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Hyperparameter Optimization of LLM Fine-Tuning

Bayesian and Partition-based approaches

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Summary

01
Introduction

Large Language Models

Summary

- State-of-the-art of Natural Language Processing (NLP) problems
- Architecture : Transformers block, mixed with classical layers (MLP, Conv)
- Huge size : Billions of parameters (1B to 405B for Llama 3)
- 2 phases of training : pre-training and **fine-tuning**

Self Attention

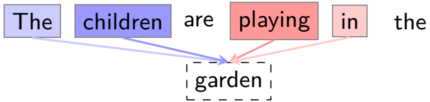

Figure: Self Attention mecanism illustration

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

Fine-Tuning

Following a first phase of pre-training, Fine-tuning is used to correct behavior or add in-domain data to a model, with limited ressources.

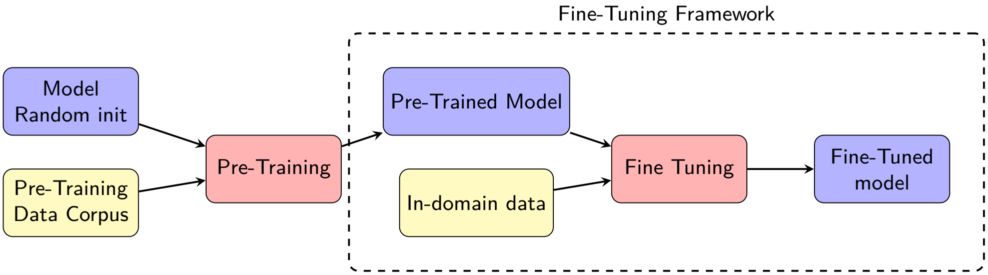

Figure: Pre-training and Fine-tuning generic workflow

Parameters Efficient Fine-Tuning (PEFT)

Set of methods aims to reduce the computation cost of fine-tuning. 2 main approachs : *Additive* and **reparametrization**.

Reparametrization

Use lower-cost proxy as trainable weights, and merge at the end.

Addivitive

Add part of the model, often linear layer, to train these. One con is to add inference to generation.

Quantization

To reduce further the cost of computing during the training, quantization can also be used. This can be combined with either of precedent approaches.

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. With LoRA, $W = W_0 + \frac{\alpha}{r} B.A$

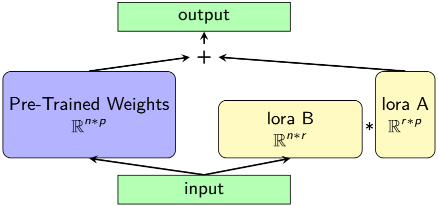

Figure: LoRA Decomposition

LoRA hyperparameters

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

Hyperparameter Optimization (HPO)

Objectives

- Better performance than manual tuning
- Ease popularization of the Fine Tuning

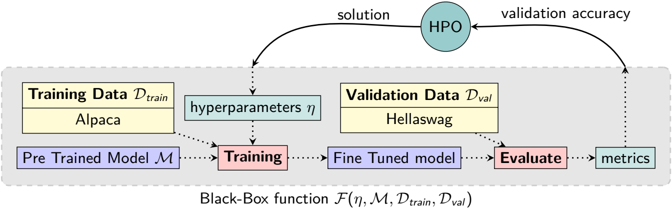

Figure: HPO workflow

Related Works

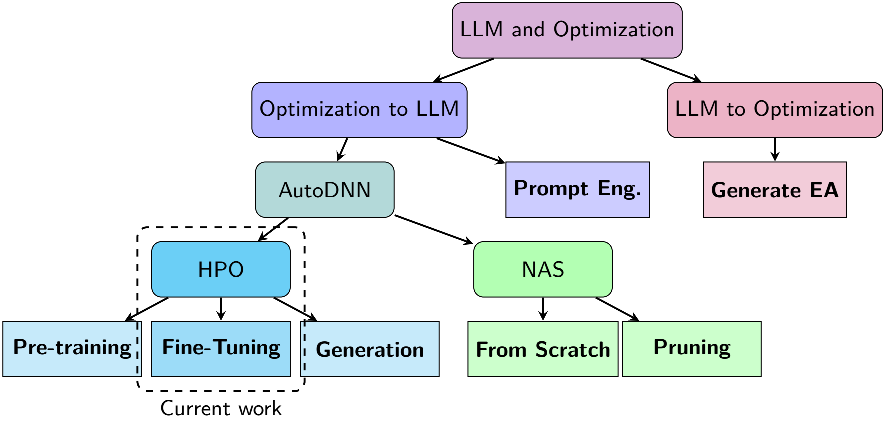

Figure: Summary of links between LLM and Optimization

02
Problem Definition

Problem Definition

Problem Formulation

The HPO problem can be defined as

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

This function can be characterized as an **expensive, mixed-variable, noisy, blackbox** function.

3 phases of an optimization problem

- **Search Space** $\mathcal{H}$: all variables and how to handle them
- **Search Strategy** $\arg\min$: how to search for the minimum of the function
- **Performance Evaluation Strategy** $\mathcal{F}(.)$: how to evaluate a given solution

Search Space

Hyperparameters

Hyperparameters	Optimization range		Type	Conversion
	Lower Bound	Upper Bound		
Learning Rate	-10	-1	log.	$f(x) = 10^x$
LoRA Rank	1	64	int.	$f(x) = \text{round}(x)$
LoRA scale (α)	1	64	int.	$f(x) = \text{round}(x)$
LoRA Dropout	0	0.5	cont.	$f(x) = x$
Weight Decay	-3	-1	log.	$f(x) = 10^x$

Table: Summary of Hyperparameter Search Space

- Conversion and naming convention is taken from LitGPT framework.
- Variable conversion for handling mixed-variables with continuous algorithms
- No *A-priori* knowledge on hyperparameters importance

Search Strategy

Algorithms for LLM HPO are *Global Optimization* algorithms. Can be classified as :

- **Exploratory**(GS, Random Search, LHS) : sample the search space
  no exploitation, give a lower bound
- **Metaheuristics** (Genetic Algorithm, ILS, PSO) : bio-inspired heuristics
  evaluation greedy, cannot be used for expensive function
- **Bayesian Optimization** (Gaussian Process, TS) : Use a surrogate to enhance exploitation
  innate sequential nature, strong exploitation
- **Partition-Based Optimization**(FDA, SOO, DiRect) : partition the search space
  massively parallel, slow convergence

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

2 ways to evaluate LLM Fine-Tuning :

- **Loss (validation/test)** : dataset and model dependant, difficult to compare to other models.
- **Accuracy on Benchmark dataset (GLUE, MMLU)** : can be used to compare to other models throughout the training.

Complementary approaches

- Multi-fidelity : reduce the cost and the reliability of early evaluations. (ex : BOHB algorithm)

03
Design and Implementation

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-3.2-1B
- 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

Optimization algorithms

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: Ω, f, K, $n_{\max}$

// initiate

$x_{0,0} \leftarrow \mathrm{center}(\Omega)$
$f_{0,0} \leftarrow f(x_{0,0})$
$\mathcal{T}_1 \leftarrow \{x_{0,0}, f_{0,0}, \Omega\}$
$n \leftarrow 1$
while $n < n_{max}$ **do**
  $\nu_{\max} \leftarrow -\infty$
  for $h \leftarrow 0$ **to** $depth(\mathcal{T}_n)$ **do**
    $j \leftarrow \arg\max_{j \in \{j \mid (h,j) \in L_n\}} f(x_{h,j})$ // select function
    if $f(x_{h,j}) > \nu_{max}$ **then**
      $\Omega_{h+1,j+1}, \ldots, \Omega_{h+1,j+K} \leftarrow \mathrm{section}(\Omega_{h,j}, K)$
      for $i \leftarrow 1$ **to** K **do**
        $n \leftarrow n + 1$
        $x_{h+1,j+i} \leftarrow \mathrm{center}(\Omega_n)$
        $f_{h+1,j+i} \leftarrow f(x_{h+1,j+i})$ // Scoring function
        $\mathcal{T}_n \leftarrow \{(x_{h+1,j+i}, f_{h+1,j+i}, \Omega_{n+1})\}$ // add_leaf function
        $\nu_{\max} \leftarrow f_{h,j}$
      end
    end
  end
end
return best of $x_{h,j}, f(x_{h,j})$

Figure: SOO Algorithm

Optimization algorithms II

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: Ω, f, K_D, $\mathcal{O}$, f_{acq}, n_{init}, n_{opt}

// initiate function

for $i \leftarrow 1$ **to** n_{init} **do**

 $\lambda' \leftarrow \text{LHS}(\Omega, \mathcal{D})$ // Sample one point

 $\mathcal{D} \leftarrow \mathcal{D} \cup \{(\lambda', f(\lambda'))\}$ // Add solution and evaluation to set of data

end

for $i \leftarrow 1$ **to** n_{opt} **do**

 $\mu_D, K_D \leftarrow \text{Update}(K_D, \mathcal{D})$

 $K_D \leftarrow \text{Fit}(\text{GP}(K_D), \mathcal{D})$

 $\lambda' \leftarrow \text{Optimize}(f_{\text{acq}}(K_D), \mathcal{O})$ // Generate new point

 $\mathcal{D} \leftarrow \mathcal{D} \cup \{(\lambda', f(\lambda'))\}$ // scoring function

end

return best of $\{(\lambda^*, f(\lambda^*)) \in \mathcal{D}\}$

Optimization algorithms III

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.

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

Algorithm 3.4: BamSOO scoring

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if $\mathcal{UCB}(x_{h+1,j+i}, \mu, \sigma) \geq f^+$ **then**
  $g_{h+1,j+i} \leftarrow f(x_{h+1,j+i})$
  $t \leftarrow t + 1$
end
else
  $g_{h+1,j+i} \leftarrow \mathcal{LCB}(x_{h+1,j+i}, \mu, \sigma)$
end
if $g_{h+1,j+i} > f^+$ **then**
  $f^+ \leftarrow g_{h+1,j+i}$
end
$n \leftarrow n + 1$
$\mathcal{T}_n \leftarrow \{(x_{h+1,j+i}, f_{h+1,j+i}, \Omega_{h+1,j+i})\}$
return best of $x_{h,j}, g(x_{h,j})$

04
Computation 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 40 minutes.
Each algorithms have a budget of 50 evaluations, including the 10 sampling evaluation of BO.

Sampling experiment : Latin Hypercube Sampling I

Objective : explore the search space and make a reference for other algorithms.

Analysis

- Top scores :
  Hellaswag : 47.9%
  MMLU : 37.6%
- High range for Hellaswag, allowing to discriminate efficiently between solutions.

Running time : arround 36 hours

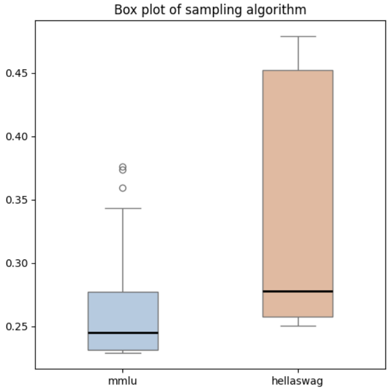


Figure: Distribution of score for sampling experiment

Sampling experiment : Latin Hypercube Sampling II

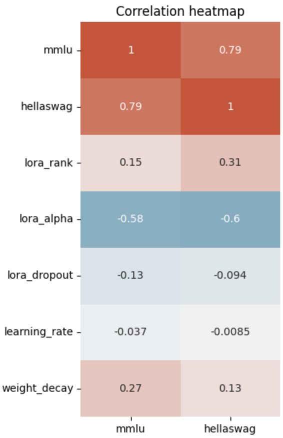


Figure: Correlation between variables and metrics

Correlation between metrics

With 79% of correlation, Hellaswag and MMLU accuracy are relevant as validation/testing metrics.

Correlation between variables and metrics

High factor variables : LoRA alpha the Lora rank / weight decay.

TO DO : verify with other experiment the relevance of using dropout and learning rate.

BO (waiting for results)

Score evolution

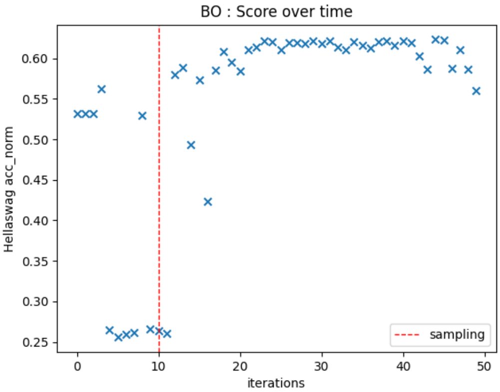


Figure: Score over time

Results

Best score : 62.3%, achieved after X iterations.
Wait for MMLU to look at overfitting

Behavior

- 0 -> 10 : sampling (LHS)
- 10 -> 25 : converge to high score
- 25 -> 40 : high score
- 40 -> 50 : search unexplored space

BO (waiting for results) II

Exploitation of the search space

rank, alpha and learning rate seem to converge fast
weight decay converge slowly to the top during high score phase
dropout does not converge, linked with weak correlation to metrics => relevant Hyperparameter ??

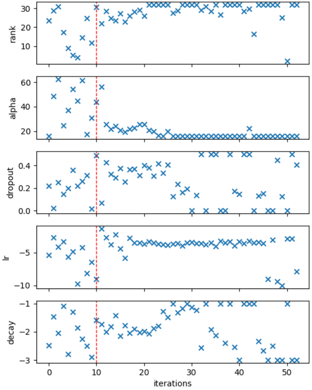
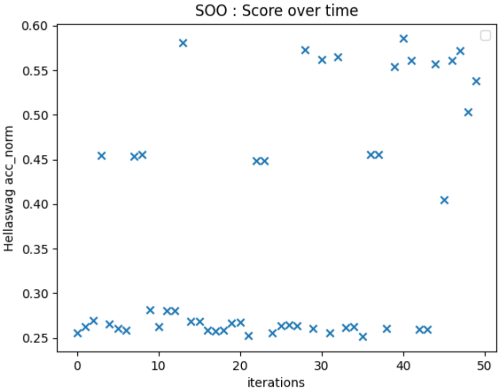


Figure: Variables over time

SOO(waiting for results)

Score evolution



Results

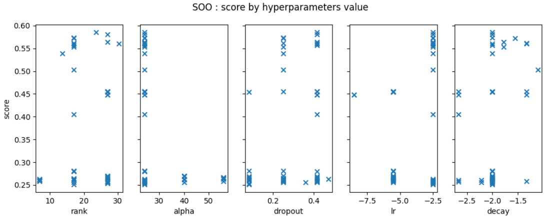
Best score : 58.4%

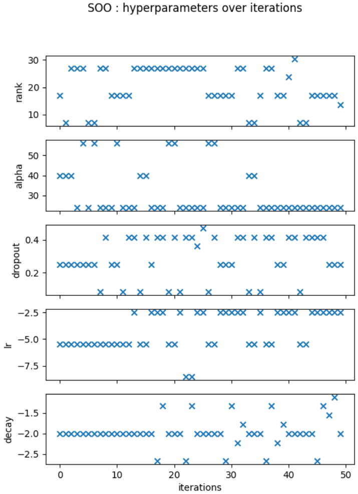
Behavior

Slow convergence, need more than 50 iterations to converge to more depth. Max depth : 6 A lot of unpromising point to explore

SOO(waiting for results) II

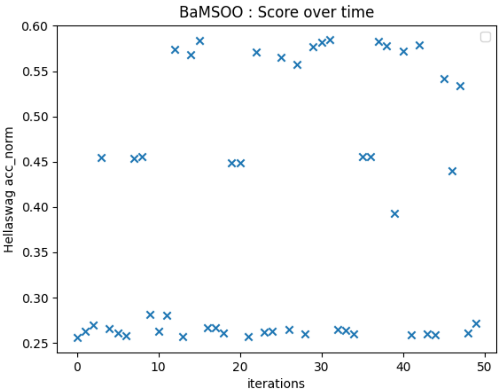
Score by variables and Varibles over iterations





BaMSOO

Score evolution



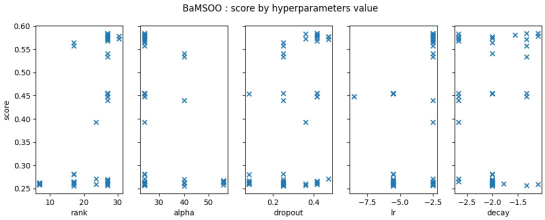
Results

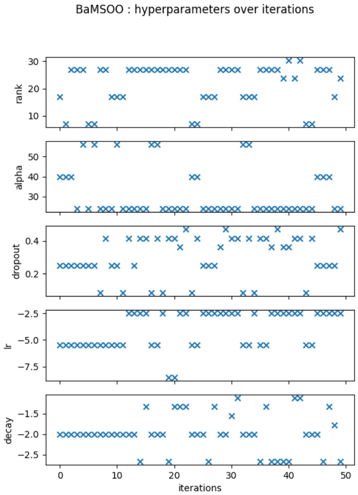
Best score : 58.5%

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

BaMSOO II

Score by variables and Varibles over iterations





Comparison (waiting results)

Datasets	Lower (LHS)	Upper	BO	SOO	BaMSOO
Hellaswag	47.9	69.8*	X	X	X
MMLU	37.6	49.3	X	X	X

Table: Bounds on accuracy for validation and testing dataset

05
Conclusions and Perspectives

Conclusion

review

On a sequential comparaison, BO-GP algorithms is the most efficient between theses 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 inate 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.

Perspective

- Expand search space : add dimensions (Adam momentum, precision, matrices to apply LoRA)
- use more training datasets
- make a distributed implementation

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Thank You.