Thompson Sampling for best arm identification:

- may be viewed as a fix of TS for BAI
- is a inspiration for others (non-Bayesian) Top Two algorithms
- ... which are near optimal in theory and very good in practice

Perspective:

- Understand better the good anytime performance
- Top Two for more complex pure exploration problems?





Robbins, H. (1952).

Some aspects of the sequential design of experiments. Bulletin of the American Mathematical Society, 58(5):527–535.



Russo, D. (2016).

Simple Bayesian algorithms for best arm identification. In Proceedings of the 29th Conference on Learning Theory (COLT).



Shang, X., de Heide, R., Kaufmann, E., Ménard, P., and Valko, M. (2020). Fixed-confidence guarantees for bayesian best-arm identification. In International Conference on Artificial Intelligence and Statistics (AISTATS).



Thompson, W. (1933).

On the likelihood that one unknown probability exceeds another in view of the evidence of two samples.

Biometrika, 25:285-294.