Novel Approaches For Tuning Models' Hyper Parameters

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1 INTRODUCTION

Hyperparameters are crucial in machine learning, as they determine if the model will be efficient and accurate. Usually, a tuning process is used to find good combinations of hyperparameters. This tuning process used to be very time-consuming as it historically consisted of training the model with all combinations of hyperparameters among the space of all possibilities for grid-search, and of a random set of combinations for random search. Then results were compared to choose the best combination. Now notice that the space of possibilities grows exponentially with the number of hyperparameters. Furthermore, for complex deep-learning problems a single training can take days.
Thus new approaches are needed to find good hyperparameters faster. In this project, we would like to choose a few deep-learning problems as they are usually long to train and compare different tuning approaches [1]. We would like to empirically quantify and qualify the speed for each method as well as the efficiency of the parameters found.

Project Plan:

1. Choose and describe optimization algorithms that are going to be compared during the project.
2. Implement a benchmark tool to measure the results of various optimization algorithms.
3. Choose a batch of different machine learning problems (more precisely, deep-learning problems).
4. Analyze the results and determine if any approach performs better in average in terms of efficiency or in terms of speed than random search, which is the commonly used algorithm.

2 DESCRIBE TRADITIONAL AND NOVEL OPTIMIZATION ALGORITHMS FOR HYPERPARAMETER TUNING

We will in a first time describe current approaches, then main concepts and tools used behind more recent optimization methods. Finally we will describe novel approaches proposed by RayTune.

2.1 Overview of traditional methods

The historical approach was Grid search. It consists of testing all hyperparameters combinations on the validation set to find the combination with the best metrics. Time budget then only depends on the granularity of the combinations tested. As an example, if there are d parameters, each with n possibilities, the space of different possibilities/combinations is n^d. This is exponential in function of the number of hyperparameters, so very inefficient for large d. Note that grid search is trivially parallel.

The most commonly used approach with grid search for hyperparameters optimization is Random search: It consists of trying randomly some combinations in the space of possibilities which should (should because random) find a decent combination in a reasonable amount of time. It is better than Grid search for the following reasons: If only a small number of hyperparameters a have a big influence on results out of d hyperparameters each having n possible different values, then, GridSearch tests with n different values each parameter. So there are only n^a useful trials (combinations where an important parameters changes) out of n^d different combinations. The proportion of useful tests out of all tests is:

$$\frac{n^a}{n^d} = n^{a-d} \tag{1}$$

That is exponentially inefficient in function of dimensions with low impact. Now random search is going to make all d parameters change at each trial (since random), so n^d useful tests since all a dimensions changes for every trial. The proportion of useful training is:

$$\frac{n^d}{n^d} = 100\% \tag{2}$$

A second interesting property about random search is that independently of the shape of the space, random

[1]using the Ray Tune library

search is statistically assured to find a good solution if there is one, as long as there are enough trials. Imagine that a proportion of $x\,\%$, $x \in \mathbb{R}\backslash\{\ 0 \leq x \leq 100\}$ of the combination space will provide very good results (x is often very small). We are interested in finding **at least one** solution in this subspace. Now let's define the $p_x(n)$, the **probability** that all n search are **not** in the subspace of interesting results (the subspace is $\frac{100}{x}$ times smaller than the original space). Since all trials are i.i.d:

$$p_x(n) = (1 - \frac{x}{100})^n \tag{3}$$

Table 1 Table with example values of **1 -** $p_x(n)$ with varying values of n and x.
Please remember that x is in percentage of the whole space size. The most distant value we rounded to 1 was 0,99995

$x\backslash n$	10	100	1000	10000
0,01	0	0,01	0,095	0,632
0,1	0,01	0,095	0,632	1
1	0,096	0,634	1	1
10	0,651	1	1	1
100	1	1	1	1

We clearly see on table 1 that $1 - p_x(n)$ converges to 1 as n goes large. Thus we find a combination is in the chosen subspace with probability which tends to 1 as n goes large, this, independently of the subspace shape. Note that random search is also trivially parallel.
Please look at Bergstra & Bengio (2012) for more details.

2.2 Tools and concepts used by the novel tuning algorithms

New kinds of optimization methods have been proposed since a couple of years: The global idea is rather to try different parameters via grid search or random search, then to select a set of parameters in an **adaptive manner**: Once one knows the results of a first set, he shall choose next set smartly. These methods aim to identify good configurations more quickly. We will here explain and describe all approaches proposed by the Ray Tune python library.

But first, as they will be widely used in the described approaches, let's explain some of the main tools and concepts used in those different optimization methods.

- SHA: SuccessiveHalvingAlgorithm has a very intuitive concept: given n combinations, it trains all n models, select the best $\frac{n}{2}$ (sometime $\frac{n}{3}$), and then starts again with the $\frac{n}{2}$ best combinations. The best (last) model is found in $2 \times n$ trainings as $\sum_{i=0}^{\infty} \frac{1}{2^i} = 2$.
  Grid search is in only n trainings, but the strength of SHA is that the time allocated for a training can be much smaller since best models are going to get more and more training time. SHA's conceptual interest is to stop the training of model with low potential. This is one of the simplest adaptive algorithm. See Li et al. (2017).

- ASHA: Stands for AsynchronousSuccessiveHalvingAlgorithm . It allows parallelisation and asynchronisation of SHA, hence permitting a trivial parallelisation of HyperBand. See Li et al. (2018).

- MSR: Median Stopping Rule is very close conceptually to SHA. It simply stops a trial as its performance is below the median performance of all other trials after an equal training. It suffers the same problem as SHA: it needs to train all models at least once, which can be very long.

- BO: Bayesian Optimisation uses the principle of Bayesian inference: it exploits all observed trials results to infer the probability results of not yet observed trials. The probability representation of the objective function using previous observations is called the surrogate.

  It often is a ***Gaussian process*** , as it is very useful to guess the values of unexplored trials: For a distribution of the result estimation $\mathbf{N}(\mu, \sigma)$, if the σ is large, then exploration is interesting as an unknown maximum could probably be there, and if the μ is big, then we can exploit: it could be near the maximum. The dilemma is resolved by taking the **maximum** of the potential function

$$f(x) = \mu(x) + k \times \sigma(x) \tag{4}$$

  where k is the weight of exploration and x is a combination of hyperparameters.

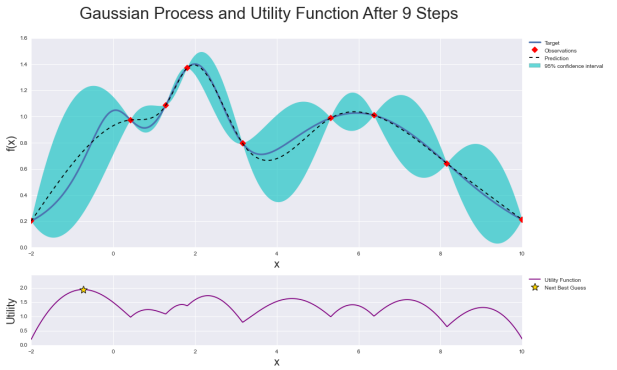


Figure 1. Here is a BO process, see Gamboa (2019).

We can observe in Figure 1 a Bayesian Optimisation in process, with the blue curve being the real

function, the black one the predicted function, and the blue area the incertitude about the predicted function. On the bottom in purple is the potential function.

Gaussian process is a logical surrogate function: it updates predictions after new observations, and chooses to observe next the combination with the best potential. It tries to **maximize** $p(P|O)$, the probability of having a good prediction given observations. See Balandat et al. (2019).

Other surrogate functions exists such as the ***Tree-structured Parzen Estimator (TPE)*** : using Bayes rule

$$p(P|O) = \frac{p(O|P) \times p(P)}{p(O)} \tag{5}$$

It is interested in $p(O|P)$ and $p(P)$ to find $P(P|O)$ rather than directly in $P(P|O)$.
Here is the TPE algorithm explained: After a random initialization, models are separated in two groups, best performing ones, and the others, and let y be the threshold. Then let's have densities l and g from Parzen estimators's model such that

$$p(o|P) = \begin{cases} l(o) & o < y \\ g(o) & o \geq y \end{cases} \tag{6}$$

o an observation. The expected improvement if x is chosen as next observed model then is $\frac{l(x)}{g(x)}$, so we have to choose x that maximises $\frac{g(x)}{l(x)}$. See Bergstra et al. (2011) and Falkner et al. (2018).

Note that the same mechanisms can be used to predict the expected remaining gains (if we continue the algorithm), hence Bayesian optimisation allows early termination. It also allows parallelism, but as a trade off for performances, as the model will have more information at any point in sequential mode than in parallel mode.

- Multi-armed Bandit Problem: This optimisation problem consists of optimizing gains when K cash machines are available, and it is only possible to use one cash machine per turn.
The interest of this problem is to find the trade-off between exploration: trying an untested cash machine with the hope of discovering an even worthier one, and the exploitation: choosing the yet discovered best cash-machine.
We define the regret as the difference between the reward sum in case of an optimal strategy and the sum of collected rewards. When we speak of optimizing hyperparameters, cash machines are models, and gains are efficiency results of the models.
Here are some known algorithm which tries to find the best trade-off:

The simplest algorithm "greedy" consists of maximising exploitation: always choose the model with best performances.

Another simple strategy is the ***epsilon first strategy*** : $\times N$ steps of random exploration followed by $(1-) \times N$ steps of exploitation of the best yet discovered models. It is very close to the epsilon strategy: probability of ϵ of exploring new models and $1-$ of exploiting.

The ***Thompson sampling algorithm*** : The intuition is that you select a combination of hyperparameters with a probability proportional to that combination being the best. This adaptive algorithm is very similar to SHA or MSR, intuitively, we invest trainings in models with high potential, which is going to confirm or infirm quickly and with strong evidence that it indeed has strong potential. We can see in Figure 2 the strong advantage of finding a good optimization method. See Dimmery et al. (2019).

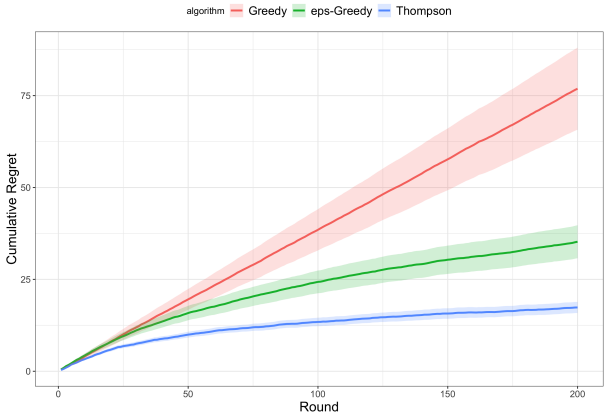


Figure 2. We can see that regret is clearly sub-linear for Thompson algorithm [5]

- PBT: Population-Based Training trains n models in parallel with different random combinations. Once all models are trained with budget B, they are tested and models with bad results copy the hyperparameters of most performing models plus some noise, intending to outperform best models by finding even better combinations. This is the only approach that modifies hyperparameters of models during training.

Summing up, it first starts by creating n models in parallel with random hyperparameters.
Then it starts a **while Loop**. It trains all n with budget B, then only the best a models are kept, and the $n - a$ other take hyperparameters close to the best models. Back to **Loop** until convergence . This algorithm is promising as it is similar to

random search with the difference it reallocates training budget smartly in zones with high potential.

- HyperBand. This method is using a bandit based optimisation: The problem of SHA is that training all n combinations can be much too long. If you only have a budget B to spent all trainings, Hyperband proposes to evaluate some random subsets m of combinations, and, using the SHA algorithm, to spent budget $\frac{B}{log(m)}$ for i from 0 to $log(m)$ randomly among all $\frac{m}{2^i}$ models, as long as it the budget is at least r and at least one model is trained with budget at least R, R is a random input of the program ($R > r$) , and r a function of R and i. The complexity then is $B \times log(R)$.

  Intuitively if a model requires a long time before having converging results, we would prefer a small n, to give enough budget to each model so it has relevant results. Equivalently, if the models are not noisy and train quickly, we want n to be as large as possible. HyperBand finds the solution to the latter Bandit problem by proposing random R and random sets of configuration m in a SHA with limited budget B. It balances very aggressive evaluations with many configurations with small budget, and very conservative evaluations with bigger budgets. It has infinite arm since the space of hyperparameters combinations needs to be infinite, which is usually the case (continuous). It also provides early stopping, meaning the algorithm stops as soon as it does not notice any significant improvement. Please see Li et al. (2017).

2.3 Description of Tuning algorithms proposed by Ray-Tune

- AxSearch: Ax can optimize continuous configurations (integer included) using Bayesian optimization improved using matern kernel to manage very noisy models. It optimizes discrete configurations (only several choices) as a multi-armed bandit problem, solved using the Thompson sampling algorithm and empirical Bayes. We shall not use this latter algorithm as it is an optimisation algorithm for a small number of possibilities, opposed to deep-learning problems which could have a lot of combinations of hyperparameters. Balandat et al. (2019), Dimmery et al. (2019).

- DragonflySearch uses Bayesian optimisation adapted for expensive large scale problems with high dimensional spaces. It also provides a parallel approach. The main idea is the following: it is known that BO is very successful for low dimensional models ($d < 10$). And it is said to be exponentially difficult in function of dimensions. So the dragonfly algorithm is going to decompose the result function

$$g(x) = g_1(x_1) + g_2(x_2) + ... + g_n(x_n) \quad x_i \in X_i \quad (7)$$

  where X_i is a set of very low dimensionality randomly chosen such that every X_i is disjoint with any X_j, and all f_i is independent with any g_j, and g_i are considered as sampled from a Gaussian process. Then it is proved that the overall potential function described in our paragraph about BO is simply the sum of each potential function, resulting in a huge performance improvement. That is:

$$\begin{aligned} f(x) &= f_1(x_1) + f_2(x_2) + ... + f_n(x_n) \\ et \quad & f_i(x_i) = \mu_i(x_i) + k \times \sigma_i(x_i) \end{aligned} \quad (8)$$

  One now simply has to observe the maximum of f. See Kandasamy et al. (2020).

- SkoptSearch is using regular BayesianOptimizationSearch. Louppe & Kumar (2016).

- HyperOptSearch performs especially well in case of mixed search space, which may include both continuous, discrete, and conditional dimensions. It is using BO with either a Gaussian Process or the Tree-structured Parzen Estimators algorithm as surrogate function. See Bergstra et al. (2011).

- BayesOptSearch is using regular BayesianOptimizationSearch as well.

- TuneBOHB is named after Bayesian Optimisation concatenated with HyperBand. The interest is to take the best of the two worlds as Hyperband has strong performance and scalability, but samples configurations randomly (without learning from previous observations, although BO is very good at this). It uses Bayesian optimisation with TPE instead of Gaussian process as it would scale better in high dimensional space.

  BOHB uses HB algorithm to determine the number and the budget of each configuration, but replaces the random selection of combinations by a BO algorithm for most samples (with probability $1 - \rho$) based on all observations so far. the combination is still selected with probability $p$at random. It can use the parallel properties of both TPE and HB to provide efficient parallelism. It is said by his authors to always beat or match both methods.
  We can observe on Figure 3 how TuneBOHB is always better than both random search, BO, and

HyperBand. See Falkner et al. (2018).

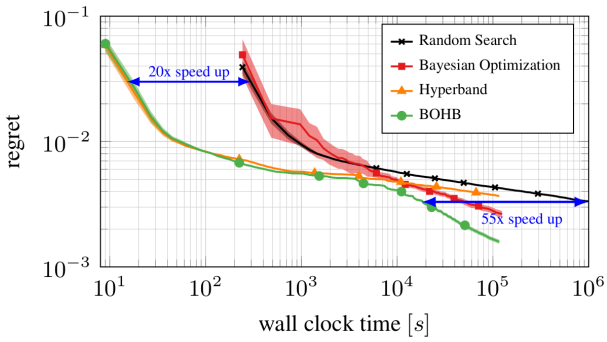


Figure 3. Comparative plot of HB, BO, BOHB and random search for a deep learning problem according to [11]

- NevergradSearch: this Facebook open project proposes several algorithms. Here is a selection of three evolutionary algorithm:

  TwoPointsDE : Differential Evolution algorithm is the following:
  First n models are trained with random combinations.
  Then loop until convergence or end of time budget:
  (1) For every models x,
  (2) choose 3 other distinct models a, b, c.
  (3) Then for any dimension of x, keep same value with high probability, and take a combination of a, b, c 's value otherwise (mutation), in a way that at least one dimension changes.
  (4) Then keep the best model between old x and new x (selection).
  This is the historical algorithm. Facebook's algorithm only differs from the facts there are only 2 others models a and b instead of a, b, c. See Storn & Price (1997).

  CMA : This algorithm uses two different concepts: First exploration: by updating the average of the distribution in a way that maximizes the likelihood of actual good models. The Covariance matrix is incremented to increase the likelihood of previous search steps.
  The second concept is that it adaptively increases or decreases the variance depending on last steps. If the model is in an exploration phase, variance will increase until it finds the best combinations, but if we are close to best results (exploitation), the variance becomes very small, hence allowing fast convergence. See Hansen (2006).

  PSO : This algorithm imitates birds or ants movement. First initialize n models with random combination of hyperparameters; let's call it position in the d-dimension space, and assign to each model an additional information: it's best position so far. Let g be the best position of all models so far. Then on each loop every model is going to have on every dimension a speed, functions both of it's best position times a normal distribution sample and of the best position of the swarm times a normal distribution sample. Then update the *position* as last *position* + *speed*.
  See Kennedy & Eberhart (1995).

- ZOOptSearch: its particularity is that is focused on derivative-free optimization.
  The goal is to find the minimum of a function f without having any other informations than $f(x)$ (performance of combination x) given x.

  The classification model will classify combinations as either good (k best) or bad, by using a parallel to axis hyper-rectangle, of same dimension as the combination space, that contains all good combinations. Then **loop** on the following: (1) Choose a combination either randomly from the d dimension rectangle with probability λ, or from the whole space with probability 1-λ, (2) evaluates its efficiency and (3) replace the worst of the k best solution with this new solution, then (4) replace a random bad solution with the worst of the k solutions (the one just replaced).
  Finally (5) update the classifier and go back to loop.
  The asynchronous process is accomplished by parallelising the loop on different threads, but it needs to update the model after each evaluation. Liu et al. (2019).

- SigOptSearch: What they are doing is not clear at all for me, I have not been able to find any concept they were using.

Table 2 Characteristic of all approaches.

Tuning Algorithm	Parallelism	Adaptive algorithm	Efficient despite ineffective parameters	Early termination	Main Concept
GridSearch	✓				Extensive search
RandomSearch	✓		✓		Random search
AxSearch		✓	✓	✓	BO or Bandit Based
DragonflySearch	✓	✓	✓	✓	BO
SkoptSearch		✓	✓	✓	BO
HyperOptSearch	✓	✓	✓	✓	BO with TPE
BayesOptSearch		✓	✓	✓	BO
TuneBOHB	✓	✓	✓	✓	BO and HyperBand
NevergradSearch		✓	✓		Population based
ZOOptSearch	✓	✓	✓		Zeroth Optimization (ASRACOS)
SigOptSearch	✓	✓	✓	✓	Unknown

2.4 Discussion

In a nutshell, we can regroup the algorithms by the concept they use: *AxSearch*, *DragonflySearch*, *SkoptSearch*, *HyperOptSearch* and *BayesOptSearch* uses Bayesian Optimisation, except *HyperOptSearch* uses TPE as a surrogate function, *dragonflySearch* is specialized for large scale problems (in case of high dimensional optimisation, it provides improved parallelism, and cheap approximations functions), and *AxSearch* also proposes a Bandit based solution in case of discrete spaces of very small size. *NevergradSearch* is the only population based optimizer which is promising. *ZooptSearch* proposes a derivative-free optimization. Finally *TuneBOHB* uses both concepts from Bayesian optimisation and Bandit-Based optimization, which is intuitively powerful as they complete each other's weakness. You can find in Table 2 a sum up of informations related to all algorithms

We decide to consider from now on only one optimization algorithm of each kind. That is: *DragonflySearch*, *AxSearch*, *SkOptSearch*, *NevergradSearch*, *ZooptSearch* and *TuneBOHB*.

These optimization algorithms will be compared between them and with *RandomSearch* and *GridSearch* by studying the metrics we will talk about in next section.

3 BENCHMARK TOOL

3.1 metrics

Before implementing the benchmark tool, we would like to think about the comparisons metrics we will use to compare all algorithms. It is mostly about comparing either test error or test accuracy as a function of time or trials:

- One of the most common approach is to compare the test error/accuracy of the best set of hyperparameters chosen by every optimization algorithm as a function of total number of trials/the time needed to find these hyperparameters.
- An enhancement of the protocol above would be to divide the number of trials into several occurrences, to have test accuracy of the best trials, but also the distribution of performance as a boxplot. with lower and upper quartiles, whiskers above and below to show the position of the most extreme data point, two black lines across the top of the figure to mark the upper and lower boundaries of a 95% confidence interval. See Bergstra & Bengio (2012).
- Finally, an other approach is to use metrics from the validation set instead of the test set. The idea consists of finding the expected best validation accuracy (the average result from the best validation trial) in function of the number of assignments. The limitation of this method clearly is over fit, which is hopefully infrequent in NN. Dodge et al. (2019) also informs about the variance by adding an area σ wide around the validation accuracy.

We will process our data the following way: we define as best trial for trial number n, the trial with best validation accuracy for all trials from *0* to n.

This means the plot for validation value should always be increasing for classification accuracy (decreasing for Regression), but plot for test value could be decreasing (increasing for regression) because a new trial with

a better validation accuracy could have a worst test accuracy.
We are only interested in the yet best trial because what we want from a search algorithm is that it gives the best hyperparameter combination the fastest possible. So we are interested in the best test accuracy over all yet trained trials, as a function of the number of trials done.

3.2 Toy Benchmark

We implement a first version of our benchmark tool. This version is very extensive as we allow various combinations for tuning optimization. To compensate with this extensiveness, we choose some very simple datasets, and do very few iterations (max 20 epochs). This toy benchmark has three goals: First to verify that every functionality works, that models are indeed learning, second to understand which factors are important. Third to see how all algorithms perform relatively to each others. We could then focus on the important factors with some harder datasets and more complicated problems as a second (and last) batch. We conduct a large scale optimizer benchmark, with different datasets, and different labeling categories, as search algorithm's performances can highly depend on the test problem.

Here is a short description of every labels:
Model Inputs: We wanted to have at least an input category of every kind to perform an extensive comparison, so we have both Image, Table, and Text input.
Model Output: Similarly, we seek extensiveness so we propose classification, regression and generation. Classification is the task of putting the input in one class, regression is the task of finding one or few real values from the input, and generation consists of creating credible output data looking like the input data, despite being new.
We don't do all combinations here by lack of time, but we do:
Image classification with two datasets: MNIST: LeCun et al. (2010) and Fashion MNIST: Xiao et al. (2017). These are about finding back the digits and the clothes category respectively from a black and white image of low quality.
Image generation with the MNIST dataset, so here it is about creating back some images of digits.
Table Regression with both boston: Harrison Jr & Rubinfeld (1978) and diabete datasets: Kahn (1994). These are about finding the value of houses and the diabete progression measure respectively from a table of datas.
Text Regression is using the IMDB dataset: Maas et al. (2011) a huge movies review dataset to predict if the writer either liked or didn't liked the movie. It is a regression task because we will compute the error on the prediction: how far is the continuous prediction to the real label (either 0 or 1).
Text Classification using the TREC dataset: Buckley (1995) which consists of classifying text questions into one of 6 different categories of questions.
Models: We will use a lot of different models, still for extensivness. Unfortunately, we can not use every model with every input category. As an example CNN, which pre-treats the input in smaller parts, is usefull for images and text, as the model has to extract the informations, but is useless in tables, where the information is already presented in an optimal way.
We will shortly enumerate the particularities of every model:
GAN is the most complicated: On the one hand there is a generator that tries to create outputs looking like inputs, and there is a discriminator, that tries to make the difference between the real inputs and the outputs of the generator. The generator is trained by whether or not it succeeds to fool the discriminator, and the discriminator by whether of not he successfully discriminated the given input. Here we only used MNIST Dataset as it is a very simple dataset. The metric we will use is the Inception Score which quantifies how good is the generation. For this purpose we will develop an Auxiliary Classifier GAN, which means that the discriminator will have the additional task to try to find the label of the image, this is necessary to compute the Inception Score. The auxiliary classifier will be a CNN. Goodfellow et al. (2014)
CNN is used for visual and text datasets as they first pre-process the data to reduce its dimensionality through pooling, or by performing convolution, which consists of not taking into account a single value, subset of the whole input (for example a pixel for an image), but to also take into account near values. First used by LeCun et al. (1989)
RNN's particularity is that the connections of it's nodes form a directed graph. This allows it to have memory. It is hence very indicated for texts datasets as we would like to remember the influence of every word when going through the sentence.
We do the distinction between two RNN models:
LSTM stands for Long Short Term Memory and has three gates: "forget gate" adds new input to stored information and decide if some need to be forgotten, "input gate" pre-processes the data in function of it's importance to calculate the cell value, and then "output gate" decides which informations should be given to next node (memory). LSTM introduced here: Hochreiter & Schmidhuber (1997)
GRU stands for Gated Recurrent Unit and has only two gates: first a "reset gate" that decides which previous informations (important previous words in a sentence) should be kept, and then an "update gate" that decides

if a new information should be kept in memory of not (if new word provides important information). GRU were first introduced by: Cho et al. (2014).
MLP is a regular feedforward neural network with multiple layers and non linear activation functions.
Logistic Regression is a very simple model, the most likely to underfit as it is a single layer neural network with logistic function. We will use it for table regression.
Optimizer: Finally, the optimizer is the thing that makes the model train by updating the network weights. The most know is **SGD**: Stochastic Gradient Descent. It takes it roots from an algorithm developed by Robbins & Monro (1951). It maintains a single and fixed learning rate for all weight updates. **Adam** proposes to keep the principle of gradient Descent, but allows a per-parameter learning rate, and also allows a learning rate evolution, as training in the begining is often too slow. It was invented by Kingma & Ba (2014). We will compare this optimizer with **AdaBelief**, which is new and promising. It is an amelioration of Adam as in the case of a large gradient and a small variance, Adam would use a small learning rate, although AdaBelief would keep a big learning rate by noticing that variance is small. Which is intuitively what we prefer because small variance gives us a big confidence that our direction is correct. It has been very recently developed by Zhuang et al. (2020).
In our benchtest, search algorithms will also have to find best values from:
The activation function, which defines output of a node given an input. We often want it to be continuous and differentiable.
The leaning rate controls how fast the weights of the nodes in the network should learn.
The weight decay is a way to penalize complexity to reduce risk of overfitting.
The LR dropout randomly set the LR of a certain a proportion of nodes to zero. This is efficient to avoid bad local minima.
The number of layers is important to avoid overfit, underfit, and to have better results.
And finally the dimensions of hidden layers.

We use the same trial scheduler for every search: it is ASHA, as it is the scheduler recommended by ray-tune, being the most compatible among all search algorithms (among all but BOHB). It stands for Asynchronous Successive HAlving. So it is a parallelized version of **SHA**, which stops trials that are not goods enough. Finally we wish to present the different ways that exists to calculate the metrics. See Table 3.

Table 3 Here y is a label data, and $\bar{y}$ is the output of the model.
We also define T_p the true positive, T_n the true negative, F_p the false positive and F_n the false negative. D_{KL} is the Kullback–Leibler divergence.

name	formula	best	worst
classification			
accuracy	$\frac{T_p+T_n}{n}$	1	0
precision	$\frac{T_p}{T_p+F_p}$	1	0
recall	$\frac{T_p}{T_p+F_n}$	1	0
f1	$\frac{2*precision*recall}{precision+recall}$	1	0
log_loss	$-(y*log(\bar{y})$ $+(1-y)log(1-\bar{y}))$	0	$+\infty$
regression			
MAE	$\frac{\sum_i \lvert y_i-\bar{y}_i\rvert}{n}$	0	$+\infty$
MSE	$\frac{\sum_i (y_i-\bar{y}_i)^2}{n}$	0	$+\infty$
RMSE	$\sqrt{MSE}$	0	$+\infty$
R2 score	$1-\frac{MSE}{\sigma^2}$	1	-∞
Generation			
Inception Score	$e^{E[D_{KL}(p(y\lvert\bar{(}y)*p(y))]}$	#Class	1
Also all classification metrics from generated output			

As one picture says more than a thousands words, you can simply look at Figure 4 to understand how the toy benchmark works. As a sum up we have several layers which are respectively (in order according to the figure): model input, problem category, NN category, optimizer, Search algorithm. We also gave the same trial scheduler to all problems but BOHB: it is the ASHA scheduler.

Notes on the benchmark:
After testing this benchmark, we noticed we were not able to make Dragonfly work, which is regrettable.
The goal here is to compare the difference of results between each search algorithm, and especially to see if learning search algorithms can provide significantly better results than random search in significantly shorter time. We are interested in the relative difference

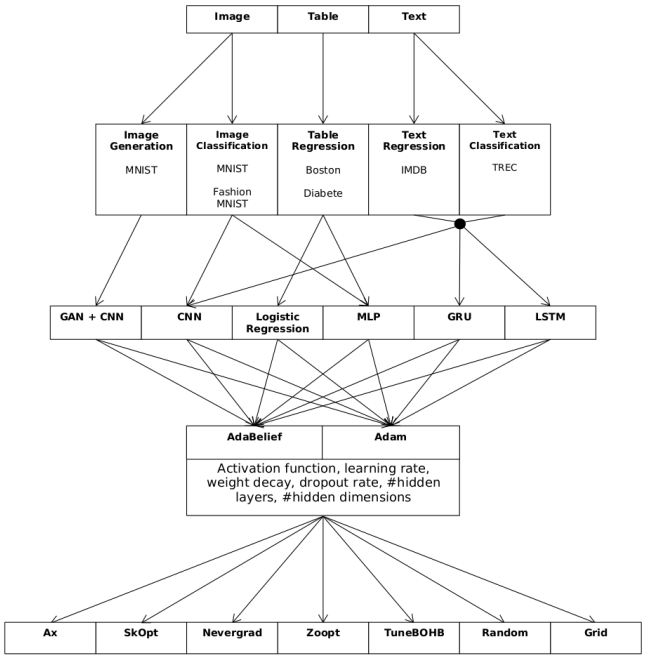


Figure 4. Plan of the toy benchmark and all the combinations it allows

between results of every search algorithms.
We would not be surprised if results are below "good" results in the literature because we don't train on a lot of epoch, and also because we have simple models. But we don't care as we want to compare disparities. Still, to get on order of idea, best literature we are aware of claims an accuracy of 99.72% on MNIST Dataset without preprocessing, while we get X% In our best results
We end up with an 8 dimension parameter space:

- Learning rat:e from 10e-8 to 0.1.
- Weight decay: from 10e-8 to 0.1.
- Sigmoid function: either relu, tanh, or sigmoid.
- Number of hidden dimiensions: from 32 to 1024.
- Number of hidden layers: from 1 to 3.
- Dropout probability: from 0 to 0.5.
- Optimizer: either Adam or AdaBelief.
- Model: which neuronal model will learn.

We will do a detailed analysis on one dataset of each category in this section, followed by an global analysis over all datasets. It is still possible to see in Appendix A a shorter analysis for datasets in redundant categories. Although we have described 3 population based algorithm, they are all using NeverGrad, so as this is only the first benchmark we will only use one of the three (the best one according to the authors) to reduce information overload, it is CMA.

3.3 Detailed analysis on boston dataset

For the detailed Analysis on boston dataset, we give 256 trials to every search algorithm (so 256 different combinations of hyperparameters). Each of these trials can learn on up to 20 epochs, but it can also be stopped before by the scheduler (all search algorithms have the same scheduler but BOHB). The scheduler stops a trial if it starts overfitting, or if it gives very bad results in the first epochs, hence has no potential and is a waste of execution time.
We repeated this process 4 times so we reduce influence of noise, and also so we can quantify variance.
Our analysis will rely on the metrics we presented in section 3.1.
To sum up, these metrics were:

1. Plot of the best test MSE, ie from best hyperparameter combination found so far, as a function of number of trials / time.
2. Plot of the best test MSE from best hyperparameter found so far, as a function of number of trials / time, including boxplot to have interesting informations about variance, quartiles, and outbound values.
3. Plot of the best expected validation accuracy from best hyperparameter found so far, as a function of number of trials, including variance information.

We can plot all of these informations on a single figure per algorithm. Note we decided to use a variance area for the second point " 2." instead of boxplots for obvious clarity/visibility reasons.

3.3.1 General Informations

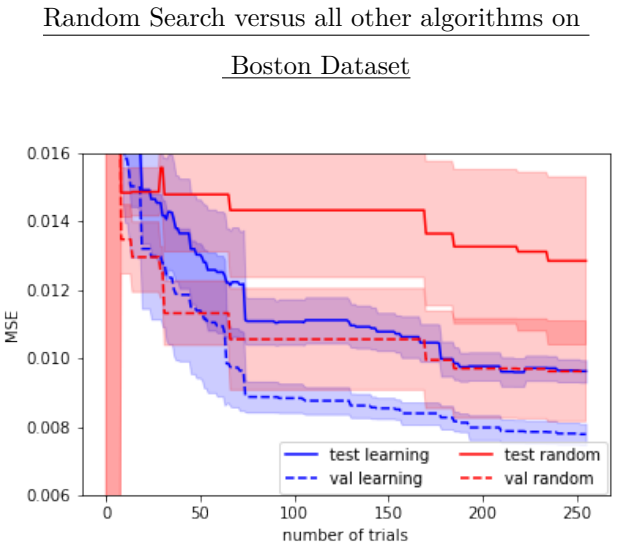


Figure 5. Here we plot the averaged test and val MSE of Random Search, and we compare it with the mean of all other algorithms (learning algorithms). Color areas are σ wide

As an introduction figure, we show in figure 5 the comparison between the random search test and validation MSE, with the mean of all other algorithms's test and validation MSE.
Note that test MSE is the value we are interested in in real life, but here we want to compare the search algorithms, so it is interesting to compare validation accuracy as well as it is the metric that optimizer, scheduler, and especially search algorithm use to learn and decide new hyperparameter combinations.
We were afraid that plotting boxplots would cause information overload, so we will add color areas that are σ wide instead. (σ is the standard deviation)
As we predicted, validation MSE is always decreasing, but test MSE is sometimes increases (a little).
Also we notice that validation MSE is always below test MSE, this is because the model is selected on his validation MSE, so there is a positive bias on it.

3.3.2 Test and validation MSE

We see in figure 6 that random-search has a test MSE that is nearly two times worst than all other learning algorithms.
Also we learn that most of the improvement happens in the 64 first trials. We also see in figure 9 that random search has as bad results for validation MSE as well.
These two plots permit an overall comparison. NeverGrad, Zoopt, and Bayes seems to be the best, and Random is the worst by far.

3.3.3 Variance per Search Algorithm

To reduce information overload, we will plot the recommended metrics only for the top 3 performing algorithms and random search. All axis are the same.
See in figure 7 the plot for BayesOpt, in figure 8 for NeverGrad, in figure 10 for Random, and in figure 11 for Zoopt.

We also understand from this data that validation loss has similar signification than test loss as the difference between the two is close for all algorithms.

We see that random and zoopt have the biggest variance. and that variance is otherwise pretty low.
There is a huge variance during the first 5 trials, for all search algorithms, but NeverGrad finds very quickly a very good solution (after 64 trials). Random doesn't converge and keep improving slowly up to the 256 trials).
Variance for random search is huge, this is expected as it is random by definition so the best trial is subject to a maximized variance. This is not desired as it means we could be unlucky and have very bad results despite searching for a lot of trials. This is another reason why NeverGrad is preferable as it has a very small variance.
This dataset is still particularized by the big variance of all models.

Test MSE

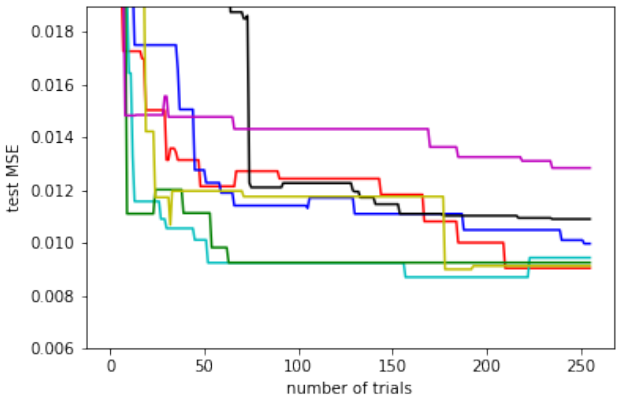


Figure 6. Here we plot the average test loss of the best trial obtained so far per search algorithm as a function of the number of trial. This is the plot presented as "metric *1.*"

Validation MSE

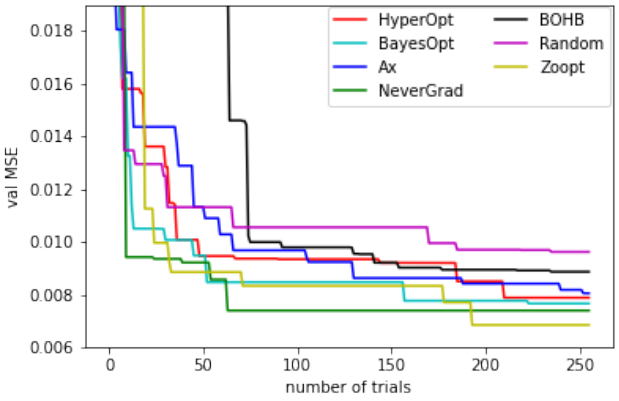


Figure 9. Here we plot the average validation loss of the best trial obtained so far per search algorithm as a function of number of trial.

Tests and Validation MSE per algorithms with σ narrow area on Boston Dataset

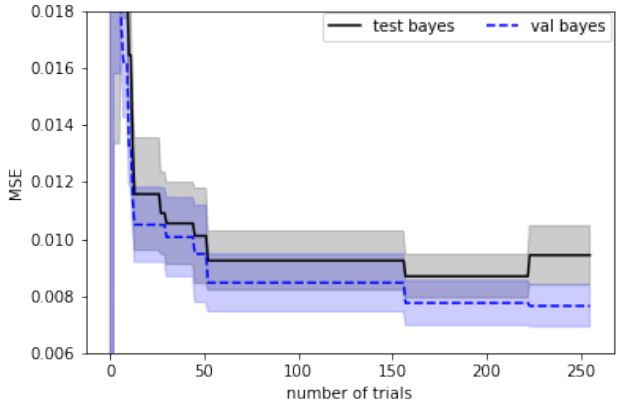


Figure 7. Validation, Test, Variance MSE with Bayes

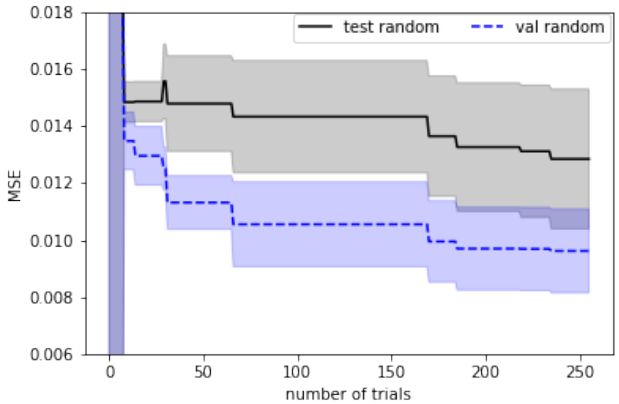


Figure 10. Validation, Test, Variance MSE with Random

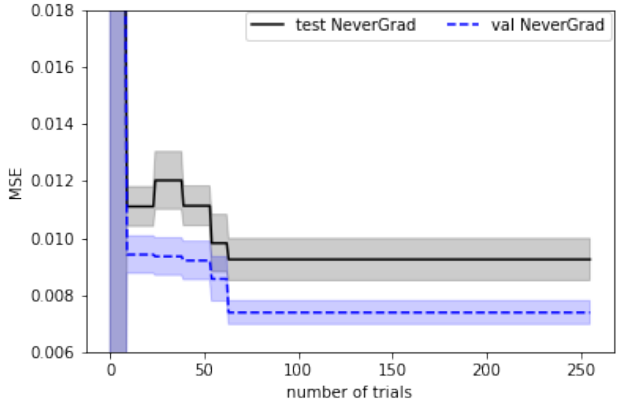


Figure 8. Validation, Test, Variance MSE with NeverGrad

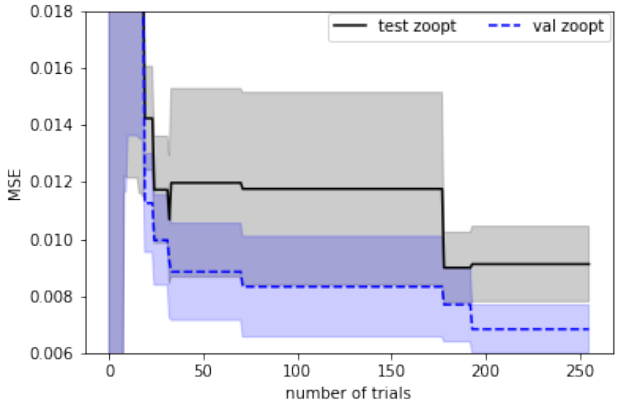


Figure 11. Validation, Test, Variance MSE with Zoopt

3.4 Detailed analysis on TREC dataset

For the detailed Analysis on TREC dataset, we give 128 trials to every search algorithm (as we learned with boston dataset that most of the learning happens during the 128 first trials). Each of these trials can learn on up to 20 epochs.
We repeated this process 5 times so we reduce influence of noise, and also so we can quantify variance.

3.4.1 General Informations

Random Search versus all other algorithms

on TREC dataset

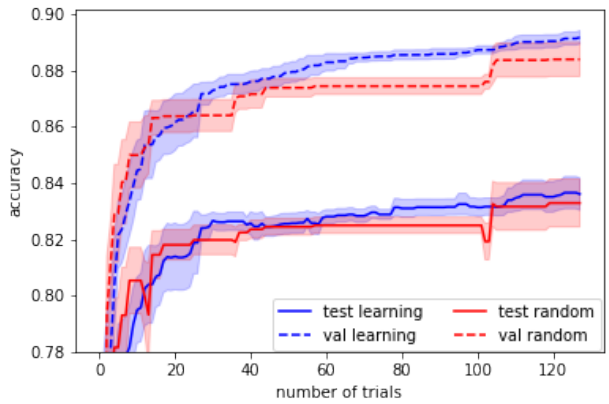


Figure 12. Here we plot the averaged test and val accuracy of Random Search, and we compare it with the mean of all other algorithms (learning algorithms). Color areas are σ wide

As an introduction figure, we show in figure 12 the comparison between the random search test and validation accuracy, with the mean of all other algorithms's test and validation accuracy.
We observe that validation accuracy is way above test accuracy for all search algorithms. Random is once again less goods than the average of other training algorithms.

3.4.2 Test and validation accuracy

These two plots permit an overall comparison. NeverGrad, Zoopt, and Bayes seems to be the best, and Random is the worst by far.

3.4.3 Variance per Search Algorithm

To reduce information overload, we will plot the recommended metrics only for the top 4 performing algorithms. All axis are the same.
See in figure 14 the plot for HyperOpt, in figure 15 for Ax, in figure 17 for BOHB, and in figure 18 for Random.

Random is once again one of the worst: it is the worst by far in terms of validation accuracy, and isbelow the average in term of test accuracy. Also note that the difference between test and validation accuracy is very high here, so difference of results of accuracy among search algorithms seems relatively smaller. What we mean here is that there is still a 3% test accuracy difference between the best algorithm (BOHB) and the average of the other algorithms, but this improvement seems small compared to the 5% gap between test accuracy and validation accuracy.

Test Accuracy

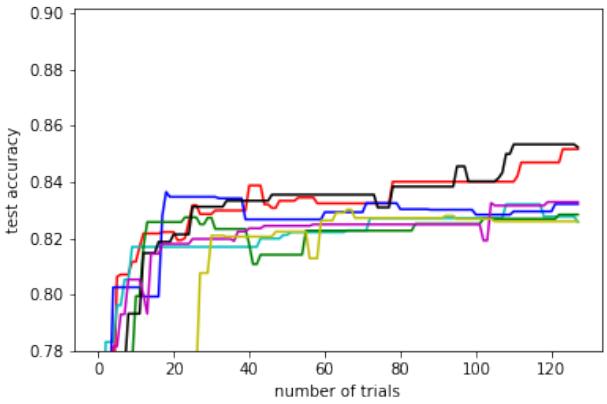


Figure 13. Here we plot the average test accuracy of the best trial obtained so far per search algorithm as a function of the number of trial.

Validation accuracy

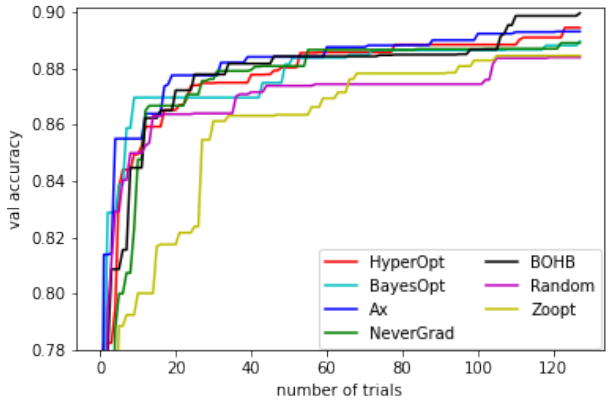


Figure 16. Here we plot the average validation accuracy of the best trial obtained so far per search algorithm as a function of number of trial.

Tests and Validation MSE per algorithms with σ narrow area on TREC Dataset

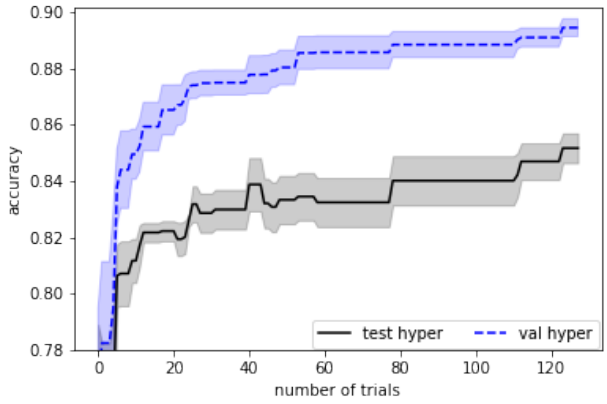


Figure 14. Validation, Test, Variance accuracy with Hyper

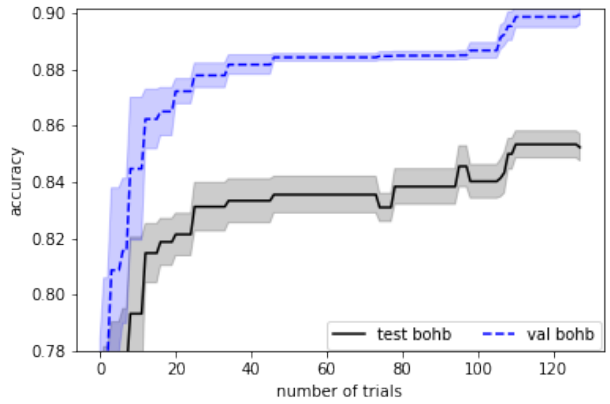


Figure 17. Validation, Test, Variance accuracy with BOHB

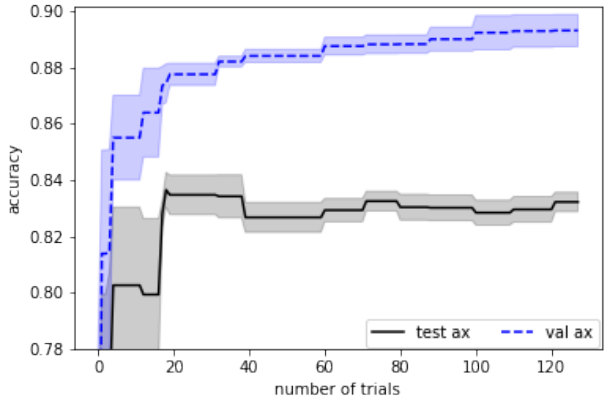


Figure 15. Validation, Test, Variance accuracy with Ax

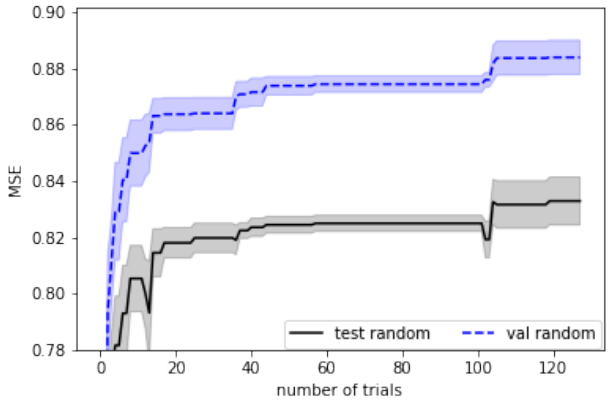


Figure 18. Validation, Test, Variance accuracy with Random

3.5 Detailed analysis on FMNIST dataset

For the detailed analysis on FMNIST dataset, we give 128 trials to every search algorithm. Each of these trials can learn on up to 20 epochs.
We repeated this process 4 times so we reduce influence of noise, and also so we can quantify variance.

3.5.1 General Informations

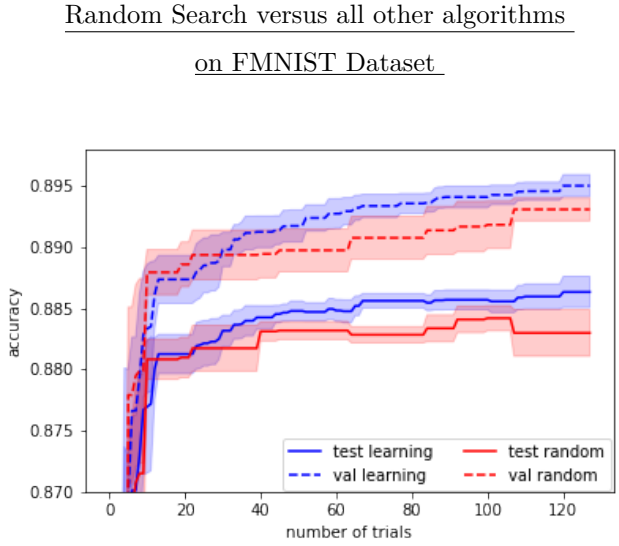


Figure 19. Here we plot the averaged test and val accuracy of Random Search, and we compare it with the mean of all other algorithms (learning algorithms). Color areas are σ wide

As an introduction figure, we show in figure 19 the comparison between the random search test and validation accuracy, with the mean of all other algorithms's test and validation accuracy.
Random seems to be way below the average of other learning algorithms once more.

3.5.2 Test and validation accuracy

These two plots permit an overall comparison. HyperOpt seems to be the best by far, followed closely by BayesOpt and BOHB. Random is clearly the worst.

3.5.3 Variance per Search Algorithm

To reduce information overload, we will plot the recommended metrics only for the top 4 performing algorithms. All axis are the same.
See in figure 38 the plot for HyperOpt, in figure 39 for Bayes, in figure 41 for BOHB, and in figure 42 for Random.

Variance is small once more

Test Accuracy

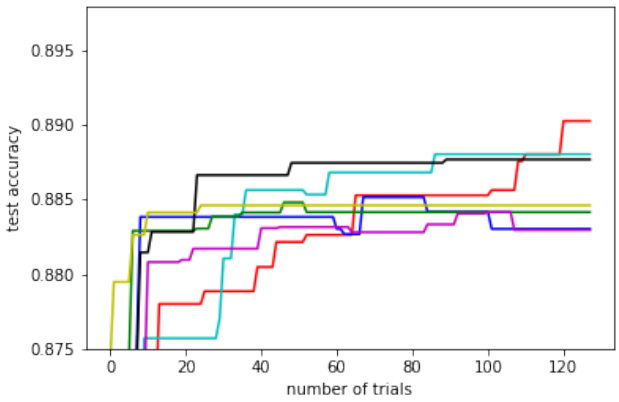


Figure 20. Here we plot the average test accuracy of the best trial obtained so far per search algorithm as a function of the number of trial.

Validation accuracy

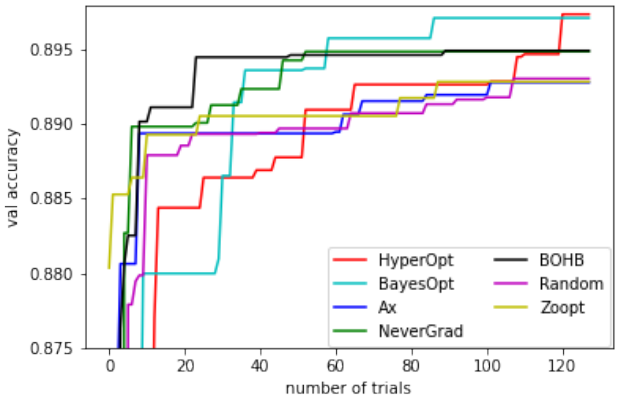


Figure 23. Here we plot the average validation accuracy of the best trial obtained so far per search algorithm as a function of number of trial.

Tests and Validation MSE per algorithms with σ narrow area on FMNIST Dataset

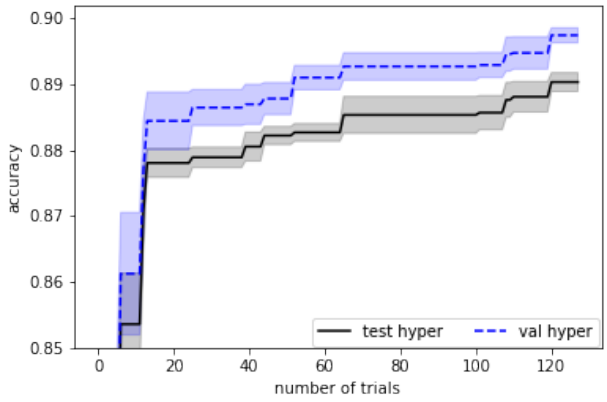


Figure 21. Validation, Test, Variance accuracy with Hyper

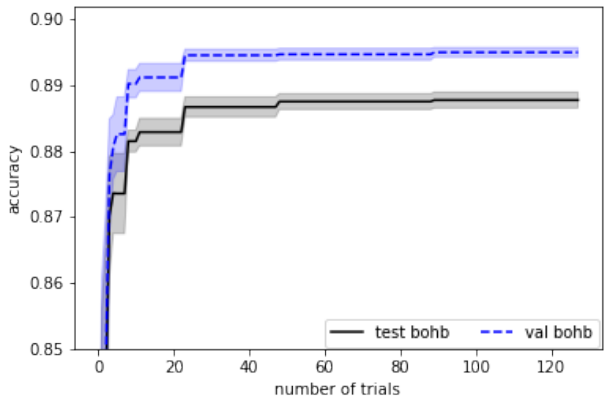


Figure 24. Validation, Test, Variance accuracy with BOHB

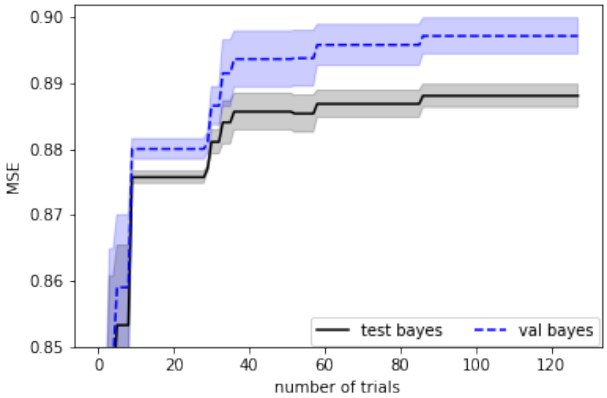


Figure 22. Validation, Test, Variance accuracy with Ax

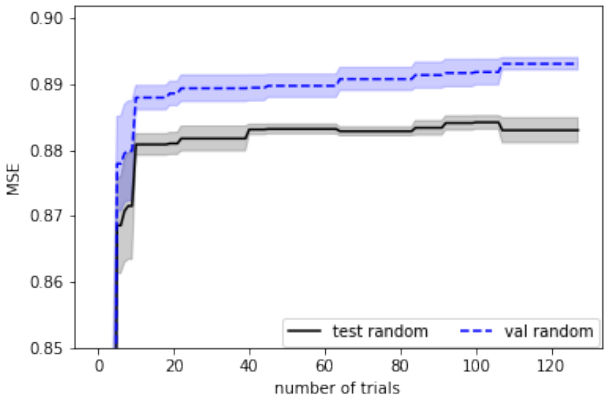


Figure 25. Validation, Test, Variance accuracy with Random

3.6 Detailed analysis on IMDB dataset

For the detailed Analysis on IMDB dataset, we give 128 trials to every search algorithm. Each of these trials can learn on up to 4 epochs.
We repeated this process 4 times so we reduce influence of noise, and also so we can quantify variance. Note that we used the entire IMDB dataset, with 200 000 cinema reviews. Despite reducing length of reviews to 200 first words, training was so long that we used free GPU from Google Collab.
We used MAE.

3.6.1 General Informations

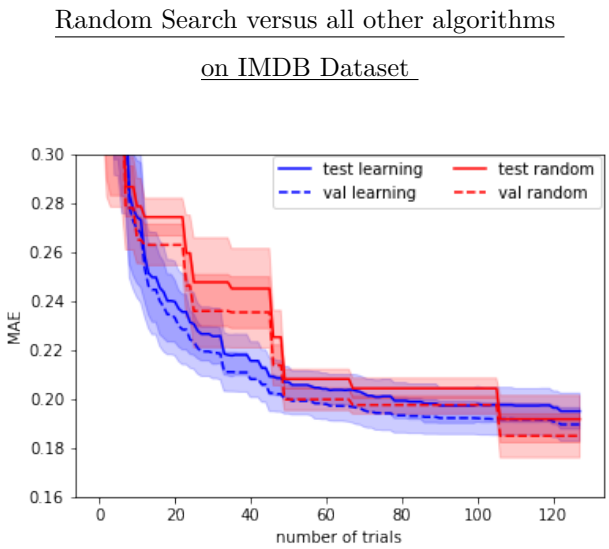


Figure 26. Here we plot the averaged test and val accuracy of Random Search, and we compare it with the mean of all other algorithms (learning algorithms). Color areas are σ wide

As an introduction figure, we show in figure 26 the comparison between the random search test and validation accuracy, with the mean of all other algorithms's test and validation accuracy.
For the first time, random is better than the average of the learning algorithms.

3.6.2 Test and validation accuracy

We see in figure 37

We also see in figure 40
We understand that HyperOpt and BayesOpt are really better, and random is slightly better than the average. Zoopt is catastrophic for this dataset.

3.6.3 Variance per Search Algorithm

To reduce information overload, we will plot the recommended metrics only for the top 4 performing algorithms. All axis are the same.
See in figure 38 the plot for HyperOpt, in figure 39 for Bayes, in figure 41 for Ax, and in figure 42 for Random.

Here Hyper convergers very quicly, Ax seems to overfit, which is a pitty as it could have perform good otherwise. Random continuously improves as expected.

Test Accuracy

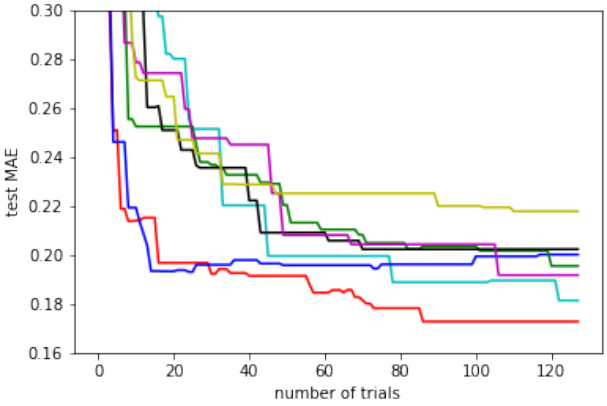


Figure 27. Here we plot the average test accuracy of the best trial obtained so far per search algorithm as a function of the number of trial.

Validation accuracy

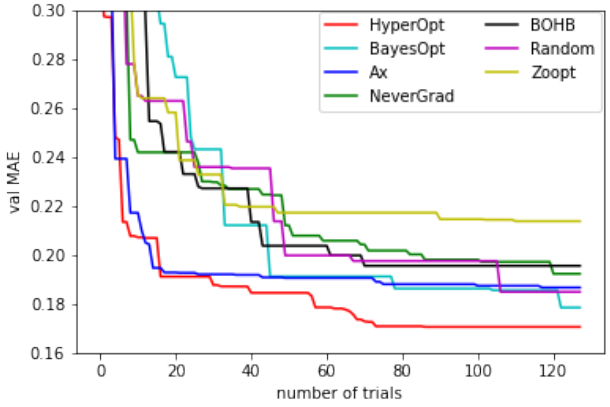


Figure 30. Here we plot the average validation accuracy of the best trial obtained so far per search algorithm as a function of number of trial.

Tests and Validation MSE per algorithms with σ narrow area on IMDB Dataset

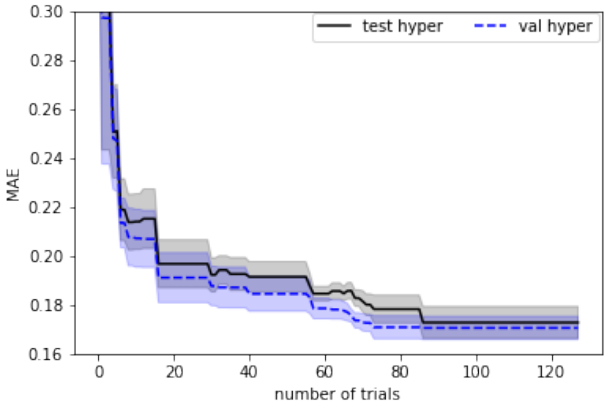


Figure 28. Validation, Test, Variance accuracy with Hyper

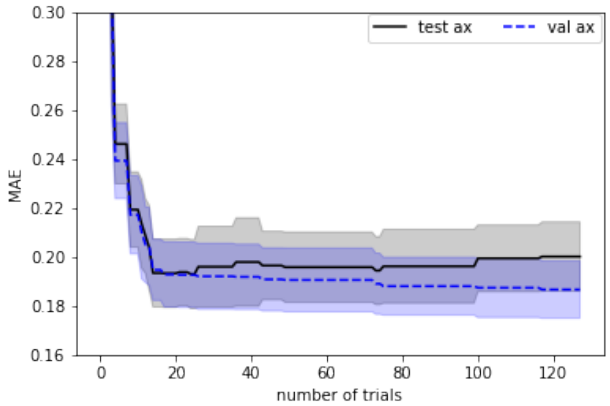


Figure 31. Validation, Test, Variance accuracy with BOHB

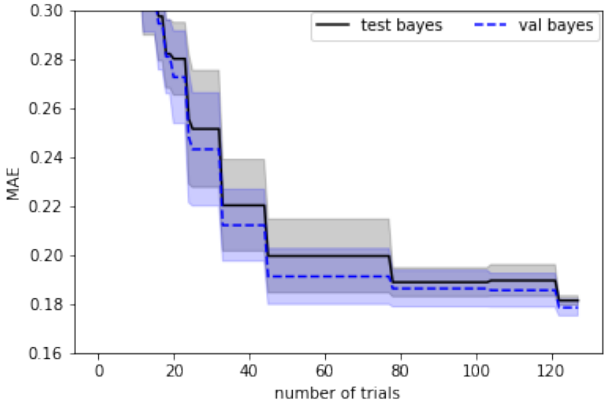


Figure 29. Validation, Test, Variance accuracy with Ax

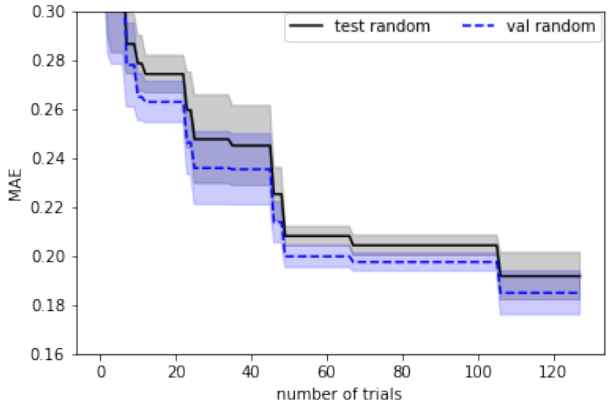


Figure 32. Validation, Test, Variance accuracy with Random

3.7 Detailed analysis on GAN with MNIST dataset

Gan are very different to regression or classification tasks as we did in the rest of this benchmark. We think it is important to have also a very different problem to see how the search algorithms will perform in a completely different context: Indeed we changed the search space: it is now about optimizing the learning rate, the first beta parameter, the weight decay, and the optimizer for two different models: the generator and the discriminator. Following the same philosophy, we used a different scheduler: we used a population based scheduler, this means bad trials will take hyperparameter values near from well performing trials. For short, population based scheduler will do intensive exploitation as a lot of trials are going to take hyperparater combinations near known good combinations. So we expect the search algorithm to still have added value on exploration. Note we couldn't test BOHB as it is the only search algorithm to use it's own scheduler, but we used TwoPointsDE instead. As GAN don't use the concept validation or test dataset, we will provide slighly different plots, as well as quantitative results from best and worst trials. We also cannot plot an Inception Score for a given trial, as we would not know what valueto give to a trial. Should it be the Inception Score when it has the hyperparameters given by the search algorithm? Or once the PB scheduler chose between giving him a better known combination and letting the trial keep his original one? Or should it be the score once it has finished to train? We thought the best way to handle this specific particularity was to plot as x-axis not only the **score of every trial once they have finished training**, but rather **score of every trial every time they train once** (and can potentially be scheduled). So if n is the number of time a trial train, our plot should contain n times more values on the x-axis then before for the same number of trial search by a search algorithm.
Each trial could learn up to 100 times, and a search consist of 128 trials. We repeated the experiment 4 times to reduce noise and compute variance.

3.7.1 Overall Inception Score

As an introduction figure, we show in figure 26 the Inception Score of all scheduler. Once again, random is below average, and Bayes and Hyper Are clearly better. HyperOpt's curve is really intrigging as it is bellow all others and only goes outo the others at the end, we will explain why in 3.7.2.

3.7.2 Quantitative results:

We will show in this section quantitative results of the GAN:

As we can observe, Inception Score of 1 really looks like nothing, and almost look like a random input.

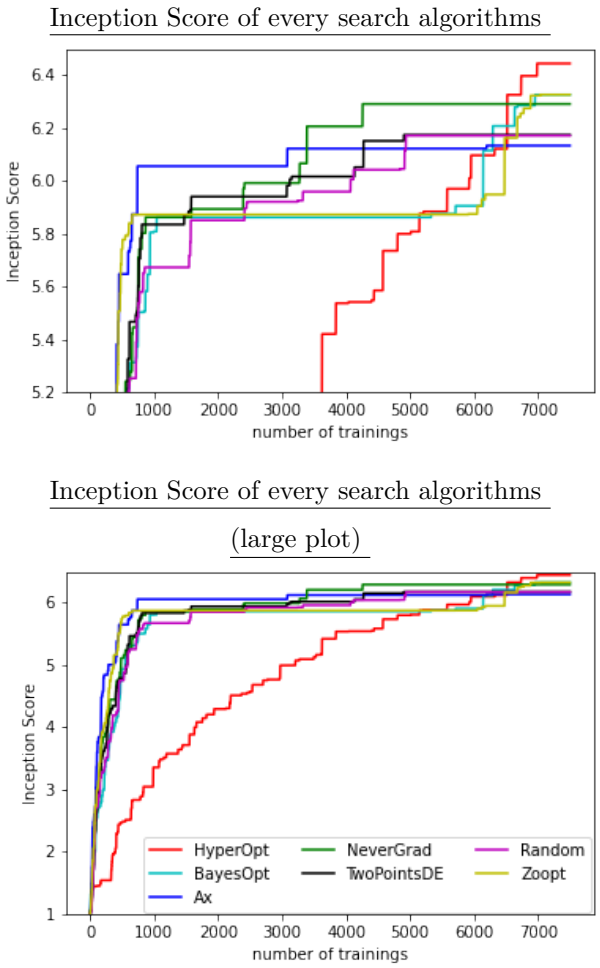


Figure 33. Here we plot the best obtained Inception score among all trials trained among all search algorithms, as a function of number of trial trainings.

Inception Score of 6 is way closer: the backgroud is uniformly black, and most shapes actually look like digits. But progress seems to be still possible.

3.7.3 Variance per Search Algorithm

Variance is small on plot 37 and 40. Once again, random is bellow average, and the best 3 algorithms are Hyper, Bayes, and NeverGrad. HyperOpt actually has one of the biggest variance.

We see on plots 38,39,41,42 the Inception Scores as function of trials training for the 3 best search algorithms and random search. It is extremely interesting as we learn when an algorithms decides to explore, and when he exploits. As an exemple, BayesOpt start very quickly by exploiting, in order to have very quickly some good results. Then he explores back, and do a longer exploitation which leads at the end to better results. Random and Nevergrad have the same strategy to alternate periodicaly between shoth exploration time followed

Figure 34. 64 input digits from MNIST dataset

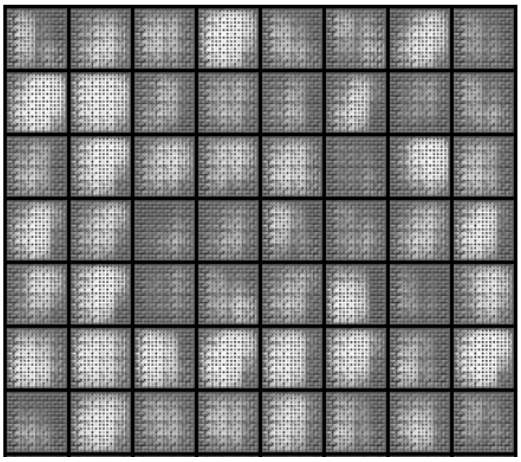


Figure 35. 64 output from our generator with Inception Score of 1

Figure 36. 64 output from our generator with Inception Score of 6

by short exploitation time. HyperOpt has this unique strategy to do a unique very long exploration, and then a unique very long exploitation. This later strategy turns out to be the best. Note that this strategy of long exploration first was not observed on other dataset as HyperOpt usually converged very quicly to some very good results. So it might be an optimisation strategy in case of PBT scheduling.

Inception Score for Hyper

Zoopt, random and Ax

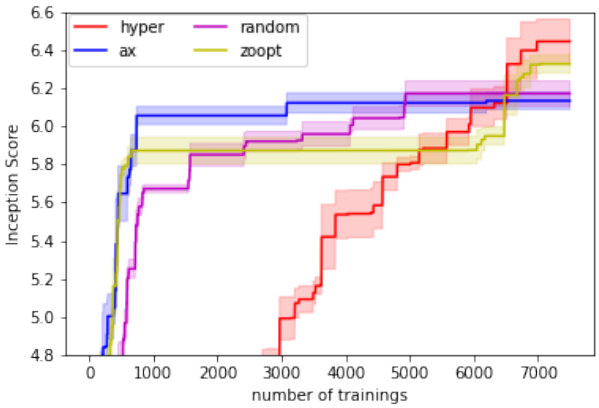


Figure 37. Here we plot the best obtained Inception score among all trials trained among all search algorithms, as a function of number of trial trainings with variance area $\sigma wide$.

Inception Score for Bayes

2pointsDE and NeverGrad

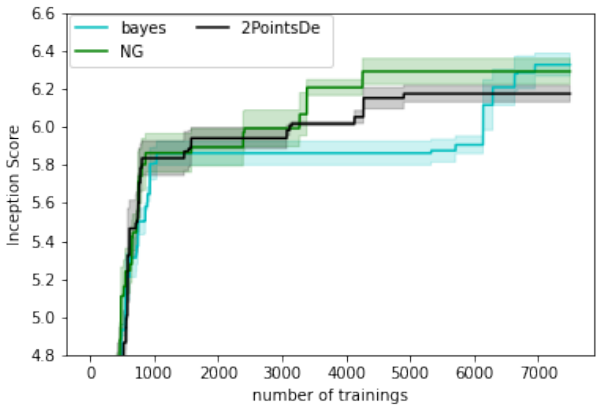


Figure 40. Here we plot the best obtained Inception score among all trials trained among all search algorithms, as a function of number of trial trainings with variance area $\sigma wide$.

Distribution of trials's Inception Score per algorithms

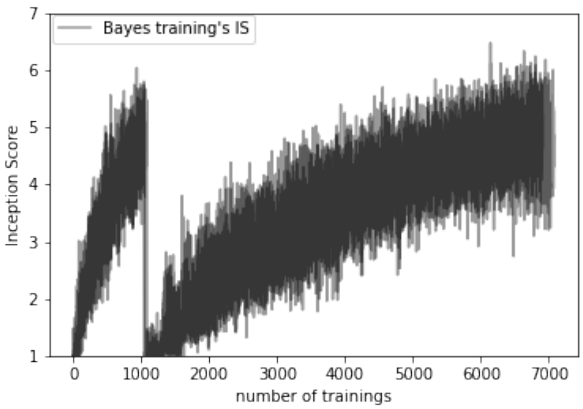


Figure 38. Distribution of trial's Inception Score on Bayes

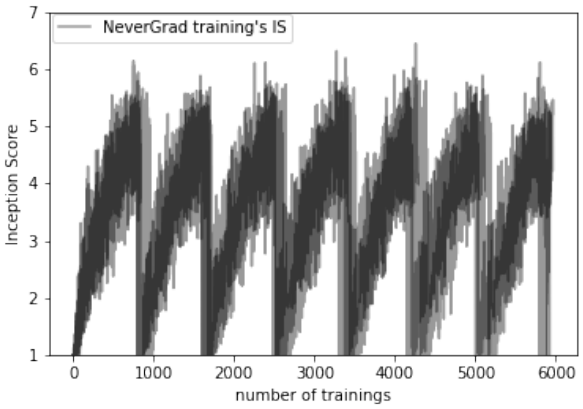


Figure 41. Distribution of trial's Inception Score on NeverGrad

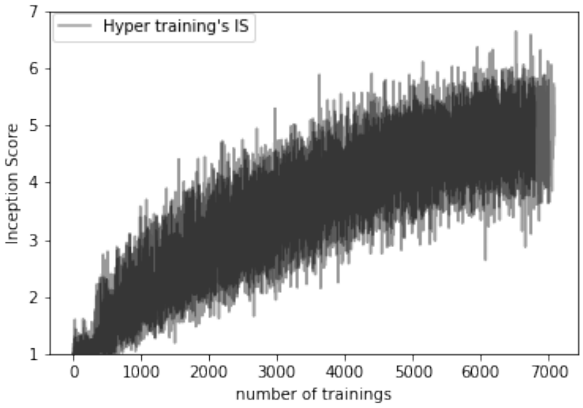


Figure 39. Distribution of trial's Inception Score on Hyper

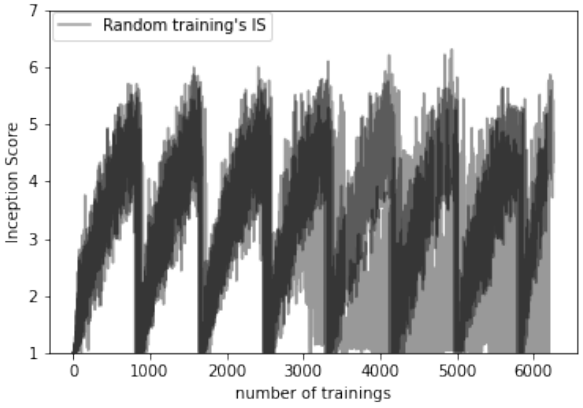


Figure 42. Distribution of trial's Inception Score on Random

3.8 OVERALL Analysis

3.8.1 Time Analysis

Parallel case:

We here want to study the time it takes for a search algorithm to do search the best hyperparameter combination for one dataset. So to make 256 or 128 models learn up to 20 epochs. We first study the parallel case, as all searches from all datasets but IMDB were made in a parallel environment with 8 CPUS. Remember that all Search Algorithms have schedulers that schedules their trials, and for example make a model learn up to 20 epochs only if it has a chance to beat the current best model. We are going to compare the time that takes a search algorithm compared to the time Random Search took. Search algorithms can have a big influence in the time it takes as they can limit parallelism, because they could need to learn from trials in a sequential way.

We see on figure 43 in blue the search time relative to the search time of random search in a parallel case. We can see that most algorithms take a time very close from the reference of Random Search (which parallelises perfectly). Two algorithms take really more time: there is AxSearch and BOHB. We can explain these difference: BOHB is the only search algorithms using its own scheduler so it is not surprising that it takes different time. But it is more surprising that despite the time he is granted he was not able to match the other search algorithms.

And AxSearch is the only Search algorithms that explicitly limits parallelism: To enforce sequential treatment of the information, it explicitly used no more than 3 of the 8 thread. As all other algorithms used all 8 threads, it is logical that Ax is about 8/3 slower which is what we observe in the figure.

We provide in page 22 plots of trial accuracy as a function of training time, for each search algorithm in the parallel environment, note that these plots mostly depend on the scheduler, but since the scheduler makes his decisions based on the results obtained by the search algorithm, there are noticeable differences.

Intuitively, we would like to have a tendency curve with a very high accuracy at the smallest execution time. Ax is the best considering this criteria.

sequential case: For IMDB dataset we used Google Collab Free GPU, which are fast and perform sequential trial search. We can see in red in figure 43 the time distribution. We observe less disparities in the distributions.

Surprisingly, some algorithms are faster than random, which should be the fastest. This is because random choses CNN, GRU, and LSTM model uniformely (each with probabiliy 1/3). But other algorithms can typiccaly be faster if they choose CNN more often. Indeed CNN are very fast compared to RNN, as RNN have a run time proportional to the number of words per input (200!). We can observe on page 23 plots of trial accuracy as a function of training time, for each search algorithm in the sequential environment As we can observe, Random really has the smoothest curve, which is bad, opposed better algorithms such as HyperOpt,Ax, Nevergrad, who reach for small trial time some good configurations.

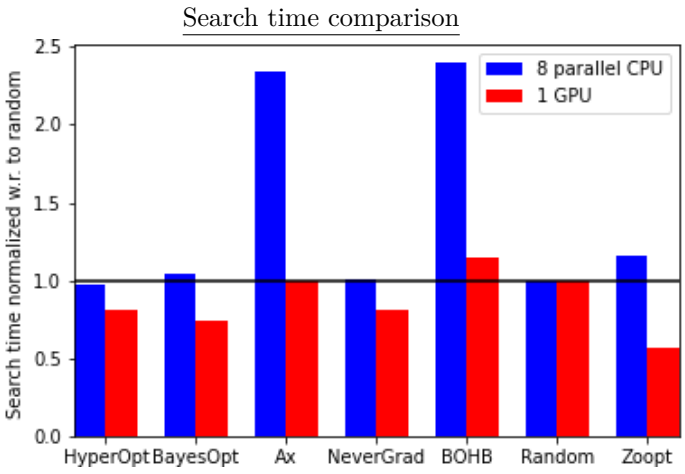
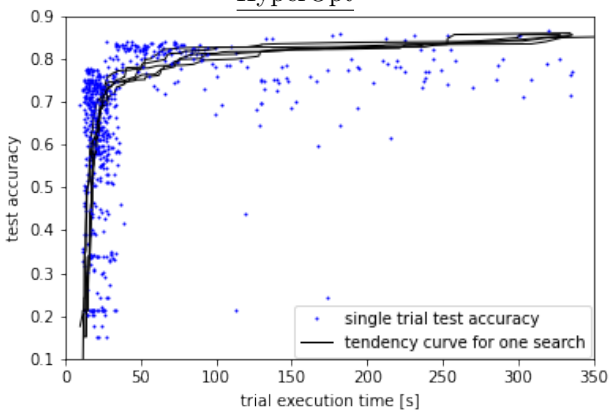


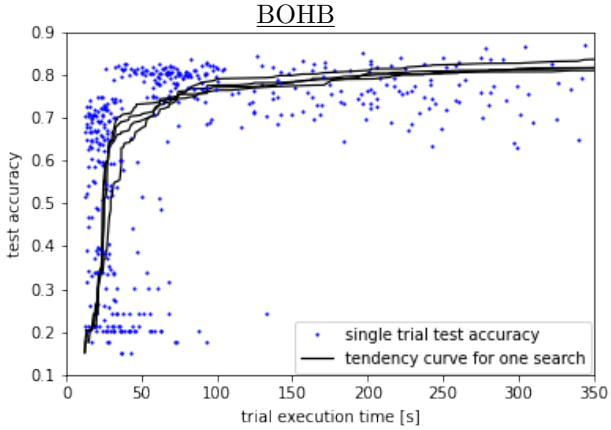
Figure 43. Relative execution time comparison among all search algorithm of a search

Test accuracy per trial as a function of execution time with tendency curves (parallel environment)

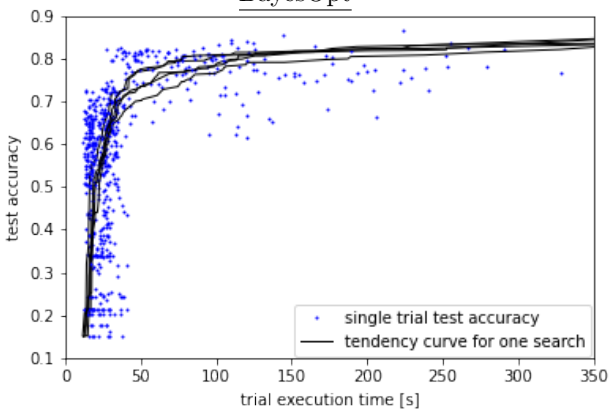
HyperOpt



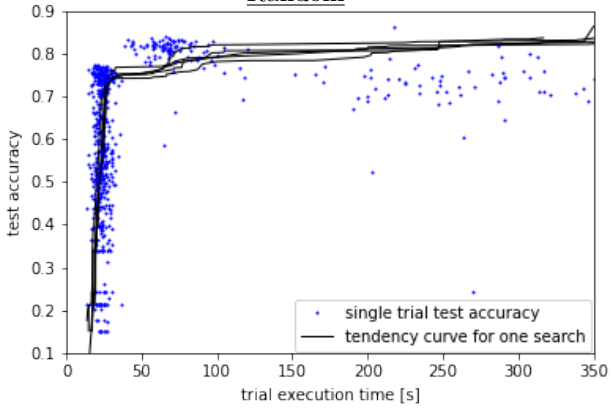
BOHB



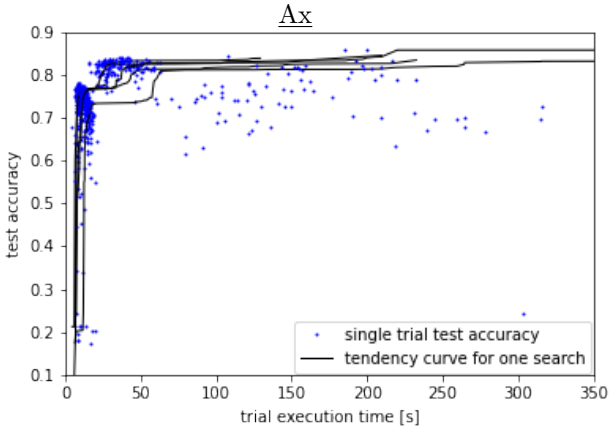
BayesOpt



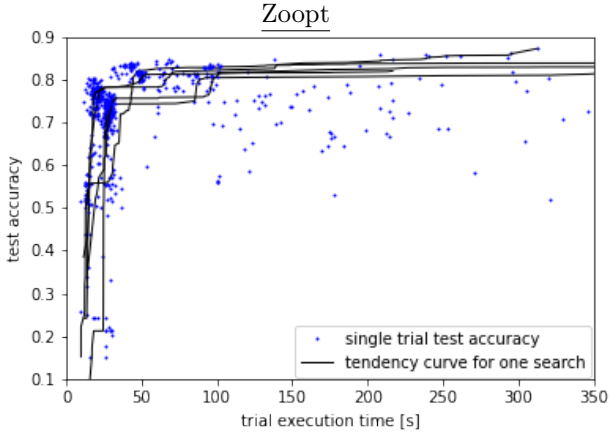
Random



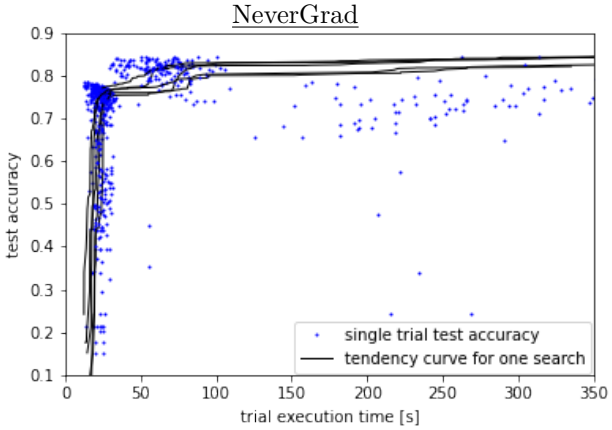
Ax



Zoopt

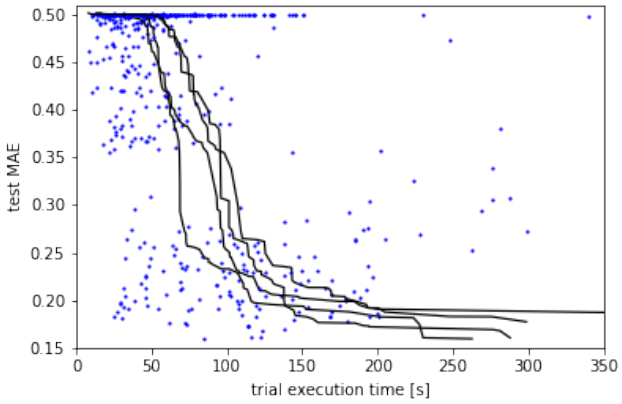


NeverGrad

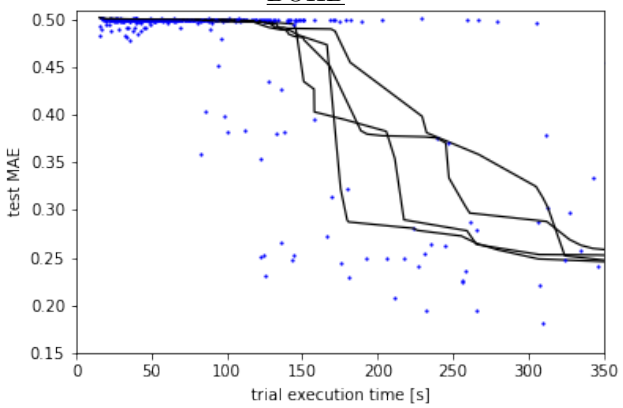


Test MAE per trial as a function of execution time with tendency curves (sequential environment)

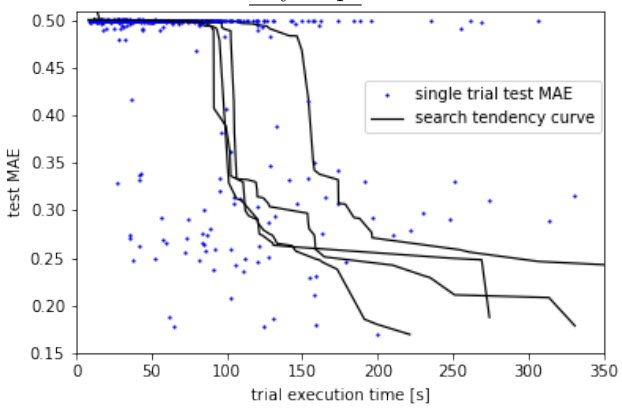
HyperOpt



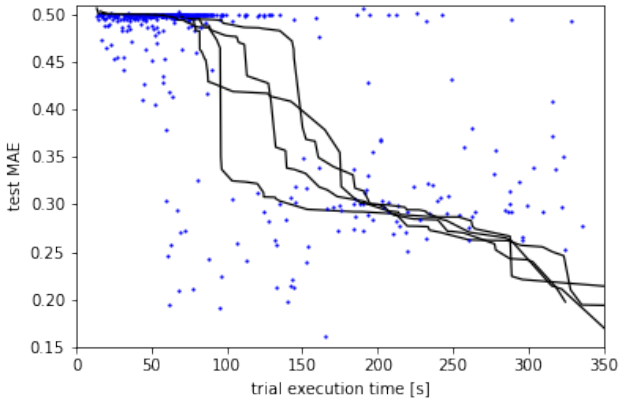
BOHB



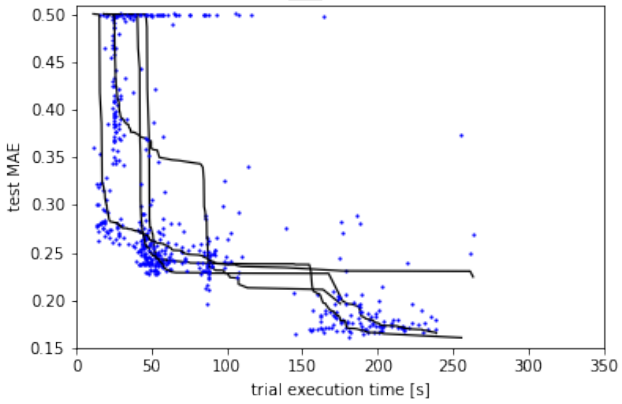
BayesOpt



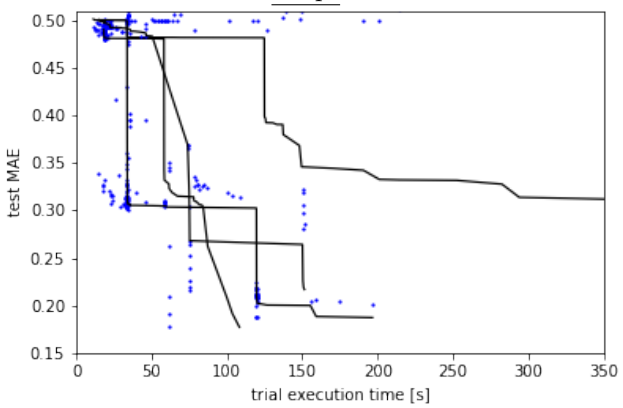
Random



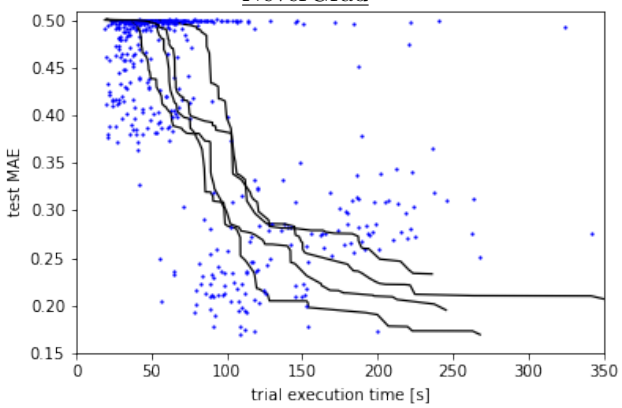
Ax



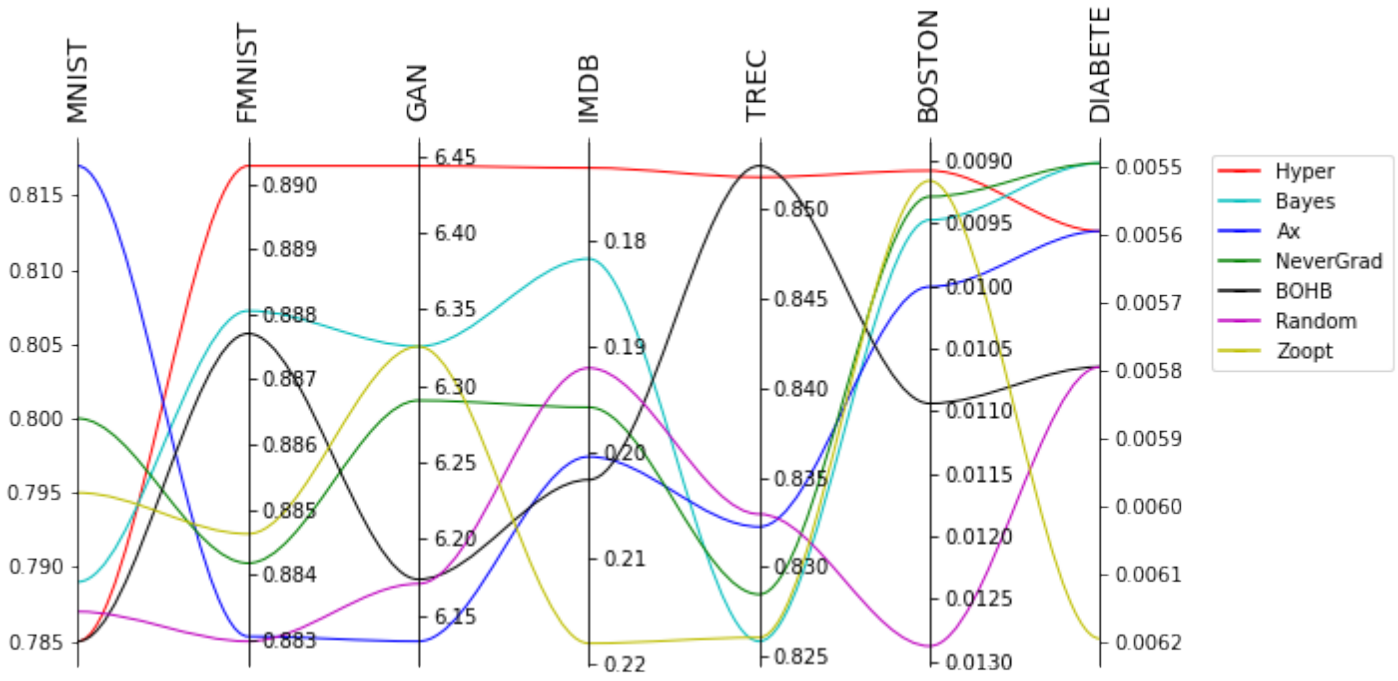
Zoopt



NeverGrad



Overall dataset performance comparison for all algorithms



3.8.2 Dataset overall performance

We finally can compare search algorithms among all datasets. A clear tendency is that HyperOpt is really above all other algorithms. Bayes is clearly second. Last place goes to random which is what we expected. You can see in appendix A the results for MNIST and DIABETES, as well as other for FMNIST and Boston, for much smaller number of epochs, and there Hyper was far less good. So our conclusion is that hyper is the best when the trials it manages have enough epochs.

4 BATCH OF COMPLEX MACHINE LEARNING PROBLEMS

5 CONCLUSION

A :APPENDIX. ON TOY BENCHMARK ANALYSIS

A.1 Fashion MNIST Analysis

FMNIST is compared with each search algorithms managing 256 trials, but going only up to 4 iterations.
1. Visual validation and global informations
We use tensor flow to get a visual impression on tendencies of hyperparameters distribution among trials. On figure 44, we compare this distribution with a learning algorithm and random search. We expect random search to give uniform distribution, and the learning algorithms to have very specific distribution, with a lot of trials having the same (good) hyperparameters. We can use tensorflow for this purpose.

As explained on the figure, we understand some informations: to get good validation accuracy in fashion mnist in our benchmark, learning rate is good to be high (in [0.05-0.1]), as well as weight decay (in [0.05-0.09]). The best sigmoid function is Tanh, the number of dimension must be high (most values in [200-240]), the number of hidden layers low (1 hidden layer: this is probably because we have so few iterations. Thus we tend to underfit). Most interestingly, Adam and MLP seems to be not efficient compared to AdaBelief and CNN, and this seems to be the major factor for obtaining good results: in the last image form figure 5, ALL trials with accuracy above 0.7 used Adabelied and

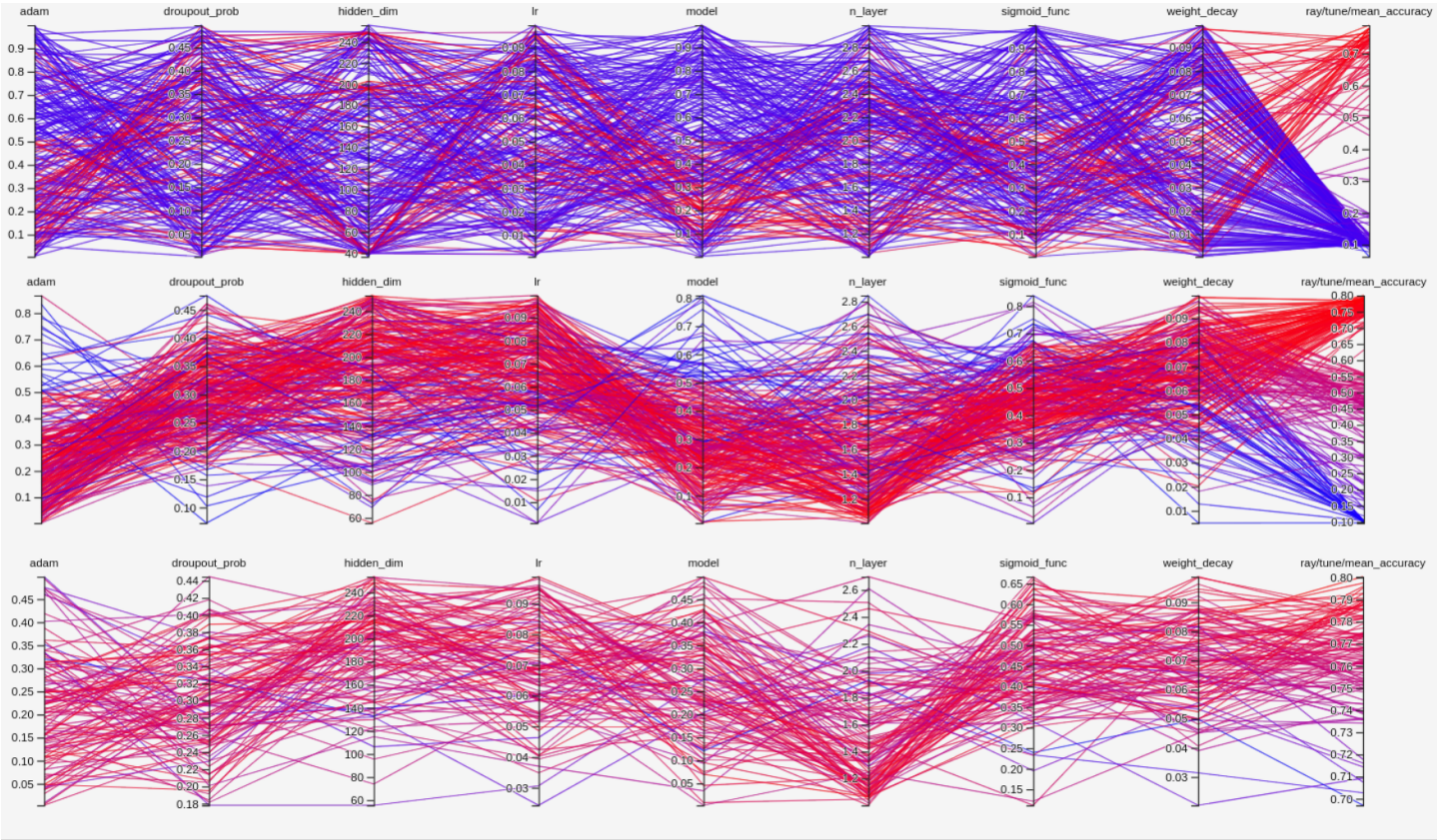


Figure 44. We here see the the distribution of hyperparameters per search algorithms. Every line is a trial. red or blue indicates whether it provides good or bad accuracy. The former is from random search. It corresponds very much to what we expected: we have a very wide and uniform looking distribution. The middle one is from AxSearch, and is similar to the other learning algorithms: we have basically all trials going in the same good position, with still some wide to search for new combinations (exploration). Finally the last one is still from AxSearch once we keep only "good" trials (the one with more than 70 % accuracy). This allows us to understand which are the good values for this problem. Take care as the scale is different for the last one.

CNN.
Dropout probability shall be in [0.2-0.4].
This figure is a good news at it proves our benchmark works at it should.

The most interesting thing is to compare RandomSearch with all other algorithms.
We can see that random search is the worst. We can compare these values on 256 Trials training on 4 epochs with the one we had for the same dataset with 128 trials and 20 epochs: Best accuracy is 82% here against 89% for 20 epochs, which is a huge difference. Note that good result in the literature is of 93% for classification for FMNIST so we are not very far: Mani et al. (2019).

Table 4 Here is a little sum up of the informations. Mean of 10 bests goal is to reduce the variance of the noisy information that validation accuracy is.

name	mean	mean of 10 bests	best
BayesOpt	0.251	0.774	0.789
Random	0.25	0.772	0.787
Ax	0.597	0.798	0.817
NeverGrad	0.539	0.793	0.8
BOHB	0.492	0.778	0.785
HyperOpt	0.23	0.768	0.785
Zoopt	0.142	0.773	0.795

2. validation accuracy repartition over time

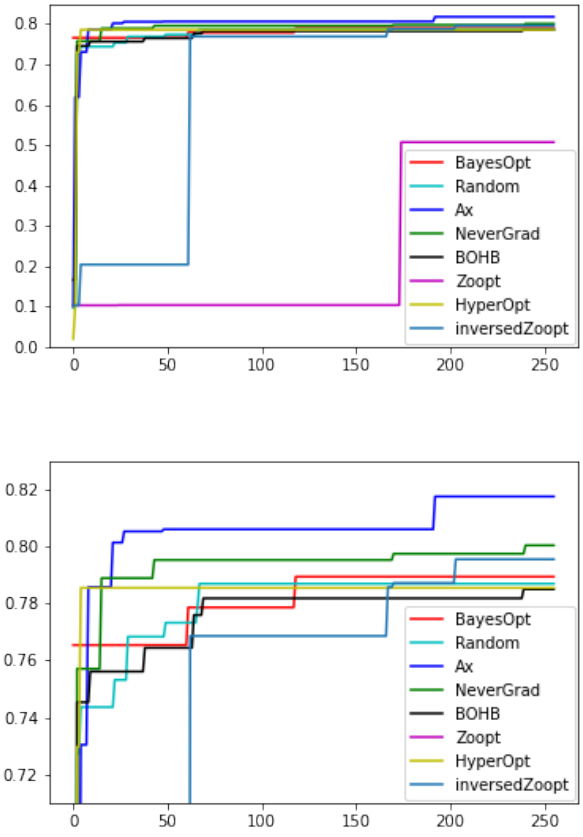


Figure 45. Here we plot the max validation accuracy already obtained (so maximum validation accuracy between this trial and all previous trials) as a function of trials number.
The objective being to be as much on the upper left as possible. The lower image is the same plot with a focus on the accuracy in [0.71;0.83]. We see that Ax and NeverGrad are really both better and faster than random for this dataset.

3. test accuracy

Here HyperOpt trial overfit badly, BayesOpt and Ax are really good, and Random is once again bellow the average.

Table 5 Here we compare the validation accuracy of the best trial from each search algorithm to the test accuracy of a model with same hyperparameters.

name	validation	5 steps	10 steps	20 steps
BayesOpt	0.789	0.806	0.848	0.851
Random	0.787	0.781	0.823	0.835
Ax	0.817	0.75	0.81	0.852
NeverGrad	0.8	0.8	0.825	0.839
BOHB	0.785	0.781	0.815	0.83
HyperOpt	0.785	0.774	0.765	0.611 **!**
Zoopt	0.795	0.8157	0.837	0.84
Correlation		-0.405	0.107	0.396
μ of 20 Random		0.789	0.828	0.844
σ of 20 Random		0.012	0.014	0.01
μ of difference		-0.007	0.024	0.014
σ of difference		0.027	0.026	0.077

A.2 MNIST Analysis

Here we study the MNIST dataset, that is very easy.

1. Visual validation and global informations

As explained on the figure, we understand some informations using tensorflow (in bold informations different then for fashion mnist): to get good validation accuracy in mnist in our benchmark, **learning rate is good to be low** (in [0.0001-0.02]), as well as **weight decay** (in [0.0001-0.07]). The best sigmoid function is Tanh, the number of dimension and hidden layers doesn't seem to be that important. Adam and MLP are still not efficient compared to AdaBelief and CNN. Dropout probability shall be in [0.2-0.3].

As we can see on table 6, this time random search is really less good then almost all others algorithms: between 2 and 3% less good although we are getting

Table 6 Validation accuracy for MNIST.

name	mean	mean of 10 bests	best
BayesOpt	0.383	0.945	0.963
Random	0.354	0.932	0.944
Ax	0.888	0.959	0.969
NeverGrad	0.765	0.961	0.972
BOHB	0.348	0.944	0.956
HyperOpt	0.675	0.911	0.919
Zoopt	0.697	0.938	0.963

very close to 100%, so one would have thought that the gap would be reduced.

2. validation accuracy repartition over time

3. test accuracy

Table 7 Here we compare the validation accuracy of the best trial from each search algorithm to the test accuracy of a model with same hyperparameters.

name	validation	5 steps	10 steps	20 steps
BayesOpt	0.963	0.916	0.931	0.906
Random	0.944	0.85	0.891	0.891
Ax	0.969	0.95	0.925	0.931
NeverGrad	0.972	0.869	0.875	0.881
BOHB	0.956	0.853	0.791	0.906
HyperOpt	0.919	0.775	0.825	0.763
Zoopt	0.963	0.73	0.825	0.888
μ of difference		-0.106	-0.089	-0.074
σ of difference		0.064	0.046	0.037

Main issue here is that all models have a validation

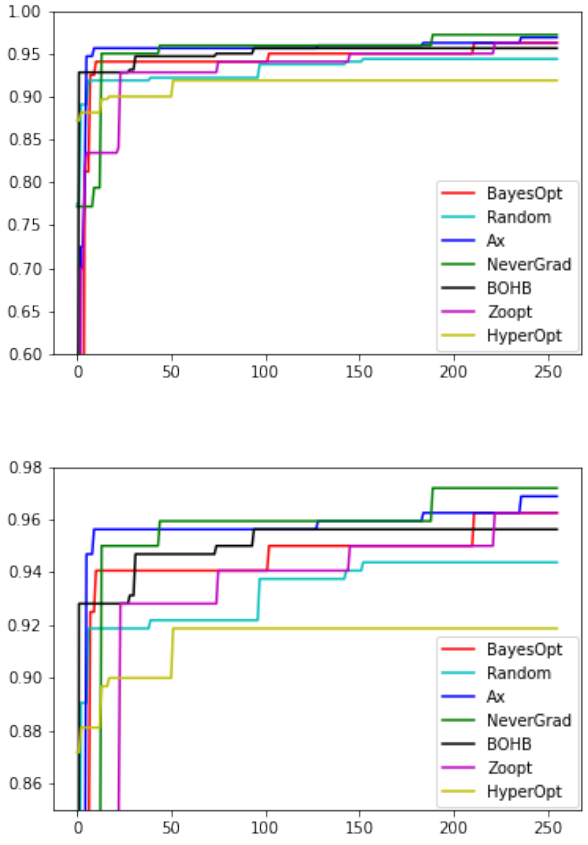


Figure 46. Here we plot the max validation accuracy already obtained as a function of trials number.
The objective being to be as much on the upper left as possible. We see that All learning algorithms but HyperOpt are really both better and faster than random for MNIST.

accuracy way above test accuracy.
It is the role of the search algorithm to handle noisy inputs, this is why all search algorithms have a similar drop of result from validation to test (see "difference"). Once again the best opponent to Random Search is AxSearch on test data.

A.3 Diabetes Analysis

Here we study the Diabetes regression dataset, that is known for being very easy. We choose MSE as loss function. Note that we normalised the data with mean 0 and std of 1. So it is normal to have very small loss as labels are smalls. **Since all loss are below 0.01, we will present loss in this section in ‰**
1. Visual validation and global informations

We understand some informations using tensorflow: to get good validation loss in diabetes in our benchmark, learning rate is good to be high (in [0.05-1]), the weight decay around 0.03. The best sigmoid function is not

relevant here as unused., the number of dimension shall be arround 140 and the best number of layers is 2. Dropout probability shall be low: in [0.1-0.2] Best model is MLP (opposed to LogReg) and Adam is preferred over Adabelief! .

Table 8 Validation loss for Diabetes, in ‰ from standard normal distribution.

name	mean	mean of 10 bests	best
BayesOpt	10.5	7.6	5.8
Random	91.2	8	6.7
Ax	10.5	8.1	6.5
NeverGrad	9.8	6.1	5.8
BOHB	3147.8	7.6	6.3
HyperOpt	400.3	8.5	6.7
Zoopt	10.6	8.5	8.1

As we can see on table 10, we had a problem of outlayer values for some of the 7 algorithms, in this case we would replace by 100000 (means are still not significant). Random search is here alos less good than other learning algorithms.

2. validation loss repartition over time

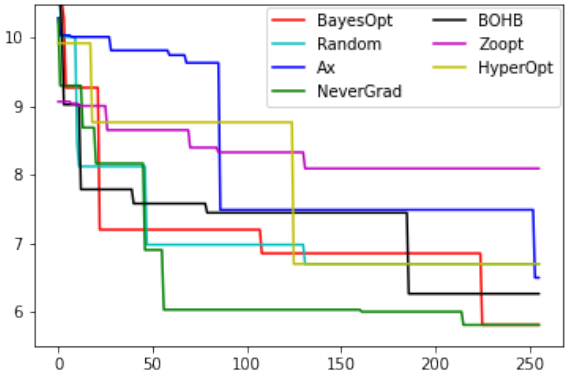


Figure 47. Here we plot the min loss accuracy already obtained as a function of trials number.
The objective being to be as much on the lower left as possible. Random is near to all other search algorithms but NeverGrad, that clearly dominates here.

3. test accuracy

Table 9 Here we compare the validation accuracy of the best trial from each search algorithm to the test accuracy of a model with same hyperparameters.

name	validation	5 steps	10 steps	20 steps
BayesOpt	5.8	7.2	5.5	5.5
Random	6.7	6.1	5.9	5.8
Ax	6.5	8	6.3	5.6
NeverGrad	5.8	8.8	6.6	5.5
BOHB	6.3	7.7	5.6	5.8
HyperOpt	6.7	7.5	5.6	5.6
Zoopt	8.1	8	6.9	6.2
μ of difference		1.1	-0.5	-0.8
σ of difference		1.1	0.6	0.5

There is a 6% difference between test accuracy of Nevergrad, and Random.
All algorithms are better than random except for BOHB and Zoopt.

A.4 Boston Analysis

Here we study the Boston regression dataset, a very known and yet complex regression dataset. We choose MSE as loss function. Note that we normalised the data with mean 0 and std of 1. **Here loss is not in ‰ anymore.**

1. Visual validation and global informations

We understand some informations using tensorflow. To get good validation loss in boston in our benchmark, learning rate is good to be moderate (in [0.02-0.04]), the weight decay around 0.04. The best sigmoid function is not relevant here as unused., the number of dimension shall be high: arround 200 and the best number of layers is 1 or 2. Dropout probability shall be around 0.35. Most trials use LogReg as it provides low loss, but lowest loss are performed with MLP.

Table 10 Validation loss for Boston with standard normal distribution.
extreme values would replaced by 100000 (means are still not very significant).

name	mean	mean of 10 bests	best
BayesOpt	17365	0.147	0.016
Random	25942	0.395	0.179
Ax	7910	0.372	0.022
NeverGrad	4264	0.241	0.122
BOHB	13429	0.118	0.034
HyperOpt	10581	0.124	0.021
Zoopt	8751	1.65	0.154

Random search is notably less good then all other search algorithms but Zoopt and NeverGrad.

2. validation loss repartition over time

3. test accuracy

This can be because of the loss that is squared, but bad algorithms from validation error are far worst (random and nevergrad), and good algorithms are better. Loss of random search is 8 times worst than BayesOpt's loss. Random and NeverGrad are so bad because they both chose LogReg. We have no overfitting at all. We can compare with Boston dataset with 20 epochs: error was then 10 times smaller!

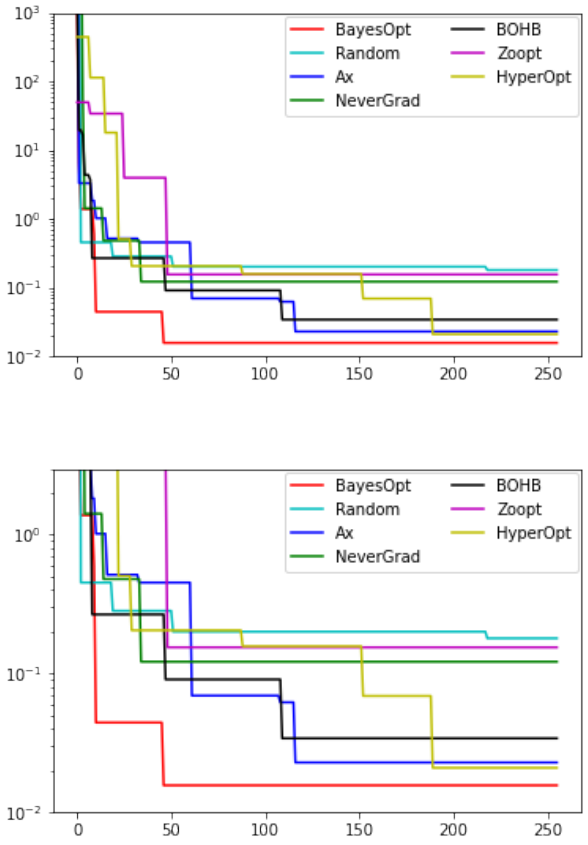


Figure 48. Here we plot the min loss accuracy already obtained as a function of trials number.
The objective being to be as much on the lower left as possible. Be careful as it is a log scale on the y-axis .

Table 11 Here we compare the validation accuracy of the best trial from each search algorithm to the test accuracy of a model with same hyperparameters.

name	validation	5 steps	10 steps	20 steps
BayesOpt	0.016	0.403	0.035	0.014
Random	0.179	6.036	0.855	0.124
Ax	0.022	0.169	0.069	0.034
NeverGrad	0.122	2.352	0.833	0.154
BOHB	0.034	0.045	0.025	0.021
HyperOpt	0.021	0.022	0.02	0.016
Zoopt	0.154	1.51	0.221	0.024

B : APPENDIX. ON POPULATION BASED SCHEDULING

Analysis of schedulers are not officially part of our project, but we still propose here a very small analysis as we think these concepts can have a very important impact to optimize the hyperparameter tuning.
We will compare the number of hyperparameter searches that can be done in function of the number of trainings in the following cases: without scheduler, with PBT scheduler, with Median scheduler, with ASHA scheduler.

B.1 Without scheduler:

Let's compare a regular search of ***n* trials** trained on ***m* iterations** each.
Any of our search algorithm try to do the following: Learning from results of all trials i for i going from *0* to *j*, to choose the optimal hyperparameter combination for trial *j*.
This implies that the search algorithm will only take the best combination between n explorations (or n hyperparameter searches) while doing $n \times m$ trainings.

B.2 PBT scheduler:

B.2.1 Simplified operating explanation:

The population based scheduler starts with the n exploration chosen by the search algorithm [2]. It then waits that all trials have done the same number of iteration before perturbing all of them.
Concretely, the PBT scheduler uses the $n \times m$ trainings to do $n \times m$ searches (perturbations[3]) as there are m iterations, and n perturbations per iterations. That is a speedup in *O(m)* compared to the last paragraph.

B.2.2 Exponential speed-up:

We explained above that PBT does $n \times m$ searches if trials are independent (every trial does m mutations without considering results of other trials). We will now show that PBT Sheduler is much stronger as it has another functionality: best trials are copied to worst trials.

This implies that trial's results are not independent anymore. For every iterations, every trial's hyperparameters will be randomly perturbed, so they are indeed n new combinations for each iteration. But then the worst half of trials copy best half trials trained model and their hyperparameters at every iterations.

The search over n new combinations comes from the *n/2* best trials found at last iteration, the n trials from last iteration were themselves issued from the *n/2* best trials from antepenultimate trial. Hence, at every iteration the n trials come from the best half space of trials in last iterations, themselves coming from the half best space of antepenultimate iteration. Thus we are doing at ith iteration n searches over a space that has been refined and halved i time, effectively a subspace of the original space that is 2^i times smaller!
Note we made the simplification that the threshold was at half to simplify.

We showed that PBT scheduler with $n \times m$ trainings does exactly the equivalent of a random search algorithm[4] with $n_1 = (\frac{n}{2})^m$ trials (against n) if the search algorithm halves its worst half trials at every iterations.

Obviously PBT is not that effective as we made two assumptions:

- if a trial x is better then a trial y at iteration i, x is better than y for every iterations.
- Perturbations are local (only exploit) and hence that they would never go back to a space that was previously evicted for being in the worst half.

We can redo the calculations without the second assumption:
In reallity, PBT's perturbations are local (exploitation) with probability p_1 and sometimes completely random over the whole search space (exploration) with probability $1 - p_1$. Also, let's says that a local perturbation has probability p_2 to go back to a previously evicted space. We define p the probability that a perturbation go back to a previously evicted space.
$p = (1 - p_1)p_2 + p_1$
$p = 0 \iff p_1 = 0 \quad and \quad p_2 = 0$
$p = 1 \iff p_1 = 1 \quad or \quad p_2 = 1$
We are only doing n(1-p) exploitation at every iterations against n before, so the total real number of perturbations is $(\frac{n(1-p)}{2})^m$. The reason why we don't want to have p too close to 0 is that it permits exploration that is good to mitigate the first assumption.

Nevertheless, PBT scheduling have important drawbacks:

[2]: Note that this assumption reduces the importance of the search algorithm as he performs his n explorations based on information from trials trained only once.

[3]We here make the assumption that perturbations and searches from Search Algorithms are similar.

[4]: it does the equivalent of random search because here the perturbations are random, an interesting idea would be to develop a PBT scheduling algorithm with Bayesian Optimisation based perturbations, as we showed that these are far better than random.

- It is slighly more complex to implement.
- It uses more memory, as all good trials are stored in memory, in order to allow bad trials to copy good trials.
- It is much slower for the same number of iterations, as all trials must be saved to memory periodically, and eventually be replaced by another better trial.

If memory is a bottleneck, we suggest the following to reduce significantly the use of memory: We will save memory by not saving the models, hence not doing any copies. We can retrain worst half trials from best half trials at every iterations, then for iteration i, $\frac{n}{2}$ trials do one training, and the other $\frac{n}{2}$ do i trainings. In total the number of trainings is:

$$n + \sum_{i=1}^{m} \frac{n}{2}(1+i) = n + \frac{n}{2}(m + \frac{m(m-1)}{2}) \quad (9)$$

which results in $O(n \times m^2)$ trainings instead of $O(n \times m)$ trainings.

We showed that PBT scheduler permitted to do $(\frac{n(1-p)}{2})^m$ searches when doing $n \times m$ trainings, hence providing an speed up of $\frac{(\frac{n(1-p)}{2})^m}{m \times n} = O(\frac{n^{m-1}}{m})$, and $O(\frac{n^{m-1}}{m^2})$ for a memory free case

B.3 Median scheduler:

Let's compare how other schedulers compare to PBT sheduler. A simple scheduler is the median scheduler, that simply stops at every iteration the worst half of the trials. For n trials, the total number of trainings follows $\sum_{i=0}^{m} \frac{n}{2^i} = 2n$ so it allows to do $2 \times n$ trainings instead of $n \times m$. A speed-up of O(m)

B.4 ASHA Scheduler:

The scheduler we often used in this project is the ASHA scheduler. ASHA is constructed with a bracket parameter k. The search starts with n trials, after 1 iteration, the n/k best trials are kept, and next selection happens in k iterations. Then, every selection keep the q/k best trials and next selection is in k times more iterations. The number of steps is $log_k(n)$, the number of iterations for step i is k**i and the number of trials is n/k**i. The overall number of trainings is $\sum_{i=0}^{log_k(n} , \quad m = \sum_{i=0}^{log_k(n)} k^i = n$ Which is in $O(log_k(n) \times n)$. We have a speedup of $O(\frac{m}{log_k(n)}) = O(\frac{n}{log_k(n)})$.

Ray tune proposes the edge case k=1 per default which works the following: parameter it simply stop a trial if it is less good than the best yet obtained trial when it had been trained with as many iterations. This imply that the first random trial is necessarily totally trained as it will be the comparison reference for other trials. Then let's say that trials are random, second trial has probability 1/2 to be better than the first random trial, third trial has probability 1/3, nth has probability 1/n the number of training is $\sum_{i=0}^{n} \frac{m}{i}$ which is in $O(m \times log(n))$.
The speedup is in $O(\frac{n}{log(n)})$ and is worst for any algorithm better than random search as trials will be better and better as the search algorithm learns. We are glad to see that the edge case k=1 have similar speed up.

B.5 Discussion:

We propose here a quick comparison of the three schedulers we presented with random search and HyperOptSearch. All sheduler were given 2 constraints to find the best combination: a total training time of 15min, and a maximum of 100 iterations per trials.

We advise to use unconditionally PBT scheduler in the following cases: huge search space, huge number of iterations, huge number of trials, scalable comparison of the trials in function of the iterations, memory is not a bottleneck.

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