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Expolving programs through LLMs

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Bernardino Romera-Paredes

PPSN 2024

Discover new and verifiably correct algorithms outperforming SOTA results in impactful problems

Previously: AlphaTensor

Why searching in the program/function space?

Generality

● No Structure

Does not rely on existing structure for any specific problem.

● Universal Interface

Can be applied to any fundamental problems with solutions in programming language space

Interpretability

● Code Output

Output is a computer program which is *interpretable* plus much *faster* and *safer* to execute than a black box neural net.

Scalability

● Concise Representation

Scale to much larger instances of a problem as opposed to traditional search because search space scales better with problem dimensions.

Article | Open access | Published: 14 December 2023

Mathematical discoveries from program search with large language models

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Nature 625, 468-475 (2024) Cite this article

Can LLMs find and code algorithms?

Write a very efficient program in Python that finds largest independent sets in a sparse graph

Can LLMs find and code algorithms?

Write a very efficient program in Python that finds largest independent sets in a sparse graph

def find largest independent sets (graph): ""Finds the largest independent sets in a sparse graph. graph: A sparse graph.

Python

Args:

Returns:
A list of the largest independent sets in the graph.
*** Returns:

 $#$ Initialize the list of independent sets. independent sets = $[1]$

Iterate through the vertices of the graph. for vertex in graph.vertices:

 $#$ Create a new independent set containing the current vertex. $independent_set = set([vertex])$

Iterate through the neighbors of the current vertex. for neighbor in graph.neighbors(vertex):

If the neighbor is already in the independent set, remove it. if neighbor in independent set: independent_set.remove(neighbor)

Add the independent set to the list of independent sets. independent_sets.append(independent_set)

Return the list of independent sets. return independent sets

Use code with caution. Learn more

This program works by first initializing a list of independent sets. Then, it iterates through the vertices of the graph. For each vertex, it creates a new independent set containing the current vertex. Then, it iterates through the neighbors of the current vertex. If any of the neighbors are already in the independent set, it removes them. Finally, it adds the independent set to the list of independent sets. The program then returns the list of independent sets.

 Ω

This program is efficient because it only iterates through the vertices and neighbors of the graph once. It also uses a set to store the independent sets, which is a fast data structure for storing and retrieving elements.

LLM+Evaluator: towards solving problems in NP "in practice"

Many problems admit a fast **evaluator**, but **solving** the problem is hard.

Largest independent set

Find largest independent set in a graph

 \rightarrow NP-hard problem

Particular focus on a structured graph (*cap-set graph*), with high mathematical significance

"*Perhaps my favourite open question"*

 Terence Tao

FunSearch finds constructions that improve over existing state-of-the-art

Two properties of a cap set candidate

- \bigcirc We can verify its correctness \bigvee
	- → Is the set of points a cap set, i.e. are there not more than 3 points in a line?
- \bigcirc We can measure how good it is \mathcal{X}
	- → How many elements are in the cap set?

→ We can write an efficient **evaluate** function

Search space size ~3³⁹⁰⁰

FunSearch finds constructions that improve over existing state-of-the-art

Search space size ~3³⁹⁰⁰

FunSearch finds constructions that improve over existing state-of-the-art

Search space size ~3³⁹⁰⁰

FunSearch finds constructions that improve over existing state-of-the-art

FunSearch also improves over existing state-of-the-art on other problems in maths:

- **● Shannon capacity of cycle graphs**
- **● Corners problem**

Solution space vs program space

Raw list of nodes

Solution space vs program space

Raw list of nodes **Program** that outputs a list of nodes

Solution space vs program space

Raw list of nodes **Program** that outputs a list of nodes

"The program supplied by the LLM is far conceptually richer than a mere list of vectors. **I am learning something** — e.g. this idea of classifying by number of reflections is novel."

Jordan Ellenberg, author of a breakthrough in this area and author of NYT bestseller "How Not to be Wrong: The Power of Mathematical Thinking"

Actionable interpretability

symmetric solutions

Why is searching in function space working surprisingly well?

Why is searching in function space working surprisingly well?

Our hypothesis: Most problems we care about are structured → solutions have small *Kolmogorov complexity*.

[Kolmogorov complexity](https://en.wikipedia.org/wiki/Kolmogorov_complexity) (KC) : $KC(y)$ = length of the shortest computer program that outputs y

KC("abababababababab") << KC("kasjiovmoisoeimpsl")

FunSearch's implicit prior is encouraging solutions with concise functional description.

By searching in the program space, we are implicitly looking for objects with small KC.

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Online bin-packing problem

What is the most resource efficient way to pack items onto bins?

Largest independent set

Find largest independent set in a graph

 \rightarrow NP-hard problem

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Online bin-packing problem

What is the most resource efficient way to pack items onto bins?

It sits at the core of many real-world problems, from loading containers with items to allocating compute jobs in data centers to minimize costs.

FunSearch delivers automatically tailored programs that outperformed established heuristics

FunSearch for online bin packing

FunSearch for online bin packing


```
def heuristic(item: float, bins: np.ndarray) -> np.ndarray:
  """Online bin packing heuristic discovered with FunSearch."""
 score = 1000 * np.ones(bins.shape)# Penalize bins with large capacities.
 score - bins * (bins-item)
 # Extract index of bin with best fit.
 index = np.arange(bins)# Scale score of best fit bin by item size.
 score[index] * = item# Penalize best fit bin if fit is not tight.
 score[index] = (bins[index] - item)**4return score
```
FunSearch for online bin packing

def heuristic(item: float, bins: np.ndarray) -> np.ndarray: """Online bin packing heuristic discovered with FunSearch.""" $score = 1000 * np.ones(bins.shape)$ # Penalize bins with large capacities. score $-$ bins * (bins-item) # Extract index of bin with best fit. $index = np.arange(bins)$ # Scale score of best fit bin by item size. $score[index] * = item$ # Penalize best fit bin if fit is not tight. $score[index] = (bins[index] - item)**4$ return score

FunSearch for tailoring programs

This showcases how FunSearch can be used to **automatically** produce programs / strategies that are **adapted** to a specific use case

Unlike neural networks - based approaches, the output of FunSearch is code:

- It is easier to deploy (no need for specialized hardware)
- It is easier to debug
- More understandable
- More predictable
- More scalable

FunSearch principles

LLMs by themselves cannot solve complex problems

They often come up with plausible but wrong outputs But we can couple it with Python runtime to provide grounding

We need to do search in the space of functions

<u>o</u>

Search based on evolutionary algorithms

Score map of functions


```
 # Trivial implementation
return [(0,)*n]
```
Score map of functions

Sample a large number of **mutations** from the LLM

```
def solve_v0(n):
     # Trivial implementation
    return [(0,)*n]
```

```
def solve_v1(n):
     # Improve over `solve_v0`
     (To be completed by LLM)
```
Very unlikely to reach

Score map of functions

Chaining mutations

FunSearch


```
@funsearch.evolve
def get_selection_score(state):
  return 0.0
```
Specification

@funsearch.run def evaluate(params): load_dataset(params) … # Greedy algorithm begins score = get_selection_score(state) … # Greedy algorithm ends eval_score = compute_eval_score(score) return eval_score

FunSearch

FunSearch

Maintaining diversity with islands $\ddot{\ddot{\Sigma}}$

Maintaining diversity with islands \triangle

Maintaining diversity with islands \triangle

Maintaining diversity with islands \triangle

Some more details

Pretrained LLMs

- Trade-off between capabilities and speed: Codey (Palm 2)
- No gradients were computed in the making of these experiments

Distributed system

We asynchronously connect 15 LLM samplers to 100s evaluators and a central programs database.

Skeleton

def solve(n):

```
 """Builds a cap set using `priority` function."""
 # Precompute all priority scores.
 elements = utils_capset.get_all_elements(n)
scores = [priority(e], n) for el in elements]
 # Sort elements according to the scores.
elements = elements[np.argsort(scores, kind='stable')[::-1]]
 # Build `capset` greedily, using scores for prioritization.
capset = [] for element in elements:
   if utils_capset.can_be_added(element, capset):
     capset.append(element)
 return capset
```
@funsearch.evolve

```
def priority(element, n):
   """Returns the priority with which we want to add `element` 
to the cap set."""
   return 0.0
```
Ablation experiments

Using admissible sets (asymptotic cap set)

Ablation experiments

Using admissible sets (asymptotic cap set)

For which problems is FunSearch useful?

1. Efficient evaluator is available

2. Smooth scoring feedback \rightarrow it is possible to gradually improve the solution

3. Prior information about the problem \rightarrow good skeleton

This is just the beginning

In this work we have striven for **simplicity**, creating a strong and simple base that we can build on in the future.

This, together with LLMs getting more powerful, faster and cheaper make us highly confide

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