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FUNSEARCH: PROGRAM SEARCH USING LLMS

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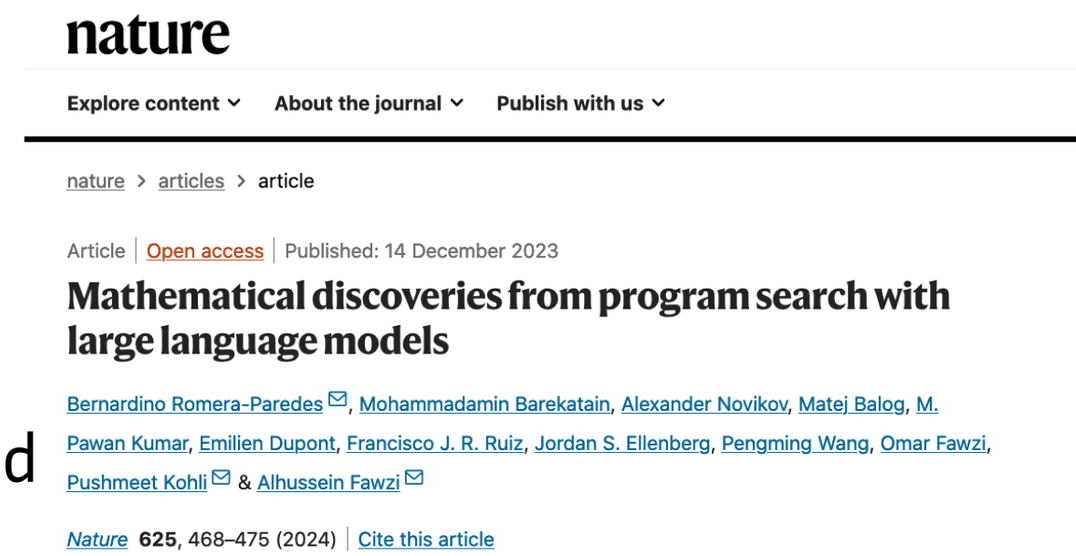
Collaboration with Google DeepMind



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Mathematical discoveries from program search with large language models

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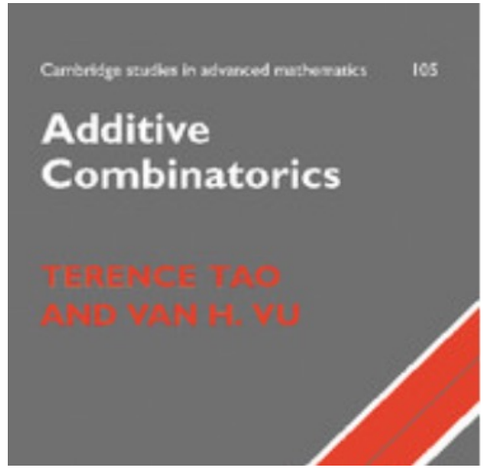
The cap set problem

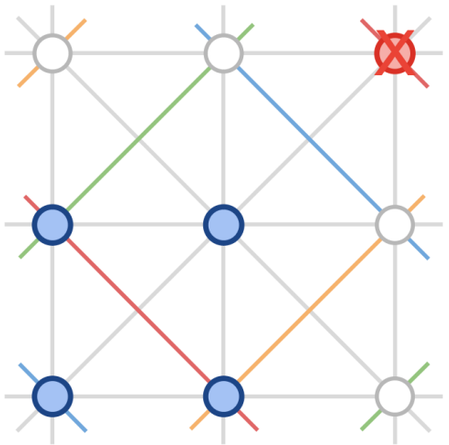
Additive combinatorics

- A group G, e.g., $G = \mathbb{Z}, G = \mathbb{Z}_N$
- Objective: construct a large set $A \subset G$ with no arithmetic progressions



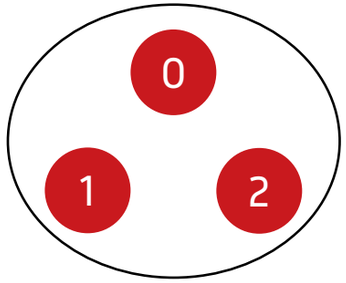
The cap set problem

- A cap set: A subset $A \subset \mathbb{Z}_3^n$ with no arithmetic progressions of length 3
- Main question: as $n \longrightarrow \infty$: $|A| \sim c^n$ how large can c be?
  - Lower bound: Trivial $c \geq 2$, important work: $c \geq 2.217$
    [Edel, *Design, Codes and Cryptography*, 2002]
  - Upper bound: Trivial $c \leq 3$, first improvement: $c \leq 2.75$
    [Ellenberg, Gijswijt, *Annals of Mathematics*, 2017]
- Also of interest for finite n
  - $n = 4$ card game SET
  - Open for $n = 8$ [Encyclopedia of Integer Sequences, https://oeis.org/A090245CT]
- Relation to other problems:
  - Algorithms for matrix multiplication
  - Circuit complexity



Cap set for n=2

Cap sets are independent sets of a simple hypergraph

$H =$ 

Cap set = Independent set in $H^{\boxtimes n}$

Dimension *n*	1	2	3	4	8	…	n → ∞
#nodes	3	9	27	81	6561	…	3^n
#edges	1	12	117	1080	~ 7,000,000		~ 9^n
Prev. best construction	2	4	9	20	496	…	2.217^n

As a computational problem

- Maximum independent set NP-hard in general
- Hypergraph is of exponential size in n
- Any generic algorithm: doubly exponential in n

Approach we take here:

- Describe an independent set by a **program** instead of a list of vertices
- Search for code describing a large indep set

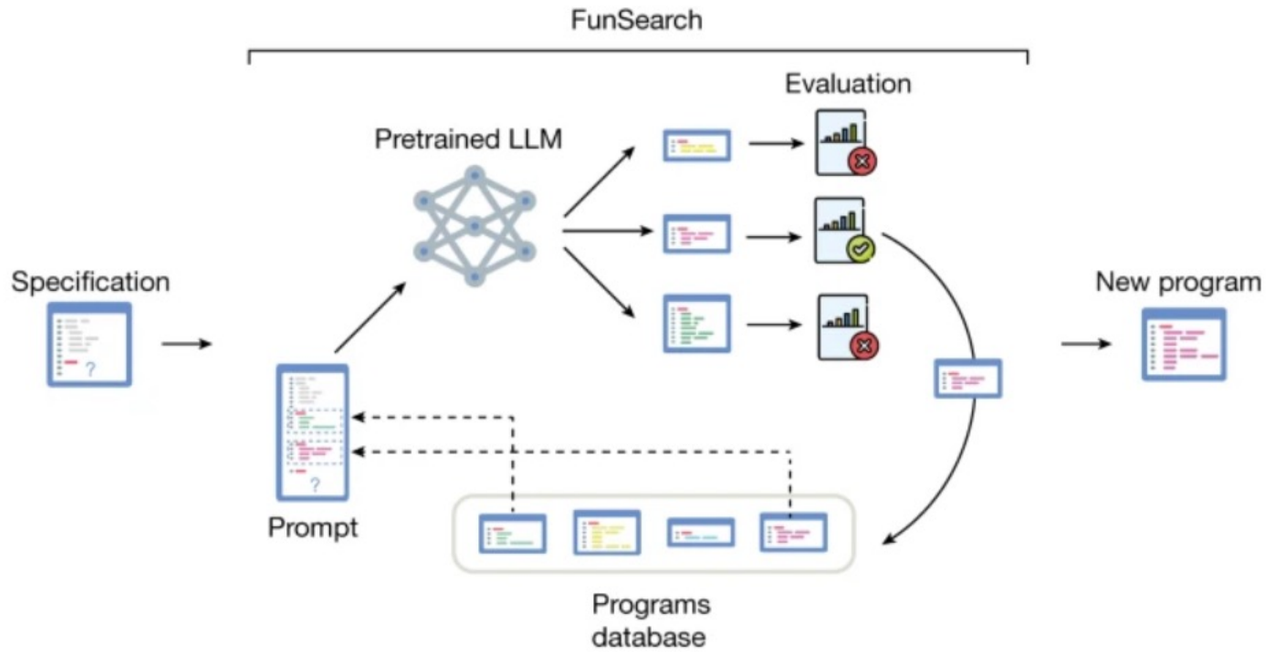
FunSearch (search in the function space)

- Asking LLM directly does not work (we do not trust it)

FunSearch combines

- Trusted & fast verification (problem is in NP)
- Large language model (generates meaningful programs)

Fig. 1: Overview of FunSearch.



FunSearch applied to the cap set problem

Choosing a good skeleton is crucial

- We do not search for a program outputs the list directly
- Instead, define a greedy algorithm: adding vertices in order defined by `priority`
- Search for `priority` function
- `evaluate` will output the size of the independent set generated by greedy algorithm with `priority`

Why?

- Boilerplate code factored out
- Guaranteed to give a cap set

a

```python
"""Finds large cap sets."""
import numpy as np
import utils_capset

# Function to be executed by FunSearch.
def main(n):
  """Runs `solve` on `n`-dimensional cap set and
  ↪  evaluates the output."""
  solution = solve(n)
  return evaluate(solution, n)

def evaluate(candidate_set, n):
  """Returns size of candidate_set if it is a cap
  ↪  set, None otherwise."""
  if utils_capset.is_capset(candidate_set, n):
    return len(candidate_set)
  else:
    return None

def solve(n):
  """Builds a cap set of dimension `n` using
  ↪  `priority` function."""
  # Precompute all priority scores.
  elements = utils_capset.get_all_elements(n)
  scores = [priority(el, 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

# Function to be evolved by FunSearch.
def priority(element, n):
  """Returns the priority with which we want to add
  ↪  `element` to the cap set."""
  return 0.0
```

Results

Dimension *n*	1	2	3	4	8	…	n → ∞
#nodes	3	9	27	81	6561	…	3^n
#edges	1	12	117	1080	~ 7,000,000		~ 9^n
Prev. best construction	2	4	9	20	496	…	2.217^n
Using FunSearch	2	4	9	20	**512**		**2.220^n**

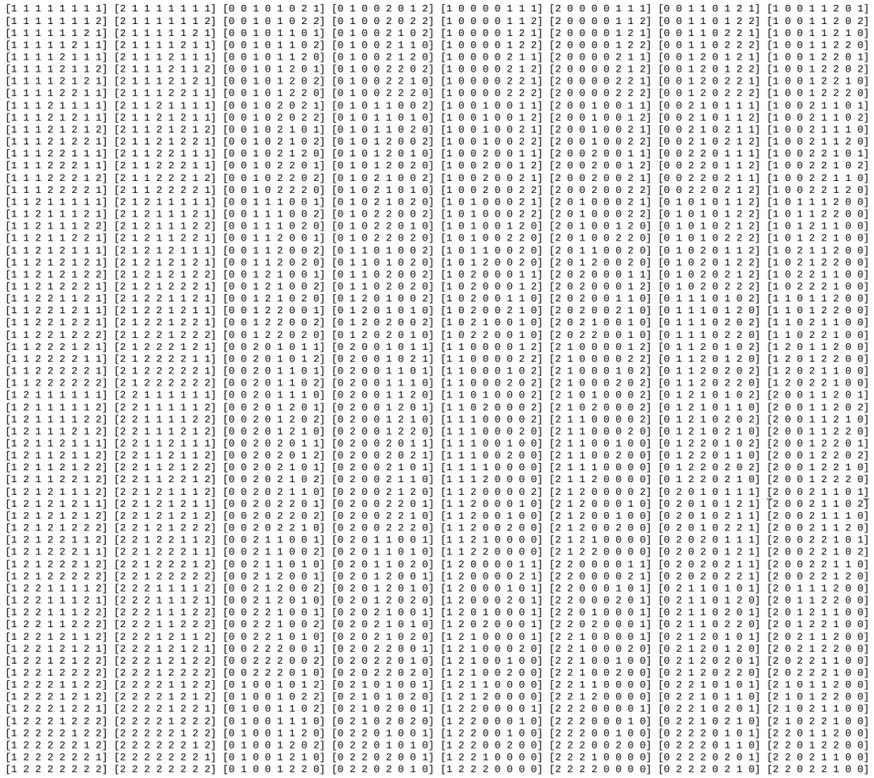
Based on finding a finite construction (“admissible set”) that implies the asymptotic bound

Why working well here?

- Problem is very structured. Can hope for a structured solution
- Scales better than traditional search methods, e.g., SAT solvers

Raw search space vs function space

Raw list of vertices



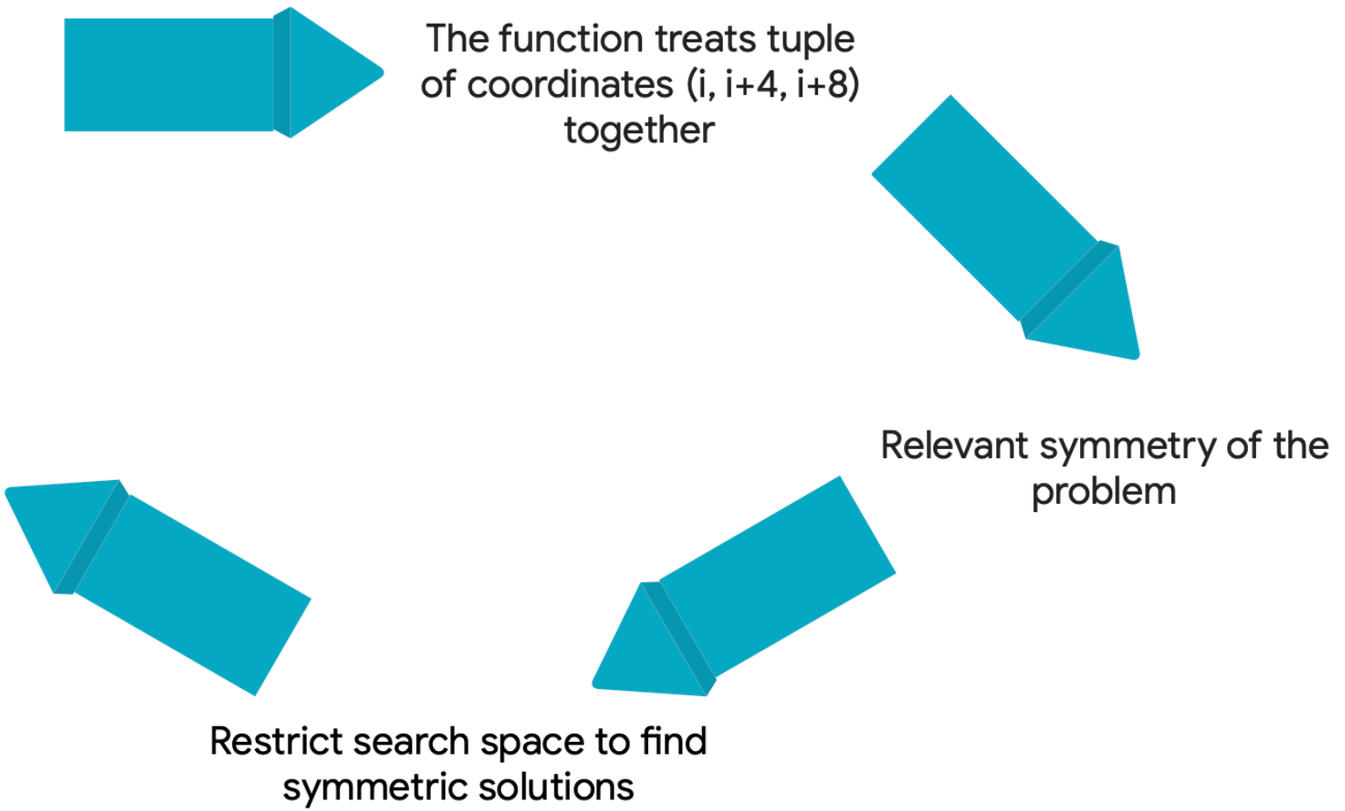
Program that outputs list of vertices (simplified by hand)

```python
def get_capset(n: int) -> CapSet:
  """Returns a 512-cap in AG(8, 3)."""
  V = np.array(list(itertools.product(range(3), repeat=n)), dtype=np.int32)
  reflections = lambda v: sum(1 for i in range(1, n // 2) if v[i] == v[-i])

  # First we list 128 weight-8 vectors with >= 2 reflections.
  weight8_points = [v for v in V
                    if np.count_nonzero(v) == 8  # Weight is 8.
                    and reflections(v) >= 2]  # At least 2 reflections.

  # Then we list 256 weight-4 vectors with allowed support and <= 1 reflections.
  allowed_supports = [
      (0, 1, 2, 3), (0, 1, 2, 5), (0, 1, 2, 7), (0, 1, 2, 6), (0, 1, 3, 7),
      (0, 1, 6, 7), (0, 3, 6, 7), (0, 5, 6, 7), (0, 1, 5, 7), (1, 3, 4, 6),
      (1, 4, 5, 6), (0, 2, 3, 6), (2, 3, 4, 7), (2, 4, 5, 7), (0, 2, 6, 7),
      (0, 2, 5, 6), (1, 2, 4, 7), (1, 2, 4, 6), (1, 3, 4, 7), (1, 4, 6, 7),
      (1, 4, 5, 7), (2, 3, 4, 6), (2, 4, 6, 7), (2, 4, 5, 6),
  ]
  weight4_points = [
      v for v in V
      if np.count_nonzero(v) == 4  # Weight is 4.
      and tuple(i for i in range(n) if v[i] != 0) in allowed_supports
      and reflections(v) <= 1]  # At most 1 reflection.

  # Finally we add 128 weight-5 vectors with <= 1 reflections.
  allowed_zeros = [(0, 4, 7), (0, 2, 4), (0, 1, 4), (0, 4, 6),
                   (1, 2, 6), (2, 6, 7), (1, 2, 7), (1, 6, 7)]
  weight5_points = [
      v for v in V
      if np.count_nonzero(v) == 5  # Weight is 4.
      and tuple(i for i in range(n) if v[i] == 0) in allowed_zeros
      and reflections(v) <= 1  # At most 1 reflection.
      and (v[1] * v[7]) % 3 != 1 and (v[2] * v[6]) % 3 != 1]  # Mod conditions.

  return weight8_points + weight4_points + weight5_points
```

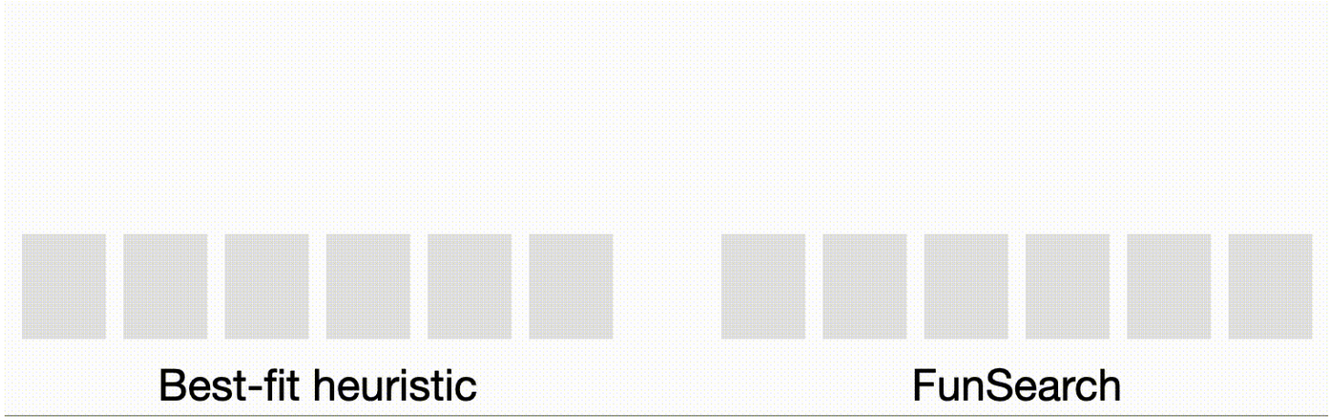
Programs can be more insightful

Actionable interpretabiliy

```python
def priority(el: tuple[int, ...], n: int, w: int) -> float:
    score = 0.0
    for i in range(n):
        if el[i] == 1:
            score -= 0.9 ** ( i % 4 )
        if el[i] == 2:
            score -= 0.98 ** (30 - ( i % 4 ))
        if el[i] == 1 and el[i - 4] == 1:
            score -= 0.98 ** (30 - ( i % 4 ))
        if el[i] == 2 and el[i - 4] != 0:
            score -= 0.98 ** (30 - ( i % 4 ))
        if el[i] == 2 and el[i - 4] == 1 and el[i - 8] == 2:
            score -= 0.98 ** (30 - ( i % 4 ))
            score -= 6.3
        if el[i] == 2 and el[i - 4] == 2 and el[i - 8] == 1:
            score -= 0.98 ** (30 - ( i % 4 ))
        if el[i] == 2 and el[i - 4] == 1 and el[i - 8] == 1:
            score -= 6.3
        if el[i] == 2 and el[i - 4] == 0 and el[i - 8] == 2:
            score -= 6.3
        if el[i] == 1 and el[i - 4] == 1 and el[i - 8] == 0:
            score -= 2.2
    return score
```



Another application: online bin packing




```python
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.argmin(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
```

	OR1	OR2	OR3	OR4	Weibull 5k	Weibull 10k	Weibull 100k
First Fit	6.42%	6.45%	5.74%	5.23%	4.23%	4.20%	4.00%
Best Fit	5.81%	6.06%	5.37%	4.94%	3.98%	3.90%	3.79%
FunSearch	**5.30%**	**4.19%**	**3.11%**	**2.47%**	**0.68%**	**0.32%**	**0.03%**

Summary

Search paradigm

Meaningful creativity of LLM + Formal verification skeleton

What caracteristics of the problem were important?

- Fast evaluation with signal of performance
- Search is difficult
- Searching for “short” programs

In 2026, this approach is applied very widely

- AlphaEvolve helped in advancing hundreds of maths problems
- Scaling this approach has computational/engineering cost

FunSearch to find Sum-of-Squares proofs (work with Mostafa Taheri)

Polynomial optimization

- Many problems can be formulated as: compute $min_{x \in R^d} P(x)$ or prove $P(x) \geq \gamma \; \forall x \in R^d$.
- Combinatorial optimization, control and robotics, quantum information,...
- If $P(x) - \gamma = \sum_i R_i(x)^2$, then R_i provide a proof that $min_{x \in R^d} P(x) \geq \gamma$.
- Searching for an SoS is a convex problem (semidefinite program):

$$P(x) - \gamma = \vec{b^t} \, Q \, \vec{b}$$

where $\vec{b}$ is a vector of monomials and $Q \geq 0$

Example

$$P(x) = (x_1 + x_2)^2 + (x_3 + x_4)^2 + (x_4 + x_5)^2$$

$$\vec{b} = (\mathbf{x_1}, \mathbf{x_2}, \mathbf{x_3}, \mathbf{x_4}, \mathbf{x_5})$$

$$Q = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 2 & 1 \\ 0 & 0 & 0 & 1 & 1 \end{pmatrix}$$

Q has many zeros

→ Find $\vec{b}$ to reduce size of convex problem

Example application: Entanglement witness

W is an entanglement witness if it is positive on product states:

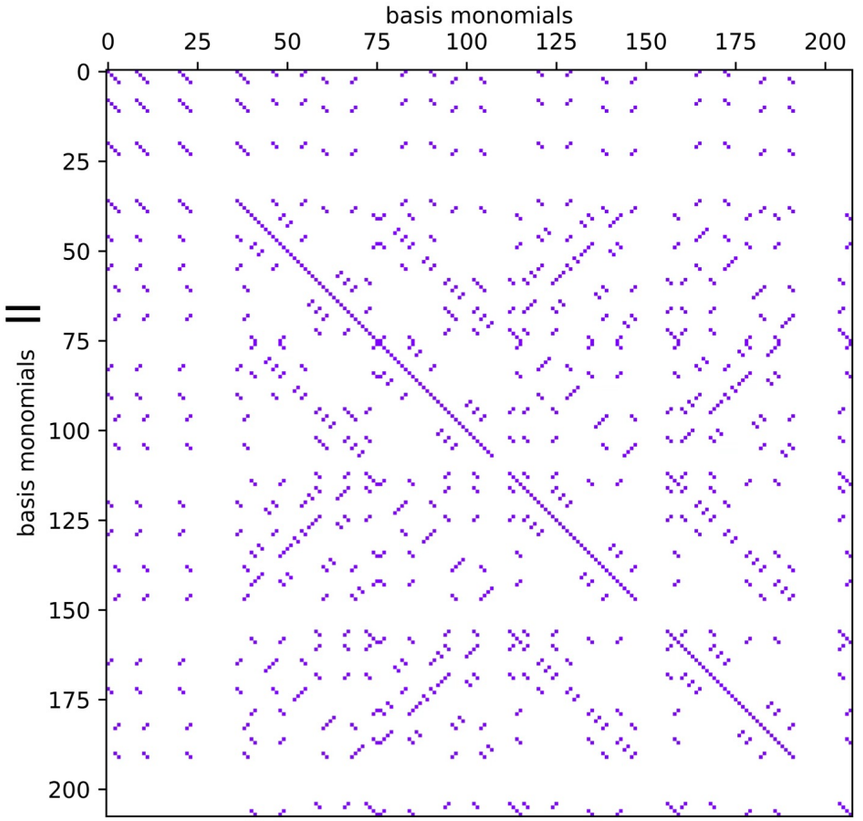
$$P(x,y) = \langle x| \otimes \langle y|\, W\, |x\rangle \otimes |y\rangle \geq 0$$

If $\mathrm{tr}(W\rho) < 0$, then ρ is entangled

Example:

$$W = (|22\rangle - |00\rangle)(\langle 22| - \langle 00|) + (|22\rangle - |11\rangle)(\langle 22| - \langle 11|)$$
$$+(|33\rangle - |01\rangle)(\langle 33| - \langle 01|) + (|33\rangle - |10\rangle)(\langle 33| - \langle 10|)$$
$$+|23\rangle\langle 23| + |32\rangle\langle 32| - |22\rangle\langle 22| - |33\rangle\langle 33|$$

$Q =$



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Search problem: Good basis sets

Given P find $\vec{b}$ or family $\{\overrightarrow{b_1}, \overrightarrow{b_2}, \dots\}$ such that

$$P(x) - \gamma = \sum_i \overrightarrow{b_i^t}\, Q_i\, \overrightarrow{b_i}$$

so that the number of variabls in Q_i is small

Gain from a family $\{\overrightarrow{b_1}, \overrightarrow{b_2}, \dots\} \cong \frac{|\#monomials|\text{^}2}{\sum_i |\overrightarrow{b_i}|^2}$

Example

$$P(x) = (x_1 + x_2)^2 + (x_3 + x_4)^2 + (x_4 + x_5)^2$$

$$\overrightarrow{b_1} = (x_1, x_2), \overrightarrow{b_2} = (x_3, x_4), \overrightarrow{b_3} = (x_4, x_5)$$

$$Q_1 = Q_2 = Q_3 = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

Number of variables: 9

Results (preliminary)

- Use same approach: search for code describing $\{\overrightarrow{b_1}, \overrightarrow{b_2}, \dots\}$
- For entanglement witness W: found a more concise sum-of-squares decomposition
- Another related family:

$$X(\alpha) := I_d \otimes I_d + \alpha d\,|\phi\rangle\langle\phi|\,, \qquad X_k(\alpha) := |\phi_k\rangle\langle\phi_k| \otimes X(\alpha)\,.$$

$$P(x,y) := \langle xy|\,X_2(\alpha)\,|xy\rangle \qquad \max_{\gamma} \text{ s.t. } \quad P - \gamma \in SOS$$

α	Full SDP			FunSearch			Fine-tuned FunSearch		
	Gain	Value	time(s)	Gain	Value	time(s)	Gain	Value	time(s)
-0,6	1	-0,14	85	30,11	-0,477	0,08	16	-0,14	0,36
-0,7	1	-0,18	71	30,11	-0,566	0,08	16	-0,18	0,37
-0,8	1	-0,22	87	30,11	-0,655	0,08	16	-0,22	0,37
-0,9	1	-0,26	73	30,11	-0,74	0,08	16	-0,26	0,37
-1,0	1	-0,30	74	40,65	-1,22	0,08	16	-0,30	0,36

- With open language models that run on local computers and open source ShinkaEvolve framework

Please reach out if you are interested in similar problems