

Scalable Hyperparameter Optimization for LLM Fine-Tuning



Bayesian and Partition-based optimization


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Summary

1. Introduction
2. Review of Related Works
3. Problem Definition
4. Methodology
5. Experiments
6. Conclusion

01 Introduction



Large Language Models

Summary

- ▶ State-of-the-art of Natural Language Processing (NLP) problems
- ▶ Architecture : Transformers[16] block, mixed with classical layers (MLP, Conv)
- ▶ 2 phases of training : pre-training and fine-tuning

Self Attention

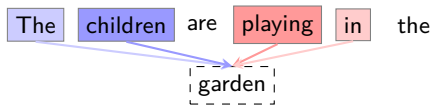


Figure: Self Attention mechanism illustration

Self attention is the key of LLM, used to compute the context of each token.



Fine Tuning

Parameters Efficient Fine-Tuning (PEFT)

Set of methods aims to reduce the computation cost of fine-tuning. Can change the structure like the 2 following, or just reduce the cost like Quantization (reduce the precision of calculus). These methods are often hyperparameter-dependent.

Low Rank Adaptation (LoRA)[7]

Use of low rank matrices of the weights matrices, which will be the only ones trained, to reduce the cost of gradient computations.

Adapter Layer

Add layer inside the model, and train only these. One con is to add inference for predicting.

Fine-Tuning workflow

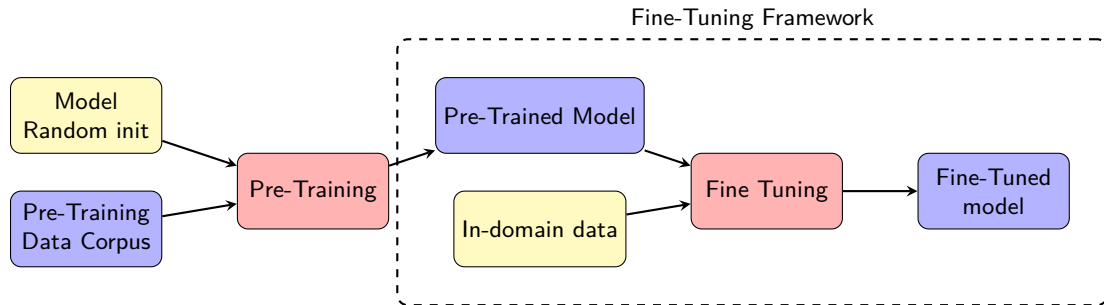


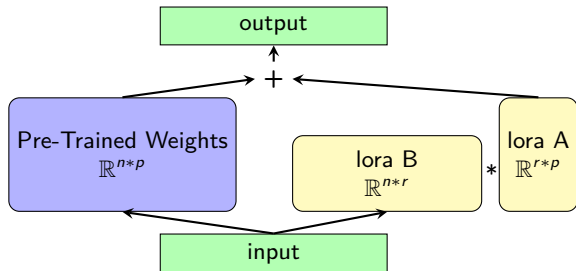
Figure: Pre-training and Fine-tuning generic workflow



Low Rank Adaptation (LoRA)

Principle

Merging Fine-tuning layers with pre-trained ones can be written as $W = W_0 + \Delta W$, with W_0 the pre-trained weights and ΔW the fine-tuned ones.



LoRA hyperparameters

- ▶ rank : the common dimension between A and B .
- ▶ alpha : apply a weighting between fine-tuning and pre-trained weights

Figure: LoRA Decomposition

02

Review of Related Works





Prompt Engineering

Prompt : process of interacting with an artificial intelligence (AI) system by providing specific instructions or queries to achieve a desired outcome.

Example with article [5], when a second LLM is used to modify the prompt.

Pros

Don't need to deal with architecture,
weights : act like the LLM is a generating
blackbox

Cons

Low impact, locate this work as the
end-user, not so much usable



LLM applied to Optimization

Multiples articles show the use of LLM to develop or code optimization algorithms, in particular Evolutionnary Algorithm. One intersting impact is to popularize the development of optimization algorithm.

Pros

Extend the fields of Meta-Heuristics, with new kinds of operators.

Cons

Low impact, don't achieve remarkable performance.



Auto DNN

Sub-domains

- ▶ **HyperParameter Optimization(HPO)** : Automatically define best hyper-parameters, from training to inference
- ▶ **Neural Architecture Search(NAS)** : Define the best architecture, from scratch or from pruning an existing one

Metrics

- ▶ Performance metrics : Accuracy, Latency
- ▶ Ressource metrics : inference time, memory usage, energy consumption

Summary

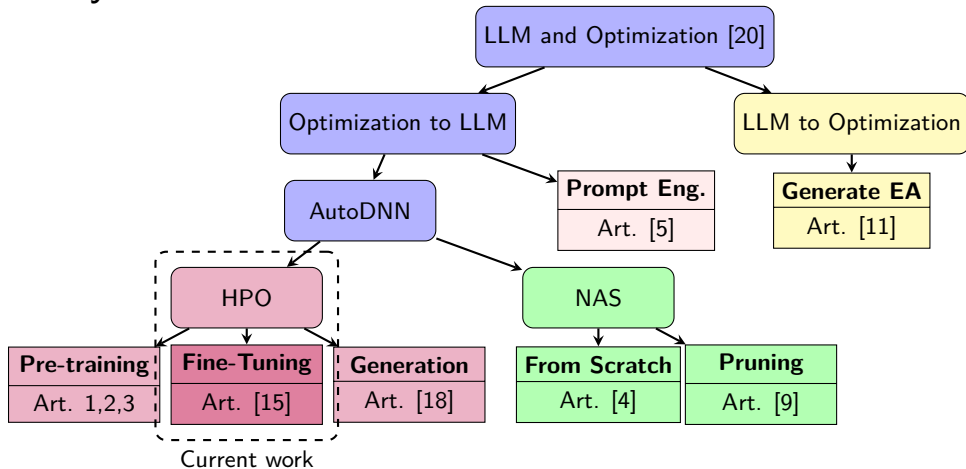


Figure: Summary of links between LLM and Optimization

03

Problem Definition





Problem Definition

This problem can be characterized the optimization of an **expensive, mixed-variable, noisy, blackbox** function.

Problem Formulation

The HPO problem can be defined as

$$\eta^* \in \arg \min_{\eta \in \mathcal{H}} \mathcal{F}(\eta) \quad (1)$$

Search Space \mathcal{H}

\mathcal{H} is the set of all values the solution tuple η can take. This stage includes method to handle the mixed-variables aspect of the problems.

Search Strategy

With η_i all the tested solutions, the search strategy is the method used to define the next solution η_{next} to evaluate.

Performance Evaluation Strategy

\mathcal{F} represent the objective function, and many can be chosen according to a problem. Also includes method like multi-fidelity that affect the fidelity of the evaluation.

Search Space

Hyper-parameters

Hyper-parameter	Optimization range		Conversion
	Lower Bound	Upper Bound	
Learning Rate	-10	-1	$f(x) = 10^x$
LoRA Rank	2	512	$f(x) = \text{round}(x)$
LoRA scale (α)	1	64	$f(x) = \text{round}(x)$
LoRA Dropout	0	0.5	$f(x) = x$
Weight Decay	-5	-1	$f(x) = 10^x$

Table: Summary of Hyperparameter Search Space

Conversion and naming convention is taken from litgpt framework.



Search Strategy I

The search strategy of an optimization problem can be seen as a balance between the exploration, i.e. going to unexplored regions, and exploitation, i.e. going close to promising areas. Here are the fields of optimization to tackle HPO problems.



Exploratory Method

Grid Search and Random Search

These 2 methods are the simplest way possible of exploring the search space, without exploiting the acquired knowledge. Useful to assess the pertinence of the optimization algorithm.

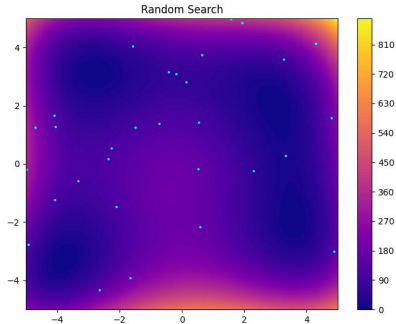


Figure: Random Search

Meta-heuristics

Meta-heuristics are mostly algorithms inspired by nature, divided in 2 approaches : population evolution or individual evolution. For the first one, methods like Genetic Algorithm (GA) allow the fitting of the population to a problem, with evolutionary operators like crossover, mutation or selection. For the second one, like Intensive Local Search (ILS), the methods iterate through the search space with only one solution by iteration.

These methods aren't fit to HPO problems applied to LLM, due of their needs of numerous evaluations, begin computationally prohibitive.



Partition Based Optimization

Partition Based Optimization

Sets of methods that apply partition to the search space, to favor (partition again) or penalize (discard region) these partitions. E.g.: DIRECT[8], Fractals[3], SOO[12]
Useful for parallelization abilities

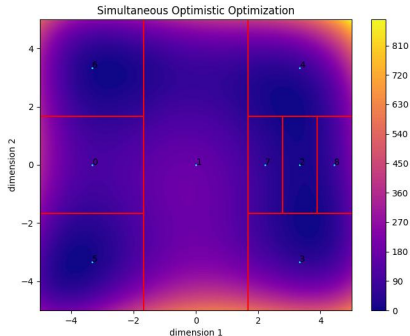


Figure: SOO

Surrogate-Model Based Optimization (SMBO)

Methods based on creating a **surrogate** model of the objective function, using the knowledge from already evaluated solutions. The acquisition function, i.e. the function of the surrogate model, is used to balance exploration and exploitation.

E.g.: Bayesian Modeling, Gaussian Process (GP), Tree Parzen Estimator (TPE).

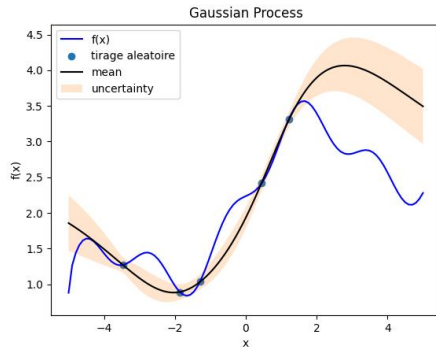


Figure: Gaussian Process



Partition and Surrogate-Model based optimization : the hybridation

The partition based methods are by nature parallel, by the generation of a tree-search of possible solutions. The SMBO achieve to reduce the number of evaluation by using an acquisition function to discard or favor a possible solution. The hybridation would result in a parallelization-able Bayesian modeling, allowing to extract the best of the two fields.

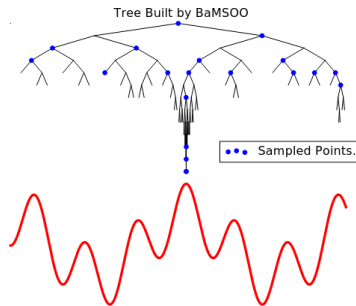


Figure: BaMSOO [19]



Performance Evaluation Strategy

Evaluation context

In this part, there are many options, like the number of epochs (if not an hyperparameters), the precision of the model, the datasets of training or evaluation.

Objective function


For this problem, there are 2 ways to evaluate a solution :

- ▶ **Loss (validation or testing)** : the loss is computed through the training, and we can keep a small part of the datasets unused to use it the evaluate the model. Cons : dataset dependant, difficult to put in global context
- ▶ **Benchmark dataset (GLUE[17], MMLU[6])** : the accuracy on a literature benchmark dataset can be used to evaluate the training. It's interesting, since it's a good measure of generalization, since the model has not read this type of questions. Warning : the benchmark used during the optimization can't be used as a final testing.

Multi-fidelity approaches can be used to reduce the cost of evaluation in earlier steps. Algorithms like Bayesian Optimization and HyperBand (BOHB[2]) achieve cost-efficient optimization by reducing the part of the datasets in early stages.

04

Methodology





Global HPO workflow

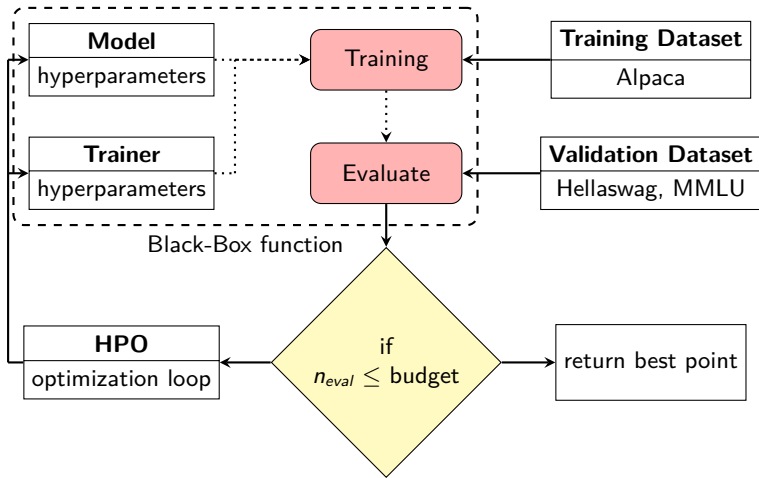


Figure: HPO workflow



Optimization : generate the new solution |

Frameworks

BoTorch for all gaussian processes, everything in python.



Optimization : generate the new solution II

Partition Based Algorithm : Simultaneous Optimistic Optimization (SOO)

Perform a K-inary partition
of the space, evaluating
every center of partition
during the expansion of a
node.

Algorithm 3.3: SOO

```

Input:  $\Omega, f, K, n_{\max}$ 
// initiate
1  $x_{0,0} \leftarrow \text{center}(\Omega)$ 
2  $f_{0,0} \leftarrow f(x_{0,0})$ 
3  $\mathcal{T}_1 \leftarrow \{x_{0,0}, f_{0,0}, \Omega\}$ 
4  $n \leftarrow 1$ 
5 while  $n < n_{\max}$  do
6    $\nu_{\max} \leftarrow -\infty$ 
7   for  $h \leftarrow 0$  to  $\text{depth}(\mathcal{T}_n)$  do
8      $j \leftarrow \arg \max_{j \in \{j | (h,j) \in L_n\}} f(x_{h,j})$  // select function
9     if  $f(x_{h,j}) > \nu_{\max}$  then
10       $\Omega_{h+1,j+1}, \dots, \Omega_{h+1,j+K} \leftarrow \text{section}(\Omega_{h,j}, K)$ 
11      for  $i \leftarrow 1$  to  $K$  do
12         $n \leftarrow n + 1$ 
13         $x_{h+1,j+i} \leftarrow \text{center}(\Omega_n)$ 
14         $f_{h+1,j+i} \leftarrow f(x_{h+1,j+i})$  // Scoring function
15         $\mathcal{T}_n \leftarrow \{(x_{h+1,j+i}, f_{h+1,j+i}, \Omega_{n+1})\}$  // add_leaf function
16         $\nu_{\max} \leftarrow f_{h,j}$ 
17      end
18    end
19  end
20 end
21 return best of  $x_{h,j}, f(x_{h,j})$ 

```

Optimization : generate the new solution III

Surrogate Model Based Optimization : Bayesian Optimization with Gaussian Process (BO-GP)

Use Gaussian Process as a surrogate for the objective function, and optimize it to found the most promising point to evaluate

Algorithm 3.2: BO

Input: $\Omega, f, K_D, \mathcal{O}, f_{\text{acq}}, n_{\text{init}}, n_{\text{opt}}$
// initiate function

```
1 for  $i \leftarrow 1$  to  $n_{\text{init}}$  do
2    $\lambda' \leftarrow \text{LHS}(\Omega, \mathcal{D})$  // Sample one point
3    $\mathcal{D} \leftarrow \mathcal{D} \cup \{(\lambda', f(\lambda'))\}$  // Add solution and evaluation to set of data
4 end
5 for  $i \leftarrow 1$  to  $n_{\text{opt}}$  do
6    $\mu_D, K_D \leftarrow \text{Update}(K_D, \mathcal{D})$ 
7    $K_D \leftarrow \text{Fit}(\text{GP}(K_D), \mathcal{D})$ 
8    $\lambda' \leftarrow \text{Optimize}(f_{\text{acq}}(K_D), \mathcal{O})$  // Generate new point
9    $\mathcal{D} \leftarrow \mathcal{D} \cup \{(\lambda', f(\lambda'))\}$  // scoring function
10 end
11 return best of  $\{(\lambda^*, f(\lambda^*)) \in \mathcal{D}\}$ 
```

Optimization : generate the new solution IV

Hybridation : Bayesian Multi-Scale Optimistic Optimization(BaMSOO)

Replace the scoring of SOO with a BO-GP based approximation to determine if it's relevant to evaluate the point.

$$\begin{aligned} \mathcal{UCB}(x|\mathcal{D}_t) &= \mu(x|\mathcal{D}_t) + B_N * \sigma(x|\mathcal{D}_t) \\ \text{with } B_N &= \sqrt{2 \log(\pi^2 N^2 / 6\eta)}, \eta \in (0, 1) \end{aligned} \quad (2)$$

Algorithm 3.4: BamSOO scoring

```
1 if  $\mathcal{UCB}(x_{h+1,j+i}, \mu, \sigma) \geq f^+$  then
2   |  $g_{h+1,j+i} \leftarrow f(x_{h+1,j+i})$ 
3   |  $t \leftarrow t + 1$ 
4 end
5 else
6   |  $g_{h+1,j+i} \leftarrow \mathcal{LCB}(x_{h+1,j+i}, \mu, \sigma)$ 
7 end
8 if  $g_{h+1,j+i} > f^+$  then
9   |  $f^+ \leftarrow g_{h+1,j+i}$ 
10 end
11  $n \leftarrow n + 1$ 
12  $\mathcal{T}_n \leftarrow \{(x_{h+1,j+i}, f_{h+1,j+i}, \Omega_{h+1,j+i})\}$ 
13 return best of  $x_{h,j}, g(x_{h,j})$ 
```



Evaluate the solution

Use LitGPT framework with it's CLI to perform an evaluation of a solution. All models and datasets are taken from HuggingFace Hub.

Training


- ▶ Model : Llama-3.2-3B
- ▶ dataset : Alpaca
- ▶ 1 epochs of training
- ▶ Fully Sharded Data Parallelism (FSDP) as distributed strategy

Evaluating

Based on lm_eval library

- ▶ validation dataset : Hellaswag
- ▶ testing dataset : MMLU

05 Experiments





Experimental Setup

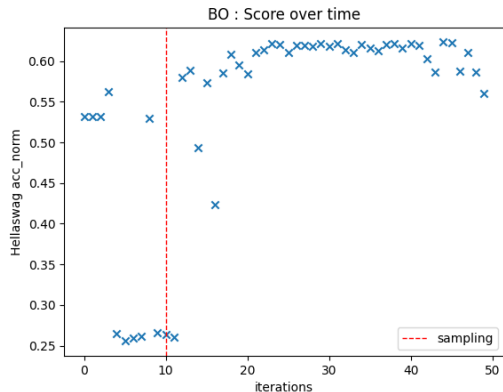
Experiments presented in this paper were carried out using the Grid'5000 testbed, supported by a scientific interest group hosted by Inria and including CNRS, RENATER and several Universities as well as other organizations (see <https://www.grid5000.fr>).

One evaluation on chuc cluster, using 4*A100 40G of VRAM GPU, is taking around 1 hour. Each algorithms have a budget of 50 evaluations, including the 10 sampling evaluation of BO.

Hellaswag bounds

- ▶ Upper bound : best accuracy on Hellaswag : 95.3%. Done with GPT4 model, with 10-shot evaluation
- ▶ Lower bound : Sampling without exploitation : 55,7%. Using one-shot LHS, with 10 picks to evaluate.

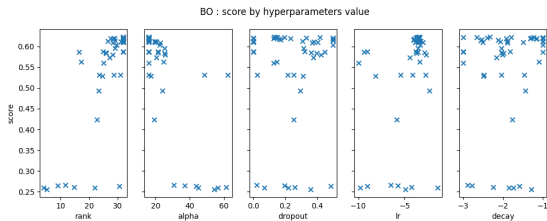
Score evolution



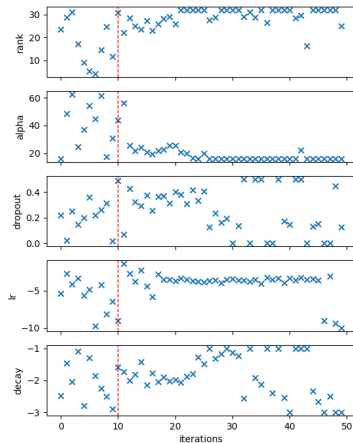
Results

Best score : 62.3%

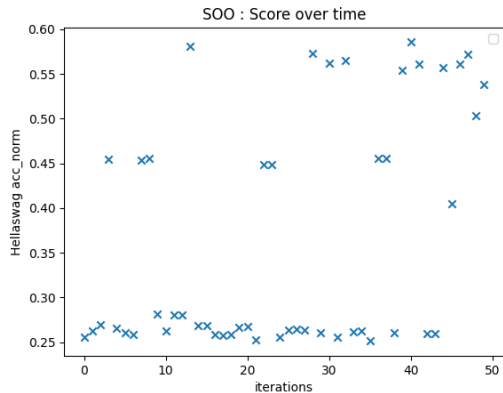
Score by variables and Variables over iterations



BO : hyperparameters over iterations



Score evolution

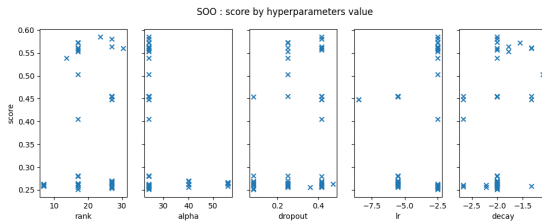


Results

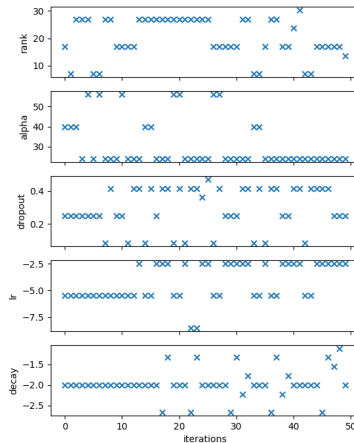
Best score : 58.4%

Slow convergence

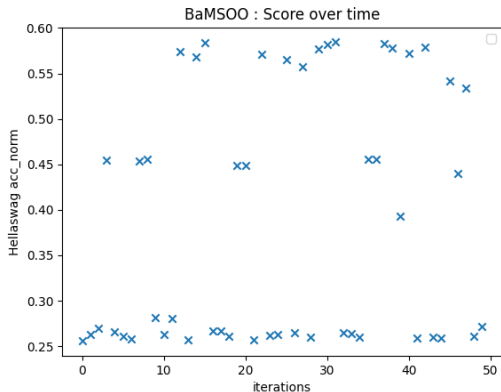
Score by variables and Variables over iterations



SOO : hyperparameters over iterations



Score evolution



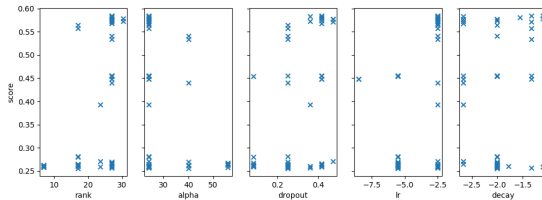
Results

Best score : 58.5%

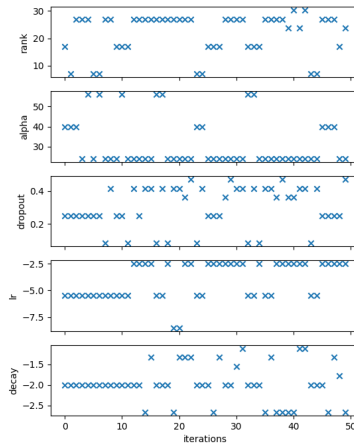
Not so much approximations, need to increase η in equation 2 to speed the convergence

Score by variables and Variables over iterations

BaMSOO : score by hyperparameters value



BaMSOO : hyperparameters over iterations





Conclusion

On a sequential comparison, BO-GP algorithms is the most efficient between these 3 algorithms, even considering the exploitation made by BamSOO algorithms. But this kind of performance needs to efficiently scale to be able to be usable with very expensive function, especially if the evaluation can't be distributed.

With it's acceleration using GP, BaMSOO keep most of the SOO abilities, in particular it's parallelism innate abilities, but achieve to be efficient with a smaller number of evaluation. To be able to effectively compare theses approaches, it's necessary to look at higher dimensionnal problem.



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Thank You.

