

# Hyperparameter Optimization of LLM Fine-Tuning



Bayesian and Partition-based approaches


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# Summary

1. Introduction
2. Problem Definition
3. Design and Implementation
4. Computation Experiments
5. Conclusions and Perspectives

# 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

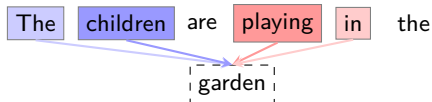


Figure: Self Attention mechanism illustration

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 resources.

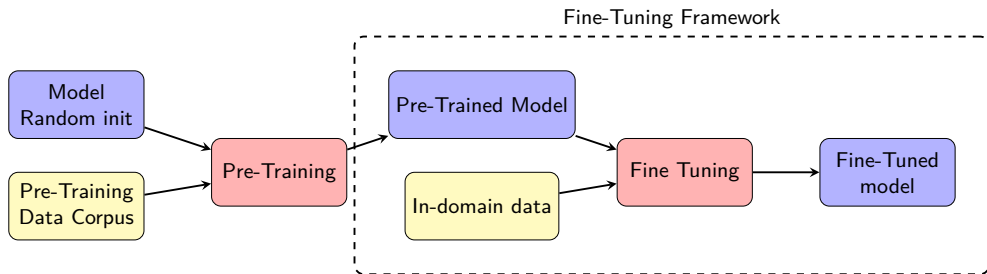


Figure: Pre-training and Fine-tuning generic workflow



## Parameters Efficient Fine-Tuning (PEFT)

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

### **Reparametrization**

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

### **Additive**

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  $\Delta W$  the fine-tuned ones. With LoRA,  $W = W_0 + \frac{\alpha}{r} B.A$

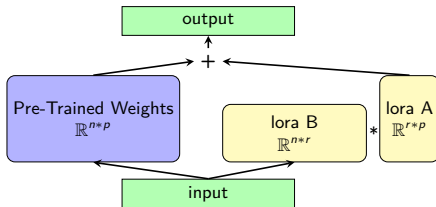


Figure: LoRA Decomposition

## LoRA hyperparameters

- ▶ rank  $r$  : the common dimension between  $A$  and  $B$ .
- ▶ alpha  $\alpha$  : 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

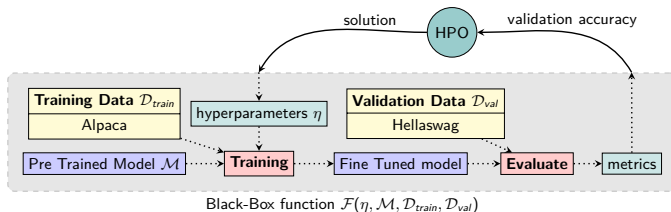


Figure: HPO workflow



## Related Works

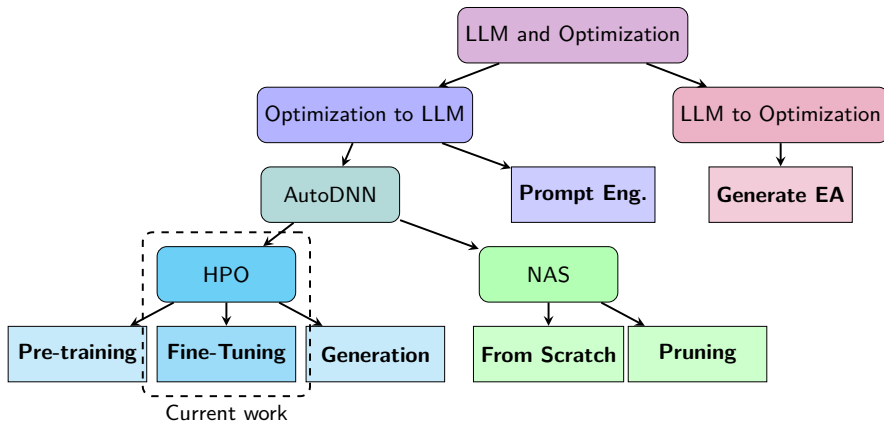


Figure: Summary of links between LLM and Optimization

# 02

## Problem Definition





# Problem Definition

## Problem Formulation

The HPO problem can be defined as

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

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**  $\mathcal{F}(\cdot)$  : 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 ( $\alpha$ )	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
- ▶ **Surrogate-Model based Optimization** (Bayesian Optimization with 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

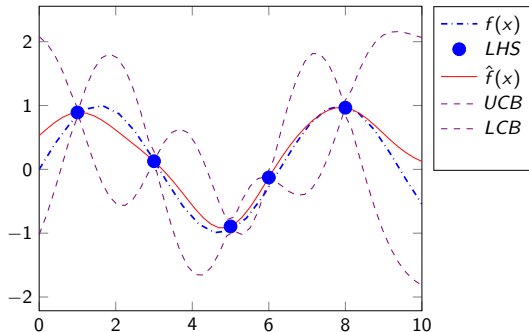




## SMBO : Bayesian-Optimization based on Gaussian-Process (BO-GP)

### Principe :

- ▶ Build a surrogate of the objective function
- ▶ Optimize the surrogate to find the most promising point to evaluate

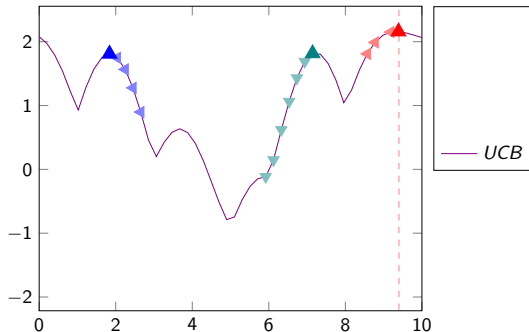




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# PBO : Simultaneous Optimistic Optimization(SOO)

## Partition Based Algorithm : Simultaneous Optimistic Optimization (SOO)

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

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### Algorithm 3.3: SOO

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```
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  $x_{h,j}, f(x_{h,j})$ 
```

---



## Hybridization : Bayesian Multi-Scale Optimistic Optimization (BaMSOO)

### 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.

$$UCB(x|\mathcal{D}_t) = \mu(x|\mathcal{D}_t) + B_N * \sigma(x|\mathcal{D}_t) \quad (2)$$

with  $B_N = \sqrt{2 \log(\pi^2 N^2 / 6\eta)}$ ,  $\eta \in (0, 1)$

---

#### Algorithm 3.4: BamSOO scoring

---

```


1 if  $UCB(x_{h+1,j+i}, \mu, \sigma) \geq f^+$  then
2    $g_{h+1,j+i} \leftarrow f(x_{h+1,j+i})$ 
3    $t \leftarrow t + 1$ 
4 end
5 else
6    $g_{h+1,j+i} \leftarrow LCB(x_{h+1,j+i}, \mu, \sigma)$ 
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  $x_{h,j}, g(x_{h,j})$ 

```

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# 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 : around 36 hours

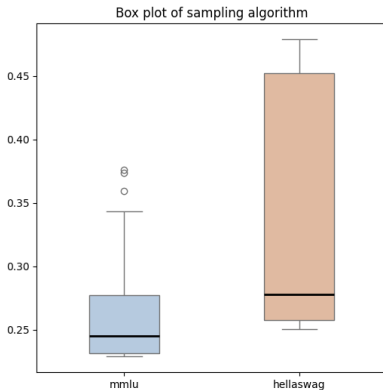
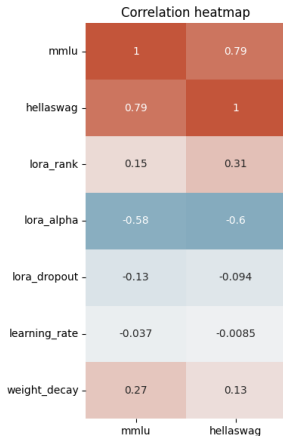


Figure: Distribution of score for sampling experiment



## Sampling experiment : Latin Hypercube Sampling II



### 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.

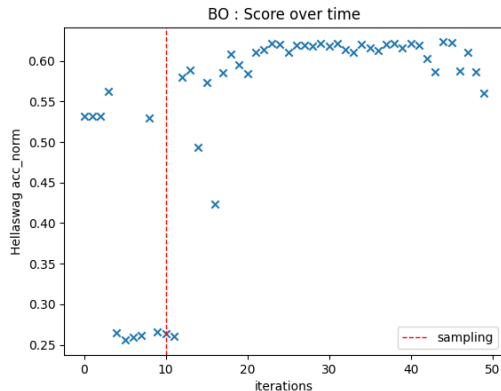
**Figure:** Correlation between variables and metrics





## BO (waiting for results) I

### Score evolution



### 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

Figure: Score over time



## 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 ??

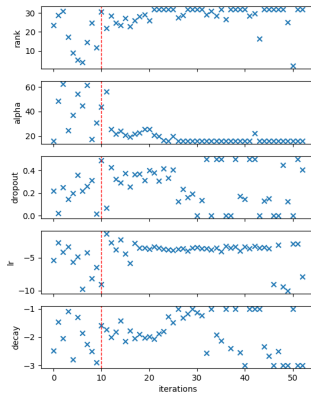
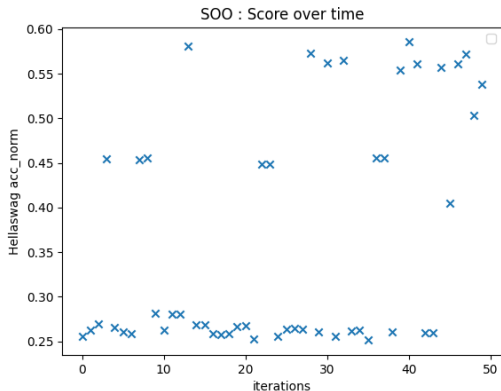


Figure: Variables over time



## SOO(waiting for results) |

### Score evolution



### Results

Best score : 58.4%

### Behavior

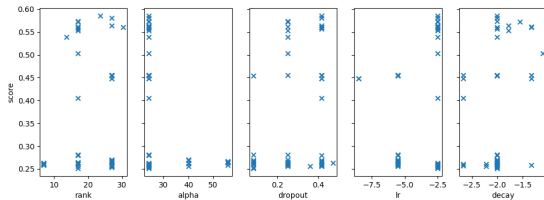
Slow convergence, need more than 50 iterations to converge to more depth.  
Max depth : 6 A lot of unpromising point to explore



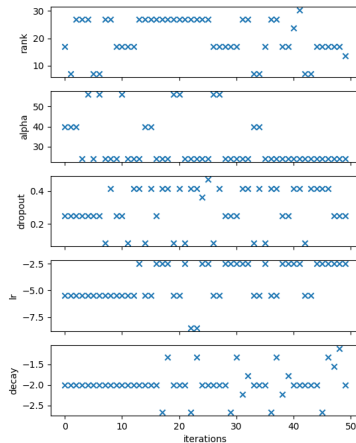
# SOO(waiting for results) ||

## Score by variables and Variables over iterations

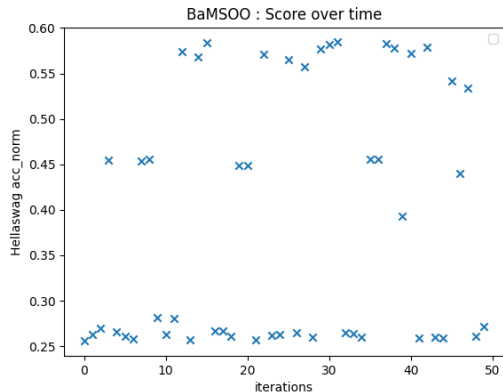
SOO : score by hyperparameters value



SOO : hyperparameters over iterations



## Score evolution



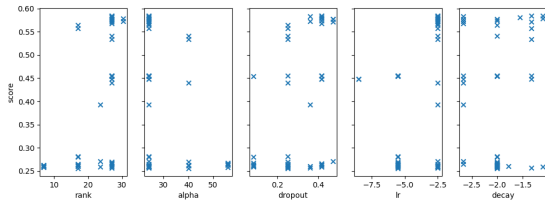
## Results

Best score : 58.5%

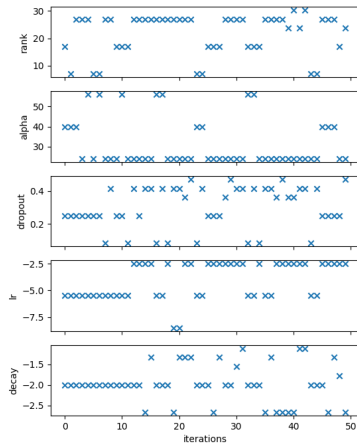
Not so much approximations, need to increase  $\eta$  in equation 2 to speed the convergence

## Score by variables and Variables over iterations

BaMSOO : score by hyperparameters value



BaMSOO : hyperparameters 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 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 its acceleration using GP, BaMSOO keeps most of the SOO abilities, in particular its parallelism capabilities, but achieves to be efficient with a smaller number of evaluations.

To be able to effectively compare these approaches, it's necessary to look at higher dimensional problems.

## Perspective

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



## Bibliography I

- [1] Mike Conover et al. *Free Dolly: Introducing the World's First Truly Open Instruction-Tuned LLM*. 2023. URL: <https://www.databricks.com/blog/2023/04/12/dolly-first-open-commercially-viable-instruction-tuned-llm> (visited on 06/30/2023).
- [2] Stefan Falkner, Aaron Klein, and Frank Hutter. "BOHB: Robust and Efficient Hyperparameter Optimization at Scale". In: *CoRR* abs/1807.01774 (2018). arXiv: 1807.01774.
- [3] Thomas Firmin and El-Ghazali Talbi. "A fractal-based decomposition framework for continuous optimization". *working paper or preprint*. July 2022.
- [4] Jiahui Gao et al. "AutoBERT-Zero: Evolving BERT Backbone from Scratch". en. In: *Proceedings of the AAAI Conference on Artificial Intelligence* 36.10 (June 2022). Number: 10, pp. 10663–10671.
- [5] Qingyan Guo et al. *Connecting Large Language Models with Evolutionary Algorithms Yields Powerful Prompt Optimizers*. [arXiv:2309.08532 \[cs\]](https://arxiv.org/abs/2309.08532). Feb. 2024.



## Bibliography II

- [6] Rohan Taori and Ishaan Gulrajani and Tianyi Zhang and Yann Dubois and Xuechen Li and Carlos Guestrin and Percy Liang and Tatsunori B. Hashimoto. *Stanford Alpaca: An Instruction-following LLaMA model*. publisher : GitHub. Dec. 2024.
- [7] Dan Hendrycks et al. "Measuring Massive Multitask Language Understanding". In: *arXiv preprint arXiv:2009.03300* (2020).
- [8] Dan Hendrycks et al. *Measuring Massive Multitask Language Understanding*. arXiv:2009.03300 [cs]. Jan. 2021.
- [9] Edward J. Hu et al. *LoRA: Low-Rank Adaptation of Large Language Models*. 2021. arXiv: 2106.09685 [cs.CL].
- [10] Donald R. Jones, Cary D. Perttunen, and Bruce E. Stuckman. "Lipschitzian Optimization Without the Lipschitz Constant". In: *Journal of Optimization Theory and Applications* 79.1 (1993), pp. 157–181.
- [11] Aaron Klein et al. "Structural Pruning of Large Language Models via Neural Architecture Search". en. In: (Oct. 2023).



## Bibliography III

- [12] Guillaume Lample, Hugo Touvron, Lucas Beatching, et al. *LLaMA 3: Open and Adaptable Foundation Models*. <https://github.com/meta-llama/llama3>. 2024.
- [13] Siyi Liu, Chen Gao, and Yong Li. *Large Language Model Agent for Hyper-Parameter Optimization*. [arXiv:2402.01881 \[cs\]](https://arxiv.org/abs/2402.01881). Feb. 2024.
- [14] Rémi Munos. “Optimistic Optimization of a Deterministic Function without the Knowledge of its Smoothness”. In: *Advances in Neural Information Processing Systems 24 (NeurIPS)*. 2011, pp. 783–791.
- [15] OpenAI. *GPT-4 Technical Report*. <https://openai.com/research/gpt-4>. 2023.
- [16] Rohan Taori et al. *Stanford Alpaca: An Instruction-following LLaMA model*. [https://github.com/tatsu-lab/stanford\\_alpaca](https://github.com/tatsu-lab/stanford_alpaca). 2023.
- [17] Christophe Tribes et al. *Hyperparameter Optimization for Large Language Model Instruction-Tuning*. [arXiv:2312.00949](https://arxiv.org/abs/2312.00949). Jan. 2024.
- [18] Ashish Vaswani et al. “Attention is All you Need”. In: *Advances in Neural Information Processing Systems*. Ed. by I. Guyon et al. Vol. 30. Curran Associates, Inc., 2017.

## Bibliography IV

- [19] Alex Wang et al. “GLUE: A multi-task benchmark and analysis platform for natural language understanding”. In: *Proceedings of the 2018 EMNLP Workshop BlackboxNLP: Analyzing and Interpreting Neural Networks for NLP*. 2018, pp. 353–355.
- [20] Chi Wang, Xueqing Liu, and Ahmed Hassan Awadallah. “Cost-Effective Hyperparameter Optimization for Large Language Model Generation Inference”. en. In: *Proceedings of the Second International Conference on Automated Machine Learning*. ISSN: 2640-3498. PMLR, Dec. 2023, pp. 21/1–17.
- [21] Ziyu Wang et al. “Bayesian multi-scale optimistic optimization”. In: *Proceedings of the 17th International Conference on Artificial Intelligence and Statistics 33* (2014), pp. 1005–1013.
- [22] Xingyu Wu et al. *Evolutionary Computation in the Era of Large Language Model: Survey and Roadmap*. arXiv:2401.10034. May 2024.
- [23] Rowan Zellers et al. *HellaSwag: Can a Machine Really Finish Your Sentence?* arXiv:1905.07830 [cs]. May 2019.

*Thank You.*

