# NLP CAFÉ @ CTS 

Tree of Thoughts: Deliberate Problem Solving with Large Language Models

| Shunyu Yao <br> Princeton University | Dian Yu <br> Google DeepMind | Jeffrey Zhao <br> Google DeepMind | Izhak Shafran <br> Google DeepMind |
| :---: | :---: | :---: | :---: |

21 Sept 2023<br>Constantin Orasan

https://dinel.org.uk
https://arxiv.org/abs/2305.10601

## WHOHASN'THEARD OF LLMs?

Prompt $\Rightarrow$ LLM $\Rightarrow$ Answer


(d) Tree of Thoughts (ToT)

Thought $=$ "a coherent language sequence that serves as an intermediate step towards problem solving"

## W H Y ?

- Tries to combat the usual "token-level decisions one by one and in a left-to-right fashion."
- Justification in human cognition: two modes of taking decisions
- fast automatic unconscious mode
- slow deliberate conscious mode
- Thought are seen as high-level semantic units that allow the LLM to self-evaluate the progress towards a solution
- Search heuristics via the LLM, rather than hard coded/learnt from data

We first formalize some existing methods that use large language models for problem-solving, which our approach is inspired by and later compared with. We use $p_{\theta}$ to denote a pre-trained LM with parameters $\theta$, and lowercase letters $x, y, z, s, \cdots$ to denote a language sequence, i.e. $x=$ $(x[1], \cdots, x[n])$ where each $x[i]$ is a token, so that $p_{\theta}(x)=\prod_{i=1}^{n} p_{\theta}(x[i] \mid x[1 \ldots i])$. We use uppercase letters $S, \cdots$ to denote a collection of language sequences.

Input-output (IO) prompting is the most common way to turn a problem input $x$ into output $y$ with LM: $y \sim p_{\theta}\left(y \mid \operatorname{prompt}_{I O}(x)\right)$, where $\operatorname{prompt}_{I O}(x)$ wraps input $x$ with task instructions and/or fewshot input-output examples. For simplicity, let us denote $p_{\theta}^{\text {prompt }}$ (output $\mid$ input) $=p_{\theta}$ (output $\mid$ prompt(input)), so that IO prompting can be formulated as $y \sim p_{\theta}^{I O}(y \mid x)$.

We first formalize some existing methods that use large language models for problem-solving, which our approach is inspired by and later compared with. We use $p_{\theta}$ to denote a pre-trained LM with parameters $\theta$, and lowercase letters $x, y, z, s, \cdots$ to denote a language sequence, i.e. $x=$ $(x[1], \cdots, x[n])$ where each $x[i]$ is a token, so that $p_{\theta}(x)=\prod_{i=1}^{n} p_{\theta}(x[i] \mid x[1 \ldots i])$. We use uppercase letters $S, \cdots$ to denote a collection of language sequences.

Chain-of-thought (CoT) prompting [35] was proposed to address cases where the mapping of input $x$ to output $y$ is non-trivial (e.g. when $x$ is a math question and $y$ is the final numerical answer). The key idea is to introduce a chain of thoughts $z_{1}, \cdots, z_{n}$ to bridge $x$ and $y$, where each $z_{i}$ is a coherent language sequence that serves as a meaningful intermediate step toward problem solving (e.g. $z_{i}$ could be an intermediate equation for math QA ). To solve problems with CoT, each thought $z_{i} \sim p_{\theta}^{C o T}\left(z_{i} \mid x, z_{1 \cdots i-1}\right)$ is sampled sequentially, then the output $y \sim p_{\theta}^{C o T}\left(y \mid x, z_{1 \cdots n}\right)$. In practice, $\left[z_{1 \cdots n}, y\right] \sim p_{\theta}^{C o T}\left(z_{1 \cdots n}, y \mid x\right)$ is sampled as a continuous language sequence, and the decomposition of thoughts (e.g. is each $z_{i}$ a phrase, a sentence, or a paragraph) is left ambiguous.

We first formalize some existing methods that use large language models for problem-solving, which our approach is inspired by and later compared with. We use $p_{\theta}$ to denote a pre-trained LM with parameters $\theta$, and lowercase letters $x, y, z, s, \cdots$ to denote a language sequence, i.e. $x=$ $(x[1], \cdots, x[n])$ where each $x[i]$ is a token, so that $p_{\theta}(x)=\prod_{i=1}^{n} p_{\theta}(x[i] \mid x[1 \ldots i])$. We use uppercase letters $S, \cdots$ to denote a collection of language sequences.

Self-consistency with CoT (CoT-SC) [33] is an ensemble approach that samples $k$ i.i.d.chains of thought: $\left[z_{1 \cdots n}^{(i)}, y^{(i)}\right] \sim p_{\theta}^{C o T}\left(z_{1 \cdots n}, y \mid x\right)(i=1 \cdots k)$, then returns the most frequent output: $\arg \max _{y} \#\left\{i \mid y^{(i)}=y\right\}$. CoT-SC improves upon CoT, because there are generally different thought processes for the same problem (e.g. different ways to prove the same theorem), and the output decision can be more faithful by exploring a richer set of thoughts. However, within each chain there is no local exploration of different thought steps, and the "most frequent" heuristic only applies when the output space is limited (e.g. multi-choice QA).

## TREE OF THOUGHTS (ToT)

- Human problem-solving: people search through a combinatorial problem-space - a tree where nodes represent partial solutions and branches correspond to opeators that modify the solutions
- Existing uses of LLMs do not
- Explore alternative solutions (branches)
- Incorporate any type of planning, lookahead or backtracking

A specific instantiation of To $T$ specifies:

1. How to decompose the intermediate process into thought steps;
2. How to generate potential thoughts from each state;
3. How to heuristically evaluate states;
4. What search algorithm to use

## TREE OF THOUGHTS (ToT)

1. Thought decomposition: explicitly requires to decompose the problem into intermediate thought steps

A thought should be "small" enough so that LLMs can generate promising and diverse samples, yet big enough so that it can be evaluated towards problem solving

|  | Game of 24 | Creative Writing | 5x5 Crosswords |
| :---: | :---: | :---: | :---: |
| Input | 4 numbers (4910 13) | 4 random sentences | 10 clues (h1. presented;..) |
| Output | An equation to reach 24 $(13-9) *(10-4)=24$ | A passage of 4 paragraphs ending in the 4 sentences | 5x5 letters: SHOWN; WIRRA; AVAIL; ... |
| Thoughts | $\begin{aligned} & 3 \text { intermediate equations } \\ & (13-9=4 \text { (left } 4,4,10) ; 10- \\ & 4=6 \text { (left } 4,6) ; 4 * 6=24) \end{aligned}$ | A short writing plan (1. Introduce a book that connects...) | Words to fill in for clues: (h1. shown; v5. naled; ...) |
| \#ToT steps | 3 | 1 | 5-10 (variable) |

Table 1: Task overview. Input, output, thought examples are in blue.

## TREE OF THOUGHTS (ToT)

2. Thought generator: generate k candidates for the next thought step

- Sample: if the space is rich (generate some text)
- Propose: what's next in the sequence given some constraints

3. State evaluator: assesses whether there is progress towards the solution with the help of the LLM (no rules or ML)

- Value each state independently: give a score to each state (0-10, sure/likely/impossible), promote good states, eliminate bad states
- Vote across states: compare different solutions and vote for the most promising one

4. Search algorithm: how to explore the search space

- Breadth-first search
- Depth-first search


Figure 2: ToT in a game of 24. The LM is prompted for (a) thought generation and (b) valuation.

## PROMPTS

```
# 5-shot
standard_prompt = '''Use numbers and basic arithmetic operations (+ - * /) to obtain
24.
Input: 4 4 6 8
Answer: (4 + 8)* (6-4) = 24
Input: 2 9 10 12
Answer: 2 * 12* (10 - 9) = 24
Input: 4 9 10 13
Answer: (13 - 9) * (10 - 4) = 24
Input: 1 4 8 8
Answer: (8 / 4 + 1) * 8 = 24
Input: 5 5 5 9
Answer: 5 + 5 + 5 + 9 = 24
Input: {input}
```

' ' '

```
cot_prompt = '''Use numbers and 9 - 3 = 6 (left: 4 6)
basic arithmetic operations (+ - * 4 4 * 6 = 24 (left: 24)
only allowed to choose two of the Answer: 4 * (9 - (13 - 10)) = 24
remaining numbers to obtain a new
number.
Input: 4 4 6 8
Steps:
4 + 8 = 12 (left: 4 6 12)
6 - 4 = 2 (left: 2 12)
2 * 12 = 24 (left: 24)
Answer: (6 - 4) * (4 + 8) = 24
Input: 2 9 10 12
Steps:
12 * 2 = 24 (left: 9 10 24)
10-9 = 1 (left: 1 24)
24* 1 = 24 (left: 24)
Answer: (12 * 2) * (10 - 9) = 24
Input: 4 9 10 13
Steps:
13-10 = 3 (left: 3 4 9)
```

```
propose_prompt = '''Input: 2 8 8 14
```

Possible next steps:
$2+8=10$ (left: 81014 )
$8 / 2=4$ (left: 48 14)
$14+2=16$ (left: 8 16)
$2 * 8=16$ (left: 81416 )
$8-2=6$ (left: 6814 )
$14-8=6$ (left: 26 8)
$14 / 2=7$ (left: 78 8)
$14-2=12$ (left: 8 12)
Input: \{input\}
Possible next steps:
' ' '
value prompt = '''Evaluate if given numbers can reach 24 (sure/likely/impossible)

## 1014

$10+14=24$
sure
1112
$11+12=23$
$12-11=1$
$11 * 12=132$
$11 / 12=0.91$
impossible
4410
$4+4+10=8+10=18$
4 * $10-4=40-4=36$
$(10-4) * 4=6 * 4=24$
sure
4911
$9+11+4=20+4=24$
sure
578
$5+7+8=12+8=20$
$(8-5) * 7=3 * 7=21$

I cannot obtain 24 now, but numbers are within a reasonable range
likely
566
$5+6+6=17$
$(6-5) * 6=1 * 6=6$
I cannot obtain 24 now, but numbers are within a reasonable range
likely
101011
$10+10+11=31$
$(11-10) * 10=10$
101010 are all too big impossible

133
$1 * 3 * 3=9$
$(1+3) * 3=12$
133 are all too small
impossible
\{input
' ' '

```
value_last_step_prompt = '''Use
sure
numbers and basic arithmetic
operations (+ - * /) to obtain
24. Given an input and an answer, Answer: (4 + 8) * (6 - 4) + 1 =
give a judgement
(sure/impossible) if the answer
is correct, i.e. it uses each
input exactly once and no other
numbers, and reach 24.
Input: 4 4 6 8
Answer: (4 + 8) * (6 - 4) = 24
Judge:
sure
Input: 2 9 10 12
Answer: 2 * 12 * (10 - 9) = 24
Judge:
sure
Input: 4 9 10 13
Answer: (13 - 9) * (10 - 4) = 24
Judge:
```

| Method | Success |
| :--- | :--- |
| IO prompt | $7.3 \%$ |
| CoT prompt | $4.0 \%$ |
| CoT-SC $(\mathrm{k}=100)$ | $9.0 \%$ |
| ToT (ours) $(\mathrm{b}=1)$ | $45 \%$ |
| ToT (ours) $(\mathrm{b}=5)$ | $\mathbf{7 4 \%}$ |
| IO + Refine $(\mathrm{k}=10)$ | $27 \%$ |
| IO (best of 100$)^{2}$ | $33 \%$ |
| CoT (best of 100$)^{2}$ | $49 \%$ |

Table 2: Game of 24 Results.


Figure 3: Game of 24 (a) scale analysis \& (b) error analysis.

## CREATIVE TEXT WRITING



Figure 4: A step of deliberate search in a randomly picked Creative Writing task. Given the input, the LM samples 5 different plans, then votes 5 times to decide which plan is best. The majority choice is used to consequently write the output passage with the same sample-vote procedure.
standard_prompt = ''
Write a coherent passage of 4 short paragraphs. The end sentence of each paragraph must be: \{input\}
' ' '
cot_prompt = '''
Write a coherent passage of 4 short paragraphs. The end sentence of each paragraph must be: \{input\}

Make a plan then write. Your output should be of the following format:

Plan:
Your plan here.

Passage:
Your passage here.
' ' '

```
vote_prompt = '''Given an instruction and several choices,
decide which choice is most promising. Analyze each choice
in detail, then conclude in the last line "The best choice
is {s}", where s the integer id of the choice.
```

'' '
compare_prompt = '''Briefly analyze the coherency of the following two passages. Conclude in the last line "The more coherent passage is 1", "The more coherent passage is 2 ", or "The two passages are similarly coherent".
' ' '
score_prompt = '''Analyze the following passage, then at the last line conclude "Thus the coherency score is \{s\}", where s is an integer from 1 to 10.


Figure 5: Creative Writing results.

## To T "ON THE CHEAP"

Imagine three different experts are answering this question.
They will brainstorm the answer step by step reasoning carefully and taking all facts into consideration

All experts will write down 1 step of their thinking, then share it with the group.
They will each critique their response, and the all the responses of others
They will check their answer based on science and the laws of physics
Then all experts will go on to the next step and write down this step of their thinking.
They will keep going through steps until they reach their conclusion taking into account the thoughts of the other experts
If at any time they realise that there is a flaw in their logic they will backtrack to where that flaw occurred
If any expert realises they're wrong at any point then they acknowledges this and start another train of thought
Each expert will assign a likelihood of their current assertion being correct
Continue until the experts agree on the single most likely location
The question is ...

## ToT"ON THE CHEAP"

1. Carlos is at the swimming pool.
2. He walks to the locker room, carrying a towel.
3. He puts his watch in the towel and carries the towel tightly to a lounger at the poolside.
4. At the lounger he opens and vigorously shakes the towel, then walks to the snack bar.
5. He leaves the towel at the snack bar, then walks to the diving board.
6. Later Carlos realises he has has lost his watch. Where is the single most likely location of the watch?

See: https://youtu.be/2InW1PSB2_g?si=DmL6beEdU-0qQVdP


