Large Language Model for Automatic Algorithm Design

Fei Liu, Zhichao Lu, Zhenkun Wang, and Qingfu Zhang

1 A Brief Introduction of the Topic

Algorithm design plays a pivotal role in computational optimization and decision-making. Traditionally, this process has been characterized by intensive trial-and-error methodologies, heavily reliant on deep domain expertise. The emergence and rapid advancement of Large Language Models (LLMs) over the past three years have revolutionized numerous fields, including algorithm design. The integration of LLMs into the algorithm design process, referred to as LLM for Algorithm Design (LLM4AD), has shown promising results in enhancing and automating complex algorithm design tasks [1-11].

Among existing LLM4AD works, Evolutionary Computation (EC) has gained much attention. This exploration has been carried out on two sides: 1) the use of LLMs to design EC algorithms [6,8,9,10], and 2) the application of LLMs within an EC framework to develop algorithms [1,2,3,4,5,11].

This tutorial is designed to offer an introduction to the fundamentals, developments, and practical applications of LLM4AD, particularly emphasizing its applications with/for EC. Attendees will gain insights into how LLMs can be leveraged to streamline and enhance the algorithm design process across various domains.

2 An Outline of the Tutorial

The tutorial will be structured into three main sections, each designed to build upon the previous, ensuring a cohesive learning experience:

- **Introduction to LLM-based Algorithm Design** (60 mins)
    - Introduction to the capabilities and functionalities of LLMs in algorithm design.
    - Single-objective evolutionary optimization with LLMs for algorithm design.
    - Multi-objective evolutionary optimization with LLMs for algorithm design.
- **Applications and Case Studies** (30 mins)
    - Design of single- and multi-objective continuous optimization algorithms using LLMs.
    - Design of combinatorial optimization algorithms using LLMs, focusing on real-world applications such as routing and scheduling.
    - Design of reinforcement learning agents via LLMs, demonstrating adaptive strategies in dynamic environments.
- **Code Demonstrations and Hands-on Sessions** (30 mins)
    - An introduction to LLM4AD, a Python-based algorithm design platform using LLMs.
    - Code demonstrations hosted on Google Colab, providing participants with practical experience in implementing LLM4AD solutions.
    - Step-by-step guidance on applying LLM4AD to the discussed application cases, enabling attendees to explore the potential of LLMs in real time.

3 Expected Length of the Tutorial

Two hours

4 Level of the Tutorial

Introductory

5   Reference

[1] **Fei Liu**, Xialiang Tong, Mingxuan Yuan, Xi Lin, Fu Luo, **Zhenkun Wang**, **Zhichao Lu**, and **Qingfu Zhang**. Evolution of Heuristics: Towards Efficient Automatic Algorithm Design Using Large Language Model. In Forty-first International Conference on Machine Learning (ICML). 2024.

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[3] Rui Zhang, **Fei Liu**, Xi Lin, **Zhenkun Wang**, **Zhichao Lu**, and **Qingfu Zhang**. Understanding the Importance of Evolutionary Search in Automated Heuristic Design with Large Language Models. In International Conference on Parallel Problem Solving from Nature (PPSN), pp. 185-202. 2024.

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[5] Ping Guo, **Fei Liu**, Xi Lin, Qingchuan Zhao, and **Qingfu Zhang**. L-AutoDA: Large Language Models for Automatically Evolving Decision-based Adversarial Attacks. In Proceedings of the Genetic and Evolutionary Computation Conference (GECCO) Companion, pp. 1846-1854. 2024.

[6] Yuxiao Huang, Shenghao Wu, Wenjie Zhang, Jibin Wu, Liang Feng, and Kay Chen Tan. Autonomous Multi-objective Optimization using Large Language Model. arXiv preprint arXiv:2406.08987. 2024.

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[8] Shengcai Liu, Caishun Chen, Xinghua Qu, Ke Tang, and Yew-Soon Ong. Large language models as evolutionary optimizers. In 2024 IEEE Congress on Evolutionary Computation (CEC). 2024.

[9] Niki van Stein, and Thomas Bäck. LLaMEA: A Large Language Model Evolutionary Algorithm for Automatically Generating Metaheuristics. arXiv preprint arXiv:2405.20132. 2024.

[10] **Fei Liu**, Xi Lin, **Zhenkun Wang**, Shunyu Yao, Xialiang Tong, Mingxuan Yuan, and **Qingfu Zhang**. Large Language Model for Multi-objective Evolutionary Optimization. The International Conference on Evolutionary Multi-Criterion Optimization (EMO). 2025.

[11] Shunyu Yao, **Fei Liu**, Xi Lin, **Zhichao Lu**, **Zhenkun Wang**, and **Qingfu Zhang**. Multi-objective Evolution of Heuristic Using Large Language Model. The 39th Annual AAAI Conference on Artificial Intelligence (AAAI). 2025.

6   Name and Brief Biography of the Organizers

6.1   Orgnizers

Name	Title	Affiliation	Email
Fei Liu	Postdoctoral Researcher	City University of Hong Kong	fliu36-c@my.cityu.edu.hk
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Qingfu Zhang	Chair Professor	City University of Hong Kong	qingfu.zhang@cityu.edu.hk

6.2   Biographies

Fei Liu is a Postdoctoral Researcher at the Department of Computer Science, City University of Hong Kong, Hong Kong. He received his BSc degree and MSc degrees from Northwestern Polytechnical University, China in 2017 and 2020, and Ph.D. degree from the Department of Computer Science, City University of Hong Kong, Hong Kong in 2024. His main research interests include computational intelligence, optimization, and their applications. More information is available at https://feiliu36.github.io/.

Zhichao Lu is an Assistant Professor at the Department of Computer Science, City University of Hong Kong, Hong Kong. He received bachelor's and Ph.D. degrees in electrical and computer engineering from Michigan State University, East Lansing, MI, USA, in 2013 and 2020, respectively. His current research focuses on the intersections of evolutionary computation, learning, and optimization, notably on developing efficient, reliable, and automated machine learning algorithms and systems. He received the GECCO2019 best paper award. More information is available at https://www.cs.cityu.edu.hk/ zhichalu/.

Zhenkun Wang is an Assistant Professor with the School of System Design and Intelligent Manufacturing, Southern University of Science and Technology, Shenzhen, China. He received the Ph.D. degree in circuits and systems from Xidian University, Xi'an, China, in 2016. From 2017 to 2020, he was a Postdoctoral Research Fellow with the School of Computer Science and Engineering, Nanyang Technological University, Singapore, and with the Department of Computer Science, City University of Hong Kong, Hong Kong. His research interests include evolutionary computation, optimization, machine learning, and their applications. More information is available at https://faculty.sustech.edu.cn/?tagid=wangzk3.

Qingfu Zhang is a Chair Professor at the Department of Computer Science, City University of Hong Kong, Hong Kong. His main research interests include evolutionary computation, optimization, neural network, data analysis, and their applications. Prof. Zhang has been a highly cited researcher in computer science since 2016. More information is available at https://www.cs.cityu.edu.hk/ qzhan7/index.html.