HANOI UNIVERSITY OF SCIENCE AND TECHNOLOGY

GRADUATION THESIS

Evolutionary Computation and Large Language Model for Automatic Heuristics Design

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ABSTRACT

Automatic Heuristic Design (AHD) is an active research area due to its utility in solving complex search and NP-hard combinatorial optimization problems in the real world. Recent advances in Large Language Models (LLMs) introduce new possibilities by coupling LLMs with Evolutionary Computation (EC) to automatically generate heuristics, known as LLM-based Evolutionary Program Search (LLM-EPS). While previous LLM-EPS studies obtained great performance on various tasks, there is still a gap in understanding the properties of heuristic search spaces and achieving a balance between exploration and exploitation, which is a critical factor in large heuristic search spaces. This research addresses this gap by proposing two diversity measurement metrics and performing an analysis of previous LLM-EPS approaches, including FunSearch, EoH, and ReEvo. Results on black-box AHD problems reveal that while EoH demonstrates higher diversity than FunSearch and ReEvo, its objective score is unstable. Conversely, ReEvo's reflection mechanism yields good objective scores but fails to optimize diversity effectively. In light of these findings, HSEvo was introduced as an adaptive LLM-EPS framework that strikes a balance between diversity and convergence through the use of a harmony search algorithm. Experimentation demonstrated that HSEvo achieved high diversity indices and good objective scores while remaining cost-effective. These results underscore the importance of balancing exploration and exploitation and understanding heuristic search spaces in designing frameworks in LLM-EPS.

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LIST OF ABBREVIATIONS

Abbreviation	Definition
ACO	Ant Colony Optimization
AHD	Automatic Heuristic Design
AI	Artificial Intelligence
BPO	Bin Packing Online
CDI	Cumulative Diversity Index
COPs	Combinatorial Optimization Problems
EC	Evolutionary Computation
EP	Evolutionary Programming
ES	Evolution Strategies
GA	Genetic Algorithm
GLS	Guided Local Search
GP	Genetic Programming
HHs	Hyper-Heuristics
HS	Harmony Search
LLM-EPS	LLM-based Evolutionary Program Search
LLMs	Large Language Models
MST	Minimum Spanning Tree
NCO	Neural Combinatorial Optimization
OP	Orienteering Problem
SDI	Shannon Diversity Index
SWDI	Shannon-Wiener Diversity Index
TSP	Traveling Salesman Problem

INTRODUCTION

NP-hard Combinatorial Optimization Problems (COPs) frequently arise in real-world scenarios. Examples include groups of problems such as routing and logistics, scheduling and planning, network design, and others. To address these problems, heuristic methods are among the most commonly employed approaches due to their superior efficiency in terms of time and resources needed to find solutions that approximate the optimal. Over the past few decades, significant efforts have been dedicated to designing effective search methods, resulting in techniques such as simulated annealing, tabu search, and iterated local search, among many others. These manually crafted methods have been successfully applied in numerous real-world applications.

However, due to the diverse nature of practical problems, each application comes with its constraints and objectives, often requiring customization or the selection of specific search methods tailored to the situation at hand. Manually creating, tuning, and configuring search methods for particular problems is not only labor-intensive but also demands deep expertise. This represents a bottleneck in many application domains. Consequently, AHD has emerged as a promising solution, aiming to automate the selection, tuning, or construction of efficient search methods for specific classes of problems.

The goal of AHD is to address the difficulties involved in the creation of manual heuristics by utilizing computational methods to automatically generate or enhance heuristics. Among the various approaches within AHD, both Hyper-Heuristics (HHs) [1], [2] and Neural Combinatorial Optimization (NCO) [3]–[5] have gained substantial attention for their potential to address the limitations of traditional heuristic development.

HHs operate within predefined heuristic spaces curated by human experts, selecting or generating heuristics from these established sets. While HHs have demonstrated success, their performance is inherently limited by the scope and quality of the predefined heuristic space, often restricting the discovery of novel or more effective heuristics.

On the other hand, NCO employs neural networks to learn patterns and predict solutions for COPs. By leveraging data-driven models, NCO seeks to generalize across problem instances, offering a more dynamic approach to heuristic development. Despite its promise, NCO faces significant challenges. Effective generalization across diverse problem instances requires robust inductive biases [6], which