



Bandits and Hyper-parameter Optimization: From Practice to Theory

X. Shang¹, R. de Heide², P. Ménard¹, E. Kaufmann³, M. Valko⁴

¹ Inria Lille, Sequel team

² CWI

³ CNRS, CRIStAL

⁴ Google DeepMind

What — Hyper-parameter optimization

Problem

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

What — Hyper-parameter optimization

Problem

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

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

What — Hyper-parameter optimization

Problem

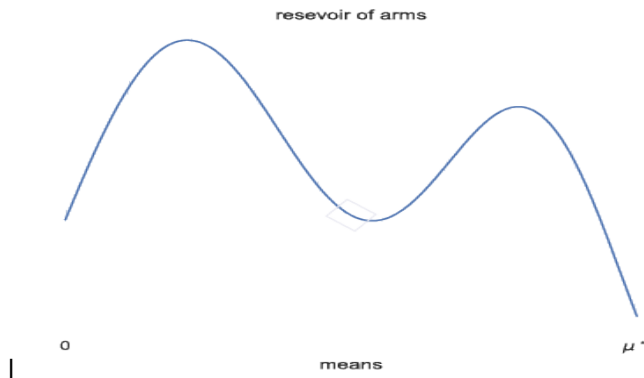
We tackle **hyper-parameter tuning** for *supervised learning* tasks:

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

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

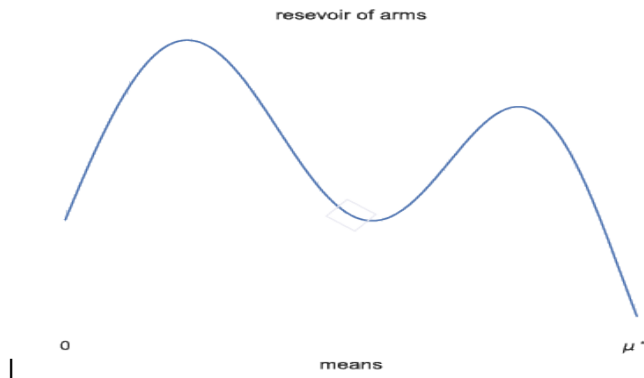
How — Best-arm identification

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



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 .



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 μ^*

D-TTTS (Dynamic Top-Two Thompson Sampling) \rightsquigarrow a dynamic algorithm built on 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: $\forall i \in \mathcal{A}, \theta_i \sim \text{Beta}(S_i + 1, N_i - S_i + 1)$
- 4: $I^{(1)} = \arg \max_{i=0, \dots, m} \theta_i$ {Thompson sampling}
- 5: **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: $\forall i \in \mathcal{A}, \theta_i \sim \text{Beta}(S_i + 1, N_i - S_i + 1)$
- 4: $I^{(1)} = \arg \max_{i=0, \dots, m} \theta_i$ {Thompson sampling}
- 5: **if** $U(\sim \mathcal{U}([0, 1])) > \beta$ **then**
- 6: **while** $I^{(2)} \neq I^{(1)}$ **do**
- 7: $\forall i \in \mathcal{A}, \theta'_i \sim \text{Beta}(S_i + 1, N_i - S_i + 1)$
- 8: $I^{(2)} \leftarrow \arg \max_{i=0, \dots, m} \theta'_i$
- 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: $\forall i \in \mathcal{A}, \theta_i \sim \text{Beta}(S_i + 1, N_i - S_i + 1)$
- 6: $I^{(1)} = \arg \max_{i=0, \dots, m} \theta_i$ {Thompson sampling}
- 7: **if** $U(\sim \mathcal{U}([0, 1])) > \beta$ **then**
- 8: **while** $I^{(2)} \neq I^{(1)}$ **do**
- 9: $\forall i \in \mathcal{A}, \theta'_i \sim \text{Beta}(S_i + 1, N_i - S_i + 1)$
- 10: $I^{(2)} \leftarrow \arg \max_{i=0, \dots, m} \theta'_i$
- 11: **end while**
- 12: $I^{(1)} \leftarrow I^{(2)}$
- 13: **end if** {TTTS}
- 14: $Y \leftarrow \text{evaluate arm } I^{(1)}$; $X \sim \text{Ber}(Y)$
- 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 $\text{Beta}(t - |\mathcal{L}_{t-1}|, 1)$.

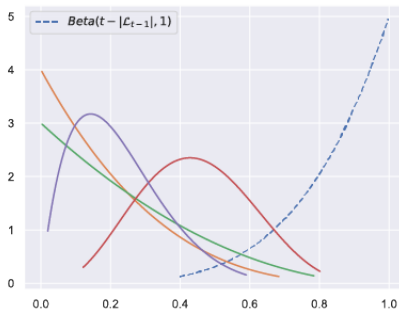


Figure: Posterior distributions of 4 arms and the pseudo-arm

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;
2. the flexibility of this Bayesian algorithm allows to propose a **dynamic** version for the infinite BAI;

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;
2. the flexibility of this Bayesian algorithm allows to propose a **dynamic** version for the infinite BAI;

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 λ'
sample an arm'	train the classifier g_λ
reward	cross-validation loss

Experiments — Setting

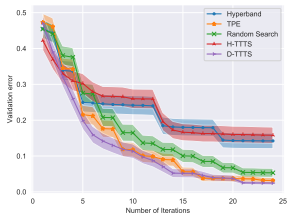
Classifier	Hyper-parameter	Type	Bounds
SVM	C	\mathbb{R}^+	$[10^{-5}, 10^5]$
	γ	\mathbb{R}^+	$[10^{-5}, 10^5]$

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

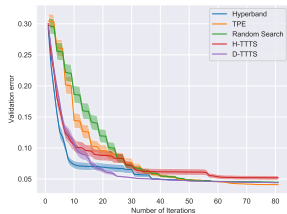
Classifier	Hyper-parameter	Type	Bounds
MLP	hidden_layer_size	Integer	[5, 50]
	alpha	\mathbb{R}^+	[0, 0.9]
	learning_rate_init	\mathbb{R}^+	$[10^{-5}, 10^{-1}]$

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

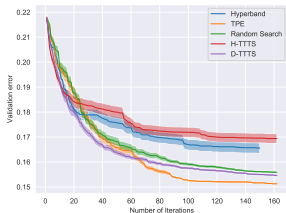
Experiments — Some results



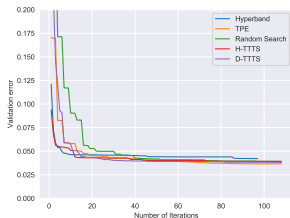
(a) wine



(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:  $\beta$ 
2: for  $n = 1, 2, \dots$  do
3:    $\forall i \in \mathcal{A}, \theta_i \sim \Pi_n$ 
4:    $I^{(1)} = \arg \max_{i=0, \dots, m} \theta_i$ 
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:        $I^{(2)} \leftarrow \arg \max_{i=0, \dots, m} \theta'_i$ 
9:     end while
10:     $I^{(1)} \leftarrow I^{(2)}$ 
11:  end if
12:  evaluate arm  $I^{(1)}$ 
13:  update  $\Pi_n$ 
14: end for
```

What we know about TTTS... (Posterior convergence)

Theorem (Russo 2016)

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

$$\lim_{n \rightarrow \infty} -\frac{1}{n} \log(1 - \alpha_{n, l^*}) = \Gamma_{\beta}^*,$$

where

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

What we know about TTTS... (Complexity)

Definition

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

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

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

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

What we know about TTS... (Complexity)

Definition

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

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

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

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

In particular, for Gaussian bandits...

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

What we want to know about TTTS

- ▶ Can we remove the *boundedness* assumption of the prior?

What we want to know about TTTS

- ▶ Can we remove the *boundedness* assumption of the prior?
- ▶ What can we say about the sample complexity in the fixed-confidence setting?

What we want to know about TTTS

- ▶ Can we remove the *boundedness* assumption of the prior?
- ▶ What can we say about the sample complexity in the fixed-confidence setting?

Lower bound

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

$$\liminf_{\delta \rightarrow 0} \frac{\mathbb{E}[\tau_\delta]}{\ln(1/\delta)} \geq \frac{1}{\Gamma_\beta^*}.$$

What we want to know about TTS

- ▶ Can we remove the *boundedness* 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

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

Theorem (Shang, Heide, et al. 2020)

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

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

Main result — Sample complexity

Theorem (Shang, Heide, et al. 2020)

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

$$\limsup_{\delta \rightarrow 0} \frac{\mathbb{E}[\tau_\delta]}{\log(1/\delta)} \leq \frac{1}{\Gamma_\beta^*}.$$

Main result — Sample complexity

Theorem (Shang, Heide, et al. 2020)

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

$$\limsup_{\delta \rightarrow 0} \frac{\mathbb{E}[\tau_\delta]}{\log(1/\delta)} \leq \frac{1}{\Gamma_\beta^*}.$$

Recall (Lower bound)

$$\liminf_{\delta \rightarrow 0} \frac{\mathbb{E}[\tau_\delta]}{\ln(1/\delta)} \geq \frac{1}{\Gamma_\beta^*}.$$

Sample complexity sketch - δ -correctness

Stopping rule

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

Sample complexity sketch - δ -correctness

Stopping rule

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

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

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

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

Sample complexity sketch - δ -correctness

Stopping rule

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

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

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

Theorem (Shang, Heide, et al. 2020)

The TTS 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

$$\limsup_{\delta \rightarrow 0} \frac{\mathbb{E} [\tau_{\delta}]}{\log(1/\delta)} \leq \frac{1}{\Gamma_{\beta}^*},$$

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

Sample complexity sketch — Sufficient condition for β -optimality

Lemma

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

$$\limsup_{\delta \rightarrow 0} \frac{\mathbb{E} [\tau_{\delta}]}{\log(1/\delta)} \leq \frac{1}{\Gamma_{\beta}^*},$$

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

$$T_{\beta}^{\varepsilon} \triangleq \inf \left\{ N \in \mathbb{N} : \max_{i \in \mathcal{A}} |T_{n,i}/n - \omega_i^{\beta}| \leq \varepsilon, \forall n \geq N \right\}$$

Sample complexity sketch - Core theorem

Theorem (Shang, Heide, et al. 2020)

Under *TTTS*, $\mathbb{E} \left[T_{\beta}^{\varepsilon} \right] < +\infty$.

The proof is inspired by Qin et al. (2017), but some technical novelties are introduced. In particular, our proof is much more intricate due to the randomized nature of the two candidate arms...

Alleviate the computational burden?

```
1: Input:  $\beta$ 
2: for  $n = 1, 2, \dots$  do
3:    $\forall i \in \mathcal{A}, \theta_i \sim \Pi_n$ 
4:    $I^{(1)} = \arg \max_{i=0, \dots, m} \theta_i$ 
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:        $I^{(2)} \leftarrow \arg \max_{i=0, \dots, m} \theta'_i$  {Re-sampling phase}
9:     end while
10:     $I^{(1)} \leftarrow I^{(2)}$ 
11:  end if
12:  evaluate arm  $I^{(1)}$ 
13:  update  $\Pi_n$ 
14: end for
```


Alleviate the computational burden?

- 1: **Input:** β
- 2: **for** $n = 1, 2, \dots$ **do**
- 3: $\forall i \in \mathcal{A}, \theta_i \sim \Pi_n$
- 4: $I^{(1)} = \arg \max_{i=0, \dots, m} \theta_i$
- 5: **if** $U(\sim \mathcal{U}([0, 1])) > \beta$ **then**
- 6: $I^{(2)} \leftarrow \arg \min_{i \neq I^{(1)}} W_n(I^{(1)}, i) \{\text{T3C}\}$
- 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

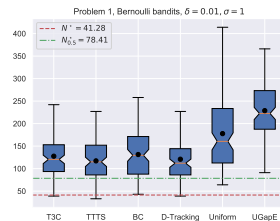
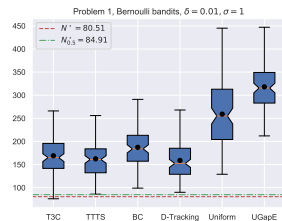
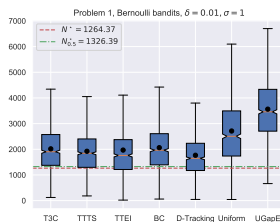
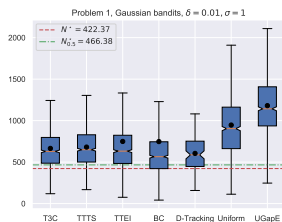
$$\limsup_{\delta \rightarrow 0} \frac{\mathbb{E}[\tau_\delta]}{\log(1/\delta)} \leq \frac{1}{\Gamma_\beta^*}.$$

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].

Thank you!



Zohar Karnin, Tomer Koren, and Oren Somekh. “Almost optimal exploration in multi-armed bandits”. In: *30th ICML*. 2013.



Emilie Kaufmann and Wouter Koolen. “Mixture martingales revisited with applications to sequential tests and confidence intervals”. In: 2018.



Daniel Russo. “Simple Bayesian algorithms for best arm identification”. In: *29th CoLT*. 2016.



Xuedong Shang, Rianne de Heide, Pierre Ménard, Emilie Kaufmann, and Michal Valko. “Fixed-confidence guarantees for Bayesian best-arm identification”. In: *23rd AISTATS*. 2020.



Xuedong Shang, Emilie Kaufmann, and Michal Valko. “A simple dynamic bandit algorithm for hyper-parameter optimization”. In: *6th ICML Workshop on AutoML*. 2019.