End-of-studies internship ST30
Optimization and fine tuning of Large Langage Models (LLM)

Student
DAVOUSE **Nathan**

School Representative
MAKBOUL **Salma**

Academics Programs
Industrial Engineering
Systems Optimization and Safety

Semester
Fall 2024

Abstract (150 words)

This internship took place at INRIA Lille, within the BONUS research team. The aims of this internship was to explore the applications of optimization algorithms to the current hot topic of Neural networks: Large Language Model (LLM). In particular, I worked more specifically on Hyperparameter Optimization (HPO) applied to LLM fine-tuning. The work was split in three stages:

- Definition of the subject: explore the specific literature to understand stakes and how it works.
- Implementation of the algorithms: develop HPO algorithms and use them for LLM fine-tuning.
- Experiments: refine the implementation along the results, to obtain relevant outcomes.

This semester was also a first immersion in a research and academic field, allowing me to fine tune my professional project.

Company : **Inria Lille**

Adress : **172 avenue de Bretagne, 59000 Lille**

Tutor : **El-Ghazali Talbi**

Keywords

- **Applied Research**
- **Transport and Telecommunications**
- **Informatic**
- **Mathematical Optimization**
- **Software - Research**

utt UNIVERSITÉ DE TECHNOLOGIE TROYES

Inria

Intentionnaly left blank

Acknowledgements

Personal acknowledgements

First and foremost, I would like to express my gratitude to my tutor, Mr. Talbi, for his guidance and for giving me the opportunity to work on this subject, which allows me to go out of my primary field of study. I also extend my thanks to the whole BONUS research team for their warm welcome and support throughout the internship.

On a more personal note, I am deeply thankful to my girlfriend for her patience and willingness to listen as I tried to explain the intricacies of my work during the internship. Her encouragement meant a great deal to me during this journey.

Lastly, I would like to acknowledge several people at the University of Technology of Troyes (UTT) for their essential contributions to my experience. I am especially grateful to Ms. Makboul for her support, guidance, and advice regarding my professional development. My thanks also go to Ms. Goffroy from the corporate relations department for her responsiveness and assistance during the internship process. Finally, I am indebted to all the professors who took time to answer my questions about academic careers, particularly Mr. Afsar, Mr. Hnaien and Ms. Yalaoui, whose help was crucial in securing this internship opportunity.

Offical acknowledgements

This work was partially supported by the EXAMA (Methods and Algorithms at Exascale) project under grant ANR-22-EXNU-0002.

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).

Note on the use of AI : ChatGPT has been used to write this report of text polishing (correct remaining English mistakes, reformulates sentences, maintain consistence in the terms used across the document) and as a help to write some of LaTeX components.

Summary

List of Tables

List of Figures

List of Algorithms

Glossary

acquisition function Representation of a surrogate model for the objective function. 17, 25

black-box objective function An objective function that can not be expressed analytically. 12, 20, 21

decoder-only LLM model with only the decoder part of the transformer. 8, 10, 21, 22

dropout probability probability of removing a neuron during backpropagation. 23, 24

encoder-decoder LLM model using the whole transformer architecture. 10

encoder-only LLM model with only the encoder part of the transformer. 10

exascale Very high performance computing resources. 14, 38

fine-tuning 2nd step of LLM training. 1, 4, 8–10, 19–23, 30, 35, 39

HellaSwag Validation Dataset for LLM Fine Tuning. 23, 31, 32, 34

himmelblau well-known non-convex function, equation 2.6 . 14–16

HuggingFace Deep Learning Hub with models and datasets. 22, 23

hyperparameter Parameters not learned by the model. 1, 4, 5, 10, 11, 13, 14, 16, 19, 21–24, 29, 35, 37, 39

instruction tuning Fine-tuning with Instruction and behavior dataset. 9, 19

learning rate value used to weight the gradient reduction during backpropagation. 22–24

LitGPT PyTorch based framework for training LLM. 22, 23

LlaMa Meta sets of LLM models. 10, 21, 22

LoRA rank value used for scaling the reduction of Low Rank Adaptation (LoRA). 23, 24

LoRA scale Value used to weight the influence of fine-tuning. 23, 24

multi-fidelity Optimization approach were the solution is not always fully evaluated. 12

performances estimation strategy All configurations to evaluate a solution. 12

pre-training 1st step of training LLM. 8, 9, 19

PyTorch Tensor-based framework for machine learning. 22

PyTorch Lightning automated deep learning training framework. 22

search space The sets of possible solutions for an optimization problem. 11–16, 19, 20, 23–25, 27, 28, 38 The ways to generate the solutions to evaluate in the search space. 12.

transformer Neural networks layers type using attention mechanisms. 4–8, 10

weight decay value used to reduce the value of weights during training, to prevent overfitting. 22–24

Acronyms

Adam Adaptive Moment Estimation. 5, 22
AdamW Adaptive Moment Estimation with Weight Decay. 22
AI Artifical Intelligence. 1
ANN Artificial Neural Networks. 5, 14, 22, 35, 37
Auto-DNN Automated Deep Neural Networks. 4, 11, 12, 17
Auto-ML Automated Machine Learning. 11, 13

BaMSOO Bayesian Multi Scale Optimistic Optimization. 26–28, 30, 33, II
BO Bayesian Optimization. 17, 24, 25, 27, 29, 30, 32–35, 37–39
BO-GP Bayesian Optimization using Gaussian Process. 24, 27, 31
BONUS Big Optimization aNd Ultra-Scale computing. 1, 3

CLI Command Line Interface. 22, 23
CNN Convolutional Neural Networks. 5

DDP Distributed Data Parallel. 14, 22
DIRECT DIviding RECTangle. 16
DNN Deep Neural Network. 4–6, 11, 13, 14, 20
DP Data Parallel. 14

EA Evolutionnary Algorithm. 5, 15
EI Expected Improvement. 25

FDA Fractal Decomposition Algorithm. 16
FLOPS Floating-Point Operations per Second. 3
FSDP Fully-Sharded Data Parallel. 14, 22

GA Genetic Algorithms. 15
GP Gaussian Process. 17, 24–26, 28
GPT Generative Pre-Trained. 8, 10, 22
GPU Graphics Processing Unit. 14
GS Grid Search. 14–16

HPC High Performance Computing. 14, 37
HPO Hyperparameter Optimization. 1, 4, 10, 11, 13, 14, 16, 19, 22, 23, 31, 35, 37, 39

ILS Iterated Local Search. 15, 16
INRIA National Research Institute for Computer Science and Automation. 1–3

LCB Lower Confidence Bound. 27, 28
LHS Latin Hypercube Sampling. 14, 24, 30, 31, 34, IV
LLM Large Language Model. 1, 4, 6–14, 17–20, 22, 30, 35, 37, 39
LoRA Low Rank Adaptation. 9, 22, 23, 29
LTSM Long Short-Term Memory. 7

MCQ Multi-Choice Question. 22
MCTS Monte Carlo Tree Search. 25
MHA Multi-Head Attention. 6, 8, 22
ML Machine Learning. 17
MLP Multi-Layer Perceptron. 5
MSE Mean-Squared Error. 5
MVOP Mixed Variable-size Optimization Problem. 12

NAS Neural Architecture Search. 1, 4, 11–13
NLP Natural Language Processing. 4, 6, 7
NN Neural Networks. 19

OOP Object Oriented Programming. 27

PBO Partition Based Optimization. 14, 16, 24, 25, 38
PEFT Parameter Efficient Fine-Tuning. 9, 20, 22, 37
PEPR Priority Research Program and Equipment. 1, 3
POC Proof-of-Concept. 14

QC Quality Control. 17

RS Random Search. 14–16

SA Simulated Annealing. 15, 16
SCM Supply Chain Management. 17, 18
SGD Stochastic Gradient Descent. 5
SMBO Surrogate-Model Based Optimization. 17, 24, 26
SOO Simultaneous Optimistic Optimization. 16, 24–28, 30, 32, 33
SOTA State-of-the-art. 6, 22

$\mathcal{UCB}$ Upper Confidence Bound. 26–28

VAE Variational Auto-Encoder. 5

w.r.t. with respect to. 13, 14

Introduction

From September 09, 2024, to February 21, 2025, I joined the Big Optimization aNd Ultra-Scale computing (BONUS) team at the INRIA Center of the University of Lille, under the supervision of Mr. El-Ghazali Talbi. Adding a Master's degree in Systems Optimization and Safety to my Industrial Engineering curriculum, the intrinsic question was : do I want to continue in this academic track ? From a carreer path point of view, this internship was designed to answer this question.

As one of the greatest french institute for research in digital science and technology, INRIA is a leading figure for such an internship. It was within the framework of the Priority Research Program and Equipment (PEPR) called *Numérique pour l'Exascale (NumPEx)*, and in particular the Exa-MA axis, that I carried out this internship. Introduced by the Neural Architecture Search (NAS) problem, the focus of my internship was to apply optimization algorithms to a recent paradigm in Artifical Intelligence (AI) and industrial world : Large Language Model (LLM).

After a first phase presenting the INRIA, we will continue with a focus on the subject of the internship, and the context in which it is embedded, to fully understand the stakes and the environment. Then, a second phase will adress the methodology of the internship, to give an insight into the research process and the skills needed to navigate it effectively. This phase allow the final chapter to handles the results, and the prospectives approach of the internship.

Chapter 1
Company's presentation

What is research but a blind date with knowledge?

Will Harvey

National Research Institute for Computer Science and Automation (INRIA),is one of the leading public institutions involved in academic research in France. Today, more than 3,800 scientists, working in 220 project teams, are involved in digital research at INRIA. Since its creation, INRIA's mission has been to ensure French sovereignty and autonomy in IT-related fields, while transferring knowledge to the industrial world.

INRIA is made up of 10 research centers, spread across France, which work in a dozen areas, including :

- High-performance computing
- Digital Education
- Artificial intelligence
- Digital health
- Data science
- Software

To support this, the institute is developing a large number of partnerships, playing its role as a research vector. These partnerships include, first and foremost university partnerships; the research centers are attached to universities, in order to contribute in the training of tomorrow's scientists. We can also add institutional research partners, such as CNRS or CEA in France, and many others in France, and many others in Europe, which enable us to take on large-scale projects. projects. And last but not least, our industrial partnerships help to keep the Institute going. These range from the 170 start-ups incubated on INRIA premises over the past 20 years, to industry giants such as Microsoft, for example, who collaborate in the joint Microsoft-Research / INRIA joint research center[19]

1.1 INRIA history

INRIA was founded in 1967, under the name "Institut de Recherche en Informatique et Automatique" (IRIA), as part of the *Plan Calcul*[38]. This project, launched by the French government in 1966, was designed to ensure France's autonomy and sovereignty in the field of information technology. A few years later, in the 70s, INRIA led the *Cyclades* project, participating in the networking of computers, and contributing to what would later become the Transmission Control Protocol (TCP).

In 1979, the institute affirmed its commitment to a national structure, and became INRIA, with the opening of centers in Rennes, Sophia-Antipolis, Nancy and Grenoble. The same dynamic led to the creation of Simulog, the first start-up incubated at INRIA, reaffirming the Institute's commitment to innovation in the broadest sense of the term.

In the early 2000s, INRIA, like the rest of the world, was strongly influenced by the development of the Web and its applications. In particular, INRIA was responsible for the European node of the W3C (World Wide Web Consortium). Since then, INRIA has diversified its research, supporting research into digital health and developing significant expertise in software engineering.

1.2 INRIA center of Lille University

The INRIA center at the University of Lille was born from a partnership between INRIA and the University of Lille, in 2007. It first set up a site in Villeneuve d'Asq [1], close to the scientific city campus, in a location shared with Polytech Lille and Centrale Lille, then a second site in Lille [2], in the Euratechnologies park. It currently houses 385 employees, including 260 researchers and 50 engineers, divided into 15 project teams. In line with national priorities, while at the same time asserting its specialties, the center focuses on 5 themes:

- Data Science
- Software Engineering
- Cyber Systems Physics
- Digital Health
- Digital Sobriety

1.3 BONUS team

The BONUS team is part of the INRIA center at the University of Lille, located on the Lille site, and comprises around 15 headcounts, including 4 researchers. It focuses on large-scale optimization problems, which are characterized by: 1) a large number of problem dimensions 2) the possibility of multi-objective optimization 3) very high solution evaluation costs 4) the need for supercomputers. To address these issues, the team has divided its research into 3 areas:

- Decomposition-based optimization: defining and solving sub-problems to approximate the larger problem
- Optimization supported by machine learning: machine learning, and by extension artificial intelligence, concentrates a set of problems that require optimization.
- Large-scale computation: for these problems, the need for computation is reaching levels that seemed unimaginable just a few years ago. Parallelization and the development of suitable hardware are the key to progress.

INRIA, through its BONUS team, is involved in the PEPR NumPex[34], which aims to enable the development and use of exascale computing[3]. This internship is part of the Exa-MA priority project, which aims to develop mathematical methods and algorithms for translating simulated phenomena into equations.

[1] 40, avenue Halley - 59650 Villeneuve d'Ascq
[2] 172, avenue de Bretagne - 59000 Lille
[3] machines capable of performing at least 10^{18} FLOPS

Chapter 2
Subject Definition

Research is formalized curiosity. It is poking and prying with a purpose.

Zora Neale Hurston

In a research internship, or indeed in any research activity, it's crucial to properly define the subject of the research, and to extract a precise problematic. That's why, during my first few weeks as an intern, and in this chapter of the report, I've endeavorded to define this framework. To do so, I begin by recalling the subject as defined in my agreement (Appendix 34):

NAS for LLMs architectures is computationally prohibitive. In this work, we will investigate the use of efficient optimization algorithms (example: parallel fractal optimization) to reduce the latency of real-world commercial web-scale text prediction system. The goal of this work is to solve the NAS problem to find an architecture that when trained with data D and training algorithm A, produces a model that has similar accuracy but significantly reduced latency. The tasks composting this work are summarized below:

- Modeling and analysis of the NAS problem
- Solving of the problem using original and high-performance optimization algorithms
- Application to well known LLM such as GPT
- Application to logistics/transports problems

From there, to understand fully the problems, it's important to define what are LLMs, and what are the stakes of this fields. Then, we will take a look about the application to manufacturing or logistics contexts. Alike we will look at the Automated Deep Neural Networks (Auto-DNN) fields, with focus to NAS and HPO problems, to locate the further work in a global litterature. To complement Hyperparameter Optimization () presentation, a section will be dedicated on a taxonomy of optimization algorithms. With this, I can finally close this part with a precise search problematic, to drive my contribution.

2.1 Large Langage Model (LLM)

LLMs can be defined as Deep Neural Network (DNN) using the transformer bloc for Natural Language Processing (NLP) problems. For the next parts, it's important to understand the architecture of LLMs, after a short reminder about DNNs. Due to computation limitation, a lot of research contribution are about Fine-tuning, defined in 2.1.4. To pursue to the next section, I will finish with a light review and taxonomy of LLMs.

2.1.1 Deep Neural Network (DNN)

Like many fields, DNN comes from biology-inspired design. In 1943, Warren Mcculloch and Walter Pitts introduced the idea of logical calculus and computation, based on neural network, in article [29]. Artificial Neural Networks (ANN) aims to reproduce the cells of the brain to make a reasoning : the brain neuron is a node using a function to "activate" and the synapses are edges linking neurons to each others.

The figure 2.1 show the structure of an artifical neuron, taking input x_i and trainable weights ω_i, including the biais ω_0. The output of the neuron is expressed as : $\hat{y} = f(x, \omega) = \sigma(\sum_{i=1}^{n} x_i\omega_i + \omega_0)$, with $\sigma(.)$ the activation function.

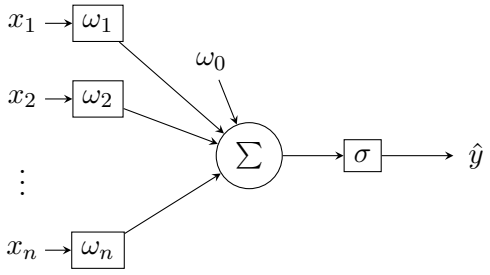


Figure 2.1: Illustration of an artifical neuron

The activation function is the key of ANN. The function need to make an output adapted to the use case (e.g. value between 0 and 1 for a probability), and to be differentiable to be able to use gradient-based optimization, the most efficient optimization method when possible. Approaches using Evolutionnary Algorithm (EA) to update weights were studied and called *meta-learning*[17], but were deprecated in favor of gradient-based methods.

With the notation of figure 2.1, and ω being the matrix of all parameters, the training of the ANN can be expressed as equation 2.1. The loss $\mathcal{L}$ is the expression of the difference between the wanted output y and the predicted output $\hat{y}$. Many formulas can be used the compute the loss, such as cross-entropy[57] or Mean-Squared Error (MSE).

$$\omega \in \arg\min_{\omega \in \mathbb{R}^n} \mathcal{L}(\hat{y}, y) \tag{2.1}$$

The optimization of equation 2.1 is done using gradient descent, and especially Stochastic Gradient Descent (SGD). For each parameter, the gradient is expressed as 2.2. Based on this, the parameter is updated with $\omega_i \leftarrow \omega_i - \eta * \Delta_{\omega_i}$.

$$\Delta_{\omega_i} = \Delta_{\omega_i}(x, y) = \frac{\partial \mathcal{L}(f(x, \omega), y)}{\partial \omega_i} \tag{2.2}$$

To accelerate the gradient descent, some optimization algorithm like Adaptive Moment Estimation (Adam) [24] use the momentum of the function, replacing $\Delta\omega_i$ with $m_t = \beta m_{t-1} + (1-\beta)[\Delta\omega_i]$. In this formula, m_t is the moment of the function $\mathcal{L}$ at the instant t, and $\beta = [\beta_1, \beta_2]$ hyperparameters of the method, with $\beta_i \in \{0, 1\}$. In this internship, I will mostly use Adam or SGD.

From simple Multi-Layer Perceptron (MLP) to more complexe architecture (Convolutional Neural Networks (CNN), Transformers,Variational Auto-Encoder (VAE)...), from dozen to

bilions of parameters, the DNN became over the years the State-of-the-art (SOTA) in many tasks like classification[56], computer vision[41], prediction [23], NLP[12] and so on.

2.1.2 Self Attention Mechanism

To understand how LLM works, it's crucial to understand the self attention mechanism. The key feature of LLM is the understanding of the context of a words to perform a generation or a classification Using Multi-Head Attention (MHA), the *transformer* cell define the importance of each word for the prediction of the next one. On the example of figure 2.2, to predict the word "garden", the important words are "children" and "playing". The multiplicity of the attention heads allow the model to understand different context with each one, represented by colors on the example.

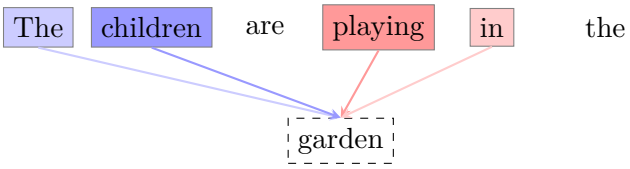


Figure 2.2: Illustration of self attention

To perform this feat, Vaswani in article [49] present the scaled dot-product attention, used to build MHA. Transformers use a scaled dot-product attention, shown in figure 2.3, between a queries(Q)/Keys(K) pair, and a value (V) vector. With d_k the dimension of the queries and keys,the attention function can be written as $Attention = \text{softmax}(\frac{QK^T}{\sqrt{d_k}})V$.

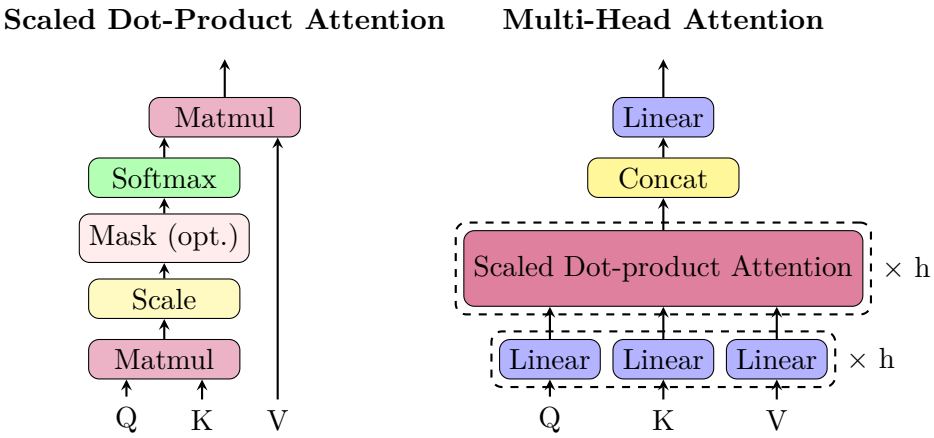


Figure 2.3: Multi-Head Attention (MHA) illustration

The 3 linear cells are matrices multiplications between an input vector of size d_i to a matrices $W^i \in \mathbb{R}d_{model}.d_i$, with $i \in Q, K, V, O$ (O being the output vector). These matrices are the trainable weights of the MHA, and will be train along the rest of the network. MHA output can be write as equation 2.3.

$$\begin{aligned} Multihead(Q,K,V) &= Concat(head_1, ..., head_h)W^O \\ with\ head_i &= Attention(QW_i^Q, KW_i^K, VW_i^V) \end{aligned} \tag{2.3}$$

The softmax function is often used to extract probabilities, since it gives values between 0 and 1, and that is take into account every values in order that the sum of softmax value is one. It can be written as : $softmax(x_i) = \frac{e^{x_i}}{\sum_{j=1}^{n} e^{x_j}}$.

2.1.3 LLM Architecture

For many years, NLP problems were approached by statistical and rules models, but they were not able to capture the context of a whole sentence to generate a word. In 2016, Google published *Google's Neural Machine Translation System* [54], a Long Short-Term Memory (LTSM) neural network, trained on a big corpus of text datas, making it like the first Large Language Model. This was an important break-through, and a proof-of-concept that neural networks can be the key of Natural Language Processing (NLP) Problems.

To perform further, what NLP needed was the ability to understand a context, to predict or understand a sentence. To do that, the transformer architecture was published in 2017 [49], and was using the self attention mechanism presented in section 2.1.2.

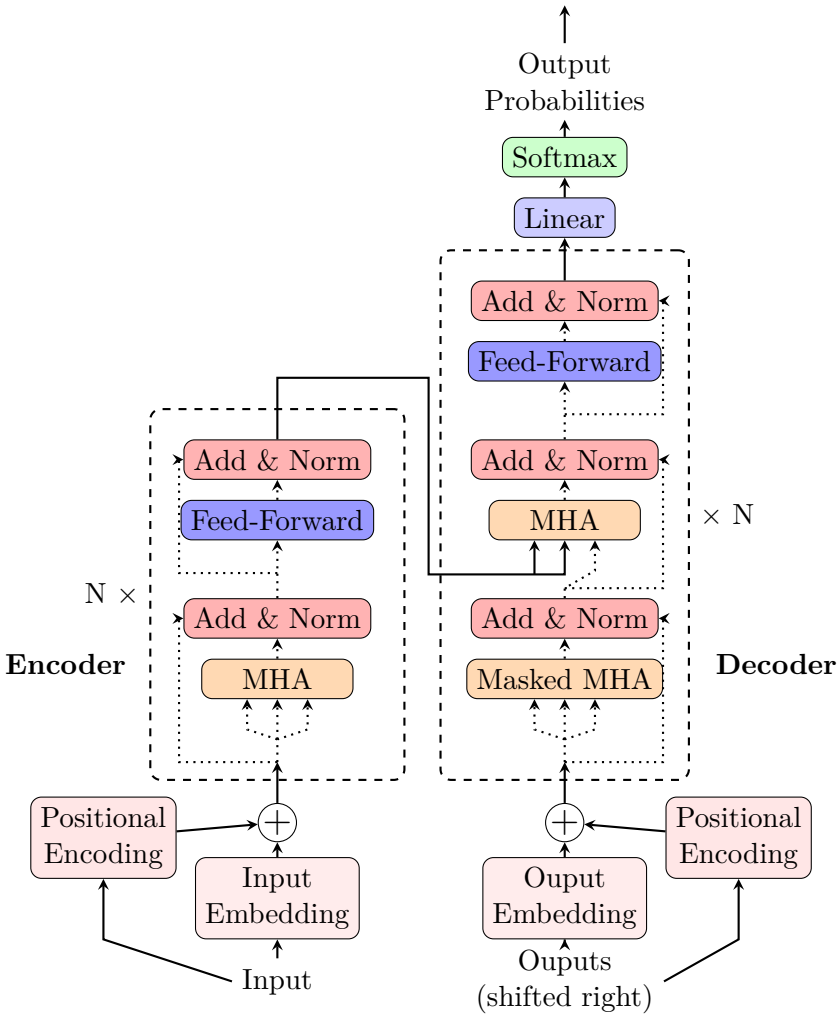


Figure 2.4: Transformers topology (inspired by [49])

Transformer architecture, as shown in figure 2.4, is composed of 3 main components : embedding (including positional encoding), encoder and decoder. The embedding consist of

representing the words in a vector space, using *tokenizer* to encode the sentence. Along with it, the positional encoding allow the model to keep the position of the token inside the model. A sinusoidal function is used for this, to stay on a relative position and not an absolute.

The encoder is a stack of MHA with feed-forward layers, with the addition of a residual connection and a normalization layer between the two. The output of the encoder is used as the input of second MHA of the decoder. Like the encoder, the decoder is a stack of MHA with feed-forward layers, but is composed of two MHA. The first one is masked, to learn only the part before the word to predict, and the second one is not masked to learn the whole sentence.

This topology is the base of LLM, with diversification on the number of layer, the number of head and the size of the embedding vector. It will be further discussed in section 2.1.5, but some model are using only part of the transformer architecture, with the rise of *encoder-only* and *decoder-only* models.

2.1.4 Fine-tuning

As of today, the training of LLMs is split is two phases : pre-training and fine-tuning. The **pre-training** is computationally very expensive, and only few companies can made one from scratch (OpenAI, Meta, Mistral ...). It also need an enormous corpus of data, often kept hidden from public. Model after pre-training are called Generative Pre-Trained (GPT) model or foundation model. At this point, LLMs are able to answer a prompt correctly, with a general amount of knowledge, but not to excel in a specific task.

Aspect	**Pre-training**	**Fine-tuning**
Objective	General-purpose learning	Task/domain adaptation
Dataset	Large, diverse	Small, specific
Scale	High resource demand	Relatively efficient
Duration	Weeks to months	Hours to days

Table 2.1: Comparison Between Pre-training and Fine-tuning for LLMs

After pre-training, the next stage, known as **Fine-tuning**, is a lighter but crucial step that adapts the general knowledge in the model to perform well on specialized tasks. Figure 2.5 and table 2.1 illustrate the scope of the fine-tuning process, in opposition to the pre-training process.

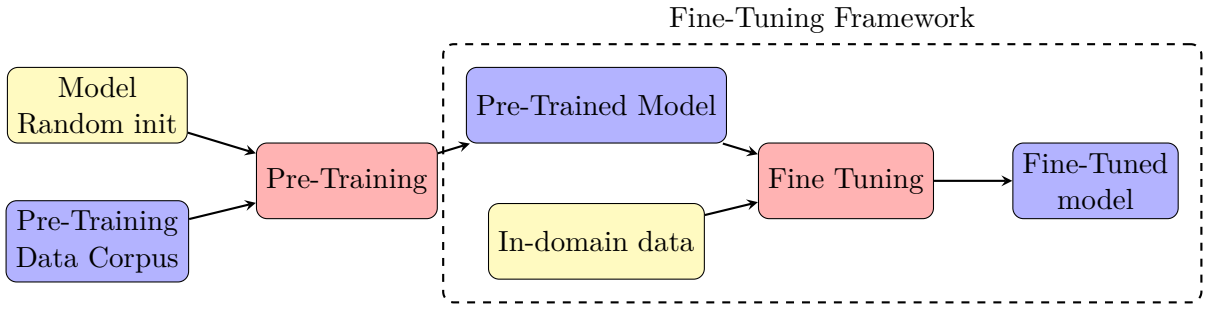


Figure 2.5: Pre-training and Fine-tuning Framework

Fine-tuning is often applied to refine the LLM responses by training it on domain-specific datasets or to improve its performance on specific tasks, such as medical diagnosis,

legal document analysis, or customer service automation. Research, including studies like [51], suggests that fine-tuning not only helps with task-specific adaptation but also enhances the model's generalization abilities. This process enables the model to transfer the foundational knowledge it learned in pre-training more effectively across a variety of prompts, making it more robust and adaptable. The table 2.1 summarize difference between fine-tuning and pre-training.

Instruction tuning is the process of fine-tuning a pre-trained LLM using datasets composed of instruction-response pairs. The goal is to enhance the model's ability to follow natural language instructions effectively. This involves training the model to generate precise, contextually relevant, and human-aligned responses to a variety of prompts. On this work, I will mostly work with instruction tuning.

Parameter Efficient Fine-Tuning (PEFT)

PEFT methods are aiming to reduce the cost of fine-tuning, and make it more accessible to a wider range of users. Article [14] make an exhaustive review of PEFT, and is the base of this paragraph. The two main approaches to PEFT are *additive* and *reparameterization* methods.

The *additive* approach aims to add news weights or layers to the models, and train only theses weights. Popular method use *adapter* layers, adding layer between layers of the model, as shown in figure 2.6. One con of this approach is the rise of the inference time implied by the addition of these layers to the model.

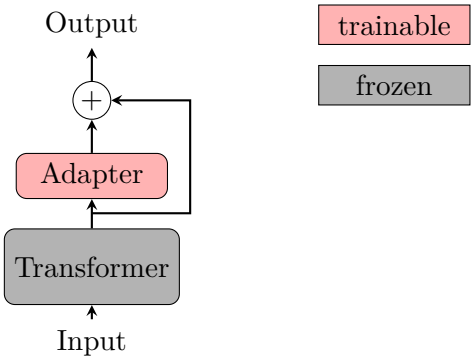


Figure 2.6: Illustration of adapter layer

The *reparameterization* approach provides a proxy for model weights, to train this proxy and then merge it with the original model. The most popular method is Low Rank Adaptation (LoRA), based on article [18]. This method use the intrinsic rank of the weight matrix W, to factorize the matrix W into 2 matrices A and B with $W = B.A$, with $W \in \mathbb{R}^{n*p}, A \in \mathbb{R}^{r*p}, B \in \mathbb{R}^{n*r}, r$ being the rank of the matrices factorization, as expressed in equation 2.4. The $\frac{\alpha}{r}$ term is used to scale the weights of the full matrix when r is changing.

$$\begin{aligned} W = W_0 + \Delta W = W_0 + \frac{\alpha}{r} B.A \\ s.t. \quad W, W_0, \Delta W \in \mathbb{R}^{n*p}, \\ A \in \mathbb{R}^{r*p} \text{ and } B \in \mathbb{R}^{n*r} \end{aligned} \tag{2.4}$$

Figure 2.7 show the illustration of the Low Rank Adaptation (LoRA) layer, with A and B being the factorization of the weight matrix. The benefits of this is the inference that aren't penalized since the model is composed of the same number of weights after the merging.

Other plus it that multiple fine-tuning could be done and they can then be merged when needed from a same base, saving only the low-rank version of the weights. One con is that it add hyperparameters, but it will be tackled in nexts sections.

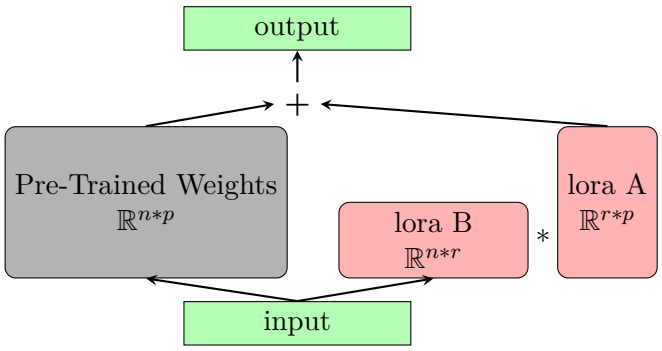


Figure 2.7: Illustration of lora layer

In the litterature, somes articles before the emergence of LLM are using the terms "fine-tuning" as the choice of hyperparameters like Hyperparameter Optimization (HPO), but in this work, it will solely mean the second phase of LLM training.

2.1.5 Review and taxonomy of LLMs

Exhaustive review of LLMs can be found, like the article [40], with details on training, datasets, architectures... On this part, I will focus on key concept and details needed to achieve sufficient understanding for this report.

LLMs Taxonomy

For this taxonomy, the criteria chosen is the downstream tasks, and the corresponding part of the Transformers Architecture used for this.
Encoder-only : LLMs using only the encoder side of the *transformer* are used to do text analysis or word classification (e.g. extract noun or verb of a sentence). The most famous one is BERT[6] or its variations, an open source model by Google.
Decoder-only : these models are used for generative tasks, using prompts to lead it's generation. Generative Pre-Trained (GPT) models, with it's web service ChatGPT [35] is a decoder-only model, and has strongly contribute to the renowned of the LLMs. We can also cite LlaMa [13] family models, open-source foundation models.
Encoder-decoder : model using standard Transformers are mainly used for translation, one of the first aim of NLP model, or summarize a text. BART[27] or T5[39] models are fairly known model for this.

The relevance of this taxonomy come from the compatibility of different optimization method with these three types of models. Different types of models won't be used and train in the same way, and won't have the same hyperparameters.

LLMs review

After seeing the functioning of LLM, it's abilities, it's import to look at its limitations, since every work based on it may be influenced by these open issues.
Debiaising data corpus: generative AI base it's representation on dataset, so it tend to reproduce the biaises of the corpus. For instance, if we ask ChatGPT to generate 10 name of

engineer, we have low probability of having parity.
Interpretability : when using neural network in general, but especially LLMs, we can't explain why it works, or why a specific generation happens, so it can not fully justify decision-taking.
Efficiency and energy consumption : the result-oriented search tend to only focus on accuracy, rather than energy consumption for a given result. This lead to an over and over increasing models size, and corresponding energy consumption to train and deploy it.
Hallucinations[4] : when asking something to the model that does not have the answer, it tend to create a false answer from scratch, and be confident on it. It lower the confidence on the generation.

2.2 Auto-DNN

Automated Deep Neural Networks (Auto-DNN), as defined in article [45], refers to the automation of the design and hte optimization of deep neural network models. This concept is linked to Automated Machine Learning (Auto-ML), but focus solely on DNN. The contribution of Auto-DNN is multiple :

- Taking the human out of the loop, to find solutions outside of human expertise and way of thinking.
- Ease the deployment of DNN models, to lessen the needs of expertise.
- Ensuring reliability and performance of the solution, with a data-driven approach.

Two populars problem of this fields emerged in the last years : **Neural Architecture Search (NAS)** and **Hyperparameter Optimization (HPO)**. In this part, I will briefly expose the general formulation of the Auto-DNN problem, and then focus on presenting NAS and HPO specificities.

2.2.1 Problem Formulation

The general Auto-DNN optimization problem can be defined, like article [45], with a quadruplet $\alpha = (V, E, \lambda_V, \lambda_\alpha)$, where V is a set of nodes denoting the neurons, E is a set of edges (i.e. connections) between neurons, λ_V the feature set of operations and λ_α the optimization features set of the DNN. Given the space of all datasets D, the space of models M, and the search space of architectures A.

For reminder, namely (x, y) the input-output pair, $f(x, \omega) = \hat{y}$ the predicted output and $\mathcal{L}(\hat{y}, y)$ the loss function of the model. Subsequently to the optimization problem of section 2.1.1, ω^* is the optimal parameters of the model.

Following the first optimization problem, a second is expressed as the Auto-DNN problem, with equation 2.5. In this equation, f is the objective function, often the negative loss function or the accuracy.

$$a^* \in \arg\max_{a \in A} f(\Theta(a, d_{train}), d_{valid}) = \arg\max_{a \in A} f(a). \tag{2.5}$$

To sum up equation 2.5, we want to optimize a, so that $f(a)$ is the best when a is used to train the model (optimize the weights). The Auto-DNN problem in characterized, is the worst

case, by theses properties :

- **Mixed Variable-size Optimization Problem (MVOP)** : Variables can be continuous (e.g. learning rate), discrete ordinal (e.g number of layers or neurons) or discrete categorical (e.g. type of activation function). The search space of the problem contains conditionnality, i.e. the size of a variables may depend on other variable (e.g. the number of neurons depend on the number of layers). These properties requires specific optimization methods, or conversion of variables, as presented in article [46].
- **Black-box objective function :** this problem is a black-box function, i.e. the function cannot be analytically formulated, and so is derivative-free.
- **Expensive evaluation :** The evaluation of a solution can take minutes to days, and even days, constraining the number of evaluations. These properties constrains optimization algorithms.
- **Noisy results :** when the same solution is evaluated, the objective function does not output the exactly same result. This property induce the need to take care not to take decisions like discarding values on only one evaluation.

Auto-DNN is an extremely broad field, and it's important to define precisely the specific problem we are treating. Following the notation of article [7] about NAS problems, theses problems are structured according to three fields : Search space, Search strategy and Performances estimation strategy. The **search space** consists of all variables, and theirs properties (range, type ...). The **search strategy** is about the optimization algorithms, defined more thoroughly in section 2.3. The **performances estimation strategy** is the definition of the loss function as expressed in equation 2.1, and all linked attributes (e.g. datasets choice). This part can also includes approach like *multi-fidelity*, modifying the evaluation along iterations.

2.2.2 Neural Architecture Search (NAS)

The Neural Architecture Search (NAS) problem is a sub-problem of the Auto-DNN problem, where the search space is the topology G as defined in the preceding section. For an exhaustive survey of NAS, one can refer to the article by T. Elsken, *Neural Architecture Search: A Survey [7]. Figure 2.8 presents the generic workflow of NAS. My contribution in this part focuses on NAS applied to LLM. Due to computational demands, the problem can be addressed using two approaches:

- **Building from Scratch**:
  A classical approach to Neural Architecture Search involves building the architecture from scratch. However, the primary drawback of this method is the significant computational cost, making it accessible only to a limited number of organizations. A remarkable example of this is Google's development of the **AutoBERT-Zero** model [10]. This approach involves discovering an entirely new topology, including new transformer-based structures.
  To mitigate the computational cost, one can constrain the search space. For instance, the number of layers can be fixed, with modifications made to their internal components, or pre-built layers can be fixed, allowing experimentation with their arrangement.
- **Pruning**:
  Pruning involves reducing the size of a model by selecting parts of the topology while aiming to minimize performance degradation. A notable example of this is presented in [25], which uses **weight sharing** methods, such as the approach proposed in [37].

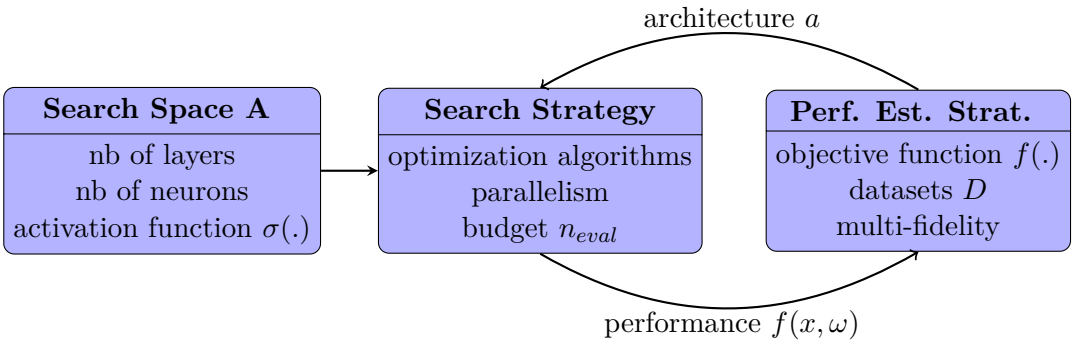


Figure 2.8: Neural Architecture Search workflow, inspired by [7]

The methods to solve NAS for LLM are quite diverse. Some methods encode topology into a continuous space, broadening the range of possible optimization techniques. Further details will be addressed in Section 2.3, but it is worth mentioning derivative-based methods like [28], which apply such techniques to NAS.

2.2.3 Hyper-parameter optimization

Like NAS, HPO can be defined as a sub-field of Auto-ML, even if HPO by itself is tackled since the 1990s [8]. In Deep Neural Network (DNN), hyperparameters can be defined as configuration settings that govern the structure of the networks and the process of training. As opposed to parameters (or weights), hyperparameters are not learnt directly from the data during the training. They are typically set before training begins and remain fixed throughout the process.

Most of the time, hyperparameters are chosen by humans, w.r.t. their expertise. HPO is the process of automating the choice of the best hyperparameters for a specific problem (a quadruplet a as defined in 2.2.1). However, manually selecting hyperparameters is often inefficient and prone to suboptimal configurations, especially as models grow in complexity. Automated HPO methods aim to address these challenges by systematically exploring the search space to identify configurations that maximize performance or minimize error for a given task.

The significance of HPO grows with the increasing complexity of modern DNN architectures. As models become larger and datasets more diverse, the choice of hyperparameters can significantly impact both model accuracy and computational efficiency. Moreover, HPO plays a critical role in enabling the deployment of models in resource-constrained environments, where trade-offs between accuracy and efficiency must be carefully balanced. Future sections will detail methodologies and frameworks designed to tackle HPO effectively in various contexts.

2.3 Optimization Algorithms taxonomy

Global optimization refers to the field of mathematical and computational methods designed to find the best solution to a problem within a defined domain, particularly when the objective function is complex, non-linear, or multi-modal. Traditional methods often struggled with problems involving multiple local optima or discontinuities. The search space $\mathcal{X}$ is generally a subspace of the real space $\mathbb{R}^n$, where n is the dimensionality of the problem.

Optimization methods aim to efficiently navigate vast and complex search space, balancing the trade-off between *exploration* (searching new regions) and *exploitation* (refining known good solutions). In the context of Hyperparameter Optimization (HPO), global optimization plays a crucial role in systematically identifying configurations that maximize model performance while minimizing computational costs. The subsequent sections categorize and detail these optimization methods.

$$f(x) = (x_1^2 + x_2 - 11)^2 + (x_1 + x_2^2 - 7)^2 \tag{2.6}$$

Equation 2.6 represent the *himmelblau* function, a well-known non-convex function with multiple local optima. It will be used as an example in the following sections if relevant. In the next subsections, I will present a taxonomy of global optimization methods, w.r.t. their relevance in the HPO problem. Before this taxonomy, section 2.3.1 will introduce the topic of the parallelism of optimization algorithm.

2.3.1 Parallel Optimization and High Performance Computing

The advent of largest DNN was possible with the development of Graphics Processing Unit (GPU) and corresponding software. Parallel computation and High Performance Computing (HPC) are what makes the uses of complex parallel architectures possible, from multicore processors passing by distributed clusters and grids to Exascale supercomputers.

To briefly explore parallel optimization, we need to classify, based on article [44], the ways to parallelize an optimization algorithm. The simpler to implement is **solution-level** parallelism, when multiples processes are used just to evaluate one solution. It's often the case when evaluating the training of an ANN, with the different strategy of distributed training (Data Parallel (DP), Distributed Data Parallel (DDP), Fully-Sharded Data Parallel (FSDP)). This approach is the one used in this work, even if the aim is to access higher levels of parallelism.

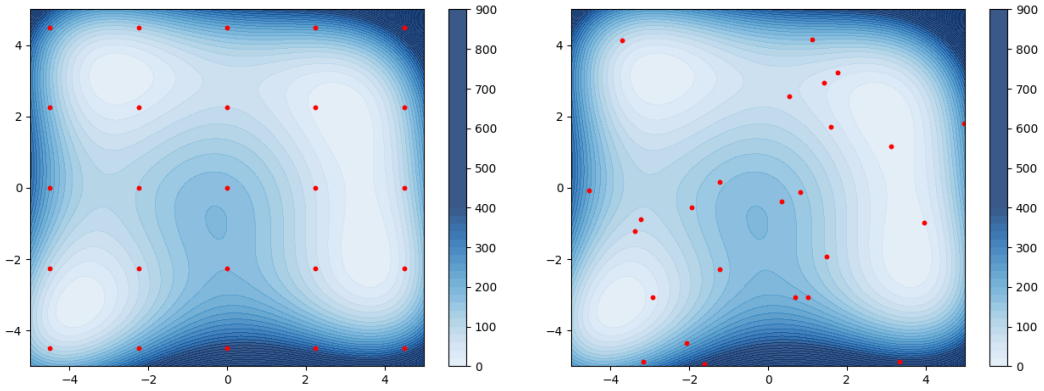
Just higher than solution-level parallelism, **iterative-level** parallelism consist to evaluate multiple solutions with multiples processes in parallel. For instance, when PBO algorithm is used, we can evaluate in parallel all the sub-regions of the same partition. The higher level is **algorithmic-level** parallelism, where all the evaluation is done in parallel. It's possible for sampling based algorithms, like GS or LHS for instance.

As said in chapter 1, my internship is funded on NumPEx project. NumPEx, through its Exa-MA (Methods and Algorithms for Exascale) subprogram, addresses computational challenges of exascale systems by developing scalable algorithms and architectures. This work aims to align with Exa-MA's goals by presenting Proof-of-Concept of a scalable optimization algorithm for LLM.

2.3.2 Exploratory Methods

Basic approaches such as Grid Search (GS) and Random Search (RS) provide straightforward solutions for HPO. GS systematically evaluates all possible combinations of hyperparameters within a predefined grid, making it simple to implement and interpret. However, this approach becomes computationally intractable in high-dimensional hyperparameter spaces due to the exponential increase in the number of configurations. On the other hand, RS selects hyper-

parameters randomly from the search space, offering a more scalable alternative to GS while maintaining simplicity. Despite its limitations, RS is often used as a baseline or guideline to compare with more sophisticated optimization methods.



(a) Grid Search (b) Random Search

Figure 2.9: Exploratory Methods on Himmelblau 2D function

Figure 2.9 show the results of the GS and RS on the *himmelblau* function, with a given budget of 25 evaluations. Con of GS is the curse of dimensionality, since with a grid of size s, the number of configurations to evaluate is d^n. RS is less dependent on the dimensionality since the number of configurations to evaluate is only fixed by the budget. With search space including a lot of good solutions in the space, RS can achieve efficient performance.

2.3.3 Metaheuristics

Metaheuristic methods, including Simulated Annealing (SA) and Evolutionnary Algorithm (EA), are designed to search more efficiently within large search spaces by mimicking natural or physical processes. SA is inspired by the cooling process of metals, where the algorithm explores the search space by gradually reducing the probability of accepting worse solutions. This allows it to escape local optima and converge to a globally optimal solution over time. EA, on the other hand, draw inspiration from biological evolution, employing operators such as mutation, crossover, and selection to iteratively improve a population of candidate solutions.

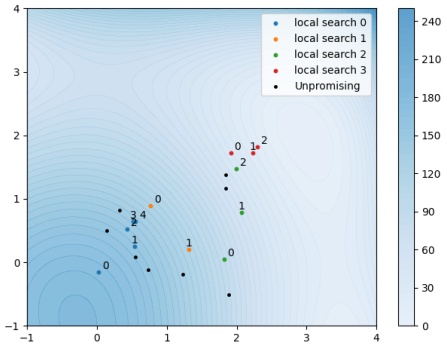


Figure 2.10: Example of Iterated Local Search (ILS) on himmelblau function

Metaheuristic can be classed on two main categories, population-based and solution-based. The first one like GA are methods working on a population of candidate solutions, while the

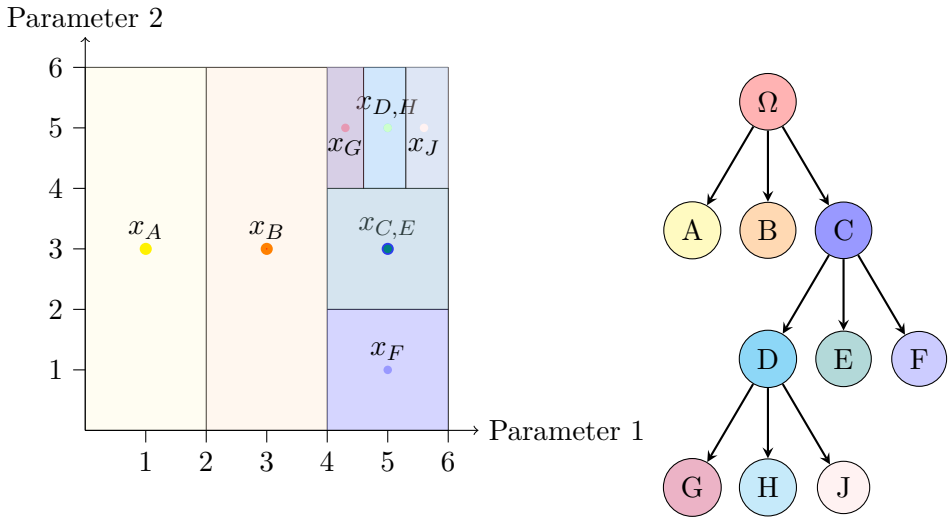
second one like SA or Iterated Local Search (ILS) are methods working on a single solution. These approaches are particularly useful for complex, non-convex search space where simpler methods like GS or RS might struggle.

Figure 2.10 show an example of ILS algorithm on himmelblau function. Like its name imply, Iterated Local Search (ILS) start with initial solution (here $(0, 0)$), and search for better solution arround this point, with a defined step. If the solution is better than existing, the solution is kept and so on. On the figure, there are 4 rounds of local search.

Even if theses methods are effective, they can be computationally expensive when dealing with expensive objective function, especially population-based methods. For a lot of methods like ILS, unpromising evaluation are just discarded without really exploiting them. This characteristic makes them less suitable for high-dimensional hyperparameter spaces, and especially for HPO.

2.3.4 Partition Based Optimization (PBO)

Partition Based Optimization (PBO) methods aim to divide the search space into smaller subspaces, focusing the search on the most promising regions. This division can be done either by penalizing less promising regions or by favorizing. Famous PBO methods are Fractal Decomposition Algorithm (FDA)[33], DIviding RECTangle (DIRECT) [21] or even Simultaneous Optimistic Optimization (SOO)[32]. One of the biggest advantages of PBO methods is their intrinsicly parallelism abilities, enabling the scalibility of the optimization process when working with large hardware resources.



(a) SOO partition (b) SOO tree

Figure 2.11: Example of a Partition Based Optimization

On figure 2.11, we can observe an example of Partition Based Optimization such as SOO, with all it's element. At right, on figure 2.11a, we saw the 3-section of the space, and x_i the center of the sub-space i, the point to evaluate to score the partition. This partition give us the figure on the left, the corresponding tree, a depth of 3 in our case. This figure summarize the key point of PBO algorithm : the geometry (here a rectangle), the partition, the scoring and the tree to selec the next sub-space to partition.

2.3.5 Surrogate-Model Based Optimization (SMBO)

Surrogate-Model Based Optimization (SMBO) approach is aimed to deal with expensive objective function, in terms of costs, times or limitations of experiments. It is originally used for mecanical engineering, or chimic experiments. In face of the costs of ML training, SMBO became the must have of Auto-DNN problem. Bayesian Optimization (BO) contains a lot of SMBO methods, using probabilistic models. Article [42] provides an exhaustive review and taxonomy of Bayesian Optimization (BO).

The global idea is to reduce the cost of the objective function by using surrogate models to predict the values of the objective function. The surrogate can be parametric like *Thompson Sampling in the Beta-Bernoulli Bandit Model*, or non-parametric like Gaussian Process (GP). The model is used to extract an *acquisition function*, which is optimize to obtain best promising point to evaluate with the real function $f(x)$. The acquisition function balance between exploration and exploitation.

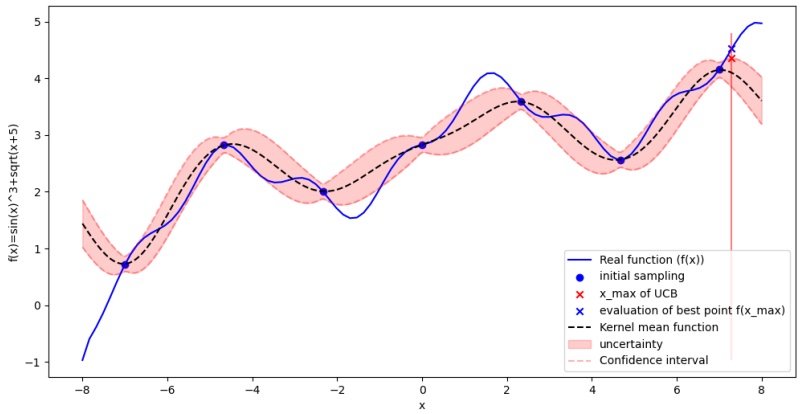


Figure 2.12: Gaussian Process example on $f(x) = \sin(x)^2 + \sqrt{x+8}$

Figure 2.12 shows an example of Gaussian Process (GP) on a simple function. Based on historic of points, the gaussian process is able to compute a mean and a variance, which is used to compute the acquisition function. The acquisition function is then used to select the next point to evaluate. More details will be discussed in section 3.4. The biggest drawback of SMBO methods are the sequential nature of the optimization process, which limits the scalability of the optimization process when working with large hardware resources.

2.4 LLMs application to manufacturing context

To link this internship to my engineering curriculum, I will explore the application for LLM to manufacturing. The application can be split in three topics : Quality Control (QC), Supply Chain Management (SCM) and predictive maintenance. Among these application, the two key-point of LLMs are the extensive reasoning, that can be used for prediction or analysis, and the performance in NLP problems, proving itself to be able to simply interact with any operator.

2.4.1 LLMs-based quality control

Quality control can be defined as "procedure or set of procedures intended to ensure that a manufactured product or performed service adheres to a defined set of quality criteria or meets the requirements of the client or customer" [52]. In this field, the last decades was really interesting from a data management point of view, since it's was the emergence of a lot of data collection : product measurement along manufacturing executive system (MES), customer feedbacks... Since a lot of structured and unstructured data is collected, deep learning can be a way to use all of these to manage quality control. We can extract few specific ways :

- Automated Inspection : LLM are more and more multimodals, and it's possible to achieve computer vision along the reasoning capacities. It's now possible to go further and use camera to control every products on a conveyor.
- Customer Feedback : LLM can be used to summarize and prioritize feedback, to be able to use precise insight on the manufacturing process.

2.4.2 LLMs-based supply chain management

Since decades, **demand forecast** is a key issue of Supply Chain Management (SCM), with many methods considering means and data collection of the company. LLM, and in specific time-LLM [20], achieve a new step in automated reasoning, and to the corpus of data taken into account. From the first method using only historical sales, it's now possible to use a wider historical data, like climate, economical situation ... LLM can also be used for **supplier evaluation**. When considering a relationship with a supplier, many information can be used to characterise it : prices, delay, defaults, reactivity ... And LLM can summarize all of this to provide insight for the choice of a supplier on a specific project.

2.4.3 LLMs-based predictive maintenance

By combining keys aspect of automated inspection and demand forecast, LLM could be a great asset in **maintenance scheduling**. One key point of these model is that they could use every possible inputs : machine logs, humain report, captures... With this, they could reach the best of humain (multi-modality) and machine (long, tedious tasks) to achieve state-of-the-art performance on these subject. More over, LLMs can be used for **root cause analysis**, to find the root of anomaly or failure and reduce the down time of the manufacture.

2.5 Search problematic

My first two weeks were focused on understanding the context of the internship, mainly by reading articles, and working on extracting a specific and precise search problematic. To do this, my main concerns were :

- Feasibility : 24 weeks could be short for a too long research plan, all the more with time-expensive experiments. I need to be able to understand and assess the problem, try and implement methods.

- Resources : be it hardware, collection of datasets or energy costs, the search problematic need to be constrained to a reasonable budget. For instance, pre-training is prohibited by resources limitations.
- Research team expertise : the team is firstly optimization oriented, so problematic only oriented to LLM won't be the priority

After a first week, the possible fields were narrowed to two tracks. The first one is based on article [25], and involve the pruning of a large pre-trained model, in order to reduce latency without losing to much accuracy. The other one [48] is Hyperparameter Optimization applied to instruction tuning.

Eventually, after reflection and discussion with my tutor, we choose to address the HPO of LLM fine-tuning. This choice was made to reduce the uncertainties when working with an already very exploratory fields, since HPO was already tackled on different type of NN.

The objective of my internship is then to work on HPO methods applied to LLM fine-tuning. This work includes :

- **Reproduce the objective function :** on a given library, implement the black box function of training and evaluate a LLM.
- **Definition of the search space :** balancing between curse of dimensionnality and research ambition, find pertinent hyperparameters to work with, and define theirs properties.
- **Selection and Implementation of Optimization algorithm :** considering litterature and available frameworks, choose relevant algorithms and implement it to the problem
- **Make experiments :** following a rigorous protocol, make experiments to determine the effects of the optimization, and analysis it
- **Formalize the contribution :** With this report and a scientific article, explicit the contribution, and formalize for furthers works

Chapter 3
Methodology

The methods we use to answer our questions shape the answers we get.

John W. Creswell

The methodology is a cornerstone of any research or project, providing a structured framework to achieve objectives systematically and effectively. It ensures clarity, reproducibility, and reliability by defining the steps, tools, and techniques used to address specific problems. A well-defined methodology not only aligns the research process with its goals but also facilitates critical evaluation by external audiences, allowing them to assess the validity and generalization of the results. In the context of this work, the chosen methodology was pivotal in navigating complex challenges, optimizing processes, and ensuring that outcomes are both credible and relevant.

To ensure my sincere approach, and contribute to open-source domain, all the code of my internship is readable on my github account[2]. It's split in two parts : *Scalable_HPO_LLM* for everything linked to the article (code, data, experiments...) and *ST30-deliverable* for every deliverable of this internship (presentation, report, defence and so on).

In this chapter, I will talk about the contextualization in academic literature, then tackle the elaboration of the black-box objective function. The definition of the search space being one of the most crucial step in global optimization, the section 3.3 will focus on this. After this preliminary work, we will enter the core of this report : optimization algorithms. Previous sections will be linked in section 3.5, for the description of the concrete implementation. A section about experimental setup, to explore the resource used during this internship, is concluding this chapter.

3.1 A Literature-Based Approach

In industrial field of works, the goal is to be better than competitor, or at least be better than the past of the company. In research fields, a contribution must aims to be better than existing, at least by one facet. In order to do this, the first step of every research project is to make an exhaustive bibliography of the domain, to understand what's already done, and what could be the contribution of the project.

Chapter 2 was the result of a first stage of bibliography, to define what's the context of this internship. With this, we have insights and contexts about DNN, LLM, fine-tuning and PEFT, and a first look at global optimization fields. In this chapter, a complementary approach will be done about specific optimization algorithms, frameworks and implementation specific details.

[2]link :`https://github.com/Kiwy3/`

At the beginning of this internship, I started my bibliography using few articles that my tutor sent me, for a first look of the subject. From theses articles, I jumped to referenced articles until I started to make a loop between articles. It allows me to find fundational article like articles [49, 45], establishing the core of the domain, and reviews like articles [7, 45], allowing to understand a global context and finding a way to classify what I read before.

To manage my bibliography, in a first time I used Notion App[1] to make a table for my bibliography, with papers charateristics (title, authors, year ...), an export of bibtex from original site and my notes. The table can be found on this link. When I started writing my article, I thought that it's wasn't pratical to copy bibtex export one by one, and I looked at others tools to manage this. It's how I found Zotero[2], with many options to ease my life like collecting article from web with only one click, and export a collection.

3.2 Blackbox Elaboration

My internship can be seen as global optimization applied to a noisy, mixed-variables, expensive black-box objective function. A black-box objective function is a process that receive an input (here a set of hyperparameters), and return one (or multiple) value(s) (here the accuracy), without any information about the internal process.

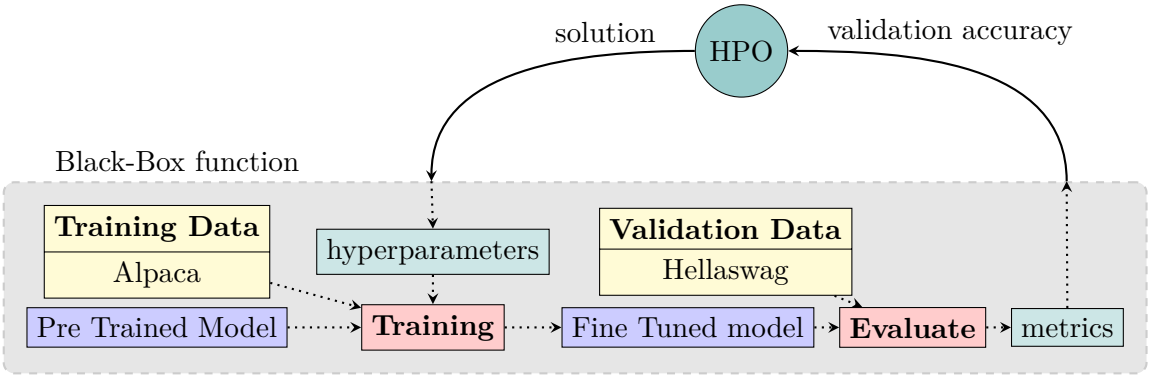


Figure 3.1: HPO workflow

The blackbox process here is described by figure 3.1. This process start by the fine-tuning of the model, using training dataset, and then evaluating the model, using the validation dataset. Next sections will explore in details the action box of figure 3.1.

3.2.1 Fine-Tuning of the Model

For fine-tuning, the first step is to choose the model to work with. For this choice, the first element was the kind of tasks we want to work with. For the biggest use case and impact, focus is done on *decoder-only* model. Then, based on article [48], and open-source model availability, I choose to work with a model of LlaMa family.

The LlaMa family, launched on February 24, 2023 with the publication of "LLaMA: Open and Efficient Foundation Language Models"[47], is a family of open-source (topology

[1] https://www.notion.so
[2] link : https://www.zotero.org/

and weights values) *decoder-only* fundational models produced and maintained by Meta AI. Latest releases from september 2024, LlaMa 3[13] set of models, include model from one billion of parameters (*LlaMa 3.2-1B*) to 405 billions of parameters (*LlaMa 3.1-405B*), and achieved State-of-the-art performances on multiple benchmarks. During the first phase of the elaboration of the fine-tuning, I work with *TinyLlama-1.1B*, a lightweight model based on LlaMa architecture. After this phase, I upgraded to *LlaMa 3.2-1B* for a better performance, but compatible with hardware constraints described in section 3.6.

After the model, the next step is the training dataset. The reference in fine-tuning training dataset is the *Alpaca* dataset[15]. It's an AI-generated dataset of 52k examples of instruction-based dialogues from the *Stanford Alpaca* project. The dataset is composed of 4 fields : *input*, *output*,*instruction* and *text*. At first, I used *Alpaca-2K* dataset, a small subset of *Alpaca* composed of 2k examples. Then, I used the full *Alpaca* dataset when I reached a stable version.

For the training of the weights, as described in 2.1.1, I use AdamW, a variant of Adam decoupling weight decay [26] from learning rate. Along with the optimizer, the training went with Low Rank Adaptation (LoRA) as a Parameter Efficient Fine-Tuning (PEFT) method, as defined in section 2.1.4. The fine-tuning follow the generic ANN training process, except only LoRA are trainable. LoRA is applied to all weights inside Multi-Head Attention, i.e. keys, values, queries and output weights, so the linear layers outside MHA are not affected.

For the implementation, at first I started from example from PyTorch Lightning documentation, then I adapted it to my needs. This approach used PyTorch as backend, providing *LightningModule* and *LightningDataModule* classes, with Distributed Data Parallel (DDP) as parallelism strategy. GPT specific function and classes were implemented in LitGPT librairy. For loading models, HuggingFace, the standard hub for model and datasets, is used to manage token with Meta interface. After few adaptations, I had python code almost usable for fine-tuning, but the file input and output at each step (after training, merging with LoRA weights, conversion for evaluation) was prone to error and file corruption.

In the last half of December, I decided to restart this part from scratch, using solely LitGPT library with it's Command Line Interface (CLI). This approach was easier to implement, and provided a more stable workflow although it reduced the training performance, using another parallel strategy (Fully-Sharded Data Parallel (FSDP)). In this approach, I managed long strings corresponding to CLI commands, and I used python *subprocess* to execute them.

3.2.2 Evaluation of the model

To evaluate an ANN, the standard way is to split the dataset into training and validation datasets. For Hyperparameter Optimization (HPO), a testing dataset is used to prevent data leakage, and prevent overfitting. The training dataset is used to train the model, and the validation dataset is used to evaluate the model. The evaluation metric can be the loss, a metric about the difference between the predicted output and the true output, or the accuracy, a metric about the percentage of correct predictions. There exists differents kind of loss, link cross-entropy, or mean-square error, to adapt to the datasets and the problem.

With LLM, the diversity of the tasks, even with a decoder-only model, is crucial. During the training, the loss or the accuracy is done with the prediction of the next word, compared to the true one. It does not represent the generalization capability of the model. To deal with it, challenge benchmarks, often using Multi-Choice Question (MCQ) on diverses thematics, were

rising. It's was enhanced by article like [51], proving the advantage of fine-tuning in terms of generalization.

Among those challenge benchmark datasets, I choose two of them : one to use during HPO and the other for testing. The HellaSwag [55] dataset is composed of 40k lines of text and 4 choice of answers, meaning random pick lead to 25% of accuracy. I use this first during HPO. The MMLU dataset [16] is the testing dataset, measuring general knowledge for a lot of fields. .

The implementation of this part is also done with LitGPT library, as a CLI like for training. Under the LitGPT part, it's using lm_eval library from HuggingFace to manage the evaluation of the accuracy.

3.3 Search Space

The search space is defined with the choice of hyperparameters, theirs bounds, theirs types and even the scale of theirs steps. Well-defined search space is crucial for a correct application of HPO : if the space is too high-dimensional, the HPO algorithm will need too many shots to converge to a good solution, if it's too small, we are missing it's relevance.

The search space is composed of 5 hyperparameters, from classical training hyperparameters to LoRA specific ones. A detailed presentation of hyperparameters is just below, but one can look at table 3.1 for a summary.

- LoRA rank : with LoRA method, the fine-tuning weights matrix $\Delta W \in \mathbb{R}^{n*p}$ is replaced by two matrices $A \in \mathbb{R}^{r*p}$ and $B \in \mathbb{R}^{n*r}$ with $\Delta W = B * A$. r is called the LoRA rank, and scale the reduction of the weights matrix. It's an integer, and it's value range from 1 to 64.
- LoRA scale (α) : when merging pre-trained weights W_0 and Lora fine-tuned weights $B * A$, the scale α is weighting the influence of fine-tuning, with $W = W_0 + \frac{\alpha}{r} * (B * A)$. It's an integer value, from 1 to 64 as guided by LoRA article and LitGpt framework.
- Learning rate : learning rate is a classical hyperparameter used in HPO, weighting the gradient of each weight when doing backpropagation. It is often tuned in a logarithmic scale, to manage effectively the exploration.
- Dropout probability : based on article [43], dropout is a method used to prevent over-fitting, by randomly fixing cells/layers to zeroes during one iteration. Being a probability, it's bounds by 0 and 1, but for this work it's between 0 and 0.5.
- Weight decay : weight decay is used to improve generalization capacity, as proved in article [26], by reducing the weights at each iterations by a small value, to force the model to use new inputs. Typically, the parameter for weight decay is set on a logarithmic scale between 10^{-3} and 10^{-1}.

For the 2 integers variables (LoRA rank and LoRA scale), to adapt to continuous optimization algorithms, the relax and round methods will be applied. It mean that the integers constraints is relaxed when generating a solution, and is rounded when evaluating a solution. Others methods like computing with lower and upper discrete value can be used, but this one was kept for simplicity and computation costs.

For the 2 variables with logarithmic scale (learning rate and weight decay), to explore with consistency the search space , the optimization algorithm will be bound between a larger range, and then convert with $f(x) = 10^x$.

Hyperparameter	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	1	64	int.	$f(x) = \text{round}(x)$
Dropout	0	0.5	cont.	$f(x) = x$
Weight decay	-3	-1	log.	$f(x) = 10^x$

Table 3.1: Summary of hyperparameter Search space

3.4 Optimization Algorithms

Linked with section 2.3, this part aims to describe the implemented algorithms, and how they are applied to the optimization problem. It start from elements of section 2.3, then describe algorithms and show examples of application.

The first approach to explore is Surrogate-Model Based Optimization (SMBO), and particularly Bayesian Optimization (BO) using Gaussian Process (GP) (BO-GP). Then considering the dimensionnality of the problem, and the PBO performance benchmark in article [9], I went with Simultaneous Optimistic Optimization (SOO) algorithm as representative of PBO methods. After theses two approachs, section 3.4.3 present an hybrid approach, combining the intrinsic parallel abilities of PBO combined to the efficiency and exploitation of BO.

3.4.1 Bayesian Optimization using Gaussian Process (BO-GP)

We saw in 2.3 that BO use a surrogate model to perform optimization. On this work, a focus is done on Gaussian Process (GP) for the BO surrogate. GP use the kernel trick to build a bayesian nonparametric regression model. It use a mean vector m_i and a covariance matrix $K_{i,j}$ to define the prior function as equation 3.1.

$$\text{f}|X \sim \mathcal{N}(m, K) \tag{3.1}$$

From the prior function and the data points $\mathcal{D}$, the GP build a posterior. The prior was representing the assumption made for the regression, the posterior represent the regression itself. On this posterior is build an acquisition function used as a surrogate for the objective function.

Algorithm 3.1 offer an overview of the BO process. To ease the first build of the surrogate, it's crucial, as proven in article [53], to sample efficiently the search space . This sampling provides information for the Gaussian Process (GP) to estimation the function. Like article [5], Latin Hypercube Sampling (LHS)[30] is used as a sampling method, for a defined budget called n_init. More detail about LHS are presented in section 4.1.1 and appendix 34.

Algorithm 3.1: 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**
  $K_D, \mu_D \leftarrow \text{Fit}(\text{GP}(K_D, \mu_D), \mathcal{D})$
  $\lambda' \leftarrow \text{Optimize}(f_{\text{acq}}(K_D), \mathcal{O})$ // Generate new point
  $\mathcal{D} \leftarrow \mathcal{D} \cup \{(\lambda', f(\lambda'))\}$ // scoring function
end
return best of $\{(\lambda^*, f(\lambda^*)) \in \mathcal{D}\}$

After this preliminary phase, a second phase is done with loop containing the update of the GP, the optimization of the acquisition function to obtain a new points to evaluate and the evaluation. After the evaluation of the point, the point is added to the history $\mathcal{D}$ and so on. The loop end based on a budget n_{opt}, with the budget $n_{max} = n_{init} + n_{opt}$

For this algorithm, the first requirements is the search space, and the objective function already described in 3.3 and 3.2 respectively. On the GP part, we need to define a Kernel function $K_{\mathcal{D}}$, an acquisition function f_{acq} and an Inner Optimizer $\mathcal{O}$. Theacquisition function is logEI, more reliable than Expected Improvement (EI), based on article [1]. The kernel and the inner optimizer are the standard implementation of Botorch, introduced in the next paragraph, with a radial basis function kernel and multi-start optimization method.

BoTorch [2] is a Bayesian Optimization library built on PyTorch, designed for efficient and scalable optimization of expensive black-box functions. Leveraging PyTorch's GPU acceleration and integration with GPyTorch [11] for GP, BoTorch enables advanced surrogate modeling and optimization. Botorch is used on this work for all tasks including GP, this part and section 3.4.3

3.4.2 Partition Based Optimization : Simultaneous Optimistic Optimization (SOO)

SOO [32] is a tree-based space partitioning method for black-box optimization, inspired by Monte Carlo Tree Search (MCTS) methods. SOO is called optimistic since it assume the existence of l such that $f(x^*) - f(x) \leq l(x, x^*)$ where x^* is the maximizer of x.The algorithm partition the space Ω by building a tree with smaller and smaller sub-space $\Omega_{h,j}$. A node (h, j), the node number j of depth h, is scored at the center of his space.

An expanded node have K children, making the tree a K-nary tree. L_n is the *open list* of the tree, to avoid expanding the same nodes over and over. At each round, SOO expand a maximum of one node by depth, meaning that each round score a maximum of $depth * (K)$ solution, enhancing the parallel evaluation of the solution. Summary of SOO is present in algorithm 3.2.

The original algorithm manage the end of the loop with the $h_{max}(n)$ function, limiting the depth of the tree search. To compare different algorithm, the stopping criterion here is n_{max}, the evaluation budget.

Algorithm 3.2: SOO

Input: Ω, f, K, $n_{\max}$

// initiate

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

3.4.3 Bayesian Multi Scale Optimistic Optimization (BaMSOO)

Surrogate-Model Based Optimization (SMBO) algorithms harness the exploitation of the informations to define a cost-reduce function to optimize. This approach ensure exploitation but have several limitations, including the parallelization difficulties.. On the other hand, Partition-based approach are massively parallel, but are computation costly in front of very expensive objective function. To overcome both limitations, hybrid methods, using surrogates and space partition, were developed.

In this work, we focus on BaMSOO[50], a SOO based algorithm (algorithm A.1). Like SOO, BaMSOO performs a K-inary partitionning of the space, using the center of the partition to evaluate.

$$\begin{aligned} \mathcal{UCB}(x|\mathcal{D}_t) &= \mu(x|\mathcal{D}_t) + B_N * \sigma(x|\mathcal{D}_t) \\ \text{with } B_N &= \sqrt{2\log(\pi^2 N^2/6\eta)}, \eta \in (0,1) \end{aligned} \tag{3.2}$$

The difference with lies primarily in the scoring $g(.)$ of the partitions (blue line in algorithm 3.2 is replaced by algorithm 3.3). In the face of an expensive objective function, BaMSOO leverages a GP surrogate to estimate the potential of a point, using the $\mathcal{UCB}$ as a measure of expected performance. Given a partition with center x and existing evaluations $\mathcal{D}_t$, the $\mathcal{UCB}$ of x, defined in Equation 3.2, is compared against the best evaluation so far, f^+. If the $\mathcal{UCB}$ is higher than f^+, the algorithm evaluates x directly using the objective function $f(.)$.

Otherwise, the partition is scored using the LCB of x, reflecting the lower bound of potential improvement. Full BaMSOO algorithm is presented in appendix A.

Algorithm 3.3: BamSOO scoring

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 $x_{h,j}, g(x_{h,j})$

To sum up, this algorithm prevent unpromising evaluations in order to allocate more budget for exploring more promising areas than SOO. This hybrid approach harness a part of BO-GP exploitation of knowledge without losing the intrinsic parallel abilities.

For the implementation of the GP components, including the calculation of LCB and $\mathcal{UCB}$ scores, the BoTorch library was employed. This choice ensures computational efficiency and robustness, as BoTorch provides a modular framework for Bayesian optimization and GP modeling, seamlessly integrating with the partition-based structure of BamSOO. By adhering to the methodology outlined in section 3.4.1, the framework ensures consistency in surrogate modeling and acquisition function computation, further enhancing the effectiveness of the algorithm in high-dimensional, continuous search spaces .

3.5 Concrete Implementation

At first, one may think that for this kind of article and experiment, the quality of the code does not really matter. But a relevant way of designing the implementation, concise classes and functions and precise documentation are what make possible for the code to live even after the article. On this part, I describe the structure and implementation on my work, with the goal of being able to give it to a PhD candidate working on close field.

To implement what's described in section 3.2 to 3.4, I used Python as my main language. After a first phase of coding only with function on a small number of file, I started to rethink everything as Object Oriented Programming (OOP). When the rework from scratch happened in December, I used this opportunity to structure my code with OOP.

Figure 3.2 is an UML class diagramm presenting the whole framework of my internship, split in tree parts : the optimization part, including all optimization algorithm seen in section 3.4, the search space part, and evaluation part.

At the left, the optimization part includes a base class for optimization algorithm, managing all recurrent tasks, especially scoring and extracting the best result. From this class is built SOO and BO classes. All theirs attributes and functions are described in section 3.4.2

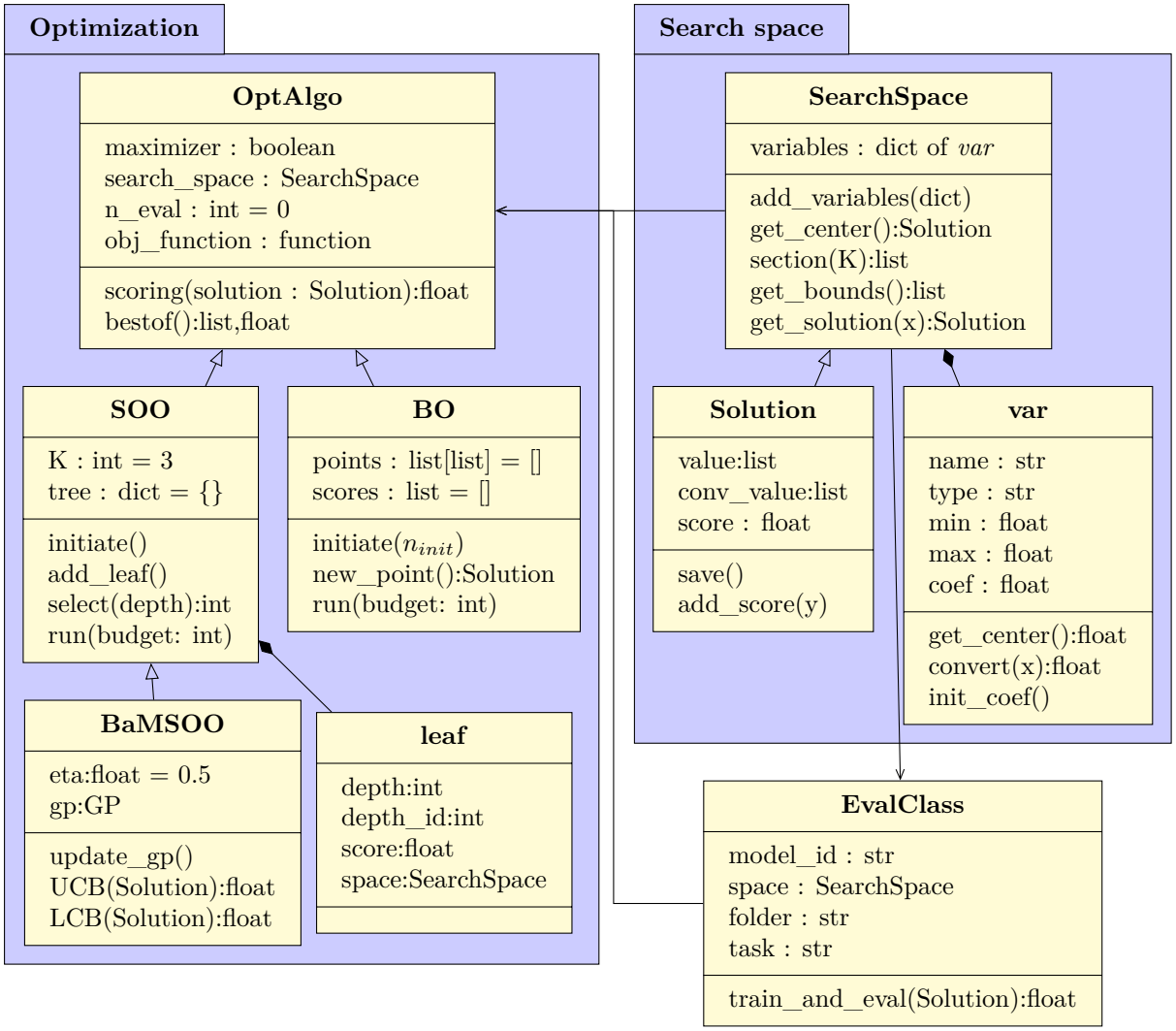


Figure 3.2: Class diagramm of the optimization framework

and 3.4.1 respectively, with comment in algorithms to precise which function is used for which line. SOO being a tree-based algorithm, a leaf class in create to manage the leaf of the tree, and especially the decomposition of the space. From SOO class, BaMSOO is built, add especially the GP surrogate, and updating the scoring function with $\mathcal{UCB}$ and LCB to adapt to algorithm 3.3.

At the top right, the search space part is firstly composed with a search space class. This class is composed on multiple var class, use to automate all function used by each variables. Then, it's used to manage the space, like section to split the space for SOO, or other functions to deal with algorithms and compatibility needs. Then, the Solution class inherit the search space class, to force a solution to be define in a search space , and then manage the conversion of the solution, with the conversion function of table 3.1.

The last part is the eval class, use to store the model id, the experiment folder, the task and then call the *train_and_eval* function when the scoring function is called. The whole structure allow an easy understanding of the framework, an easier testing and debuging process and a better reusability of each part of the code.

Along these part, all experiments are also stored as a subpackage of the whole, and then

called from the main file. This method ease the reproducibility of the experiments, and avoid import or module error from python package management.

After this rework, I worked on the documentation of my code. There are various forms of documenting my code. At first, I use *type hinting*, to show for every fonction what are the type of input and outputs, like what's mandatory in c++ for instance. After this, I write a small description for each function, and I use *docstring* to explain what each function does. On top of this, I concluded with adding small comment in specific part when needed. To finish about the reusability of my code, I wrote a *readme* file, explaining how to implement the code, and how to modify a part for reusing it.

3.6 Experiments setup

The experiments are done with Grid5000 [3], " a large-scale and flexible testbed for experiment-driven research in all areas of computer science, with a focus on parallel and distributed computing including Cloud, HPC and Big Data and AI." In specific, the *chuc* cluster, in the Lille center, composed of nodes of 4 GPU A100 with 40G of VRAM was used.

Apart from aforementioned hyperparameters (learning rate, LoRA rank ...) and configuration (weight matrix to apply LoRA), all arguments of LitGPT CLI is used with default value. The only exception is the number of epochs, fixed to 1 to reduce computation costs. For next sections, a difference will be made between variables (value inside optimization range), and hyperparameters (value used by the training function) to clarify the reading of the value.

Using this configuration, one epoch of fine-tuning is taking around 31 minutes. For the evaluation on both datasets, it's taking around 12 minutes. Based on previous articles, and evaluations durations, the total evaluation budget for experiments is 50 evaluations by each algorithms, including a sampling budget of 10 for Bayesian Optimization.

The implementation of the previous algorithm, the objective function and next experiments are all stored in github, following this link : `https://github.com/Kiwy3/BO_PBO_HPO_LLM`.

Chapter 4
Outcomes and Prospectives

I had a period where I thought I might not be good enough to publish.

Stephen King

This internship has yielded valuable insights into optimizing expensive function, and especially the optimization of hyperparameters applied to LLM fine-tuning. This chapter start with the presentation and the analysis of the results obtained following the methodology of chapter 3.

Following this presentation, a section will discuss the valorisation of this work in the academic community, i.e. the publication of an article. The scientific contribution along with the redaction of the article will be detailed, as it's crucial in an academic environment to think about the impact of one's work. Looking ahead, this chapter will discuss the challenges faced during experimentation and propose potential areas for future exploration.

4.1 Experiment Results

From what's discussed in chapter 3, three main experiments have been carried out, one by each algorithms (BO, SOO and BaMSOO). On top of these experiment, a sampling experiment will also be conducted. Details and motivation are inside section 4.1.1. Theses 4 next sections bring section 4.1.5, with a thorough analysis on all experiments.

4.1.1 Sampling experiment

This experiment is done using Latin Hypercube Sampling (LHS) algorithm. Figure 4.1 illustrate LHS. In simple, it's a random sampling of the search space, with the warranty that each interval on each dimension is sampled.

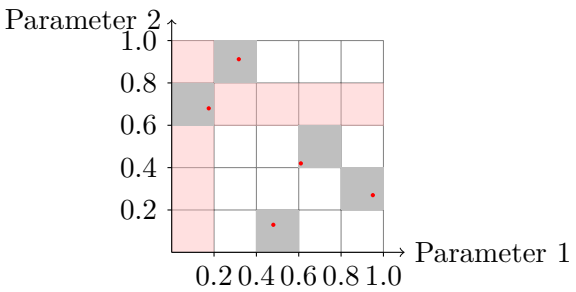


Figure 4.1: LHS illustration

LHS can also be called *non-attacking rook*, where picks are like rooks on a chessboard, where the maximum of rooks must be put without attacking other rooks. For instance, if the first sampled point is the one at $(0.17, 0.68)$, another point can't be sampled in the light-red squares.

For the sampling experiment, LHS was used with the same budget as other, i.e. 50 evaluations. Whole experiments took 36 hours. The aims of this experiments is dual: first, make a lower bound reference for others experiments, and second, explore the search space and the score behavior. To use as a lower bound, LHS achieve scores of 37.6% for MMLU, and 47.9% for Hellaswag. Theses score are inside table 4.1.

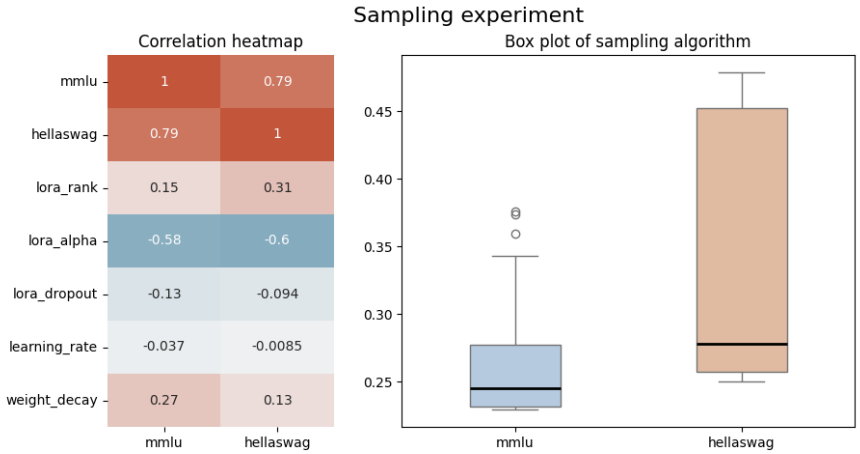


Figure 4.2: Results of Latin Hypercube Sampling experiment

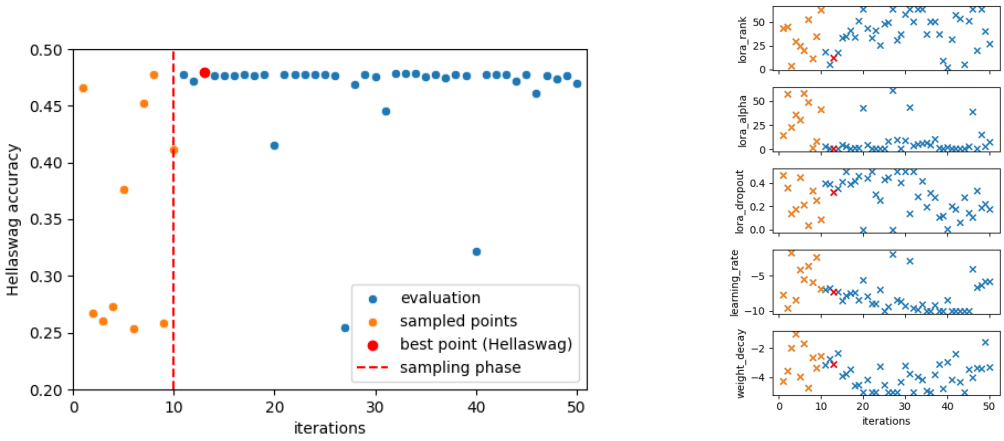
The correlation between MMLU and Hellswag tend to confirm the relevance of their choice as a pair for validation and testing dataset. It's sufficiently high to guess that most of *good* model for one will be good for the other one, but it's still less than one, making over-fitting visible if present.

For variables, it look like LoRA alpha, the scaling parameter of LoRA, is the most influent on the score, be it Hellaswag or MMLU. Next to it, LoRA Rank and weight decay are the most influent, with a difference in ranking on the metrics. With this first exploration, it look like Dropout and Learning rate are not very effectful for this problem, be it the choice of their range or the implementation.

On the distribution of the score values, it's interesting to note that Hellaswag has a broader range of score, making it useful for efficiently discriminating solutions. With a broader thinking, the sampling experiment confirm the relevance to apply HPO algorithms to the described problem. If scores were independent from variables, or all scores were the same, HPO would be useless.

4.1.2 BO-GP experiment

Figure 4.3 depicts the performance of Bayesian Optimization using Gaussian Process (BO-GP) over 50 iterations, measured in terms of the HellaSwag accuracy. This visualization highlights the evolution of the optimization process as it transitions from sampling to the exploitation, and ultimately converges towards high-performing solutions.



(a) Score over time

(b) Variable over time

Figure 4.3: Experiment using BO algorithm

During the sampling phase, as shown by figure 4.3a, evaluated solutions have the same diversity of solutions than the full sampling experiment, allowing to efficiently extract knowledge from the search space. The algorithm achieve a stable convergence to mostly high-performing solution.

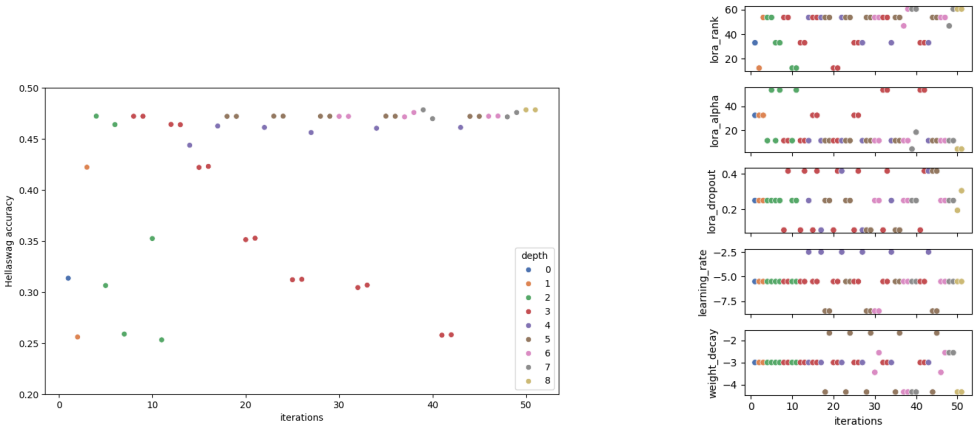
If we briefly look at figure 4.3b, it's interesting to look at the diversity of configuration to obtain high-performance, and the trend of the algorithms for each variables. For example, for LoRA alpha, or learning rate, we can observe a clear trend toward the lower bound of the optimization range. To summarize, this experiment demonstrate the effectiveness of Bayesian Optimization in efficiently exploiting the knowledge of the search space obtained in the sampling phase. The optimization process still explore area with high uncertainty, giving few low-performing solution.

4.1.3 SOO experiment

On this experiment, we observe in Figure 4.4 the behavior of SOO as it optimizes the given objective function. The figure illustrates how the algorithm navigates the search space, iteratively improving the solution by adjusting the hyperparameters. By examining the trends in performance metrics and variables evolution, we aim to analyze the convergence behavior, stability, and overall effectiveness of SOO in this setting.

Figure 4.4a depicts the accuracy of the HellaSwag dataset as a function of iterations, with marker colors representing different depth configurations. The observed trend suggests that most configurations achieve accuracies arround 0.46 throughout the optimization process. Several configurations converge toward the higher end of this range, indicating potential stability and effectiveness in learning as iterations progress.

It is evident that higher-depth configurations tend to cluster around higher accuracy values, while lower depths display more scattered behavior across the accuracy spectrum. In specific, depth 2, with a section on lora alpha seems to greatly affect the performance on the accuracy. On figure 4.4b, it's clear on the limitation of constrained-budget SOO without local exploitation at the end of the algorithms : Only a few number of values by variables are explored : around 5 by variables, making it equivalent to exploration of a search space of $6^5 = 7,776$ discrete solutions.



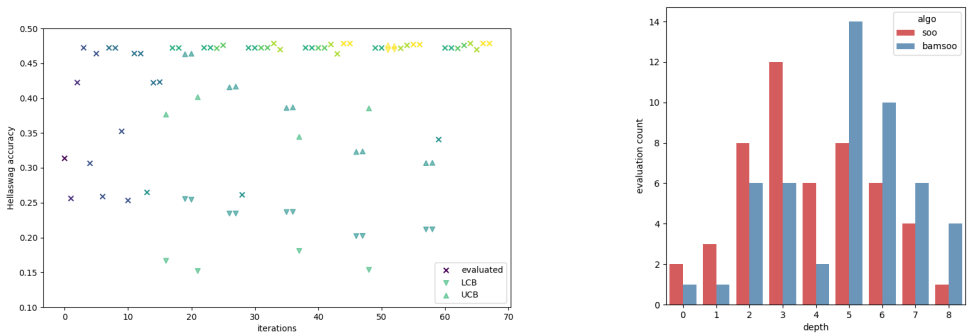
(a) Score over time (b) Variable values over time

Figure 4.4: Experiment using SOO algorithm

To summarize, SOO achieve a maximum performance closed to the precedent algorithm, but explore a restricted number of configuration, and lose time by evaluating unpromising solutions.

4.1.4 BaMSOO experiment

The last experiment of this work is using BaMSOO, with $\eta = 1$ in equation 3.2, to reduce the confidence interval and promote approximation, to avoid the evaluation of unpromising points. To look after it, figure 4.5a discriminate evaluated and approximated points, and might be compared with 4.4a to look after approximated points.



(a) Score over time (b) Depth exploration

Figure 4.5: Experiment using BaMSOO algorithm

When compared to figure 4.4a, the pair of evaluations for depth 2, with low-performing solutions seems to have mostly been approximated. On the whole experiment, 16 points were approximated, to efficiently search further than SOO. Figure 4.5b compare the budget allowed on each depth, and highlight the focus of BaMSOO for lower depth exploration. To summarize, BaMSOO achieve to speed up SOO, but is still slow in comparison with BO at first glance. Moreover, BaMSOO succeed to prevent most of low-performing evaluation of SOO.

4.1.5 Comparison and analysis

To conclude this section, it's crucial to directly compare algorithms, especially their performance, with validation and testing dataset. To look at absolute performance, and not only relative between algorithms, lower and upper bounds will be used.

Datasets	Lower (LHS)	Upper (model card)	BO-GP	SOO	BaMSOO
Hellaswag (validation)	47.90	41.5	47.91	47.84	47.84
MMLU (testing)	37.61	49.3	38.11	37.42	37.50

Table 4.1: Bounds on accuracy for validation and testing dataset

In face of such experiments, it's interesting to look at bounds of the metric, to compare the results. The lower bounds is the results of the experiment using solely LHS to pick solutions, with the same number of evaluation than algorithms. LHS being intrinsically parallel, if evaluated algorithms don't achieve better performance than a solely exploring one, their benefit isn't relevant.

For the higher bound, I will look at the higher value in the model card[1] of the model, achieved using advanced fine-tuning methods like Supervised Fine-Tuning (SFT), Rejection Sampling (RS), and Direct Preference Optimization (DPO). Values are inside table 4.1.

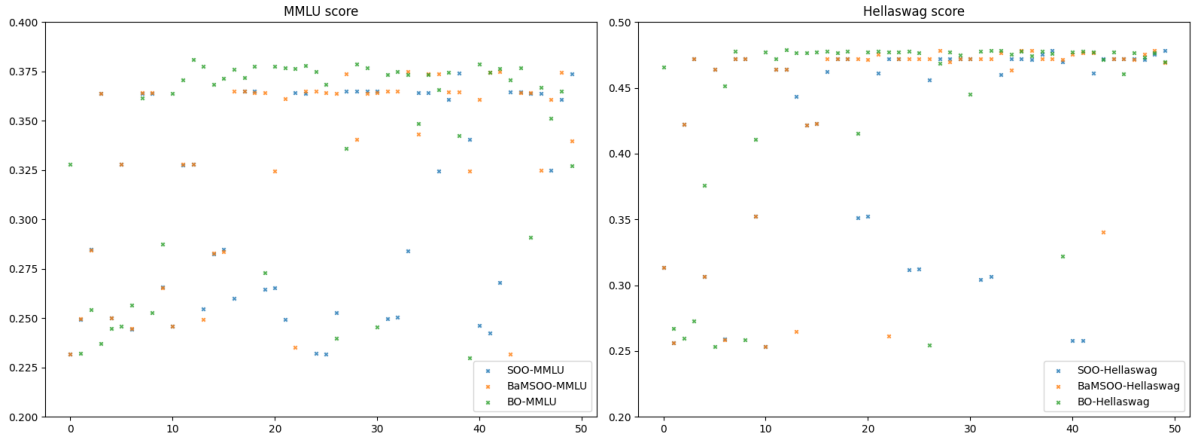


Figure 4.6: Comparison between 3 algorithms on 2 metrics

At first, what's interesting is to look at testing and upper bounds results. Since the upper bound is mostly fine-tuned with aimed for MMLU results, the HellaSwag upper bounds isn't really relevant. Considering this, the analysis of this part will mostly be done with MMLU. The best results with MMLU is Bayesian Optimization (BO), being 23% from the upper bound.

With figure 4.6, it's clear than BO algorithm is a step more performing than others algorithms for this problem, especially with the low number of low-performing solutions evaluated. Apart from this part, the whole results may suggest that the objective function, or the search space could be different, to have an higher range of results for comparison.

[1] `https://huggingface.co/meta-llama/Llama-3.2-1B`

4.2 Article Publication

After few weeks of my internship, when we were able to define cleary a subject and estimate the possible contribution, with my supervisor we decided to aim to write an article from what I worked on. This aims push me to refine clearly what would be my contribution, since a published paper should aim for this.

Under my supervisor guidance, what we aimed for was a conference article, for the International Conference on Optimization & Learning (OLA2025). With this, a long paper should be published in *Springer* indexed proceedings. At the time of writing and sending this report, the paper is under review, and the outcome is awaited. The current version can be found on github[1]

After a section on the contribution, I will adress in section 4.2.2 the redaction of the article, as it was also a crucial part of my internship.

4.2.1 The contribution

The first contribution of this work is direct and practical: the provision of usable HPO algorithms and experiments specifically tailored for LLM fine-tuning. The popularization of LLMs is a relatively recent development, and while these models are increasingly adopted by companies and end-users, the process of fine-tuning remains somewhat inaccessible due to knowledge barriers and the lack of practical resources. By providing detailed experiments and insights into HPO algorithms, this work aims to lower these barriers, enabling users to better understand and utilize fine-tuning techniques. Furthermore, this contribution supports the selection of hyperparameters : a crucial step in achieving optimal performance without excessive trials and errors.

The second contribution lies in addressing the challenge of optimizing expensive functions. The development and training of ANNs are computationally intensive processes, underscoring the importance of efficient optimization methods. This has driven significant interest in BO algorithms, originally developed for scenarios such as mechanical and aeronautical engineering, where simulations can take hours to run. However, other domains with similarly expensive functions stand to benefit from advancements in this area. Through this work, a comparative analysis was conducted between two approaches for optimization in settings with limited evaluations, providing valuable insights for both researchers and practitioners.

Finally, this work contributes to the scalability of BO algorithms. Given that this internship is part of an exascale computing project, the broader goal is to develop scalable and efficient algorithms capable of handling a wide variety of use cases. While the immediate focus has been on LLM fine-tuning, the findings and methodologies have implications that extend to other computationally intensive tasks. By addressing scalability, this work lays the groundwork for future innovations in optimization methods that can leverage the full potential of high-performance computing infrastructure.

[1] `https://github.com/Kiwy3/ST30-deliverables/blob/master/OLA_Article/OLA.pdf`

4.2.2 Redaction

The redaction process was as interesting as it was frustrating at times. At the outset, I spent considerable time analyzing the structure of numerous published articles to understand how to organize and present research effectively. This gave me a better sense of how to approach the task. Additionally, I had discussions with my supervisor to define the overall content and structure of the article, ensuring that the key aspects of the work were covered comprehensively. With this framework in mind, I began writing as early as possible, focusing on sections that did not require finalized results. This proactive approach allowed me to step back and reflect on my work as it progressed, identifying gaps and limitations in both my understanding and the way I communicated the research.

However, the final stages of the paper's completion turned out to be more challenging, as I faced a tight timeline. The latter part of the writing process felt rushed because I only obtained correct and usable results two days before the submission deadline. This created a significant constraint on my ability to test and validate the results thoroughly. The time and resources required for each experiment were substantial, which limited the number of tests I could conduct within the available timeframe. Despite these challenges, I focused on making the most of the results I had, presenting them in the most coherent and impactful way possible.

On a technical level, the redaction of the article, much like the drafting of this report, was a valuable learning experience. It helped me deepen my proficiency in using LaTeX, from creating structured tables and formatting content to incorporating figures seamlessly. Moreover, I learned how to produce high-quality illustrations and diagrams using the *TikZ* library, which enhanced the visual presentation of the article. This process not only improved my technical skills but also gave me practical experience in preparing a professional, publication-ready document that adhered to academic standards.

4.3 Challenges

This section outlines the key challenges encountered during the internship and the strategies employed to address them. The terms *challenge* can have two signification, a difficulty or like a challenge to adress (like a sport team winning a cup), and this section adress the two kinds of challenge.

Undertaking a project situated at the intersection of multiple research domains presented unique difficulties, from defining and addressing a novel research problem to managing the technical complexities of implementation and resource constraints. Each of these challenges required a combination of critical thinking, adaptability, and collaboration to overcome.

4.3.1 Adress a research problematic

The first significant challenge I faced during the initial weeks of my internship was adapting to a completely new environment and working on a subject rooted in research—a domain I had not fully encountered before. While my academic courses had involved numerous projects of varying complexity and levels of research ambition, this internship marked the first time I was required to address a genuine research problem in its entirety. This shift introduced me to the complexities of the research process and the skills necessary to navigate it effectively.

One of the initial hurdles was managing the literature review. This involved handling numerous references, reading and analyzing complex academic articles, and extracting relevant information to identify a specific research problem. Estimating the right problematic to focus on proved particularly difficult at the outset, given the broad scope and technical depth of the subject. However, with the guidance of my supervisor, I was able to refine my understanding of the domain, define a clear and well-scoped research problem, and develop a structured approach to tackle it. This process laid the foundation for the rest of the project, ensuring that my efforts were focused and aligned with the goals of the internship.

4.3.2 Work in a complex research field

The subject of my internship was as fascinating as it was complex, sitting at the intersection of several cutting-edge research fields. To approach this multidisciplinary challenge effectively, I began with a rapid yet thorough literature review of each relevant aspect. This step was essential to grasp the stakes of the subject and avoid wasting valuable time on unnecessary or redundant work. The fields I needed to familiarize myself with included LLM, encompassing ANNs and the specific nuances of Parameter Efficient Fine-Tuning, as well as Bayesian Optimization, which required an understanding of probabilistic models and optimization rules. Additionally, I had to delve into High Performance Computing (HPC), particularly the scalability of processes, which became increasingly relevant to my project's objectives.

This endeavor was particularly challenging for me because my aim was to produce work comparable to that of well-established researchers or even research teams, despite having only a short internship period of six months to achieve it. Starting from scratch, I had to quickly acquire foundational knowledge and develop expertise in these domains. Balancing the demands of mastering multiple complex fields while striving to meet the high standards of professional research pushed me to adapt and learn at an accelerated pace. This experience, while demanding, was invaluable in helping me grow both academically and professionally.

4.3.3 Technical implementation

The first significant difficulty I encountered was related to the development process itself. I lacked a well-structured approach to code development, including strategies for writing clean, efficient, and modular code, as well as systematic methods for testing it. This absence of an established process initially slowed down my progress and required me to learn best practices as I advanced through the project.

Another major challenge was working with numerous libraries for implementing the black-box objective function. The codebase involved a complex network of libraries, classes, and functions, all deeply interconnected. It was initially overwhelming to understand how these components interacted and to adapt the existing code to fit my specific requirements. This was especially challenging because my use case—Hyperparameter Optimization—was not a generic application of the libraries. As such, no pre-existing implementation was readily available to use HPO as a black-box objective function, requiring significant effort to tailor the code.

The last key challenge is about the computing resources, and the discovery of Grid'5000 plateform. I never used before python as command line, or even shell on an unix environment. Theses elements push me to learn a lot about the deployment of the code on a unix-based cluster, about virtual environment and so on. On the other hand, working with grid'5000 means

working with resource with time-limitation, with reservation. This force me to think a lot before launching an experiment, to not lose my reservation with useless experiment or small bugs.

4.3.4 Open the door of Partition-based Bayesian Optimization

As written multiple time, a key facet of this internship was the exploration of parallel Bayesian Optimization (BO), based on hybridization with Partition Based Optimization (PBO). On my main job, I explored this topic, but without looking too far, since I had many other things to do, and to not lose myself.

After the submission of my article, I talked with my tutor and one of his PhD candidate, to talk about the following of my work. There was a part about the direct continuation of my work, like expanding models, datasets, search space and so on. But there was also a more theoric work, about the parallelization of BO algorithms.

Based on articles [22, 36, 31], with the PhD candidate, we made a first litterature review of this field, to make a first unification on the field. This includes how to exploit the most of surrogates for PBO algorithms, what's the best surrogate to scale for exascale computing, and all small questions arising from them.

This work allow me to exploit a lot of reflection I had during my work, and face really interesting challenges like the specific needs of highly scalable parallel algorithm.

Conclusion

During the course of this internship, I addressed several critical challenges and contributed to advancing knowledge in the field of Hyperparameter Optimization for Large Language Model fine-tuning. My work involved implementing and experimenting with various Hyperparameter Optimization algorithms, adapting them to the unique requirements of fine-tuning, and conducting comparisons to assess their performance in optimizing expensive black-box functions. Even if results were not groudbreaking, the behavior of the algorithms in front of expensive function, the implementation of Hyperparameter Optimization (HPO) were precious to continuate this work.

Through this, I contributed to bridging the knowledge gap that often limits the accessibility of fine-tuning processes for companies and practitioners. Furthermore, I explored the scalability of Bayesian Optimization algorithms in the context of high-performance computing, aligning my work with the long-term objectives of exascale-based projects. This multifaceted approach not only deepened my understanding of the subject but also produced insights and methodologies that can aid future research and practical applications.

Throughout this internship, I gained invaluable knowledge and skills across several domains. I developed a deeper understanding of Hyperparameter Optimization, Large Language Model fine-tuning, and the intricacies of Bayesian Optimization algorithms, including their theoretical foundations and practical applications. Beyond the technical aspects, I acquired experience in navigating complex research fields, performing thorough literature reviews, and defining well-scoped research problems in collaboration with my supervisor. On a technical level, I honed my programming and development skills, learning to write modular and efficient code while adapting existing frameworks to specific use cases. Moreover, working within resource constraints and leveraging platforms like Grid'5000 strengthened my problem-solving and resource management abilities.

To conclude this report, I will expand briefly on my professional project, as I introduce since the abstract of this report. One aim of this internship was to decide if I wanted to continue these 6 months with a PhD. And after discussion, a lot of reflection and the opportunity on the right timing, I continue my cursus with a PhD in operation research, at Lille, with a topic on network design for delivery.

References

[1] Sebastian Ament et al. *Unexpected Improvements to Expected Improvement for Bayesian Optimization*. arXiv:2310.20708 [cs]. Jan. 2024. DOI: 10.48550/arXiv.2310.20708. URL: http://arxiv.org/abs/2310.20708 (visited on 01/07/2025).

[2] Maximilian Balandat et al. *BoTorch: A Framework for Efficient Monte-Carlo Bayesian Optimization*. arXiv:1910.06403 [cs]. Dec. 2020. DOI: 10.48550/arXiv.1910.06403. URL: http://arxiv.org/abs/1910.06403 (visited on 01/07/2025).

[3] Daniel Balouek et al. "Adding Virtualization Capabilities to Grid'5000". en. Pages: 18. report. INRIA, July 2012. DOI: 10/document. URL: https://inria.hal.science/hal-00720910 (visited on 01/06/2025).

[4] Yejin Bang et al. *A Multitask, Multilingual, Multimodal Evaluation of ChatGPT on Reasoning, Hallucination, and Interactivity*. arXiv:2302.04023 [cs]. Nov. 2023. DOI: 10.48550/arXiv.2302.04023. URL: http://arxiv.org/abs/2302.04023 (visited on 12/17/2024).

[5] Prapatsorn Borisut and Aroonsri Nuchitprasittichai. "Adaptive Latin Hypercube Sampling for a Surrogate-Based Optimization with Artificial Neural Network". en. In: *Processes* 11.11 (Nov. 2023). Number: 11 Publisher: Multidisciplinary Digital Publishing Institute, p. 3232. ISSN: 2227-9717. DOI: 10.3390/pr11113232. URL: https://www.mdpi.com/2227-9717/11/11/3232 (visited on 01/07/2025).

[6] Jacob Devlin et al. *BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding*. arXiv:1810.04805. May 2019. DOI: 10.48550/arXiv.1810.04805. URL: http://arxiv.org/abs/1810.04805 (visited on 11/20/2024).

[7] Thomas Elsken, Jan Hendrik Metzen, and Frank Hutter. *Neural Architecture Search: A Survey*. en. arXiv:1808.05377 [stat]. Apr. 2019. URL: http://arxiv.org/abs/1808.05377 (visited on 11/20/2024).

[8] Matthias Feurer and Frank Hutter. "Hyperparameter Optimization". en. In: *Automated Machine Learning: Methods, Systems, Challenges*. Ed. by Frank Hutter, Lars Kotthoff, and Joaquin Vanschoren. Cham: Springer International Publishing, 2019, pp. 3–33. ISBN: 978-3-030-05318-5. DOI: 10.1007/978-3-030-05318-5_1. URL: https://doi.org/10.1007/978-3-030-05318-5_1 (visited on 12/13/2024).

[9] Thomas Firmin and El-Ghazali Talbi. "A fractal-based decomposition framework for continuous optimization". July 2022. URL: https://hal.science/hal-04474444 (visited on 01/07/2025).

[10] 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. ISSN: 2374-3468. DOI: 10.1609/aaai.v36i10.21311. URL: https://ojs.aaai.org/index.php/AAAI/article/view/21311 (visited on 11/20/2024).

[11] Jacob R. Gardner et al. *GPyTorch: Blackbox Matrix-Matrix Gaussian Process Inference with GPU Acceleration*. arXiv:1809.11165 [cs]. June 2021. DOI: 10.48550/arXiv.1809.11165. URL: http://arxiv.org/abs/1809.11165 (visited on 01/07/2025).

[12] Yoav Goldberg. "A Primer on Neural Network Models for Natural Language Processing". en. In: *Journal of Artificial Intelligence Research* 57 (Nov. 2016), pp. 345–420. ISSN: 1076-9757. DOI: 10.1613/jair.4992. URL: https://www.jair.org/index.php/jair/article/view/11030 (visited on 12/17/2024).

[13] Aaron Grattafiori et al. *The Llama 3 Herd of Models*. arXiv:2407.21783 [cs]. Nov. 2024. DOI: 10.48550/arXiv.2407.21783. URL: http://arxiv.org/abs/2407.21783 (visited on 12/13/2024).

[14] Zeyu Han et al. *Parameter-Efficient Fine-Tuning for Large Models: A Comprehensive Survey*. arXiv:2403.14608 [cs]. Sept. 2024. DOI: 10.48550/arXiv.2403.14608. URL: http://arxiv.org/abs/2403.14608 (visited on 12/13/2024).

[15] 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. URL: https://github.com/tatsu-lab/stanford_alpaca (visited on 12/18/2024).

[16] Dan Hendrycks et al. *Measuring Massive Multitask Language Understanding*. arXiv:2009.03300 [cs]. Jan. 2021. DOI: 10.48550/arXiv.2009.03300. URL: http://arxiv.org/abs/2009.03300 (visited on 12/05/2024).

[17] Timothy Hospedales et al. "Meta-Learning in Neural Networks: A Survey". In: *IEEE Transactions on Pattern Analysis and Machine Intelligence* 44.9 (Sept. 2022). Conference Name: IEEE Transactions on Pattern Analysis and Machine Intelligence, pp. 5149–5169. ISSN: 1939-3539. DOI: 10.1109/TPAMI.2021.3079209. URL: https://ieeexplore.ieee.org/abstract/document/9428530 (visited on 12/17/2024).

[18] Edward J. Hu et al. *LoRA: Low-Rank Adaptation of Large Language Models*. arXiv:2106.09685. Oct. 2021. DOI: 10.48550/arXiv.2106.09685. URL: http://arxiv.org/abs/2106.09685 (visited on 11/20/2024).

[19] *Inria Joint Center*. en-US. URL: https://www.microsoft.com/en-us/research/collaboration/inria-joint-centre/ (visited on 11/25/2024).

[20] Ming Jin et al. *Time-LLM: Time Series Forecasting by Reprogramming Large Language Models*. arXiv:2310.01728 [cs]. Jan. 2024. DOI: 10.48550/arXiv.2310.01728. URL: http://arxiv.org/abs/2310.01728 (visited on 12/18/2024).

[21] D. R. Jones, C. D. Perttunen, and B. E. Stuckman. "Lipschitzian optimization without the Lipschitz constant". en. In: *Journal of Optimization Theory and Applications* 79.1 (Oct. 1993), pp. 157–181. ISSN: 1573-2878. DOI: 10.1007/BF00941892. URL: https://doi.org/10.1007/BF00941892 (visited on 12/18/2024).

[22] Kenji Kawaguchi, Leslie Pack Kaelbling, and Tomás Lozano-Pérez. "Bayesian Optimization with Exponential Convergence". en. In: arXiv:1604.01348 (Apr. 2016). arXiv:1604.01348 [stat]. URL: http://arxiv.org/abs/1604.01348.

[23] Abbas Khosravi et al. "Comprehensive Review of Neural Network-Based Prediction Intervals and New Advances". In: *IEEE Transactions on Neural Networks* 22.9 (Sept. 2011). Conference Name: IEEE Transactions on Neural Networks, pp. 1341–1356. ISSN: 1941-0093. DOI: 10.1109/TNN.2011.2162110. URL: https://ieeexplore.ieee.org/abstract/document/5966350 (visited on 12/17/2024).

[24] Diederik P. Kingma and Jimmy Ba. *Adam: A Method for Stochastic Optimization*. arXiv:1412.6980. Jan. 2017. DOI: 10.48550/arXiv.1412.6980. URL: http://arxiv.org/abs/1412.6980 (visited on 11/20/2024).

[25] Aaron Klein et al. “Structural Pruning of Large Language Models via Neural Architecture Search”. en. In: (Oct. 2023). URL: https://openreview.net/forum?id=VAwgL8kPvr (visited on 11/20/2024).

[26] Anders Krogh and John Hertz. “A Simple Weight Decay Can Improve Generalization”. In: *Advances in Neural Information Processing Systems*. Vol. 4. Morgan-Kaufmann, 1991. URL: https://papers.nips.cc/paper_files/paper/1991/hash/8eefcfdf5990e441f0fb6f3fad709e21-Abstract.html (visited on 01/07/2025).

[27] Mike Lewis et al. “BART: Denoising Sequence-to-Sequence Pre-training for Natural Language Generation, Translation, and Comprehension”. en. In: *Proceedings of the 58th Annual Meeting of the Association for Computational Linguistics*. Online: Association for Computational Linguistics, 2020, pp. 7871–7880. DOI: 10.18653/v1/2020.acl-main.703. URL: https://www.aclweb.org/anthology/2020.acl-main.703 (visited on 12/17/2024).

[28] Hanxiao Liu, Karen Simonyan, and Yiming Yang. *DARTS: Differentiable Architecture Search*. arXiv:1806.09055. Apr. 2019. DOI: 10.48550/arXiv.1806.09055. URL: http://arxiv.org/abs/1806.09055 (visited on 11/20/2024).

[29] Warren S. McCulloch and Walter Pitts. “A logical calculus of the ideas immanent in nervous activity”. en. In: *The bulletin of mathematical biophysics* 5.4 (Dec. 1943), pp. 115–133. ISSN: 1522-9602. DOI: 10.1007/BF02478259. URL: https://doi.org/10.1007/BF02478259 (visited on 11/20/2024).

[30] M. D. McKay, R. J. Beckman, and W. J. Conover. “A Comparison of Three Methods for Selecting Values of Input Variables in the Analysis of Output from a Computer Code”. In: *Technometrics* 21.2 (1979). Publisher: [Taylor & Francis, Ltd., American Statistical Association, American Society for Quality], pp. 239–245. ISSN: 0040-1706. DOI: 10.2307/1268522. URL: https://www.jstor.org/stable/1268522 (visited on 01/14/2025).

[31] Erich Merrill et al. “An Empirical Study of Bayesian Optimization: Acquisition Versus Partition”. In: *Journal of Machine Learning Research* 22.4 (2021), pp. 1–25. URL: http://jmlr.org/papers/v22/18-220.html.

[32] Rémi Munos. “Optimistic Optimization of a Deterministic Function without the Knowledge of its Smoothness”. In: *Advances in Neural Information Processing Systems*. Vol. 24. Curran Associates, Inc., 2011. URL: https://proceedings.neurips.cc/paper/2011/hash/7e889fb76e0e07c11733550f2a6c7a5a-Abstract.html (visited on 12/18/2024).

[33] A. Nakib et al. “Deterministic metaheuristic based on fractal decomposition for large-scale optimization”. In: *Applied Soft Computing* 61 (Dec. 2017), pp. 468–485. ISSN: 1568-4946. DOI: 10.1016/j.asoc.2017.07.042. URL: https://www.sciencedirect.com/science/article/pii/S1568494617304623 (visited on 11/20/2024).

[34] *Numérique pour l’Exascale (NumPEx)*. fr. URL: https://anr.fr/fr/france-2030/programmes-et-equipements-prioritaires-de-recherche-pepr/numerique-pour-lexascale-numpex/ (visited on 11/25/2024).

[35] OpenAI et al. *GPT-4 Technical Report*. arXiv:2303.08774 [cs]. Mar. 2024. DOI: 10.48550/arXiv.2303.08774. URL: http://arxiv.org/abs/2303.08774 (visited on 12/13/2024).

[36] Erick G. G. de Paz et al. “A Regression Tree as Acquisition Function for Low-Dimensional Optimisation”. en. In: *Pattern Recognition*. Ed. by Efrén Mezura-Montes et al. Cham: Springer Nature Switzerland, 2024, pp. 23–33. ISBN: 978-3-031-62836-8. DOI: 10.1007/978-3-031-62836-8_3.

[37] Hieu Pham et al. *Efficient Neural Architecture Search via Parameter Sharing*. arXiv:1802.03268. Feb. 2018. DOI: 10.48550/arXiv.1802.03268. URL: http://arxiv.org/abs/1802.03268 (visited on 11/25/2024).

[38] *Plan Calcul*. fr. Page Version ID: 218696510. Sept. 2024. URL: https://fr.wikipedia.org/w/index.php?title=Plan_Calcul&oldid=218696510 (visited on 11/25/2024).

[39] Colin Raffel et al. “Exploring the Limits of Transfer Learning with a Unified Text-to-Text Transformer”. In: *Journal of Machine Learning Research* 21.140 (2020), pp. 1–67. ISSN: 1533-7928. URL: http://jmlr.org/papers/v21/20-074.html (visited on 12/17/2024).

[40] Mohaimenul Azam Khan Raiaan et al. “A Review on Large Language Models: Architectures, Applications, Taxonomies, Open Issues and Challenges”. In: *IEEE Access* 12 (2024), pp. 26839–26874. ISSN: 2169-3536. DOI: 10.1109/ACCESS.2024.3365742. URL: https://ieeexplore.ieee.org/document/10433480/ (visited on 12/17/2024).

[41] Waseem Rawat and Zenghui Wang. “Deep Convolutional Neural Networks for Image Classification: A Comprehensive Review”. In: *Neural Computation* 29.9 (Sept. 2017). Conference Name: Neural Computation, pp. 2352–2449. ISSN: 0899-7667. DOI: 10.1162/neco_a_00990. URL: https://ieeexplore.ieee.org/abstract/document/8016501 (visited on 12/17/2024).

[42] Bobak Shahriari et al. “Taking the Human Out of the Loop: A Review of Bayesian Optimization”. In: *Proceedings of the IEEE* 104.1 (Jan. 2016). Conference Name: Proceedings of the IEEE, pp. 148–175. ISSN: 1558-2256. DOI: 10.1109/JPROC.2015.2494218. URL: https://ieeexplore.ieee.org/abstract/document/7352306/authors#authors (visited on 12/13/2024).

[43] Nitish Srivastava et al. “Dropout: A Simple Way to Prevent Neural Networks from Overfitting”. en. In: (2014).

[44] El-Ghazali Talbi. “Parallel Evolutionary Combinatorial Optimization”. en. In: *Springer Handbook of Computational Intelligence*. Ed. by Janusz Kacprzyk and Witold Pedrycz. Berlin, Heidelberg: Springer Berlin Heidelberg, 2015, pp. 1107–1125. ISBN: 978-3-662-43504-5 978-3-662-43505-2. DOI: 10.1007/978-3-662-43505-2_55. URL: http://link.springer.com/10.1007/978-3-662-43505-2_55 (visited on 11/20/2024).

[45] El-Ghazali Talbi. “Automated Design of Deep Neural Networks: A Survey and Unified Taxonomy”. In: *ACM Comput. Surv.* 54.2 (Mar. 2021), 34:1–34:37. ISSN: 0360-0300. DOI: 10.1145/3439730. URL: https://dl.acm.org/doi/10.1145/3439730 (visited on 11/20/2024).

[46] El-Ghazali Talbi. “Metaheuristics for variable-size mixed optimization problems: A unified taxonomy and survey”. In: *Swarm and Evolutionary Computation* 89 (Aug. 2024), p. 101642. ISSN: 2210-6502. DOI: 10.1016/j.swevo.2024.101642. URL: https://www.sciencedirect.com/science/article/pii/S2210650224001809 (visited on 11/20/2024).

[47] Hugo Touvron et al. *LLaMA: Open and Efficient Foundation Language Models*. arXiv:2302.13971 [cs]. Feb. 2023. DOI: 10.48550/arXiv.2302.13971. URL: http://arxiv.org/abs/2302.13971 (visited on 12/18/2024).

[48] Christophe Tribes et al. *Hyperparameter Optimization for Large Language Model Instruction-Tuning*. arXiv:2312.00949. Jan. 2024. DOI: 10.48550/arXiv.2312.00949. URL: http://arxiv.org/abs/2312.00949 (visited on 11/20/2024).

[49] Ashish Vaswani et al. "Attention is All you Need". In: *Advances in Neural Information Processing Systems*. Vol. 30. Curran Associates, Inc., 2017. URL: https://papers.nips.cc/paper_files/paper/2017/hash/3f5ee243547dee91fbd053c1c4a845aa-Abstract.html (visited on 11/20/2024).

[50] Ziyu Wang et al. *Bayesian Multi-Scale Optimistic Optimization*. arXiv:1402.7005 [stat]. Feb. 2014. URL: http://arxiv.org/abs/1402.7005 (visited on 11/20/2024).

[51] Jason Wei et al. *Finetuned Language Models Are Zero-Shot Learners*. arXiv:2109.01652 [cs]. Feb. 2022. URL: http://arxiv.org/abs/2109.01652 (visited on 11/20/2024).

[52] *What is quality control (QC)?* en. URL: https://www.techtarget.com/whatis/definition/quality-control-QC (visited on 12/18/2024).

[53] James Wilson et al. "Efficiently sampling functions from Gaussian process posteriors". en. In: *Proceedings of the 37th International Conference on Machine Learning*. ISSN: 2640-3498. PMLR, Nov. 2020, pp. 10292–10302. URL: https://proceedings.mlr.press/v119/wilson20a.html (visited on 01/07/2025).

[54] Yonghui Wu et al. *Google's Neural Machine Translation System: Bridging the Gap between Human and Machine Translation*. arXiv:1609.08144. Oct. 2016. DOI: 10.48550/arXiv.1609.08144. URL: http://arxiv.org/abs/1609.08144 (visited on 11/20/2024).

[55] Rowan Zellers et al. *HellaSwag: Can a Machine Really Finish Your Sentence?* arXiv:1905.07830 [cs]. May 2019. DOI: 10.48550/arXiv.1905.07830. URL: http://arxiv.org/abs/1905.07830 (visited on 12/05/2024).

[56] G.P. Zhang. "Neural networks for classification: a survey". In: *IEEE Transactions on Systems, Man, and Cybernetics, Part C (Applications and Reviews)* 30.4 (Nov. 2000). Conference Name: IEEE Transactions on Systems, Man, and Cybernetics, Part C (Applications and Reviews), pp. 451–462. ISSN: 1558-2442. DOI: 10.1109/5326.897072. URL: https://ieeexplore.ieee.org/abstract/document/897072 (visited on 12/17/2024).

[57] Zhilu Zhang and Mert Sabuncu. "Generalized Cross Entropy Loss for Training Deep Neural Networks with Noisy Labels". In: *Advances in Neural Information Processing Systems*. Vol. 31. Curran Associates, Inc., 2018. URL: https://proceedings.neurips.cc/paper/2018/hash/f2925f97bc13ad2852a7a551802feea0-Abstract.html (visited on 12/17/2024).

⋆ ⋆ ⋆

Chapter A
Appendix

A.1 Bayesian Multi Scale Optimistic Optimization (BaMSOO) algorithm

Algorithm A.1: BamSOO

Input: Ω,f,K,$n_{\max}$,K_D:

$x_{0,0} \leftarrow \text{center}(\Omega)$
$g_{0,0} \leftarrow f(x_{0,0})$
$\mathcal{T}_1 \leftarrow \{x_{0,0}, g_{0,0}, \Omega\}$ // Initiate the tree
$f^+ \leftarrow g_{0,0}$
$n \leftarrow 1$,$t \leftarrow 1$ // nodes and evaluation index
$\mathcal{D}_1 \leftarrow \{x_{0,0}, g_{0,0}\}$ // list of evaluated points
while $t < n_{max}$ **do**
  $\nu_{\max} \leftarrow -\infty$
  for $h \leftarrow 0$ **to** $depth(\mathcal{T}_n)$ **do**
    $j \leftarrow \arg\max_{j \in \{j|(h,j)\in L_n\}} g_{h,j}$
    if $g_{h,j} > \nu_{max}$ **then**
      $\Omega_{h+1,j+1}, \ldots, \Omega_{h+1,j+K} \leftarrow \text{section}(\Omega_{h,j}, K)$
      for $i \leftarrow 1$ **to** K **do**
        $\mu, \sigma \leftarrow \text{GP}(\mathcal{D}_t, K_D)$ // update_gp function
        $N \leftarrow N + 1$
        $x_{h+1,j+i} \leftarrow \text{center}(\Omega_n)$
        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
        $n \leftarrow n + 1$
        $\mathcal{T}_n \leftarrow \{(x_{h+1,j+i}, f_{h+1,j+i}, \Omega_{h+1,j+i})\}$
      end
      $\nu_{\max} \leftarrow g_{h,j}$
    end
  end
end
return best of $x_{h,j}, g(x_{h,j})$

A.2 Internship offer

Internship: Optimization and fine tuning of LLM (Large Langage Models)

Supervisor: Prof. E-G. Talbi
INRIA & University of Lille
Contact: el-ghazali.talbi@univ-lille.fr

This internship will be carried out in the framework of the PEPR (Programme et Equipement Prioritaire de Recherche Numpex (Exama project).

Context

Many scientific and industrial disciplines are concerned by big optimization problems (BOPs). The goal of this work is to come up with breakthrough in optimization algorithms on LLMs (Large Language Models) composed of trillions of parameters. The convergence between optimization algorithms and generative AI is an important in AI and High Performance Computing (HPC).

Inference with Large Language Models is costly and often dominates the life cycle cost of LLM-based services. Naural Architecture Search (NAS) can automatically find architectures optimizing the tradeoffs between accuracy and inference cost.

Roadmap

NAS for LLMs architectures is computationally prohibitive.

In this work, we will investigate the use of efficient optimization algorithms (example: parallel fractal optimization) to reduce the latency of real-world commercial web-scale text prediction system. The goal of this work is to solve the NAS problem to find an architecture that when trained with data D and training algorithm A, produces a model that has similar accuracy but significantly reduced latency.

The tasks composting this work are summarized below:

- Modeling and analysis of the NAS problem
- Solving of the problem using original and high-performance optimization algorithms
- Application to well known LLM such as GPT

Location: INRIA Lille

References

[1] T. Firmin, E-G. Talbi, «A framework for fractal based optimization", 2024.
[2] Raiaan, M. A. K., et al. (2024). A review on large Language Models: Architectures, applications, taxonomies, open issues and challenges. *IEEE Access*.
[3] Javaheripi, M., et al. (2022). Litetransformersearch: Training-free neural architecture search for efficient language models. *Advances in Neural Information Processing Systems*, *35*, 24254-24267.
[4] Javaheripi, Mojan, et al. "Litetransformersearch: Training-free neural architecture search for efficient language models." *Advances in Neural Information Processing Systems* 35 (2022): 24254-24267.
[5] E-G. Talbi, "Metaheuristics: from design to implementation", *Wiley*, 2009.

A.3 Latin Hypercube Sampling (LHS) algorithm

Algorithm A.2: Latin Hypercube Sampling Algorithm

Input: Number of samples N, Number of dimensions D
Output: $N \times D$ matrix of sampled points

Initialize an empty matrix M of size $N \times D$
for *each dimension* $i \in \{1, 2, \ldots, D\}$ **do**
    Divide the range $[0, 1]$ into N equally spaced intervals
    Shuffle the interval indices randomly
    for *each sample* $j \in \{1, 2, \ldots, N\}$ **do**
        Pick a random value x within the j-th interval
        Assign x to $M[j][i]$
    end
end
return M

Contents