A simple dynamic bandit algorithm for hyper-parameter tuning

Xuedong Shang xuedong.shang@inria.fr
SequeL team, INRIA Lille - Nord Europe, France
40 avenue Halley 59650, Villeneuve d'Ascq, France

Emilie Kaufmann emilie.kaufmann@univ-lille.fr
CNRS & ULille, UMR 9189 (CRIStAL), SequeL team, INRIA Lille - Nord Europe, France
40 avenue Halley 59650, Villeneuve d'Ascq, France

Michal Valko valko@google.com
DeepMind Paris
14 Rue de Londres, 75009 Paris, France

Abstract

Hyper-parameter tuning is a major part of modern machine learning systems. The tuning itself can be seen as a sequential resource allocation problem. As such, methods for multi-armed bandits have been already applied to tackle this challenge. In this paper, we view hyper-parameter optimization as an instance of best-arm identification in an infinitely many-armed bandit. We propose a new adaptive algorithm, inspired by Thompson sampling, that dynamically balances between refining the estimate of the quality of hyper-parameter configurations previously explored and adding new hyper-parameter configurations to the pool of candidates. The algorithm is easy to implement and shows competitive performance compared to state-of-the-art algorithms for hyper-parameter tuning.

1. Introduction

Training a machine learning algorithm often requires to specify several parameters. For instance, for neural network this can be the architecture of the network but also the parameters of the gradient algorithm used or the choice of regularization. These *hyper-parameters* are difficult to be learned through the training process and are often manually specified.

When it is not feasible to design algorithms with a few hyper-parameters, we can opt for *hyper-parameter optimization* (HPO). HPO can be viewed as a *black-box optimization* problem where the evaluation of the objective function is expensive as it is the accuracy of a learning algorithm for a given configuration of hyper-parameters. This vastly limits the number of evaluations that can be carried out, which calls for a design of efficient high-level algorithms that automate the tuning procedure.

Several naive but daily used HPO methods are available, such as grid search or random search. More sophisticated methods address HPO as a *sequential resource allocation problem*, by choosing in an adaptive way the next hyper-parameter(s) to explore based on the results previously obtained. For example, *evolutionary optimization* follows a process inspired by the biological concept of *evolution*, which repeatedly replaces the worst-performing hyper-parameter configurations from a randomly initialized population of solutions; see Loshchilov and Hutter (2016) for an example of using CMA-ES for hyper-parameter tuning. A major drawback of evolutionary optimization is its lack of theoretical understanding.

Bayesian optimization (BO) is another approach that leverages the sequential nature of the problem. BO depends on a prior belief for the target function, typically a Gaussian process (GP). This prior distribution can be updated to a posterior given a sequence of observations. Several algorithms exploiting this posterior distribution to decide where to sample next have been given (see, e.g., Shahriari et al., 2016, for a survey). Snoek et al. (2012) and Klein et al. (2017) provide Python packages called Spearmint and RoBO to perform hyper-parameter tuning with BO methods. Similar packages are available for PyTorch (BoTorch[1]) and TensorFlow (GPflowOpt by Knudde et al. 2017). Among BO algorithms, TPE (Bergstra et al., 2011) and SMAC (Hutter et al., 2011) were specifically proposed for hyper-parameter tuning. A shortcoming of Bayesian optimization is that most algorithms select the next point to sample based on optimizing some *acquisition function* computed from the posterior, e.g., the expected improvement (Jones et al., 1998). This auxiliary optimization task cannot be solved analytically but needs to be performed itself by optimization procedures as L-BFGS that make the process slow.

A simple model for sequential resource allocation is the stochastic multi-armed bandit model (see Lattimore and Szepesvari, 2018 for a recent survey), and some bandit tools have already been considered for global optimization and HPO: First, in the field of Bayesian optimization, the GP-UCB algorithm (Srinivas et al., 2010) is a GP extension of the classical UCB bandit algorithm (Auer et al., 2002). Then, Hoffman et al. (2014) proposed to use *best-arm identification* (BAI) tools—still with a Bayesian flavor—for automated machine learning, where the goal is to smartly try hyper-parameters from a pre-specified *finite* grid.

However, in most cases, the number of hyper-parameter configurations to explore is infinite. In this paper, we investigate the use of bandit tools suited for an *infinite* number of arms. There are two lines of work for tackling a very large or infinite number of arms. The first combines classical bandit tools with a hierarchical partitioning of the arm space, and aims at exploiting the (possibly unknown) smoothness of the black-box function to optimize (Bubeck et al., 2010; Grill et al., 2015; Shang et al., 2019). To the best of our knowledge, these methods have never been investigated for HPO. The second line of work does not assume any smoothness to be present: At each round the learner may ask for a new arm from a *reservoir distribution* ν_0 (pick randomly a new hyper-parameter configuration) and add it to the current arm pool $\mathcal{A}$, or re-sample previous arms (evaluate configuration already included in $\mathcal{A}$), in order to find quickly an arm with a good mean reward (e.g., a hyper-parameter configuration with a good validation accuracy). The *stochastic infinitely-many armed bandit* (SIAB) model is studied by Berry et al. (1997); Wang et al. (2008) for the rewards maximization problem while Carpentier and Valko (2015); Aziz et al. (2018a) study the BAI problem. While most proposed algorithms consist of querying an *adequate* number of arms from the reservoir before running a standard BAI algorithm, Li et al. (2017) propose a more robust approach called Hyperband that uses several such phases.

In this paper, we go even further and propose the first *dynamic* algorithm for BAI in a SIAB model, that may at each round either query a new arm from the reservoir or re-sample arms previously queried. Our algorithm leverages a Bayesian model and builds on

[1] https://botorch.org/

the top-two Thompson sampling (TTTS) algorithm proposed by Russo (2016). We present an extensive numerical study in which we show that our algorithm is competitive with respect to state-of-the-art HPO methods.

2. Hyper-parameter optimization framework

In this paper, we view HPO as a particular *black-box optimization problem*, for which the target function f to optimize is a mapping from a hyper-parameter configuration to some measure of failure for the machine learning algorithm trained with those hyper-parameters. Formally speaking, we are interested in solving an optimization problem of the form $\min\{f(\boldsymbol{\lambda}) : \boldsymbol{\lambda} \in \Omega\}$, where $\boldsymbol{\lambda}$ denotes a configuration of hyper-parameters chosen from a configuration space Ω. A hyper-parameter optimizer is a sequential procedure, that at each round t, selects a configuration $\boldsymbol{\lambda}_t$ to evaluate using some sampling rule, after which a (costly and *noisy*) evaluation of $f(\boldsymbol{\lambda}_t)$ is observed. Besides, at round t a hyper-parameter $\boldsymbol{\lambda}_t^\star$ configuration is recommended as a current guess for a close-to-optimal configuration. The hope is that $f(\boldsymbol{\lambda}_t^\star)$ is not far from the minimum of f.

We restrict our presentation to hyper-parameter tuning for supervised learning algorithms. Given a training dataset $\mathcal{D}_{\texttt{train}}$ containing n labeled examples in $\mathcal{X} \times \mathcal{Y}$ and a choice of hyper-parameter configuration $\boldsymbol{\lambda}$, a supervised learning algorithm (neural network, SVM, gradient boosting, $\ldots$) produces a predictor $\widehat{g}_{\boldsymbol{\lambda}}^{(n)} : \mathcal{X} \to \mathcal{Y}$. Note that there can be some randomness in the training process (e.g., if stochastic gradient descent is used) so that $\widehat{g}_{\boldsymbol{\lambda}}^{(n)}$ may still be random for a given training set and hyper-parameters. The goal is to build a predictor that generalizes well. If we had access to the distribution $\mathbf{P}$ that generated the data (i.e., assuming that data points in $\mathcal{D}_{\texttt{train}}$ are i.i.d. from $\mathbf{P}$), this generalization power would be measured by the risk $f(\boldsymbol{\lambda}) = \mathbb{E}\left[\ell\left(\boldsymbol{Y}, \widehat{g}_{\boldsymbol{\lambda}}^{(n)}(\boldsymbol{X})\right)\right]$, where ℓ is some loss function measuring the distance between two predictions and the expectation is taken on $(\boldsymbol{X}, \boldsymbol{Y}) \sim \mathbf{P}$ and the possible randomness in the training process.

In practice, however, the explicit evaluation of f is impossible, but there are several methods for proposing *noisy evaluations*. One can either compute the validation error of $\widehat{g}_{\boldsymbol{\lambda}}^{(n)}$ on a held-out validation set, $1/|\mathcal{D}_{\texttt{valid}}| \sum_{i=1}^{|\mathcal{D}_{\texttt{valid}}|} \ell(\widehat{g}_{\boldsymbol{\lambda}}^{(n)}(\mathbf{x}_i), \mathbf{y}_i)$, or a cross validation error over the training set as an approximation of the real objective.

3. Active Thompson sampling for HPO

HPO can be modeled as a BAI task in a bandit model. However, standard algorithms are not directly applicable since the search space is often continuous. We thus turn our attention to BAI in an infinitely many armed bandit (see Appendix A for a detailed discussion).

In this section we introduce a new algorithm for BAI in an infinite bandit model, that is an adaptation of Thompson sampling (Thompson, 1933). Thompson sampling can be seen as the very first bandit algorithm ever proposed, but is designed for the *rewards maximization* objective, which is quite different from BAI, as explained by Bubeck et al. (2009). Instead of using vanilla Thompson sampling, we build on the TTTS algorithm that is an adaptation of Thompson sampling for BAI in a finite MAB. Unlike the state-of-the-art algorithm SequentialHalving (SHA) that requires the knowledge of the total budget to operate, TTTS is particularly appealing as it does not. We call such an algorithm *anytime*. Besides, TTTS is proved to be optimal in a Bayesian (asymptotic) sense, as it can attain the best possible rate of decay of the posterior probability of the set of wrong models.

As a Bayesian algorithm, TTTS uses a prior distribution Π_0 over the vector of means of the K arms, $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_K)$, which can be updated to a posterior distribution Π_t after t observations. Under a Bernoulli bandit model, arm i produces a reward $Y_{t,i} = 1$ with probability μ_i, and $Y_{t,i} = 0$ with probability $1 - \mu_i$ when sampled at round t. Given independent uniform prior on the mean of each arm, the posterior distribution on $\boldsymbol{\mu}$ is a product of K Beta distributions: $\Pi_t = \bigotimes_{i=1}^{K} \texttt{Beta}(1 + S_{t,i}, N_{t,i} - S_{t,i} + 1)$, where $N_{t,i}$ is the number of selections of arm i until round t and $S_{t,i}$ is the sum of rewards obtained from that arm. At each time step t, TTTS chooses one arm from the following two candidates to evaluate: (1) it first samples a parameter $\boldsymbol{\theta}$ from Π_{t-1}, and the first candidate is defined as $I_t^{(1)} \triangleq \arg\max_{i \in \mathcal{A}} \theta_i$, (2) it repeatedly samples new $\boldsymbol{\theta}'$ until $I_t^{(2)} \triangleq \arg\max_{i \in \mathcal{A}} \theta'_i$ is different from $I_t^{(1)}$. TTTS depends on a parameter $\beta \in (0, 1)$: the algorithm selects $I_t = I_t^{(1)}$ with probability β, and $I_t = I_t^{(2)}$ with probability $1 - \beta$.

TTTS can also be used for bandit models in which the rewards are bounded in $[0, 1]$ by using a binarization trick first proposed by Agrawal and Goyal (2012): when a reward $Y_{t,i} \in [0, 1]$ is observed, the algorithm is updated with a fake reward $Y'_{t,i} \sim \texttt{Ber}(Y_{t,i}) \in \{0, 1\}$. TTTS can thus be used for BAI among a *finite* number of arms that provide rewards in $[0, 1]$. We now present a simple way of extending TTTS to deal with an infinite number of arms.

Dynamic TTTS In an infinite bandit algorithm at each round we either query a new arm from the reservoir *and sample it*, or re-sample a previous arm. In a Bayesian setting, one can also imagine that at each round an arm is queried from the reservoir and added with a uniform prior to the list of queried arms, *regardless of whether it is sampled or not.* Then at round t, D-TTTS consists in running TTTS on those t arms, out of which several are endowed with a uniform prior and have actually never been sampled.

Leveraging the fact the the maximum of k uniform distribution has a Beta$(k, 1)$ distribution and that TTTS only depends on the maxima of posterior samples, one can propose the following equivalent implementation for D-TTTS. Letting $\mathcal{L}_t$ be the list of arms that have been queried from the reservoir and sampled at least once before round t, at round t we run TTTS on the set $\mathcal{A}_t = \mathcal{L}_t \cup \{\mu_0\}$ where μ_0 is a pseudo-arm with posterior distribution Beta$(t - k_t, 1)$ where $k_t = |\mathcal{L}_t|$. This is the approach we choose in the presentation of Algorithm 1, which describes in detail the sampling rule of D-TTTS.

The remaining question is how to choose the arm to be recommended. The most natural recommendation strategy for Bayesian algorithms is the arm with the largest *posterior probability of being optimal.* Letting Θ_i be the subset of the set Θ of possible mean vectors such that arm i is optimal, $\Theta_i \triangleq \left\{\boldsymbol{\theta} \in \Theta | \theta_i > \max_{j \neq i} \theta_j \right\}$, the posterior probability that arm i is optimal after round n is defined as $\Pi_n(\Theta_i)$.

4. Experiments

We benchmark our bandit-based strategy against different types of HPO algorithms namely TPE, random search and Hyperband and a simple Thompson sampling variant of Hyperband (called H-TTTS) that we describe in Appendix B, for the tuning of classifiers (SVM and MLP) on

Algorithm 1 Sampling rule of Dynamic TTTS (D-TTTS)

```
Input: $\beta$; $B$ (total budget); $\nu_0$
Initialization: $\mu_1 \sim \nu_0$; $t = 0$; $\mathcal{A} = \{\mu_0, \mu_1\}$; $m = 1$; $S_0, N_0 = 0$; $S_1 \sim \texttt{Ber}(\mu_1)$, $N_1 = 1$
while $t < B$ do
    $\forall i = 0, \dots, m$, $\theta_i \sim \mathrm{Beta}(S_i + 1, N_i - S_i + 1)$; $U \sim \mathcal{U}([0,1])$
    $I^{(1)} = \arg\max_{i=0,\dots,m} \theta_i$
    if $U > \beta$ then
        while $I^{(2)} \neq I^{(1)}$ do
            $\forall i = 0, \dots, m, \theta'_i \sim \texttt{Beta}(S_i + 1, N_i - S_i + 1)$
            $I^{(2)} \leftarrow \arg\max_{i=0,\dots,m} \theta'_i$
        end while
        $I^{(1)} \leftarrow I^{(2)}$
    end if
    if $I^{(1)} \neq 0$ then
        $Y \leftarrow$ evaluate arm $I^{(1)}$; $X \sim \texttt{Ber}(Y)$
        $S_{I^{(1)}} \leftarrow S_{I^{(1)}} + X$; $N_{I^{(1)}} \leftarrow N_{I^{(1)}} + 1$; $S_0 \leftarrow S_0 + 1$
    else
        $\mu_{m+1} \sim \nu_0$; $\mathcal{A} \leftarrow \mathcal{A} \cup \{\mu_{m+1}\}$;
        $Y \leftarrow$ evaluate arm $m + 1$; $X \sim \texttt{Ber}(Y)$
        $S_{m+1} \leftarrow X$; $N_{m+1} \leftarrow 1$; $m \leftarrow m + 1$
    end if
    $t = t + 1$
end while
```

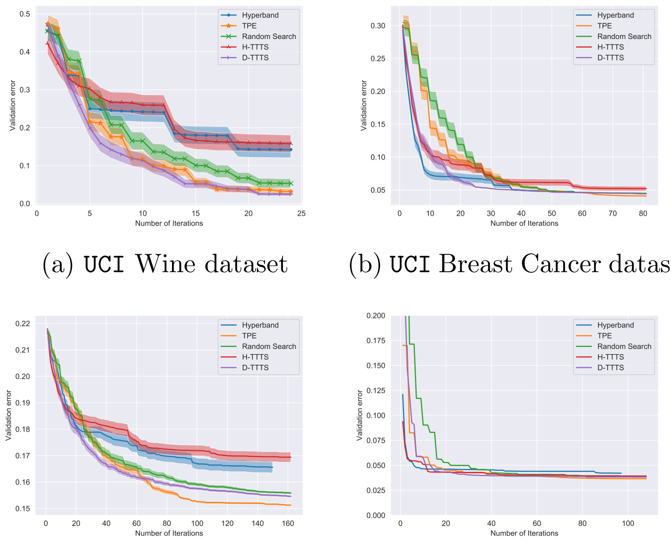
four different classification task: Wine, Breast Cancer and Adult dataset from UCI Machine Learning Repository (Dua and Taniskidou, 2017); and the classical MNIST dataset.

For all those methods, a noisy evaluation of the black-box function f (see the terminology introduced in Section 2) for a hyper-parameter configuration $\boldsymbol{\lambda}$ consists in performing a shuffled 3-fold cross-validation on $\mathcal{D}_{\texttt{train}}$. More precisely, given a random partitioning $\cup_{j=1}^{3} \mathcal{D}_{\texttt{valid}}^{j}$ of $\mathcal{D}_{\text{train}}$ where the folds have equal size, we train a classifier $\widehat{g}_{\boldsymbol{\lambda}}^{(j)}$ on $\mathcal{D}_{\texttt{train}} \backslash \mathcal{D}_{\texttt{valid}}^{j}$ for each fold j and the average validation error $e = 1/|\mathcal{D}_{\texttt{train}}| \sum_{j=1}^{3} \sum_{i \in \mathcal{D}_{\text{valid}}^{j}} \mathbb{1}\left\{\widehat{g}_{\boldsymbol{\lambda}}^{(j)}(\mathbf{x}_i) \neq \mathbf{y}_i\right\}$ is reported as a noisy estimate of the risk $f(\boldsymbol{\lambda}) = \mathbf{P}(\widehat{g}_{\boldsymbol{\lambda}}^{(n)}(\boldsymbol{X}) \neq \boldsymbol{Y})$.

Observe that both the noisy evaluation and the value of f belong to $[0,1]$, so one can introduce an "arm" with rewards in $[0,1]$ for each hyper-parameter $\boldsymbol{\lambda}$. Sampling the arm $\boldsymbol{\lambda}$ produces a reward $r = 1 - e \in [0,1]$ (with a different random partitioning and random seed for training for each selection), that is assumed to have mean $1 - f(\boldsymbol{\lambda})$. In an infinite setting, querying a new arm from the reservoir corresponds to selecting a new hyper-parameter at random from the search space. With these two notions (arm sampling and reservoir querying), our algorithm for infinite BAI can be readily applied to HPO.

For those experiments, we adapt the recommendation rule of D-TTTS to the HPO applications considered and always recommend the hyper-parameter configuration that has produced the smallest cross-validation error so far (which is the recommendation rule used by other approaches as well). For all methods, we then report as a function of time the cross-validation error for the recommended hyper-parameter configuration at this time. We stress again that, unlike in a classic bandit setting where we could use the simple regret as a performance metric, we do not have access to the ground truth generalization error in real classification tasks. Thus we only report a proxy of the error rate that we are interested in.

Experiments results (code available at https://bit.ly/2IDwuir) We first benchmark our methods on some simple `UCI` datasets using `SVM` (from `scikit-learn`) as the classifier. We optimize over two hyper-parameters: the *penalty parameter* C and the *kernel coefficient* γ for a *rbf* kernel, for whom pre-defined search bounds are both $\left[10^{-5}, 10^{5}\right]$.



(a) `UCI` Wine dataset

(b) `UCI` Breast Cancer dataset

(c) `UCI` Adult dataset

(d) MNIST dataset

Fig. 1a shows the mean cross-validation error of `SVM` run on the `UCI` Wine dataset over 24 iterations averaged on 100 replications. The task is to predict the quality score (between 0 and 10) of a wine given 11 attributes. We recall that one iteration corresponds to one arm pull. In this experiment, `D-TTTS` improves over other benchmark algorithms. Fig. 1b is the same experiment run on the `UCI` Breast Cancer dataset over 81 iterations. The task is to predict whether a patient has breast cancer based on 32 attributes. We repeat the experiment for 100 times. This time, `D-TTTS` is slightly worse than `Hyperband` at the beginning, but improves later. Finally we optimize `SVM` on a relatively more complicated `UCI` Adult dataset over 162 iterations, for which the result is shown in Fig. 1c. The task is to tell whether the income of an individual is higher than 50k or not given 14 attributes. This experiment is also run over 100 replications. `D-TTTS` is better than other algorithms at the beginning, but is outperformed by `TPE` towards the end.

We see that, although not always the best, `D-TTTS` shows a consistent, robust, and quite competitive performance in the 3 tasks.

We now carry out the classic `MNIST` digits classification task using multi-layer perceptron (`MLP`). We choose to optimize over three hyper-parameters: the *size of hidden layer* (an integer between 5 and 50), the *L2 penalty parameter* α (between 0 and 0.9) and the *initial learning rate* (bounded in $\left[10^{-5}, 10^{-1}\right]$). Fig. 1d shows the result of `MLP` run on `MNIST` over 108 iterations, this time averaged on 20 replications. D-TTTS is slightly slower than Hyperband and H-TTTS at the very beginning, but is performing well afterward.

5. Discussion

We presented a way to use Thompson sampling for BAI in an infinitely many-armed bandit model, and explained how to use it for HPO. We introduced the first fully dynamic algorithm for this problem and showed through an extensive empirical study that it is a promising approach for HPO. In the future, we would like to provide experiments on more datasets and establish theoretical guarantees to support the good performance of D-TTTS, with the hope to provide a finite-time upper bound on its error probability. We will also investigate variants of this algorithm for the non-stochastic bandit setting for which Hyperband can be used, and that allows to spend more time on training the more promising algorithms.

Acknowledgments

The research presented was supported by European CHIST-ERA project DELTA, French Ministry of Higher Education and Research, Nord-Pas-de-Calais Regional Council, Inria and Otto-von-Guericke-Universitt Magdeburg associated-team north-European project Allocate, and French National Research Agency projects ExTra-Learn(n.ANR-14-CE24-0010-01), BADASS (n.ANR-16-CE40-0002), and BoB (n.ANR-16-CE23-0003).

References

Shipra Agrawal and Navin Goyal. Analysis of Thompson sampling for the multi-armed bandit problem. In *Proceedings of the 25th Conference on Learning Theory (CoLT)*, pages 1–26, 2012.

Jean-Yves Audibert and Sébastien Bubeck. Best arm identification in multi-armed bandits. In *Proceedings of the 23rd Conference on Learning Theory (CoLT)*, 2010.

Peter Auer, Nicolò Cesa-Bianchi, and Paul Fischer. Finite-time analysis of the multi- armed bandit problem. *Machine Learning Journal*, 47(23):235–256, 2002.

Maryam Aziz, Jesse Anderton, Emilie Kaufmann, and Javed Aslam. Pure exploration in infinitely-armed bandit models with fixed-confidence. In *Proceedings of the 29th International Conference on Algorithmic Learning Theory (ALT)*, 2018a.

Maryam Aziz, Kevin Jamieson, and Javed Aslam. Pure-exploration for infinite-armed bandits with general arm reservoirs. *arXiv preprint arXiv:1811.06149*, 2018b.

James Bergstra, Rémi Bardenet, Yoshua Bengio, and Balázs Kégl. Algorithms for hyper-parameter optimization. In *Advances in Neural Information Processing Systems 24 (NIPS)*, pages 2546–2554, 2011.

Donald A. Berry, Robert W. Chen, Alan Zame, David C. Heath, and Larry A. Shepp. Bandit problems with infinitely many arms. *Annals of Statistics*, 25(5):2103–2116, 1997.

Sébastien Bubeck, Rémi Munos, and Gilles Stoltz. Pure exploration in multi-armed bandits problems. In *Proceedings of the 20th International Conference on Algorithmic Learning Theory (ALT)*, pages 23–37, 2009.

Sébastien Bubeck, Rémi Munos, Gilles Stoltz, and Csaba Szepesvari. X-armed bandits. *Journal of Machine Learning Research*, 12:1587–1627, 2010.

Alexandra Carpentier and Michal Valko. Simple regret for infinitely many armed bandits. In *Proceedings of the 32nd International conference on Machine Learning (ICML)*, pages 1133–1141, 2015.

Dheeru Dua and Karra E. Taniskidou. UCI Machine Learning Repository, 2017.

Eyal Even-dar, Shie Mannor, and Yishay Mansour. Action elimination and stopping conditions for reinforcement learning. In *Proceedings of the 20th International Conference on Machine Learning (ICML)*, pages 162–169, 2003.

Stefan Falkner, Aaron Klein, and Frank Hutter. BOHB: Robust and efficient hyperparameter optimization at scale. In *Proceedings of the 35th International Conference on Machine Learning (ICML)*, 2018.

Victor Gabillon, Mohammad Ghavamzadeh, and Alessandro Lazaric. Best arm identification: A unified approach to fixed budget and fixed confidence. In *Advances in Neural Information Processing Systems 25 (NIPS)*, pages 3212–3220, 2012.

Jean-Bastien Grill, Michal Valko, and Rémi Munos. Black-box optimization of noisy functions with unknown smoothness. In *Advances in Neural Information Processing Systems 28 (NIPS)*, pages 667–675, 2015.

Matthew W. Hoffman, Bobak Shahriari, and Nando de Freitas. On correlation and budget constraints in model-based bandit optimization with application to automatic machine learning. In *Proceedings of the 17th International Conference on Artificial Intelligence and Statistics (AIStats)*, pages 365–374, 2014.

Frank Hutter, Holger H. Hoos, and Kevin Leyton-Brown. Sequential model-based optimization for general algorithm configuration. In *Proceedings of the 5th International Conference on Learning and Intelligent Optimization (LION)*, pages 507–523, 2011.

Donald R. Jones, Matthias Schonlau, and William J. Welch. Efficient global optimization of expensive black-box functions. *Journal of Global Optimization*, 13(4):455–492, 1998.

Zohar Karnin, Tomer Koren, and Oren Somekh. Almost optimal exploration in multi-armed bandits. In *Proceedings of the 30th International Conference on Machine Learning (ICML)*, pages 1238–1246, 2013.

Aaron Klein, Stefan Falkner, Numair Mansur, and Frank Hutter. RoBO: A flexible and robust Bayesian optimization framework in Python. In *7th Workshop on Bayesian Optimization at Neural Information Processing Systems (NIPS-BayesOpt)*, 2017.

Nicolas Knudde, Joachim van der Herten, Tom Dhaene, and Ivo Couckuyt. GPflowOpt: A Bayesian optimization library using TensorFlow. *arXiv preprint arXiv:1711.03845*, 2017.

Tor Lattimore and Csaba Szepesvari. *Bandit Algorithms*. Cambridge University Press, 2018.

Lisha Li, Kevin Jamieson, Giulia DeSalvo, Ameet Talwalkar, and Afshin Rostamizadeh. Hyperband: Bandit-based configuration evaluation for hyperparameter optimization. In *Proceedings of the 5th International Conference on Learning Representations (ICLR)*, 2017.

Ilya Loshchilov and Frank Hutter. CMA-ES for hyperparameter optimization of deep neural networks. In *Workshop Track of the 4th International Conference on Learning Representations*, 2016.

Daniel Russo. Simple Bayesian algorithms for best arm identification. In *Proceedings of the 29th Conference on Learning Theory (CoLT)*, 2016.

Bobak Shahriari, Kevin Swersky, Ziyu Wang, Ryan P. Adams, and Nando de Freitas. Taking the human out of the loop: A review of Bayesian optimization. *Proceedings of the IEEE*, 104(1):148–175, 2016.

Xuedong Shang, Emilie Kaufmann, and Michal Valko. General parallel optimization without a metric. In *Proceedings of the 30th International Conference on Algorithmic Learning Theory (ALT)*, 2019.

Jasper Snoek, Hugo Larochelle, and Ryan P. Adams. Practical bayesian optimization of machine learning algorithms. In *Advances in Neural Information Processing Systems 25 (NIPS)*, pages 2951–2959, 2012.

Niranjan Srinivas, Andreas Krause, Sham M. Kakade, and Matthias Seeger. Gaussian process optimization in the bandit setting: No regret and experimental design. In *Proceedings of the 27th International conference on Machine Learning (ICML)*, pages 1015–1022, 2010.

William R. Thompson. On the likelihood that one unknown probability exceeds another in view of the evidence of two samples. *Biometrika*, 25(3/4):285, 1933.

Yizao Wang, Jean-Yves Audibert, and Rémi Munos. Algorithms for infinitely many-armed bandits. In *Advances in Neural Information Processing Systems 21 (NIPS)*, pages 1729–1736, 2008.

Appendix A. Best-arm identification for HPO

Hyper-parameter optimization can be modeled as a BAI task in a bandit model. Given a finite set of arms $\mathcal{A} \triangleq \{1, \ldots, K\}$, when we select arm i, we get an independent observation from some unknown distribution ν_i with mean μ_i. A BAI algorithm sequentially selects arms in order to identify the arm with the largest mean, $I^\star \triangleq \arg\max_{i\in\mathcal{A}} \mu_i$[2]. In the context of HPO, each arm models the quality of a given hyper-parameter configuration $\boldsymbol{\lambda}$. When the arm is sampled, a noisy evaluation of $f(\boldsymbol{\lambda})$ is received, which is the mean reward of that arm. A BAI (or pure-exploration) algorithm consists of a sequential arm selection strategy, indicating which arm I_t is selected at round t, coupled with *recommendation rule* that selects a candidate best arm $I_t^\star$ at round t. The goal is either to minimize the error probability $\mathbf{P}(\mu_{I_t^\star} \neq \mu_{I^\star})$ (Audibert and Bubeck, 2010; Karnin et al., 2013) or the *simple regret* (Bubeck et al., 2009; Gabillon et al., 2012), defined as $r_t = \mu_{I^\star} - \mu_{I_t^\star}$, possibly after a total budget B, whose knowledge may be used by the algorithm. Note that the BAI problem can also be studied from a fixed-confidence point of view (Even-dar et al., 2003).

Standard BAI algorithms are however not straightforwardly applicable to HPO when the search space can be infinite and is often continuous. To handle those interesting cases, we rather turn our attention to BAI in a infinitely many armed bandit (Carpentier and Valko, 2015). In this context, there is an infinite pool of arms, whose means are assumed to be drawn from some *reservoir distribution* ν_0. In such a model, a BAI algorithm maintains a list of arms (hyper-parameter configurations) that have been tried before. At each round it can either query a new arm from the reservoir (add a new hyper-parameter, selected at random, to the current pool), add it to the list and sample it (evaluate it), or sample an arm already in the list (re-evaluate a configuration tried before).

A natural way to perform BAI in an infinite-many armed bandit model consists in first querying a *well-chosen* number of arms from the reservoir and then running a standard BAI algorithm on those arms (Carpentier and Valko, 2015). However this ideal number may rely on the difficult of the learning task, which is hardly known in practice. The `Hyperband` algorithm (Li et al., 2017) takes a step further and successively queries several batches of arms from the reservoir, including a decreasing number of arms in each batch, while increasing the budget dedicated to each of them. `SHA` (Karnin et al., 2013), a state-of-the-art BAI algorithm, is then run on each of these batches of arms. This approach seems more robust in that it trades off between *the number of arms that is needed to capture a good arm* and *how much measurement effort we should allocate to each of them*. However, a numerical study performed by Aziz et al. (2018b) seems to reveal that an infinite bandit algorithm based on `SHA` should always query the maximal number of arms from the reservoir[3].

All the existing algorithms are still subject to a pre-defined scheduling of how many arms should be queried from the reservoir. The algorithm (`D-TTTS`) we proposed in this paper does not need to decide in advance how many arms will be queried, and is therefore fully *dynamic*.

[2] Here we present BAI problems in a standard way for which we search for an arm with the largest mean. For HPO, however, it is important to mention that we are searching for a hyper-parameter configuration that minimizes the validation error. One can easily see that it does not change the problem in principle.

[3] This reference is a preliminary draft that has been withdrawn due to technical issues in the proofs. Yet we believe the experimental section to be sound.

Remark 1 *`Hyperband` is proposed specifically for hyper-parameter tuning. Its original philosophy is to adaptively allocate* resources *to more promising configurations. Resources here can be time, dataset sub-sampling, feature sub-sampling, etc. In such a setting, the classifier is not always trained into completion given a parameter configuration, but is rather stopped early if it is shown to be bad so that we can allocate more resources to other configurations. In this case, different evaluations of a single configuration cannot be considered as i.i.d. anymore. Thus, HPO is stated as a non-stochastic infinitely-armed bandit problem. This idea of early stopping is also further investigated by combining Bayesian optimization with it (Falkner et al., 2018). However, this is out of the scope of this paper.*

Appendix B. Hyper `TTTS`

We present here another way of extending `TTTS` to deal with an infinite number of arms, namely `Hyper-TTTS` or `H-TTTS`, a variant of `Hyperband` in which `SHA` is replaced by `TTTS`. This algorithm, whose sampling rule is formally stated as Algorithm 2, runs $s_{\max}$ batches of `TTTS` with different number of arms n and each batch with a same budget $T = \lceil B/s_{\max} \rceil$ with B the total budget. The number of arms within each bracket is decreasing with an exponential rate of γ. One inconvenience of this algorithm is that $s_{\max}$ and γ still need to be tuned (in practice, we use the same tuning as the one of `Hyperband`). `D-TTTS` is thus proposed to circumvent this issue.

Appendix C. Some synthetic results

In this part, we give some synthetic experimental results comparing `D-TTTS` to `Hyperband` and to `SHA`, a state-of-the-art algorithm for finite BAI that can be adapted to the infinite setting. In those experiments, the arms are Bernoulli distributed and the reservoir distribution ν_0 is fixed to some Beta(a, b) distribution.

Infinite Sequential Halving (`ISHA`) consists in running `SHA` on a fixed number of arms drawn from the reservoir. Observe that for a total budget B, there exists a maximum number of arms $K^\star$ that can be processed by `SHA`, which satisfies $B = \lceil K^\star \log_2(K^\star) \rceil$. Following Aziz et al. (2018b), we run `ISHA` with $K^\star$ arms drawn from the reservoir.

We report in Fig. 2 the simple regret as a function of time for different algorithms and four Beta reservoir distributions. `H-TTTS` and `D-TTTS` are run with $\beta = 1/2$ which is known to be a robust choice (Russo, 2016). Each point represents the expected simple regret $\mathbb{E}[1 - \mu_{I_n^*}]$ estimated over 1000 replications for an algorithm run with budget n. `D-TTTS` is very competitive on 3 reservoirs and `H-TTTS` is sometimes better, sometimes worse than `Hyperband`. We also tried the `SiRI` algorithm (Carpentier and Valko, 2015) (with b as the tail parameter when $\nu_0 =$Beta(a, b)) but obtained worse performance and therefore do not report the results.

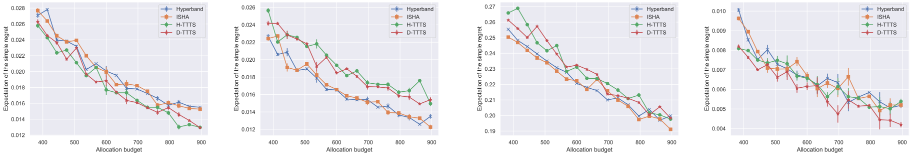
Note that in the implementation of `Hyperband` for this *stochastic* infinite bandit setting, the elimination phase of the underlying `SHA` algorithm is carried out according to the averaged loss of previous samples (as samples from an arm are i.i.d. in this setting and not a converging sequence). In the next section, we apply our algorithm to some real hyper-parameter optimization tasks.

Algorithm 2 Hyper `TTTS` (`H-TTTS`)

Input: β; γ; B; $s_{\max}$; ν_0

Initialization: $T = \lfloor B/s_{\max} \rfloor$

```
for $s \leftarrow s_{\max}$ to $0$ do
    $K = \left\lceil \frac{s_{\max}+1}{s+1} \gamma^s \right\rceil$
    $\mathcal{A} \leftarrow \{i = 1, \ldots, K : \mu_i \sim \nu_0\}$; $t = 0$
    while $t < T$ do
        sample $\boldsymbol{\theta} \sim \Pi_t$
        $I^{(1)} \leftarrow \arg\max_{i \in \mathcal{A}} \theta_i$
        sample $b \sim \text{Bernoulli}(\beta)$
        if $b = 1$ then
            $Y \leftarrow$ evaluate arm $I^{(1)}$
        else
            while $I^{(2)} \neq I^{(1)}$ do
                $\forall i \in \mathcal{A}, \theta'_i \sim \texttt{Beta}(S_i + 1, N_i - S_i + 1)$
                $I^{(2)} \leftarrow \arg\max_{i \in \mathcal{A}} \theta'_i$
            end while
            $I^{(1)} \leftarrow I^{(2)}$
            $Y \leftarrow$ evaluate arm $I^{(1)}$
        end if
        $X \sim \texttt{Bernoulli}(Y)$
        $S_{I^{(1)}} \leftarrow S_{I^{(1)}} + X$; $N_{I^{(1)}} \leftarrow N_{I^{(1)}} + 1$
        $t = t + 1$
    end while
end for
```



(a) Beta(1,1) (b) Beta(3,1) (c) Beta(1,3) (d) Beta(0.5,0.5)

Figure 2: expected simple regret as a function of the number of arms evaluations for different Beta reservoir