LLaMEA Fully-automatic design of optimisation algorithms



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Discover the world at Leiden University

LLaMEA Framework



van Stein, N., & Bäck, T. (2024). LLaMEA: A large language model evolutionary algorithm for automatically generating metaheuristics. *IEEE Transactions on Evolutionary Computation*.

LLaEA in Detail



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Human Competitive

 Beating a highly tuned modular CMA-ES and other baselines on BBOB 5d, with good performance in higher dimensions.



---- ADEM ---- AdaptiveDifferentialEvolutionHarmonySearch --- AdaptiveHybridCMAESDE ---- CMA ---- CMA ---- CMA ---- CMA

- ----- ERADS_QuantumFluxUltraRefined --- EnhancedFireworkAlgorithmWithLocalSearch
- ---- QuantumDifferentialParticleOptimizerWithElitism

Human Competitive

- Beating a highly tuned modular CMA-ES and other baselines on BBOB 5d, with good performance in higher dimensions.
- Beating expert humans on a variety of real-world **Photonics** problems. Showing great generalization power to larger problem instances. (lower is better)

Optimization of photonic structures plays a key role in the advancement of technologies in various fields such as solar energy and materials science.



Human Competitive

- Beating a highly tuned modular CMA-ES and other baselines on BBOB 5d, with good performance in higher dimensions.
- Beating expert humans on a variety of real-world Photonics problems.
 Showing great generalization power to larger problem instances.
- Winning the Many-Affine BBOB competition GECCO 2024.



Why It Beats Humans

- LLMs can exploit domain-knowledge and coding-knowledge. ullet
- Evolutionary Search enables LLMs to ground the generated solutions with evaluations and steer the code-level-search. ۲

Key-innovations: ۲

• **Self-debugging:** The LLM receives feedback on syntax and runtime errors. Solves most fatal errors.

- *Instance-based* **Any-time-performance** benchmarking drives broad generalisation.
- *Hybridised with* **HPO** \rightarrow 5× fewer LLM calls

With **LLaMEA**, **everyone** can design good optimizers **specific** to their problems

LLaMEA Framework



Human-Competitive Checklist

B. Better than peer reviewed result Beats TEVC-published CMA-ES, DE and others on full benchmarking suite.



E. Long standing problem Photonics problems are long studied and have recent domain-specific optimizers (that we beat).

G. Difficult problem Black-box optimization is GECCO's flagship benchmark. RWAs BBO such as photonics are NP-hard.

✓ H. Wins competition LLaMEA won the GECCO'24 competition on Any-time performance algorithm design.

Why choose us?



1. Generalizable results

LLaMEA has shown excellent performance in evolving algorithms for: - BBO, Bayesian and Combinatorial Optimization

2. Impact

Used for a variety of RWAs including Photonics.

- LLaMEA Already downloaded 4000+ times from pypi.

3. Accessibility

MIT-licensed GitHub repo. Fully documented and open-source.

4. Efficiency and modularity

Small LLM API budgets (~100) versus 4.5 million of DeepMind's FunSearch. Works with **any LLM** and multiple EC strategies.

Vision & Future

Methodology developments

- Benchmarking tooling for LLM-driven algorithm discovery (BLADE [1])
- Novel selection and code-diversity control mechanisms
- Etc.

Applications

- Evolving Bayesian Optimization algorithms (LLaMEA-BO, under review)
- Evolving AutoML methods
- **GPU kernel tuning** Speeding up GPU execution by 100%+ vs baseline (early results)
- **Domain specific solvers** Leveraging expert knowledge by prompting and RAG.

[1] van Stein, N., Kononova, A. V., Yin, H., & Bäck, T. (2025). BLADE: Benchmark suite for LLM-driven Automated Design and Evolution of iterative optimisation heuristics. *arXiv preprint arXiv:2504.20183*.



We leverage **LLMs** with **Evolutionary Computation** to out-design the field's best human algorithm designers and opened the tool-chain for everyone.





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