LLMs for Automated Algorithm Design

Lars Kotthoff
lk223@st-andrews.ac.uk
University of St Andrews
University of Wyoming

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Algorithm

High-level, language-independent description of step-by-step process for solving a problem.

Algorithm

High-level, language-independent description of step-by-step process for solving a problem.

And its implementation.

Algorithm Design

- Kingma, Diederik P., and Jimmy Ba. "Adam: A Method for Stochastic Optimization." In Proceedings of the 3rd International Conference on Learning Representations (ICLR). San Diego, CA, 2015 (>250,000 citations)
- Breiman, Leo. "Random Forests." Machine Learning 45, no. 1 (2001): 5–32. (>200,000 citations)
- Davis, Martin, George Logemann, and Donald Loveland. "A Machine Program for Theorem-Proving." Communications of the ACM 5 (7) (1962): 394–397. (>5,000 citations)
- ...

Algorithm Design

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- ...

Can we automate this?

Automated Algorithm Design

"[...]a constraint solver generator will be developed that, given a constraint model, will produce a highly-optimised constraint solver tailored to that model[...]"

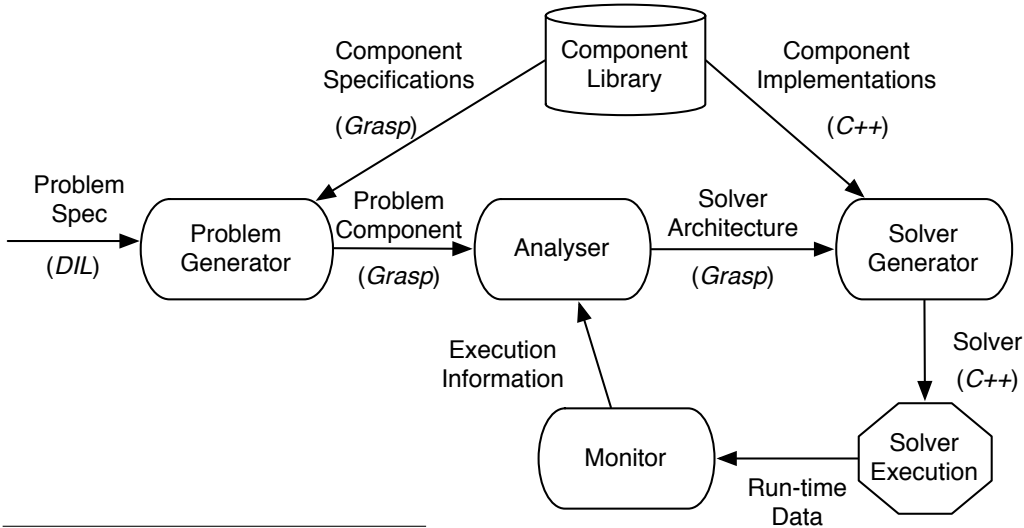
Automated Algorithm Design

"[...]a constraint solver generator will be developed that, given a constraint model, will produce a highly-optimised constraint solver tailored to that model[...]"

My PhD proposal, 2008.



Automated Algorithm Design Stone Age – Dominion



Dharini Balasubramaniam et al., "An Automated Approach to Generating Efficient Constraint Solvers," 34th International Conference on Software Engineering, June 2012, 661–71.

Automated Algorithm Design Stone Age

- Steven Minton, "Automatically Configuring Constraint Satisfaction Programs: A Case Study," Constraints 1 (1996): 7–43.
- Douglas R. Smith, "KIDS - A Knowledge-Based Software Development System," Automating Software Design, 1990, 483–514.
- David Jack Mostow, "Machine Transformation of Advice into a Heuristic Search Procedure," in Machine Learning, ed. Ryszard S. Michalski et al. (Morgan Kaufmann, 1983), https://doi.org/10.1016/B978-0-08-051054-5.50016-9.

Programming by Optimization

Levels of PbO:

Level 4: Make no design choice prematurely that cannot be justified compellingly.



Level 3: Strive to provide design choices and alternatives.



Level 2: Keep and expose design choices considered during software development.



Level 1: Expose design choices hardwired into existing code (magic constants, hidden parameters, abandoned design alternatives).



Level 0: Optimise settings of parameters exposed by existing software.



Holger H. Hoos, "Programming by Optimization," Communications of the Association for Computing Machinery (CACM) 55, no. 2 (2012): 70–80, https://doi.org/10.1145/2076450.2076469.

Automated Algorithm Design Stone Age – Problems

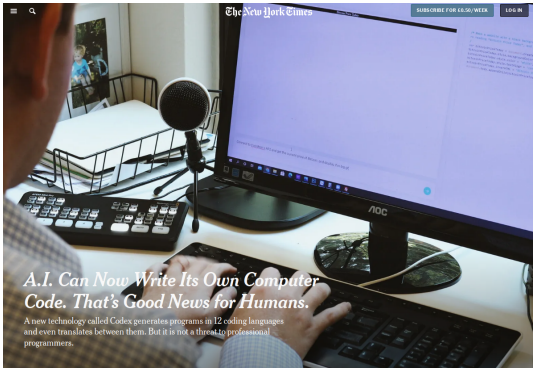
- ▷ generic and customisable systems are difficult to engineer
- ▷ design choices are hard to provide
- ▷ potentially lots of code necessary
- ▷ doesn't always improve...

Automated Algorithm Design Stone Age – Problems

- ▷ generic and customisable systems are difficult to engineer
- ▷ design choices are hard to provide
- ▷ potentially lots of code necessary
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Maybe this won't work in practice after all...

A New Hope



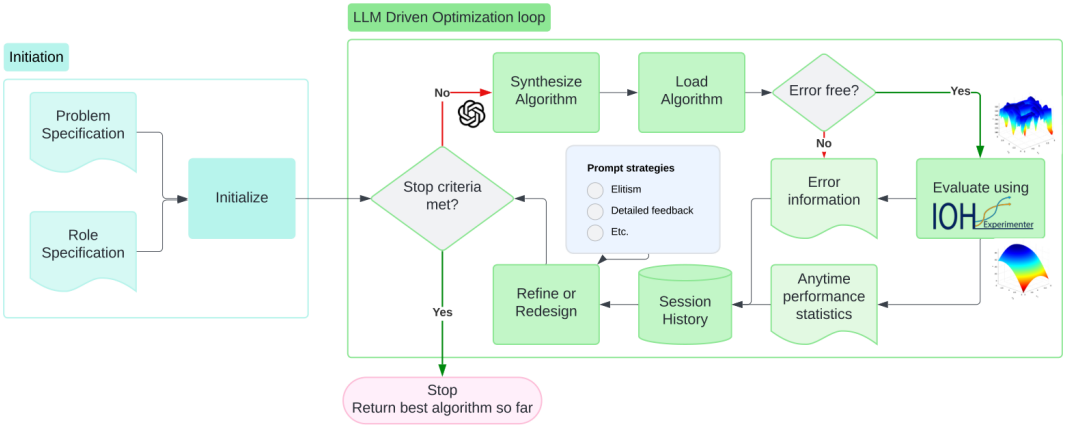
09 September 2021



LLM-Based Automated Algorithm Design

- ▷ Fei Liu et al., "Evolution of Heuristics: Towards Efficient Automatic Algorithm Design Using Large Language Model," Proceedings of the 41st International Conference on Machine Learning (Vienna, Austria), ICML'24, 2024.
- ▷ Bernardino Romera-Paredes et al., "Mathematical Discoveries from Program Search with Large Language Models," Nature 625, no. 7995 (2024): 468–75, https://doi.org/10.1038/s41586-023-06924-6.
- ▷ Niki van Stein and Thomas Bäck, "LLaMEA: A Large Language Model Evolutionary Algorithm for Automatically Generating Metaheuristics," IEEE Transactions on Evolutionary Computation 29, no. 2 (2025): 331–45, https://doi.org/10.1109/TEVC.2024.3497793.
- ▷ Yiwen Sun et al., "AutoSAT: Automatically Optimize SAT Solvers via Large Language Models," J. Artif. Int. Res. (El Segundo, CA, USA) 86 (July 2026), https://doi.org/10.1613/jair.1.20499.

LLM-Based Automated Algorithm Design



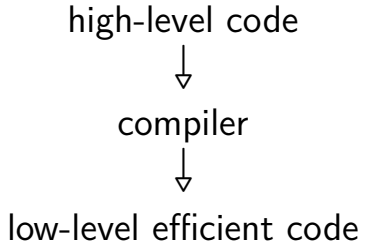
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LLM-Based Automated Algorithm Design

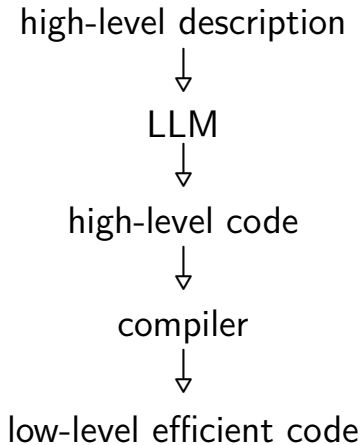
- ▷ code can be generated to solve particular problem
- ▷ can easily iterate to improve performance
- ▷ no need for algorithm to generalise

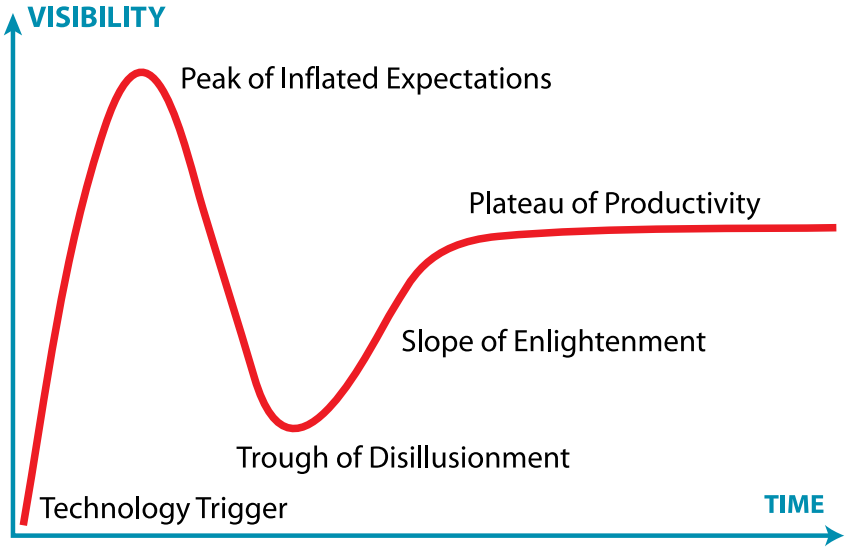
⟶ "ephemeral" implementations

We've Been There Before...

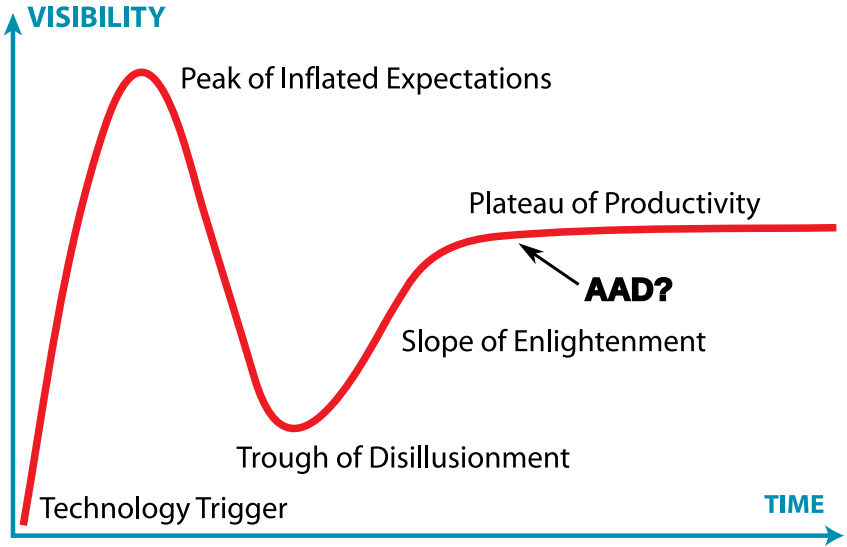


We've Been There Before...





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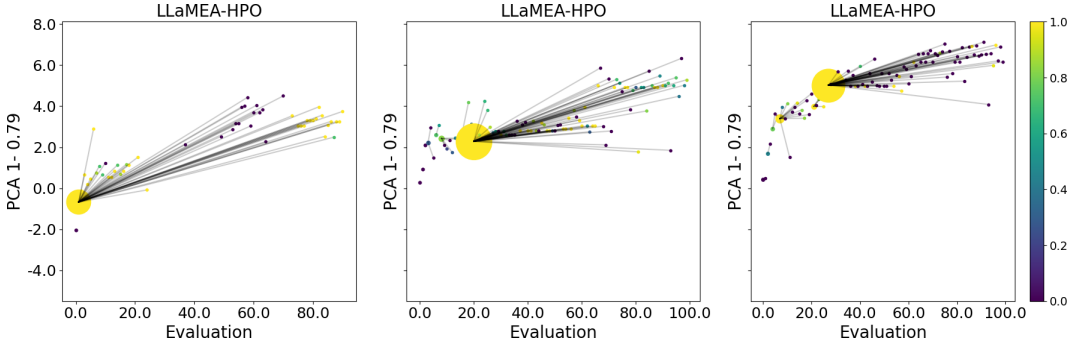
Related – Automated Verification

- more confidence that (generated) code implements the right thing
- more useful signals for LLMs to improve code
- potential for virtuous cycle

Challenges for LLM-Based Automated Algorithm Design

- cost/resource requirements
- technical debt/explanations
- guiding LLMs/agentic frameworks

Code Features for Explanations and Guidance



Niki van Stein et al., "Code Evolution Graphs: Understanding Large Language Model Driven Design of Algorithms," Genetic and Evolutionary Computation Conference (GECCO), 2025.


Thank you!
AUTOMATED ALGORITHM DESIGN SYSTEM
INPUT:
Problem Definition & Data
Dataset
Graph
Objectives
Problem Input
AI-DRIVEN GENERATION ENGINE
AI Generation Engine
SEARCH & OPTIMIZATION
Exploration
Evaluation
Iteration
Genetic Algorithms
Machine Learning
Genetic Algorithms
Genetic Algorithms
Machine Models
Genetic Algorithms
Optimization Loop
DESIGNED ALGORITHMS
Efficient
Scalable
Optimized
Efficient
Scalable
Optimized
Efficient
Graph Algorithms
Neural Architecture