Bandits and Hyper-parameter Optimization: From Practice to Theory

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Inria SequeL

What — Hyper-parameter optimization

Problem

We tackle **hyper-parameter tuning** for *supervised learning* tasks:

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↳ global optimisation task: $\min\{f(\boldsymbol{\lambda}) : \boldsymbol{\lambda} \in \Omega\}$;

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↳ global optimisation task: $\min\{f(\boldsymbol{\lambda}) : \boldsymbol{\lambda} \in \Omega\}$;

↳ $f(\boldsymbol{\lambda}) \triangleq \mathbb{E}\left[\ell\left(\mathbf{Y}, \widehat{g}_{\boldsymbol{\lambda}}^{(n)}(\mathbf{X})\right)\right]$ measures the generalization power.
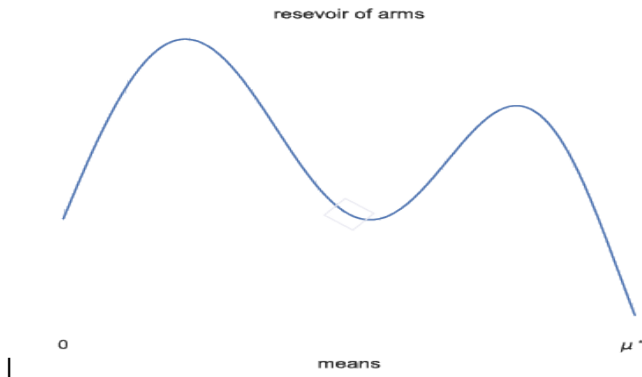
How — Best-arm identification

We see the problem as *best-arm identification* in a *stochastic infinitely-armed bandit*: arms' means are drawn from some *reservoir distribution* ν_0.

resevoir of arms

o μ^*

means

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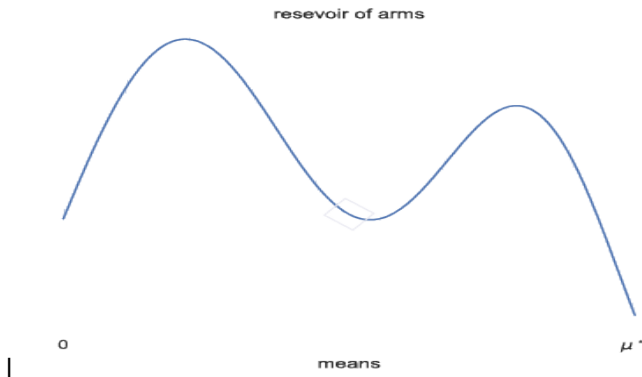
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How — Best-arm identification

We see the problem as *best-arm identification* in a *stochastic infinitely-armed bandit*: arms' means are drawn from some *reservoir distribution* ν_0.

In each round
1. (optional) query a new arm from ν_0;
2. sample an arm that was previously queried.

goal: output an arm with mean close to $\mu^\star$
D-TTTS (Dynamic Top-Two Thompson Sampling) $\rightsquigarrow$ a dynamic algorithm built on TTTS.

How — D-TTTS

In this talk...

- ▶ `Beta-Bernoulli` Bayesian bandit model
- ▶ a uniform prior over the mean of new arms

1: **Initialization**: $\mu_1 \sim \nu_0$; $\mathcal{A} = \{\mu_1\}$; $m = 1$; $S_1, N_1 = 0$
2: **while** budget still available **do**
3: $\quad \forall i \in \mathcal{A}, \ \theta_i \sim \text{Beta}(S_i + 1, N_i - S_i + 1)$
4: $\quad I^{(1)} = \arg\max_{i=0,\ldots,m} \theta_i \{ \boxed{\text{Thompson sampling}} \}$
5: **end while**

How — `D-TTTS`

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5:    **if** $U(\sim \mathcal{U}([0,1])) > \beta$ **then**
6:      **while** $I^{(2)} \neq I^{(1)}$ **do**
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8:         $I^{(2)} \leftarrow \arg\max_{i=0,\ldots,m} \theta_i'$
9:      **end while**
10:     $I^{(1)} \leftarrow I^{(2)}$
11:   **end if** $\{$ TTTS $\}$
12: **end while**

How — `D-TTTS`

1: **Initialization**: $\mu_1 \sim \nu_0$; $\mathcal{A} = \{\mu_1\}$; $m = 1$; $S_1, N_1 = 0$
2: **while** budget still available **do**
3:    $\mu_{m+1} \sim \nu_0$; $\mathcal{A} \leftarrow \mathcal{A} \cup \{\mu_{m+1}\}$
4:    $S_{m+1}, N_{m+1} \leftarrow 0$; $m \leftarrow m + 1$
5:    $\forall i \in \mathcal{A}, \theta_i \sim \texttt{Beta}(S_i + 1, N_i - S_i + 1)$
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11:      **end while**
12:      $I^{(1)} \leftarrow I^{(2)}$
13:    **end if**$\{$ TTTS $\}$
14:    $Y \leftarrow \texttt{evaluate arm } I^{(1)}$; $X \sim \texttt{Ber}(Y)$
15:    $S_{I^{(1)}} \leftarrow S_{I^{(1)}} + X$; $N_{I^{(1)}} \leftarrow N_{I^{(1)}} + 1$
16: **end while**

How — `D-TTTS` c'td

`D-TTTS` in summary...

In each round, query a new arm endowed with a `Beta(1,1)` prior, without sampling it, and run `TTTS` on the new set of arms.

How — `D-TTTS` c'td

Order statistic trick

With $\mathcal{L}_{t-1}$ the list of arms that have been effectively sampled at time t, we run `TTTS` on the set $\mathcal{L}_{t-1} \cup \{\mu_0\}$ where μ_0 is a pseudo-arm with posterior `Beta`$(t - |\mathcal{L}_{t-1}|, 1)$.
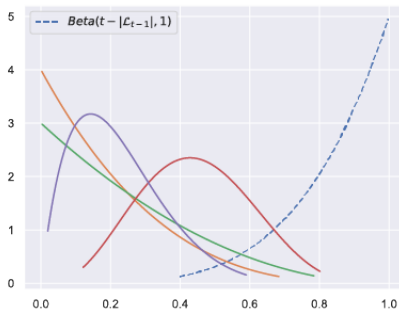

Figure: Posterior distributions of 4 arms and the pseudo-arm

Why

1. TTTS is *anytime* for finitely-armed bandits;
2. the flexibility of this Bayesian algorithm allows to propose a **dynamic** version for the infinite BAI;
3. unlike previous approaches (for infinite-armed bandits or HPO), D-TTTS **does not** need to fix the number of arms queried in advance, and naturally **adapts** to the difficulty of the task.

Why

1. TTTS is *anytime* for finitely-armed bandits;
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SiRI as an example for infinite-armed bandits

▶ choose a problem-dependent number of arms
▶ pull arms *optimistically*

Why

1. TTTS is *anytime* for finitely-armed bandits;
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Hyperband as an example for HPO

▶ equally divide the budget B into m brackets
▶ run sequential halving (Karnin et al. 2013) over a fixed number n of configurations in each bracket
▶ trade-off between B/mn and n

HPO as a BAI problem

BAI	HPO
query ν_0	pick a new configuration $\boldsymbol{\lambda}^{\cdot}$
sample an arm$^{\cdot}$	train the classifier $g_{\boldsymbol{\lambda}}$
reward	cross-validation loss

Experiments — Setting

Classifier	Hyper-parameter	Type	Bounds
SVM	C	$\mathbb{R}^+$	$\left[10^{-5}, 10^5\right]$
	γ	$\mathbb{R}^+$	$\left[10^{-5}, 10^5\right]$

Table: hyper-parameters to be tuned for UCI experiments.

Classifier	Hyper-parameter	Type	Bounds
MLP	hidden_layer_size	Integer	$[5, 50]$
	alpha	$\mathbb{R}^+$	$[0, 0.9]$
	learning_rate_init	$\mathbb{R}^+$	$\left[10^{-5}, 10^{-1}\right]$

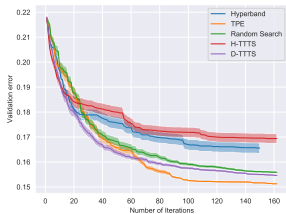Table: hyper-parameters to be tuned for MNIST experiments.
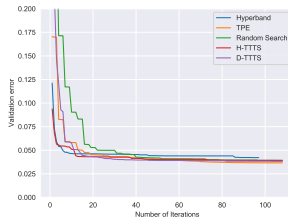
Experiments — Some results
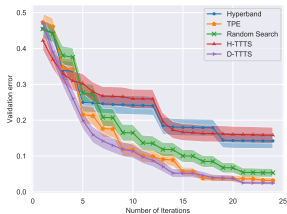
(a) wine
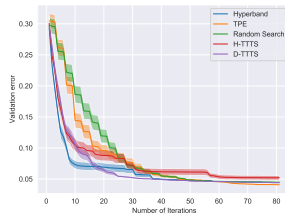
(b) breast cancer

(c) adult

(d) MNIST

What now?

▶ Extend to the non-stochastic setting;

What now?

- Extend to the non-stochastic setting;
- Theoretical guarantee?
  - Analysis of D-TTTS extremely difficult due to the dynamic nature;
  - How about take a step back to TTTS first?

More details on D-TTTS
Check out [Shang, Kaufmann, et al. 2019].

BAI for finitely-armed bandits

- sampling rule;
- stopping rule;
- recommendation rule.

What we know about TTTS... (Reminder)

1: **Input**: β
2: **for** $n = 1, 2, \ldots$ **do**
3:     $\forall i \in \mathcal{A}$, $\theta_i \sim \Pi_n$
4:     $I^{(1)} = \arg\max_{i=0,\ldots,m} \theta_i$
5:     **if** $U(\sim \mathcal{U}([0,1])) > \beta$ **then**
6:       **while** $I^{(2)} \neq I^{(1)}$ **do**
7:         $\forall i \in \mathcal{A}$, $\theta'_i \sim \Pi_n$
8:         $I^{(2)} \leftarrow \arg\max_{i=0,\ldots,m} \theta'_i$
9:       **end while**
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What we know about TTTS... (Posterior convergence)

Theorem (Russo 2016)

*Under TTTS, for **bounded** 1-dimensional exponential family priors, it holds almost surely that*

$$\lim_{n \to \infty} -\frac{1}{n} \log(1 - \alpha_{n,I^\star}) = \Gamma_\beta^\star,$$

where

$$\alpha_{n,i} \triangleq \Pi_n(\theta_i > \max_{j \neq i} \theta_j).$$

Definition

Let $\Sigma_K = \{\boldsymbol{\omega} : \sum_{k=1}^{K} \omega_k = 1, \omega_k \geq 0\}$ and define for all $i \neq I^\star$

$$C_i(\omega, \omega') \triangleq \min_{x \in \mathcal{I}} \omega d(\mu_{I^\star}; x) + \omega' d(\mu_i; x),$$

where $d(\mu, \mu')$ is the KL-divergence. We define

$$\Gamma_\beta^\star \triangleq \max_{\substack{\boldsymbol{\omega} \in \Sigma_K \\ \omega_{I^\star} = \beta}} \min_{i \neq I^\star} C_i(\omega_{I^\star}, \omega_i).$$

What we know about TTTS... (Complexity)

Definition
Let $\Sigma_K = \{\boldsymbol{\omega} : \sum_{k=1}^K \omega_k = 1, \omega_k \geq 0\}$ and define for all $i \neq I^\star$

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In particular, for Gaussian bandits...

$$\Gamma_\beta^\star = \max_{\boldsymbol{\omega}: \omega_{I^\star} = \beta} \min_{i \neq I^\star} \frac{(\mu_{I^\star} - \mu_i)^2}{2\sigma^2(1/\omega_i + 1/\beta)}.$$

What we want to know about TTTS

▶ Can we remove the *boudedness* assumption of the prior?

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- ► What can we say about the sample complexity in the fixed-confidence setting?

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- ▶ What can we say about the sample complexity in the fixed-confidence setting?

Lower bound

Under any δ-correct strategy satisfying $T_{n,I^\star}/n \to \beta$,

$$\liminf_{\delta \to 0} \frac{\mathbb{E}\left[\tau_\delta\right]}{\ln(1/\delta)} \geq \frac{1}{\Gamma_\beta^\star}.$$

What we want to know about TTTS

- Can we remove the *boudedness* assumption of the prior?
- What can we say about the sample complexity in the fixed-confidence setting?
- Can we have finite-time guarantees?

Main result — Posterior convergence

Theorem (Shang, Heide, et al. 2020)

Under TTTS, for Gaussian bandits with improper Gaussian priors, it holds almost surely that

$$\lim_{n\to\infty} -\frac{1}{n}\log(1 - \alpha_{n,I^\star}) = \Gamma_\beta^\star.$$

Theorem (Shang, Heide, et al. 2020)

Under TTTS, for Bernoulli bandits and uniform priors, it holds almost surely that

$$\lim_{n\to\infty} -\frac{1}{n}\log(1 - \alpha_{n,I^\star}) = \Gamma_\beta^\star.$$

Main result — Sample complexity

Theorem (Shang, Heide, et al. 2020)

The TTTS sampling rule coupled with the Chernoff stopping rule form a δ-correct BAI strategy. Moreover, if all the arms means are distinct, it satisfies

$$\limsup_{\delta \to 0} \frac{\mathbb{E}\left[\tau_\delta\right]}{\log(1/\delta)} \leq \frac{1}{\Gamma_\beta^\star}.$$

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Recall (Lower bound)

$$\liminf_{\delta \to 0} \frac{\mathbb{E}\left[\tau_\delta\right]}{\ln(1/\delta)} \geq \frac{1}{\Gamma_\beta^\star}.$$

Sample complexity sketch - δ-correctness

Stopping rule

$$\tau_\delta^{\mathsf{Ch.}} \triangleq \inf \left\{ n \in \mathbb{N} : \max_{i \in \mathcal{A}} \min_{j \in \mathcal{A} \setminus \{i\}} W_n(i,j) > d_{n,\delta} \right\}. \qquad (1)$$

Sample complexity sketch - δ-correctness

Stopping rule

$$\tau_\delta^{\mathsf{Ch.}} \triangleq \inf \left\{ n \in \mathbb{N} : \max_{i \in \mathcal{A}} \min_{j \in \mathcal{A} \setminus \{i\}} W_n(i,j) > d_{n,\delta} \right\}. \qquad (1)$$

Transportation cost

Let $\mu_{n,i,j} \triangleq (T_{n,i}\mu_{n,i} + T_{n,j}\mu_{n,j})/(T_{n,i} + T_{n,j})$, then we define

$$W_n(i,j) \triangleq \begin{cases} 0 & \text{if } \mu_{n,j} \geq \mu_{n,i}, \\ W_{n,i,j} + W_{n,j,i} & \text{otherwise}, \end{cases} \qquad (2)$$

where $W_{n,i,j} \triangleq T_{n,i} d\left(\mu_{n,i}, \mu_{n,i,j}\right)$ for any i,j.

Sample complexity sketch - δ-correctness

Stopping rule

$$\tau_\delta^{\mathsf{Ch.}} \triangleq \inf \left\{ n \in \mathbb{N} : \max_{i \in \mathcal{A}} \min_{j \in \mathcal{A} \setminus \{i\}} W_n(i,j) > d_{n,\delta} \right\}. \qquad (1)$$

In particular, for Gaussian bandits...

$$W_n(i,j) = \frac{(\mu_{n,i} - \mu_{n,j})^2}{2\sigma^2(1/T_{n,i} + 1/T_{n,j})} \mathbb{1}\{\mu_{n,j} < \mu_{n,i}\}.$$

Sample complexity sketch - δ-correctness

Stopping rule

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Theorem (Shang, Heide, et al. 2020)

The TTTS sampling rule coupled with the Chernoff stopping rule (1) with a threshold $d_{n,\delta}$ derived from Kaufmann and Koolen 2018 and the recommendation rule $J_t = \arg\max_i \mu_{n,i}$, form a δ-correct BAI strategy.

Sample complexity sketch — Sufficient condition for β-optimality

Lemma

Let $\delta, \beta \in (0, 1)$. For any sampling rule which satisfies
$\mathbb{E}\left[T_{\beta}^{\varepsilon}\right] < \infty$ *for all $\varepsilon > 0$, we have*

$$\limsup_{\delta \to 0} \frac{\mathbb{E}\left[\tau_{\delta}\right]}{\log(1/\delta)} \leq \frac{1}{\Gamma_{\beta}^{\star}},$$

if the sampling rule is coupled with stopping rule (1),

Sample complexity sketch - Core theorem

Theorem (Shang, Heide, et al. 2020)
Under TTTS, $\mathbb{E}\left[T_\beta^\varepsilon\right] < +\infty$.

Alleviate the computational burden?

1: **Input**: β
2: **for** $n = 1, 2, \ldots$ **do**
3:     $\forall i \in \mathcal{A}$, $\theta_i \sim \Pi_n$
4:     $I^{(1)} = \arg\max_{i=0,\ldots,m} \theta_i$
5:     **if** $U(\sim \mathcal{U}([0,1])) > \beta$ **then**
6:       **while** $I^{(2)} \neq I^{(1)}$ **do**
7:         $\forall i \in \mathcal{A}$, $\theta'_i \sim \Pi_n$
8:         $I^{(2)} \leftarrow \arg\max_{i=0,\ldots,m} \theta'_i$ {Re-sampling phase}
9:       **end while**
10:      $I^{(1)} \leftarrow I^{(2)}$
11:     **end if**
12:     evaluate arm $I^{(1)}$
13:     update Π_n
14: **end for**

Alleviate the computational burden?

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2: **for** $n = 1, 2, \ldots$ **do**
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5:     **if** $U(\sim \mathcal{U}([0,1])) > \beta$ **then**
6:       $I^{(2)} \leftarrow \arg\min_{i \neq I^{(1)}} W_n(I^{(1)}, i) \{\texttt{T3C}\}$
7:       $I^{(1)} \leftarrow I^{(2)}$
8:     **end if**
9:     evaluate arm $I^{(1)}$
10:    update Π_n
11: **end for**

Main result — Sample complexity T3C

Theorem (Shang, Heide, et al. 2020)

The T3C sampling rule coupled with the Chernoff stopping rule form a δ-correct BAI strategy. Moreover, if all the arms means are distinct, it satisfies
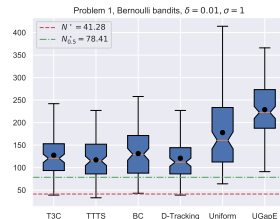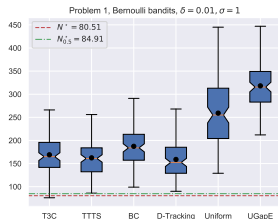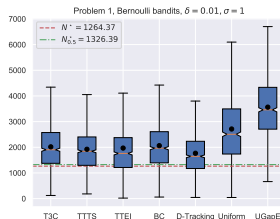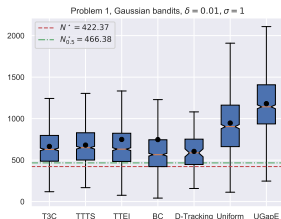
$$\limsup_{\delta \to 0} \frac{\mathbb{E}\left[\tau_\delta\right]}{\log(1/\delta)} \leq \frac{1}{\Gamma_\beta^\star}.$$

Some illustrations — Time consumption

Sampling rule	T3C	TTTS	Uniform
Execution time (s)	1.6×10^{-5}	2.3×10^{-4}	6×10^{-6}

Table: average execution time in seconds for different sampling rules.

Some illustrations — Average stopping time

Still far from the Holy Grail...

▶ Finite-time analysis (fixed-budget setting?)

Conclusion

More details on TTTS and T3C
Check out [Shang, Heide, et al. 2020].

References

Thank you!

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