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ABSTRACT

LLaMEA: Automatically Generating Metaheuristics with Large Language Models

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LLaMEA: Automatically Generating Metaheuristics with Large Language Models

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ABSTRACT

This paper summarizes our recent work published in IEEE Transactions on Evolutionary Computation (2025), entitled “LLaMEA: A Large Language Model Evolutionary Algorithm for Automatically Generating Metaheuristics”. In this work we propose a novel evolutionary algorithm framework that leverages large language models (LLMs) like GPT-4 to automatically generate, evaluate, and refine metaheuristic optimization algorithms. Evaluations on the BBOB benchmark suite demonstrate that algorithms automatically discovered by LLaMEA can outperform established state-of-the-art methods, such as CMA-ES and DE, especially on lower-dimensional optimization problems. Our results illustrate the significant potential of using LLMs for automated algorithm design, setting a new direction for evolutionary computation research.

CCS CONCEPTS

• **Computing methodologies** → *Artificial intelligence*; • **Theory of computation** → **Continuous optimization**; **Bio-inspired optimization**; **Design and analysis of algorithms**.

KEYWORDS

Large Language Models, Evolutionary Computation, Metaheuristics, Optimization, Code Generation, Automated Algorithm Discovery

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1 INTRODUCTION

Meta-heuristics, inspired by natural processes like biological evolution or swarm behaviour, have traditionally been manually designed through expert knowledge and experimentation [1]. This manual design is often inefficient, resource-intensive, and can result in incremental improvements rather than genuine innovation. Recent advances in machine learning, specifically large language models

(LLMs) such as GPT-4 [6], have demonstrated substantial capabilities in automated code generation, suggesting their potential for algorithm design automation. However, utilizing these models effectively in evolutionary computation presents significant challenges, including reliably translating natural language prompts into executable, performant code, automatically managing runtime errors, and effectively evaluating and refining generated algorithms.

In response to these challenges, we introduce LLaMEA [8], a novel evolutionary algorithm framework that systematically leverages the generative capabilities of LLMs. By integrating automated evaluation tools and automatic debugging feedback, our approach transforms algorithm design into an iterative evolutionary process, effectively navigating the complex space of meta-heuristic designs.

2 THE LLAMEA FRAMEWORK

LLaMEA operates as a fully automated evolutionary loop comprising algorithm generation, evaluation, mutation, and selection steps. Initially, an LLM generates a candidate metaheuristic based on a detailed natural language task description and a minimal code example. Generated code is executed dynamically within a controlled runtime environment, designed to automatically capture and handle syntax or runtime errors. Algorithm performance is systematically evaluated using IOHexperimenter [2], a robust benchmarking platform for optimization heuristics. Specifically, algorithms are assessed across the well-established BBOB benchmark suite [4] using the Area Over the Convergence Curve (AOCC) metric [5], which provides a measure of performance over the entire run (any-time performance).

LLaMEA employs a (1+1) evolutionary strategy, where each iteration generates one offspring algorithm from the current best-performing algorithm. If the offspring algorithm achieves improved performance, it replaces the parent, guiding iterative improvement toward optimal solutions. The evolutionary loop is maintained through continuous feedback from evaluation results to the LLM, enabling refined or significantly altered algorithm designs in subsequent iterations. This feedback loop not only corrects technical flaws but also drives algorithmic innovation by prompting the LLM to explore novel components and parameter settings.

3 EXPERIMENTAL RESULTS

On 5-dimensional BBOB benchmarks [4], LLaMEA-generated algorithms achieved performance surpassing CMA-ES [3] and DE [7]. Notably, the best algorithm found by LLaMEA consistently outperformed standard and optimized baseline algorithms, highlighting the practical effectiveness of LLaMEA.

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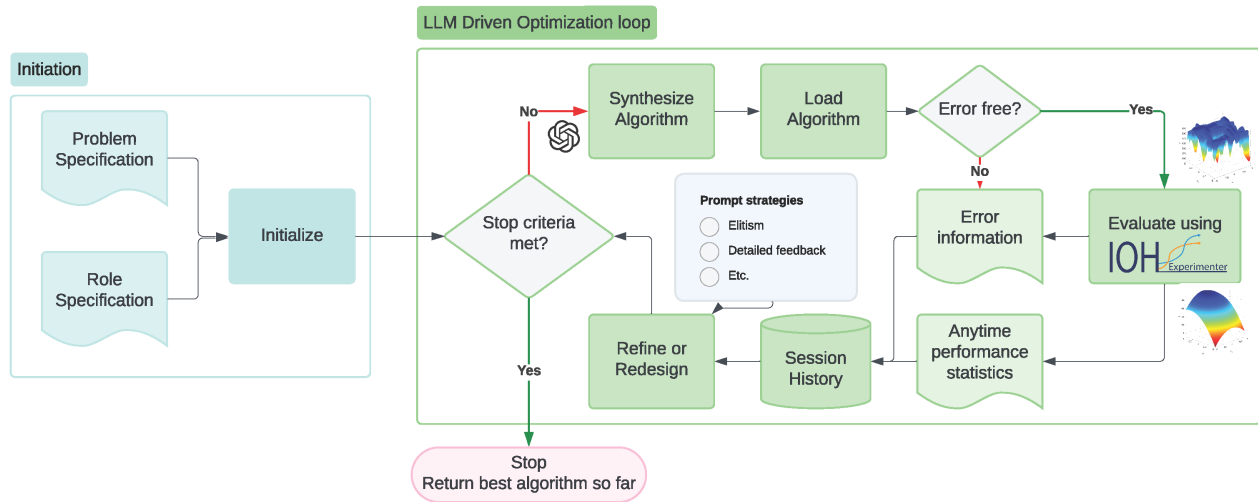


Figure 1: The proposed LLM driven algorithm discovery framework LLaMEA. From [8]

4 CONCLUSIONS

LLaMEA represents a significant advancement toward automated, efficient, and high-performing metaheuristic design. Key insights include:

- Successful automated generation of competitive optimization algorithms with minimal human intervention.
- Demonstration of robust generalization potential, particularly in lower-dimensional optimization scenarios.
- Highlighting novel algorithmic components and combinations discovered autonomously by the framework.

However, LLaMEA also has some limitations, including:

- Dependence on the quality and clarity of the initial prompts provided to the LLM.
- Potential scalability issues when applied to higher-dimensional and more complex optimization problems.
- Dependence on the quality of the LLM used.

Future research will focus on expanding LLaMEA’s capabilities to higher dimensions, to solve real-world problems and to solve problems in other domains such as automated machine learning. LLaMEA follow-up studies have already included controlling the mutation rate in LLaMEA using prompt optimization [10], exploiting problem domain specific information to efficiently solve real-world physics problems [11], and in-the-loop hyper-parameter optimization [9].

REPRODUCIBILITY STATEMENT

We provide an open-source documented implementation of our package at Github¹, including install and how-to-use guide.

¹<https://github.com/XAI-liacs/LLaMEA>

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