THOUGHTSCULPT: Reasoning with Intermediate Revision and Search

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Abstract

We present THOUGHTSCULPT, a general reasoning and search method for tasks with outputs that can be decomposed into components. THOUGHTSCULPT explores a search tree of potential solutions using Monte Carlo Tree Search (MCTS), building solutions one action at a time and evaluating according to any domain-specific heuristic, which in practice is often simply an LLM evaluator. Critically, our action space includes revision actions: THOUGHTSCULPT may choose to revise part of its previous output rather than continuing to build the rest of its output. Empirically, THOUGHTSCULPT outperforms state-of-theart reasoning methods across three challenging tasks: Story Outline Improvement (up to +30% interestingness), Mini-Crosswords Solving (up to +16% word success rate), and Constrained Generation (up to +10% concept coverage).

1 Introduction

While large language models (LLMs) such as GPT (Brown et al., 2020; OpenAI, 2024), LLaMA (Touvron et al., 2023a,b), and Claude (Anthropic, 2024) are increasingly capable at performing a variety of reasoning tasks, recent studies have revealed that the utilization of distinct prompting strategies and instructional guidance can have a notable influence on the performance of LLMs when tackling identical tasks.

Chain-of-Thought (CoT) is a prompting strategy detailed in Wei et al. (2023) that directs LLMs to produce the final task output through intermediate steps of reasoning, referred to as "intermediate thoughts." Notably, CoT has demonstrated a substantial enhancement in the problem-solving proficiency of LLMs without necessitating any model updates. Self-consistency with CoT (CoT-SC) (Wang et al., 2023a) proposes to improve output consistency by generating multiple CoTs and selecting the best outcome. Recently, extending CoT and CoT-SC, Tree-of-Thoughts (Yao et al., 2023a) and Graph-of-Thoughts (Besta et al., 2024) propose to shape the reasoning process of LLMs as a tree or an arbitrary graph structure. These approaches enable LLMs to explore different paths of thought and find better outputs by utilizing back-tracking and graph-search algorithms. However, these approaches' reasoning capabilities are often limited by the set of candidates they generate at earlier steps. They cannot revise and edit their original answers continuously in later steps. As a result, these methods may not be as effective in addressing problems that require frequent revision and modifications.

We propose THOUGHTSCULPT, a tree-based framework that emulates human reasoning by enabling LLMs to create interconnected thought networks. A key feature is its self-revision mechanism, which iteratively improves outputs while generating new thought nodes. To address the vast search space in text generation, we use Monte Carlo Tree Search (MCTS), which efficiently navigates the search space and provides high-quality solutions, though not necessarily globally optimal. Our method includes three core modules: the thought evaluator, which gives textual and numerical feedback; the thought generator, which produces solutions based on initial instructions and feedback; and the decision simulator, which simulates lines of thought within the MCTS process to assess the potential value of different paths.

We evaluate THOUGHTSCULPT on three challenging tasks for state-of-the-art language models: Story Outline Improvement, Mini-Crosswords Solving, and Constrained Generation. These tasks require advanced reasoning skills, varying degrees of exploration, and the ability for selfrevision to achieve optimal results. Compared to state-of-the-art reasoning strategies as baselines, THOUGHTSCULPT exhibits an up to 30% interestingness increase in Story Outline Improve-

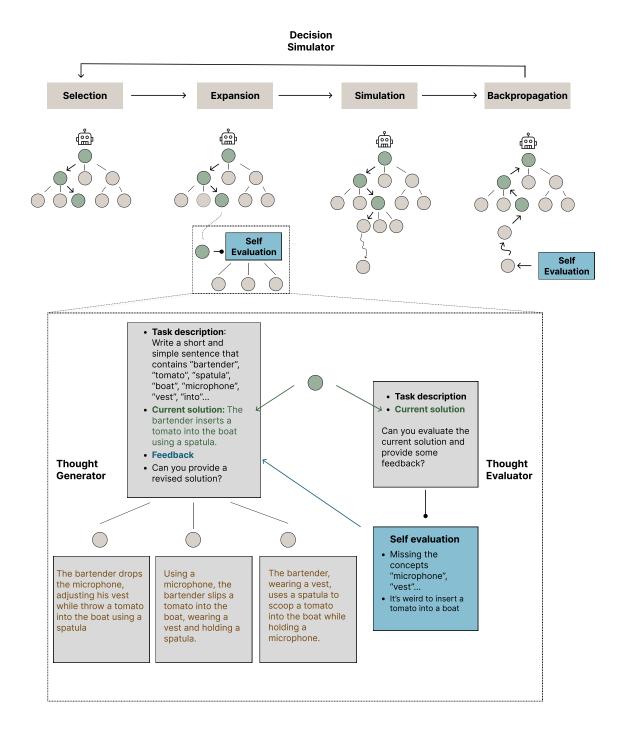


Figure 1: Illustration of THOUGHTSCULPT using Monte Carlo Tree Search on the Constrained Generation task. Each circle in the diagram represents a thought node generated by LLMs. *Selection:* choose a thought node x based on a selection algorithm. *Expansion:* A new set of child nodes X is generated using the initial instruction, the current node, and self-evaluated textual feedback. The zoom-in of the expansion phase demonstrates the use of the **Thought Evaluator** and the **Thought Generator**, which entails assessing and refining the current solution for the task 4.3. *Simulation:* a single node x' is randomly chosen from the set X. This selected node x' generates further nodes in sequence for several steps, corresponding to our **Decision Simulator**. *Backpropagation:* The numerical feedback evaluated at the last node is propagated back to the root node.

ment; up to 16% word success rate increase in Mini-Crossword Solving; and up to 10% concept coverage improvement in Constrained Generation. These findings underscore the efficacy of THOUGHTSCULPT across diverse tasks.

2 Related Works

Feedback Guided Generation. Human feedback has been shown to be effective in improving LLMs' generation (Tandon et al., 2022; Elgohary et al., 2021; Bai et al., 2022). However, human feedback is often costly and unable to be incorporated into an automated generation process. As a result, some works adopt a heuristic function to serve as an alternative to human feedback (Liu et al., 2022; Lu et al., 2022; Le et al., 2022; Welleck et al., 2022).

Madaan et al. (2023); Shinn et al. (2023); Paul et al. (2024) introduce a mechanism for LLMs to produce self-reflective feedback to improve their outputs. Along with the model-generated feedback, Chen et al. (2023) uses execution results to help improve code generation. Likewise, Kim et al. (2023) introduces a critic step to improve the model's performance in computer tasks. These approaches follow left-to-right linear processes, potentially overlooking alternative directions. In our work, each thought node having multiple children nodes allows for broader exploration, enhancing decision-making comprehensiveness.

Graph Reasoning. To facilitate broader exploration in problem-solving, Yao et al. (2023a) and Xie et al. (2023) use a tree-search procedure where each node represents a partial solution, requiring a complete solution to combine multiple nodes. This method restricts modifications to intermediate nodes, making the final output reliant on initial candidates. Besta et al. (2024) proposed a graphbased paradigm that models LLM reasoning as an arbitrary graph, allowing combinations of connecting nodes. Our approach differs by permitting review and modification of intermediate nodes, even allowing them to be revised or expanded if initially complete. This flexibility improves expressivity and enables language models to correct initial mistakes. Several concurrent works (Hui and Tu, 2024; Tian et al., 2024; Chen et al., 2024) have recently explored integrating Monte Carlo Tree Search (MCTS) with Large Language Models (LLMs). However, these approaches primarily focus on mathematical reasoning tasks or rely on

external feedback, fine-tuned policies, or reward models. In contrast, our method operates entirely at inference time, requiring no additional model training or external feedback.

LM Planning. Long-form generation and complex problem-solving often require high-level planning or outlining. Natural language outliners and structured schemas play integral roles in generating long-form content (Tian and Peng, 2022; Mirowski et al., 2022; Yang et al., 2022, 2023). There are also works that utilize LLMs to tackle complex tasks such as video games, fact-checking, housekeeping, and code optimization with planning using natural languages (Yao et al., 2023b; Huang et al., 2022a; Wang et al., 2023b; Huang et al., 2022b). Our work could also be seen as a generic task planner using LLMs that leverages Monte Carlo Tree Search to facilitate various tasks in diverse domains.

3 Method

We treat each formal output of LMs as a thought node $x \in \{x^0, x^1, ..., x^i\}$, where x^0 is the root node and the initial output provided by LMs given the task instruction *I*. For instance, a thought node can be a few lines of items (Story Outline Improvement), a couple of words (Mini-Crosswords), or a sentence (Constrained Generation). To process the thought node and look for a better output, our method consists of three modules: thought evaluator, thought generator, and decision simulator.

3.1 Thought Evaluator

The thought evaluator evaluates the status of each thought node and provides feedback for potential improvement. It not only works as a heuristic for the search algorithm but also gives potential directions and guidance to generate new candidates.

Feedback $f(x^i)$ for a node x^i consists of numerical feedback $f_{numeric}(x^i)$ and natural language feedback $f_{NL}(x^i)$. The numerical feedback will be used as the evaluation score $v(x^i)$ for the current node, and the natural language feedback will be used as context to generate child nodes.

$$f(x^{i}) = \langle f_{NL}(x^{i}), f_{numeric}(x^{i}) \rangle$$
(1)
$$f_{numeric}(x^{i}) = v(x^{i})$$
(2)

$$f_{numeric}(x^{*}) = v(x^{*}) \tag{2}$$

We present two types of natural language feedback, each beneficial for various task scenarios. Furthermore, these strategies are flexible, allowing for independent or combined utilization.

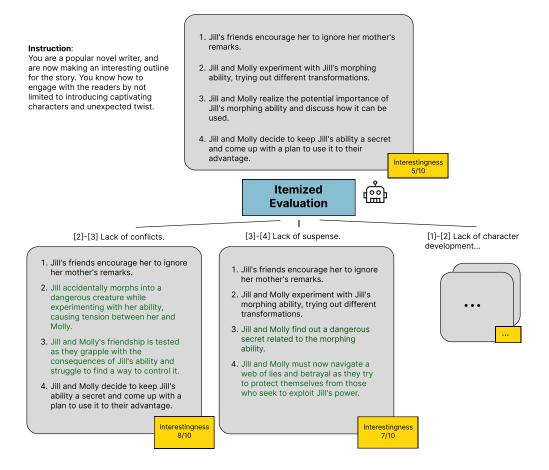


Figure 2: Illustration of our Story Outline Improvement task. A step involves employing the thought evaluator to conduct itemized evaluations of the story outline and utilizing the thought generator to generate a candidate set of improved story outlines for task 4.1.

- *Holistic Evaluation:* Evaluate the entire thought node as a unified whole to provide comprehensive feedback. This approach captures the core message and coherence of the node. The right side of the zoomed-in expansion phase in Figure 1 illustrates how the thought evaluator generates holistic feedback based on the task description and the current solution of the node.
- *Itemized Evaluation:* Evaluate each sub-unit of the thought node individually, providing targeted feedback for each component. This method results in a list of feedback specific to each sub-unit, making it ideal when the thought node can be divided into distinct elements for localized evaluation. For instance, in the story outline task shown in Figure 2, breaking the outline into separate items allows for focused assessment and refinement.

3.2 Thought Generator

Once we have evaluation feedback of the current node, we can form subsequent thought nodes that aim to improve the current output. Based on the task description I, the current solution x_{parent} , and the natural language feedback f_{NL} provided by the self-evaluator, each thought node generates kcandidate thought nodes using a pre-trained LM with a parameter θ .

A child node x_{child} will be generated as follows:

$$x_{child} \sim p_{\theta}(x|I, x_{parent}, f_{NL}(x_{parent}))$$
 (3)

The left part of the zoomed-in expansion phase depicted in Figure 1 illustrates how THOUGHTSCULPT leverages the task description, current solution, and evaluation feedback to produce a set of candidate nodes.

3.3 Decision Simulator

THOUGHTSCULPT is equipped with a decision simulator that enables it to simulate decisions at deeper layers and then backpropagate to update the score of the current decision. In other words, we are doing a rollout to get a better estimate of the reward for the node we are at. The behavior of the decision simulator is analogous to the processes in Monte Carlo Tree Search (MCTS; see Algorithm 1). It is possible to replace the decision simulator with other search algorithms such as DFS, BFS, or A* search (and we in fact run DFS as well in our experiments in Section 4), but MCTS provides a computational advantage by efficiently navigating complex search spaces, balancing exploration and exploitation to reach optimal solutions with fewer evaluations. Its incremental and iterative nature also scales well to large problem instances.

MCTS explores potential moves and stores the outcomes in a search tree. With each search iteration, the tree expands, accumulating more information. As shown in Figure 1, MCTS can be divided into four phases: selection, expansion, simulation, and backpropagation.

In the selection phase, a leaf node will be selected based on Upper Confidence Bound 1 (UCB1) Eqn 4 which prioritizes nodes that have not been explored extensively but show promise. Therefore, the UCB1 value of node x takes into account not only the heuristic score v(x) but also the total number of visits to the node itself, n(x), as well as its parent node, $n(x_{parent})$.

$$UCB1(x) = v(x) + c\sqrt{\frac{\ln n(x_{parent})}{n(x)}} \quad (4)$$

In the expansion phase, the thought generator will expand the selected leaf node by generating a set of children nodes based on the feedback provided by the thought evaluator.

In the simulation phase, a child node is picked from the newly generated set using a uniform distribution. In the subsequent iterations, however, we generate only a single node iteratively until the maximum simulation depth $d_{simulation}$ is reached.

Finally, in the backpropagation phase, we update the reward of the last node generated in the simulation back to the root node and iterate this process for $d_{rollout}$ steps. The node with the highest average reward will be chosen as the final output.

4 Experiments

We evaluate our method on three distinct tasks: Story Outline Improvement, Mini-Crossword Solving, and Constrained Generation.

We evaluate the tasks with Chain-of-Thought (CoT) (Wei et al., 2023), Self-Refine (Madaan et al., 2023), and Tree-of-Thoughts (ToT) with DFS (Yao et al., 2023a) as baselines. We use GPT-3.5 (gpt-3.5-turbo-0125) and GPT-4 (gpt-4-0125-preview) (OpenAI, 2024) as strong base LMs for the reasoning algorithms across all tasks. Both base LMs use a temperature of 0.7. To further evaluate the efficacy of our proposed approach, we conduct an ablation study by investigating the performance of our method when employing Depth-First Search (DFS) (Algorithm 2) as an alternative search algorithm to the MCTS algorithm. In addition, running THOUGHTSCULPT with DFS facilitates closer comparison with ToT, which also uses DFS. While THOUGHTSCULPT with MCTS typically performs better, we observe in our experiments below that THOUGHTSCULPT with DFS still outperforms our other baselines, demonstrating THOUGHTSCULPT's ability to generalize to other search algorithms.

4.1 Story Outline Improvement

	Base LLM		
Methods	GPT3.5	GPT4	
Initial Outline	12.0	12.0	
СоТ	50.1	28.8	
Self-refine	65.5	27.9	
ТоТ	72.1	49.9	
THOUGHTSCULPT (DFS) THOUGHTSCULPT (MCTS)	79.3 89.9	53.7 65.0	

Table 1: Average outline interestingness. Initial Outline is the starting point before rewriting with any reasoning method. THOUGHTSCULPT's outputs are judged to be interesting at a higher percentage compared to baselines.

One approach to generating long-form stories via LLMs is to adopt a high-level writing process that first designs an outline of the story and fills up the details based on the outline (Yang et al., 2022, 2023). An unengaging or uncompelling outline is unlikely to yield a captivating final draft, regardless of the subsequent detailing efforts. To address this challenge, we propose a task focused specifically on enhancing the interestingness of story outlines generated by LLMs.

Task Setup We sample 500 book descriptions from the WhatsThatBook dataset (Lin et al., 2023)

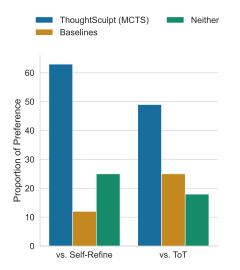


Figure 3: Proportion of outlines generated by each method that were preferred by humans in pairwise comparison. ("Neither" indicates that neither THOUGHTSCULPT nor the baseline methods were preferred.)

and generate story outlines using DOC (Yang et al., 2023) with GPT-3.5. We allocate 400 descriptions for training, 50 for validation, and 50 for testing. For each description, we generate three types of outlines: one prompted to be interesting, one prompted to be boring, and one without specific instructions. Since there is no ground truth for the interestingness of the outline, we employ an outline content evaluator to assess the final interestingness of generated or revised outlines. Neither THOUGHTSCULPT nor the baselines have access to this evaluator during outline generation. We finetune the pre-trained Flan-T5 model (Chung et al., 2022) to serve as the content evaluator, training it to rate interesting outlines as 1 and boring ones as 0. This evaluator's output serves as the score metric for the task. For evaluation, LMs revise and improve the interestingness of default outlines in the test set. The dataset includes 400 interesting and 400 non-interesting outlines for fine-tuning, 50 interesting and 50 non-interesting outlines for validation, and 50 outlines for testing algorithms.

Also, we conduct human evaluation via Prolific to assess the generated story outlines (GPT-3.5 as the base LLM), capturing subjective perceptions and cultural nuances that LLMs may miss. We recruited annotators to evaluate 100 pairs of story outlines, each pair consisting of one outline generated by THOUGHTSCULPT with MCTS and another by ToT or Self-Refine, with each pair annotated by two annotators.

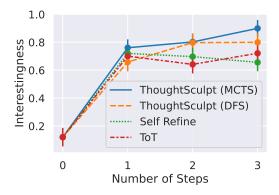


Figure 4: Average outline interestingness at each step. THOUGHTSCULPT's interestingness increases more with steps compared to baselines.

Method Setup Each method is allowed to search or iterate through a maximum depth of 3. The thought evaluator will perform an itemized evaluation on the current outline and provide an interesting score from 1 to 10 as the numerical feedback. Based on each itemized feedback, a child node will be proposed to modify the current outline in order to improve its interestingness. For THOUGHTSCULPT and ToT, each node will generate a maximum of 3 candidate child outlines. In this and all the experiments below, THOUGHTSCULPT with MCTS will have a maximum $d_{simulation}$ of 1. Figure 2 illustrates how the story outline is improved.

Results As illustrated in Table 1, all methods unsurprisingly improve the level of interestingness relative to the initial outline (sampled from default outlines with no prompting for either interesting or boring). However, overall, THOUGHTSCULPT outperforms ToT even with DFS, while THOUGHTSCULPT with MCTS demonstrates the highest average interestingness percentage across both GPT-3.5 and GPT-4 with 89.9 and 65.0 respectively.¹ As Figure 3 shown, human annotators also gave a higher preference towards THOUGHTSCULPT with MCTS outputs comparing with other baselines, agreeing with the prior evaluation results. Moreover, our strong performance comes at only a modest increase in computational cost compared to baselines.²

¹One possible explanation for why GPT-4, serving as the base LM, exhibits lower overall interestingness could be attributed to the fact that the outline content evaluator was trained on outlines generated using GPT-3.5.

 $^{^{2}}$ We compute the average token cost of THOUGHTSCULPT for this task along with other tasks in Appendix B. THOUGHTSCULPT with DFS has a cost comparable to ToT,

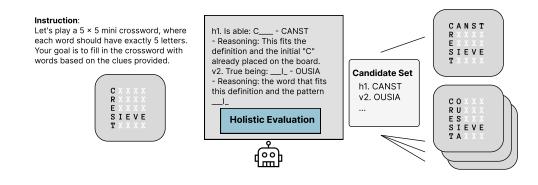


Figure 5: Illustration of a step in the deliberation process in the Mini-Crosswords task, where the current crossword board is assessed using the thought evaluator and a candidate set of words is proposed for task 4.2. One step is equal to one $d_{rollout}$

Continuous Improvement Figure 4 illustrates the progression of story outline interestingness at various steps, employing GPT-3.5 as the base LM. Among the tested methods, only THOUGHTSCULPT with MCTS has exhibited a consistent pattern of improvement over time. In contrast, both ToT and Self-refine exhibit a lack of continuous improvement. We suppose that Self-refine's limited search space and ToT's absence of a revision process contribute to this phenomenon.

4.2 Mini crosswords

We also explore our method on 5x5 mini crosswords following the setup of Yao et al. (2023a). For every puzzle, there are five horizontal (h1 to h5) and five vertical (v1 to v5) words to be filled. The task is to solve a five-by-five crossword puzzle in several steps (either filling or editing a word counts as one step). For evaluation, we check the proportion of letters, words, and games correctly filled by each reasoning method.

Method Setup Each thought node represents a (possibly partial) solution to the crossword puzzle.

while the higher-performing THOUGHTSCULPT with MCTS requires 1.2x more computation than ToT due to its additional decision simulation process.

To evaluate each thought node, the LM is prompted to evaluate each clue against the filled-in letters and suggest whether it is reasonable. For example, if the first row is filled with "AMIGO" and nothing else is filled, then the first column will be shown as "A____". Thus, in the prompt, there will be one line "v1. A Mennonite sect, named for Jacob Ammann: A____ " that asks the LM to determine whether there are potential answers. The node evaluation's prompt setup is similar to (Yao et al., 2023a)'s except that we use the evaluation feedback to generate new candidates instead of pruning branches. Based on the evaluation feedback, every candidate for a node will be generated to either suggest a new word to fill a blank space or propose a modification to a word already filled in. For each node, THOUGHTSCULPT and ToT generate a maximum of 3 candidates. In contrast to the setup in Yao et al. (2023a), where maximum search steps is set to 100, we impose a constraint on all methods to utilize only 20 search steps. This constraint aims to prevent attempts to artificially boost performance by exhaustively trying numerous word possibilities. With this restriction, each row or column of the crossword puzzle allows, on average, only two word attempts to be made

		GPT3.5			GPT4	
Methods	% word	% letter	% game	% word	% letter	% game
СоТ	10.5	34.6	0.0	15.6	40.6	5.0
Self-refine	13.5	27.4	5.0	46.5	74.8	5.0
ТоТ	19.5	36.6	0.0	39.5	64.8	5.0
THOUGHTSCULPT (DFS)	14.0	33.2	0.0	46.5	68.2	20.0
THOUGHTSCULPT (MCTS)	19.0	41.6	0.0	54.0	74.0	25.0

Table 2: Mini-crossword results of 20 puzzles for THOUGHTSCULPT and baselines (success % of letters, words, and games). THOUGHTSCULPT with MCTS is either best or closely comparable to best across the board.

within the allocated search budget. Figure 5 illustrates how THOUGHTSCULPT approaches to solve a crossword puzzle.

Results As shown in Table 8, THOUGHTSCULPT with MCTS attains the highest letter success rate using GPT-3.5 and the highest word and game success rate using GPT-4; it is also always at least comparable to the best in all cases. With limited search steps, it is surprising that ToT using GPT-4 performs worse than even Self-refine; it turns out that a self-revision mechanism is important in this task. THOUGHTSCULPT with MCTS achieves comparable performance to that reported by ToT (Yao et al., 2023a) using 100 search steps, despite employing just 20 search steps in our experiment.

4.3 Constrained Generation

CommonGen is a benchmark dataset and a constrained text generation task designed to evaluate LMs' abilities in generative commonsense reasoning (Lin et al., 2020). An example instruction for the task is shown in Appendix A.3. However, currently, the coverage test of CommonGen can be completed with 90% or higher accuracy by many LLMs with one-shot prompting. Therefore, we instead test on CommonGen-Hard as introduced by (Madaan et al., 2023). Rather than just four concepts, CommonGen-Hard requires models to generate a sentence with 20-30 concepts.

Method Setup In this task, we first provide the set of concepts required and the task description for the LM to generate an initial thought node. During the thought evaluation, the LM will be prompted to give feedback about the quality of the concepts used and whether there are any missing concepts. A child node will be generated using the feedback along with the current solution. We set a maximum depth of 3 for this task. For each node, both THOUGHTSCULPT and ToT will generate a maximum of 3 child candidates.

Methods	GPT3.5	GPT4
СоТ	44.1	96.1
Self-refine	70.0	98.5
ТоТ	54.8	98.8
THOUGHTSCULPT (DFS)	79.6	99.1
THOUGHTSCULPT (MCTS)	77.9	99.0

Table 3: Constrained Generation Results (% Coverage of Concepts). THOUGHTSCULPT outperforms all baselines on both base LMs.

Results Table 3 shows that THOUGHTSCULPT outperforms all other baselines when using either GPT-3.5 or GPT-4 as the base LM. While THOUGHTSCULPT with DFS achieves the highest coverage of 79.6% (GPT-3.5) and 99.1% (GPT-4), THOUGHTSCULPT with MCTS also demonstrates comparable concept coverage of 77.9% using GPT-3.5 and 99.0% using GPT-4. While MCTS exhibits notable exploration capabilities, it fails to surpass DFS due to the task's nature, where effective solutions are abundant as long as generated sentences correctly integrate assigned concepts. DFS, employing a greedy approach prioritizing nodes with the highest concept coverage, outperforms MCTS in this context. However, solely relying on concept coverage does not ensure appropriate concept utilization. Hence, we conduct an additional evaluation using GPT-4 to determine the preferred output based on concept coverage and appropriateness. Figure 6, comparing THOUGHTSCULPT with MCTS against THOUGHTSCULPT with DFS and a third baseline (intuitively, representing the case where neither THOUGHTSCULPT version's output is good), indicates that THOUGHTSCULPT with MCTS is significantly favored.

5 Conclusion

We introduce THOUGHTSCULPT, a framework designed to empower LLMs to handle complex tasks requiring continuous refinement and reasoning capabilities, all without necessitating any modifications or updates to the underlying model architecture.

By harnessing Monte Carlo Tree Search (MCTS), THOUGHTSCULPT enables LLMs to effectively explore vast search spaces while managing computational resource costs efficiently. Moreover, THOUGHTSCULPT facilitates a seamless self-revision process, allowing LLMs to iteratively refine and improve their outputs without the need for extensive prompt engineering. Through our experiments, we illustrate THOUGHTSCULPT's potential across diverse tasks, highlighting its versatility and broad applicability. The results underscore THOUGHTSCULPT's capacity to enhance LLM performance in challenges requiring continuous thought iteration, such as open-ended generation, multi-step reasoning, and creative ideation.

Limitations

While THOUGHTSCULPT presents a promising approach for reasoning during inference, its reliance on multiple calls to the base language model incurs a higher computational cost than most sampling methods. Consequently, in scenarios where base language models already demonstrate satisfactory performance, the adoption of THOUGHTSCULPT may not be advisable. However, THOUGHTSCULPT proves beneficial for tasks requiring intricate reasoning, potential for continual improvement, or when the base language model's performance is suboptimal. Furthermore, the incorporation of MCTS enables THOUGHTSCULPT to navigate complex search spaces, striking a balance between exploration and exploitation, and handling scalability concerns, thereby offering computational advantages over alternative search algorithms.

Ethics Statement

We affirm that all datasets utilized in our experiments have been appropriately sourced and cited, adhering to principles of academic integrity and proper attribution.

Our experiments primarily leverage GPT-3.5 and GPT-4 as the base LLMs. These models possess remarkable capabilities in generating human-like text based on prompts. However, we acknowledge the ethical concerns surrounding their potential misuse for spreading misinformation, generating harmful content, or impersonating individuals. We recognize the imperative for ethical considerations to include robust mechanisms aimed at preventing misuse and fostering responsible use of these models.

The purpose of THOUGHTSCULPT is to enhance the reasoning and complex problem-solving capabilities of Language Models (LMs). However, it is essential to acknowledge that THOUGHTSCULPT does not inherently include mechanisms to prevent LMs from generating harmful content. Therefore, we strongly advise anyone utilizing our model to exercise caution and be mindful of the potential for misuse. Users must take proactive measures to mitigate the risk of harmful content generation by implementing effective safeguards and appropriate controls.

Reproducibility

In our experiments, we aim for transparency and reproducibility by utilizing publicly accessible datasets. Furthermore, for the content evaluator utilized in the story outline improvement task, we employed Flan-T5, an open-source model. To facilitate reproducibility, our codebase will also be made available for reference and validation upon publication. However, as we access GPT-3.5 and GPT-4 through the OpenAI API, we acknowledge that reproducibility may be affected subject to OpenAI changing their API.

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A Prompts

Generally, THOUGHTSCULPT requires only three prompts: TASK_DESCRIPTION, NEW_CANDIDATE, and EVALUATE_CURRENT.

- 1. TASK_DESCRIPTION is the general instruction for the specific task. It will be placed in front of rest of the prompts.
- 2. NEW_CANDIDATE is the prompt to generate new candidates based on the evaluation feedback and the current solution.
- 3. EVALUATE_CURRENT instructs the language model to evaluate the current solution. The prompt can be tailored to ask for itemized evaluations, holistic evaluations, or both.

A.1 Task 1 Story Outline Improvement

```
TASK_DESCRIPTION = """\
# Task Description
You are a popular novel writer. You are now making an interesting outline for the
                                           story. You know how to engage with the
                                           readers by not limited to introducing
                                           interesting characters and unexpected
                                           twist.
You also know how to make the story outline coherent and consistent.
NEW_CANDIDATE = TASK_DESCRIPTION + """\
# Original Outline
{outline}
# Feedback
{feedback}
Based on the feedback and the task description, can you make a better story outline
                                           by replacing the items suggested by the
                                           feedback?
Write the outline in this format just like the original outline from [1] to [{num}]:
[1] ...
[2] ...
. . .
# Your response:
EVALUATE_CURRENT = TASK_DESCRIPTION + """ \
# Original Outline
{outline}
Do you think that this outline is good enough?
Write a score from 1 to 100 where 100 means the outline is perfect based on the task
                                           description, and provide an explanation
                                           on strengths and weaknesses. Please be
                                           specific.
# Write in this format:
[score: 1-100] [reason] xxx (50 words max)
# Example:
[score: 50] [reason] the current outline is too predictable
# Your response:
EVALUATE_CURRENT_ITEMIZED = TASK_DESCRIPTION + """ \
Here is a story outline.
{outline}
Which continuous {num_consecutive_lines} outlines items do you think are least
                                           interesting?
```

```
The interesting outline items should engage readers to read the story. Otherwise, it
                                           's boring and should be revised. The
                                           interesting level would be from 1 to 5,
                                           where 1 is the least interesting and 5 is
                                           the most interesting.
Write in this format:
Thought Process:
[reason: too repetitive/cliche plot/unsurprising/etc] [start_index]-[end_index] [
                                           interesting level: 1-10]
Example:
Thought Process:
Outline items 9 and 10 talks about the same thing over outline items 7 and 8. It's
                                           too repetitive.
[reason: too repetitive] [9]-[10] [interesting level: 5]
Can you provide {num_candidates} proposals?
# Your response:
```

Fine-tuned story outline content evaluator The content evaluator for the story outline is fine-tuned on a Flan-T5 model with a learning rate of 3e-4 and a weight decay of 0.1, trained over 5 epochs.

A.2 Task 2 Mini-Crossword Solving

```
TASK_DESCRIPTION = """\
Task Description:
Let's play a 5 x 5 mini crossword, where each word should have exactly 5 letters.
                                          Your goal is to fill in the crossword with
                                            words based on the hints provided.
.....
NEW_CANDIDATE = TASK_DESCRIPTION + """\
#Current board:
{obs}
#Strategy:
{feedback}
Given the current status of the board and the strategy, list all possible answers
                                           for unfilled or changed words, and your
                                           confidence levels (certain/high/medium/low
                                           ), using the format like this:
Use "certain" cautiously and only when you are 100% sure this is the correct word.
                                           You can list more then one possible answer
                                            for each word.
h1. [hint: ____] xxxxx (medium)
h2. [hint: ____] xxxxx (certain)
v1. [hint: ____] xxxxx (high)
. . .
Write your response in the format:
h1. [A financial loss; a negative profit; to remove bits from: D_B_{-}] DEBTS (low)
h2. [Fatuous; empty headed: ____] INANE (high)
v1. [A dice player; something that cuts into small cubes: ____] DICER (high)
v5. [An Indian tent: ____] TEPEE (medium)
```

```
Each line can only have one candidate answer.
#Your response:
EVALUATE_CURRENT = TASK_DESCRIPTION + """ \
# Current board:
{obs}
Evaluate the current board and provide a strategy on how to continue to fill in the
                                           blank or correct potential mistakes.
Write your response in the format:
v1. [reasoning and potential answers]
v2. [reasoning and potential answers]
h1. [reasoning and potential answers]
# Example:
v2. [Current answer: tough; since the filled in h1. is debit; e is conflicted with
                                           t, we could consider other options such as
                                            ENURE]
v3. [Current answer: ??? CUTUP could be a potential answer]
# Your response:
```

A.3 Task 3 Constrained Generation

```
TASK_DESCRIPTION = """\
# Instruction Given several concepts (i.e., nouns or verbs), write a short and
                                           simple sentence that contains *all* the
                                           required words. The sentence should
                                           describe a common scene in daily life, and
                                            the concepts should be used in a natural
                                           way.
# # Examples
# ## Example 1 - Concepts: "dog, frisbee, catch, throw" - Sentence: The dog catches
                                           the frisbee when the boy throws it into
                                           the air.
# ## Example 2 - Concepts: "apple, place, tree, pick" - Sentence: A girl picks some
                                           apples from a tree and places them into
                                           her basket.
.....
INSTRUCTION = """\
Your Task - Concepts: {concepts}
NEW_CANDIDATE = TASK_DESCRIPTION + """\
Instruction:
{instruct}
Here is a proposed sentence.
{solution}
Here is the feedback of outline item.
{feedback}
Based on the feedback, can you make a revised solution?
# Sentence:
EVALUATE_CURRENT = TASK_DESCRIPTION + """ \
Instruction:
{instruct}
Here is a proposed sentence.
{solution}
Do you think that the proposed sentence is good enough? Write "no need to improve"
                                           if you think 1) the sentence covers all
                                           the concepts listed in the instruction;
                                           and 2) the sentence describes a common
                                           scene in daily life.
```

Otherwise, write "still need to improve" and provide a reason.
Write in this format:
[No need to improve/still need to improve] [reason] xxx (50 words max)
Example 1:
[still need to improve] the sentence misses the concept "dog", "ladder", and "drum".
Example 2:
[still need to improve] the cat does not fly.
Your response:
"""

B Computation Efficiency

Table 4, Table 5, and Table 6 show the estimated number of input/output tokens usage and the cost of completing one case. THOUGHTSCULPT with DFS has a comparable cost to ToT while THOUGHTSCULPT with MCTS requires a greater computation since it has an additional decision simulation process.

	Input/Output Tokens	Cost per case
ТоТ	10.1k/4.9k	\$0.248
THOUGHTSCULPT with DFS	11.3k/4.6k	\$0.251
THOUGHTSCULPT with MCTS	25.0k/9.9k	\$0.547

Table 4: Token use and estimated cost for Story Outline Improvement (Base LLM: gpt-4-0125-preview)

	Input/Output Tokens	Cost per case
ТоТ	64.5k/8.9k	\$0.912
THOUGHTSCULPT with DFS	41.6k/7.1k	\$0.629
THOUGHTSCULPT with MCTS	100.2k/16.3k	\$1.491

Table 5: Token use and estimated cost for Mini-Crossword (Base LLM: gpt-4-0125-preview)

	Input/Output Tokens	Cost per case
ТоТ	7.1k/1.1k	\$0.104
THOUGHTSCULPT with DFS	7.0k/0.7k	\$0.091
THOUGHTSCULPT with MCTS	15.7k/2.0k	\$0.217

Table 6: Token use and estimated cost for Constrained Generation (Base LLM: gpt-4-0125-preview)

C Alternative Search Algorithm

Algorithm 1 THOUGHTSCULPT with MCTS1: Input: Initial node x_0 2: Output: Output node x^* 3: Initialize empty search tree T4: for $j \leftarrow 1$ to $d_{rollout}$ do5: Select a leaf node x using the tree policy UCB1 Eqn 4

- 6: Expand node x by generating a set of children nodes X_{child}
- 7: node $x \leftarrow uniformly_sampled(X_{child})$
- 8: for $k \leftarrow 1$ to $d_{simulation}$ do
- 9: node $x \leftarrow \text{generate_single_child}(x)$
- 10: end for
- 11: Evaluate reward v(x)
- 12: Propagate the reward v and number of explorations n back to x_0
- 13: **end for**
- 14: Choose the best node x^* with the highest reward v
- 15: return x^*

Algorithm 2 THOUGHTSCULPT with DFS

- 1: Input: Initial node x, Depth d
- 2: **Output:** Goal node x^*
- 3: $x \leftarrow x_0$
- 4: **if** d = 0 **then**
- 5: return x
- 6: **end if**
- 7: Expand node x by generating a set of children nodes X_{child}
- 8: for $k \leftarrow 1$ to $max_candidates$ do
- 9: Evaluate reward $v(X_{child}[k])$
- 10: **end for**
- 11: Choose the node x^* with the highest reward v in X_{child}
- 12: $DFS(x^*, d-1)$

D Output Examples

D.1 Story Outline Improvement

The examples below show the final outputs of each reasoning algorithm in the story outline improvement task. In general, THOUGHTSCULPT with MCTS displays a more complex story with a greater tendency to introduce twists and characters. The final output of THOUGHTSCULPT with MCTS may be greatly modified. Self Refine is less prone to change from the initial outline. ToT and THOUGHTSCULPT with DFS are in the middle and would like to add interesting details to the initial outlines.

D.1.1 Example 1

Initial Outline:

- 1. Jack arrives in Maine and starts attending the same high school as Leo.
- 2. Jack begins observing Leo's daily routine and interests to find common ground.
- 3. Jack strategically plans his first encounter with Leo to establish a connection.
- 4. Jack successfully befriends Leo and starts spending more time together.
- 5. Jack and Leo spend more time together, deepening their bond.
- 6. Jack and Leo's attraction becomes undeniable, leading to their first kiss.
- 7. Jack and Leo navigate the challenges of their secret relationship.
- 8. Jack and Leo's love for each other grows stronger, despite the risks involved.
- 9. The Center orders Jack to cut ties with Leo and leave Maine immediately.
- 10. Jack struggles with the decision to leave Leo and return to the Center.
- 11. Leo's father becomes a target of the Center's operation, putting Leo in danger.
- 12. Jack risks his own safety to protect Leo and his father, defying the Center's orders. Self Refine:
- 1. Jack arrives in Maine and starts attending the same high school as Leo.
- 2. Jack begins observing Leo's daily routine and interests to find common ground.
- 3. Jack strategically plans his first encounter with Leo to establish a connection.
- 4. Jack successfully befriends Leo and starts spending more time together.
- 5. Jack and Leo spend more time together, deepening their bond.
- 6. Jack and Leo's attraction becomes undeniable, leading to their first kiss.
- 7. Jack and Leo navigate the challenges of their secret relationship.
- 8. Jack and Leo's love for each other grows stronger, despite the risks involved.
- 9. The Center orders Jack to cut ties with Leo and leave Maine immediately.
- 10. Jack struggles with the decision to leave Leo and return to the Center.
- 11. A mysterious organization threatens to expose Jack and Leo's relationship, putting their lives in danger.

12. Jack must make a decision to protect Leo and himself, risking everything to defy both the Center and the new threat.

ToT:

- 1. Jack arrives in Maine and starts attending the same high school as Leo.
- 2. Jack is immediately drawn to Leo's mysterious and aloof demeanor, sparking his curiosity.
- 3. Jack discovers Leo's passion for art and secretly starts leaving anonymous gifts for him.
- 4. Leo becomes intrigued by the gifts and begins to search for the mysterious admirer.
- 5. Jack and Leo finally meet at a school art exhibition, where Leo realizes Jack's connection to the gifts.
- 6. Their initial awkward encounter slowly blossoms into a genuine friendship as they bond over their shared love for art.
- 7. Jack and Leo's friendship is tested when a scandal rocks their school, threatening to tear them apart.
- 8. Despite the challenges, Jack and Leo's bond deepens as they confide in each other and support one another.
- 9. The Center, a secretive organization Jack is a part of, reveals their true intentions and orders Jack to complete a dangerous mission that puts Leo at risk.
- 10. Jack is torn between his loyalty to the Center and his love for Leo, struggling to find a way to protect both.
- 11. Leo's life is put in grave danger when he uncovers a dark secret that implicates the Center in a series of crimes.
- 12. Jack makes the ultimate sacrifice to save Leo and expose the Center's corrupt actions, putting his own life on the line for the person he loves.

THOUGHTSCULPT with DFS

- 1. Jack arrives in Maine and starts attending the same high school as Leo.
- 2. Jack is immediately drawn to Leo, but soon realizes that Leo is hiding a dark secret.
- 3. Instead of confronting Leo right away, Jack decides to secretly follow him and discovers that Leo is actually working undercover to bring down the dangerous organization.
- 4. Jack is conflicted between his growing feelings for Leo and the danger of being involved in Leo's mission.
- 5. Jack offers to help Leo in his mission, leading to a deepening of their bond as they face increasing risks together.
- 6. Their forbidden romance blooms amidst the chaos, complicating their mission and putting them both in jeopardy.
- 7. The organization catches wind of Jack and Leo's alliance, putting both of their lives at risk.
- 8. Jack and Leo must make difficult choices to protect each other and navigate the treacherous waters of their relationship.
- 9. The Center threatens to harm Leo's family if they don't stop their investigation.

- 10. Jack and Leo are forced to go underground and make a dangerous deal to protect their loved ones.
- 11. The stakes are raised when Leo's father is kidnapped, pushing Jack and Leo to their limits in a race against time to save him.
- 12. Jack and Leo face off against the leaders of the organization in a thrilling final showdown, risking everything to bring them down and secure a future together.

THOUGHTSCULPT with MCTS:

- 1. Jack arrives in Maine and starts attending the same high school as Leo.
- 2. Jack notices a mysterious new student, Alex, who seems to be watching Leo closely.
- 3. Jack becomes curious about Alex's intentions and starts investigating their background.
- 4. Jack discovers that Alex is actually a spy from a rival organization called the Center targeting Leo.
- 5. Jack confronts Alex and warns Leo about the danger, leading to a confrontation between the three.
- 6. Jack, Leo, and Alex form an unlikely alliance to uncover the truth behind the Center's motives.
- 7. Jack and Leo's bond is tested as they navigate the complexities of trust and betrayal within their group.
- 8. The rival organization escalates their actions, putting Jack, Leo, and Alex in grave danger.
- 9. Leo sacrifices himself to protect Jack and defeat the Center, shocking everyone.
- 10. The truth behind the Center's motives is revealed, leading to a deeper understanding of the sacrifices made.
- 11. Jack and Alex must work together to honor Leo's sacrifice and take down the Center.
- 12. In a shocking revelation, it is uncovered that Leo's twin brother, who was thought to be dead, is actually the mastermind behind the Center, creating a complex dynamic between the characters.

D.1.2 Example 2

Initial outline:

- 1. The Health Department wants to close the Boys Club due to infestation of rats and cockroaches.
- 2. Closing the Boys Club means the kids will be left without a place to go.
- 3. The kids are worried about being out on the street again.
- 4. Buddy suggests organizing a bake sale to raise funds.
- 5. Johnny proposes hosting a talent show as another fundraising idea.
- 6. Rich suggests reaching out to local businesses for donations or sponsorships.
- 7. Cool suggests organizing a community car wash to raise money.
- 8. Buddy Williams suggests asking the local pet store owner if he knows anything about the rich cat.
- 9. The kids visit the pet store and ask the owner about the rich cat.
- 10. The pet store owner tells the kids about a rumor he heard of a rich cat living in a mansion nearby.
- 11. The kids decide to investigate the mansion and see if they can find the rich cat.

- 12. The townspeople share their findings and clues with the kids, who compile the information and continue the search.
- 13. The kids and townspeople follow leads and investigate potential sightings of the rich cat.
- 14. The search intensifies as more people join in, creating a sense of community and determination to find the rich cat.
- 15. After an extensive search, the kids and townspeople finally locate the rich cat, who generously donates the money needed to save the Boys Club.

Self Refine:

- 1. The Health Department wants to close the Boys Club due to infestation of rats and cockroaches.
- 2. Closing the Boys Club means the kids will be left without a place to go.
- 3. The kids are worried about being out on the street again.
- 4. Buddy suggests organizing a bake sale to raise funds.
- 5. Johnny proposes hosting a talent show as another fundraising idea.
- 6. Rich suggests reaching out to local businesses for donations or sponsorships.
- 7. Cool suggests organizing a community car wash to raise money.
- 8. Buddy Williams suggests asking the local pet store owner if he knows anything about the rich cat.
- 9. The kids visit the pet store and ask the owner about the rich cat.
- 10. The pet store owner tells the kids about a rumor he heard of a rich cat living in a mansion nearby.
- 11. The kids decide to investigate the mansion and see if they can find the rich cat.
- 12. While searching the mansion, the kids stumble upon a hidden room filled with mysterious artifacts and clues.
- 13. The artifacts lead them to a map that hints at a hidden treasure in the town.
- 14. The kids and townspeople embark on a thrilling treasure hunt, following the map's clues and facing challenges along the way.
- 15. After overcoming obstacles and working together, the kids and townspeople unearth the hidden treasure, which turns out to be the rich cat's fortune that saves the Boys Club.

ToT:

- 1. The Health Department wants to close the Boys Club due to infestation of rats and cockroaches.
- 2. Closing the Boys Club means the kids will be left without a place to go.
- 3. The kids are worried about being out on the street again.
- 4. Buddy suggests organizing a bake sale to raise funds.
- 5. Johnny proposes hosting a talent show as another fundraising idea.
- 6. Rich suggests reaching out to local businesses for donations or sponsorships.
- 7. Cool suggests organizing a community car wash to raise money.

- 8. Buddy Williams suggests asking the local pet store owner if he knows anything about the rich cat.
- 9. The kids visit the pet store and ask the owner about the rich cat.
- 10. The pet store owner tells the kids about a rumor he heard of a rich cat living in a mansion nearby.
- 11. The kids decide to investigate the mansion and see if they can find the rich cat.
- 12. While investigating the mansion, the kids stumble upon a hidden room with a mysterious map that leads to a hidden treasure.
- 13. The townspeople share their findings and clues with the kids, who now have a new mission to find the hidden treasure.
- 14. The search for the hidden treasure leads the kids and townspeople to uncover secrets about the town's history and a long-lost treasure that could save the Boys Club.
- 15. After a thrilling adventure and overcoming obstacles, the kids and townspeople finally find the hidden treasure, which not only saves the Boys Club but also brings the community closer together.

THOUGHTSCULPT with DFS

- 1. The Health Department discovers that the Boys Club is in danger of losing its funding due to budget cuts.
- 2. The kids are devastated as they learn that the Boys Club may have to shut down if they can't come up with a solution.
- 3. Buddy suggests organizing a scavenger hunt around town to raise funds and awareness for the Boys Club.
- 4. Johnny proposes creating a social media campaign to rally support and donations for the Boys Club.
- 5. Rich suggests hosting a charity concert with local musicians and performers to raise money.
- 6. Cool suggests organizing a charity auction with items donated by local businesses and community members.
- 7. The kids brainstorm and come up with a plan to combine all the fundraising ideas into one big event to save the Boys Club.
- 8. Buddy Williams suggests asking the local historian if he knows of any hidden treasures or artifacts that could help raise funds.
- 9. The kids visit the local historian and learn about a legendary treasure rumored to be hidden somewhere in town.
- 10. The historian gives the kids a map and clues to help them on their quest to find the treasure.
- 11. The kids embark on an exciting adventure to follow the map and solve the clues to locate the hidden treasure.
- 12. Along the way, they face challenges and obstacles that test their friendship and determination.
- 13. The townspeople join in the treasure hunt, adding to the excitement and suspense of the search.
- 14. After overcoming obstacles and following the clues, the kids and townspeople finally discover the hidden treasure, which turns out to be the key to saving the Boys Club.

15. The treasure not only provides the funds needed to keep the Boys Club open but also brings the community together in a heartwarming and unforgettable way.

THOUGHTSCULPT with MCTS

- 1. The Health Department wants to close the Boys Club due to infestation of rats and cockroaches.
- 2. Closing the Boys Club means the kids will be left without a place to go.
- 3. The kids are worried about being out on the street again.
- 4. Buddy suggests organizing a scavenger hunt around town to raise funds.
- 5. Johnny proposes creating a community mural project as another fundraising idea.
- 6. Luna, a mysterious new girl in town, suggests hosting a talent show to raise money, revealing her own hidden talents in the process.
- 7. Rich suggests organizing a neighborhood cleanup event to raise money.
- 8. Cool suggests hosting a movie night in the park to raise funds.
- 9. Buddy Williams suggests asking the local historian if he knows anything about a hidden treasure in the town.
- 10. The kids visit the local historian and ask about the hidden treasure.
- 11. The historian tells the kids about a legend of a lost pirate treasure buried somewhere in the town.
- 12. Luna shares a personal connection to the treasure hunt, sparking curiosity and excitement among the group.
- 13. The kids face challenges and puzzles during their treasure hunt that test their problem-solving skills and teamwork.
- 14. In a surprising twist, the treasure turns out to be a time capsule filled with memories and mementos from the town's past.
- 15. The kids realize that the true treasure was the journey itself and the bonds of friendship they formed along the way, teaching them the value of community and unity. Luna's involvement adds depth to the story and enhances the theme of unity and friendship.

D.2 Constrained Generation

The examples below show the final outputs of different reasoning strategies in Constrained Generation.

D.2.1 Example 1

Concepts: drum, clip, window, cover, graffiti, wave, vomit, hurdle, dye, sidewalk, animal, slice, swing, pottery, pineapple, fix, decorate, tire, tag, bicycle, watermelon, sign, mask, plant

Refine Children decorated pottery with vibrant dye near the graffiti-covered wall, while a masked animal rode a bicycle past a sign, waving as they passed by a tire swing hanging from a tree and a clip holding a sign on the sidewalk, avoiding a hurdle, slicing a pineapple and a watermelon to plant in the garden.

ToT A child on a swing by the sidewalk waved at a bicyclist with a tire fixed and decorated with graffiti.

THOUGHTSCULPT with DFS The children decorated the pottery with vibrant dye, while the adults fixed the tire on the bicycle near the sidewalk, as a group of friends played the drum and waved at passersby from the swing, with a clip holding a sign on the window, a slice of watermelon in hand, and a pineapple plant in the background.

THOUGHTSCULPT with MCTS A person walks down the sidewalk past a graffiti-covered window, a pottery clip lies on the ground, a bicycle rider swerves to avoid a tire, and a sign is being fixed and decorated with dye next to a pineapple stand, as a drum beats in the background, a wave crashes on the shore, an animal scurries across the path, a slice of watermelon is enjoyed under the shade of a swing, a mask-wearing individual tags a plant with a new growth, and a hurdle is cleared by a runner as they vomit from exhaustion.

D.2.2 Example 2

Concepts: plant, word, remove, toddler, hamburger, potato, set, line, place, control, eat, banner, singe, hurdle, bed, bar, alley, stove, top, air, cowboy, sharpen, pair, beat, arena, wave, singer, jacket

Refine The toddler removes the banner from the line and places it on the top of the bar to singe while the cowboy sharpens a pair of knives to beat the hurdle in the arena.

ToT The toddler eats a hamburger and potato at the place where the plant is growing, while the singer on stage waves under the banner to the cheering crowd, and the cowboy sharpens his pair of beat-up boots backstage.

THOUGHTSCULPT with DFS The toddler eagerly eats a hamburger while the cowboy sharpens his pair of scissors at the plant nursery.

THOUGHTSCULPT with MCTS The toddler removes a plant from the line, places it in the bed, eats a hamburger with a side of potato, then sets the table for a cowboy sharpening his pair of knives at the top of the bar, while a singer controls the banner in the arena, singing as the wave of music beats through the alley where a jacketed cowboy hurdles over a singe stove.

E G-Eval on Story Outline Generation

We've run an additional evaluation using the G-Eval metric (Liu et al., 2023). We provide a definition prompt of interestingness, and the result indicates that ThoughtSculpt(MCTS) outperforms other baselines when evaluated by either GPT-4 and GPT-3.5, consistent with other metrics.

	GPT-3.5	GPT-4
Self-refine	4.33	4.45
ТоТ	4.37	4.66
ThoughtSculpt (DFS)	4.47	4.71
ThoughtSculpt (MCTS)	4.60	4.73

Table 7:	G-Eval Result	(1-5 scale)
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F More search steps on Mini-Crosswords

We've shown that THOUGHTSCULPT (MCTS) could achieve a solid performance in only 20 search steps, but we have run an extended number of search steps to match the experiment setup provided by Yao et al. (2023a).

		GPT4	
Methods	% word	% letter	% game
ToT (20 search steps)	39.5	64.8	5.0
ToT (100 search steps) (Yao et al., 2023a)	60	78	20
THOUGHTSCULPT (MCTS) (20 search steps)	54.0	74.0	25.0
THOUGHTSCULPT (MCTS) (100 search steps)	66.0	83.0	35.0

Table 8: Mini-crossword results of 20 puzzles for THOUGHTSCULPT and baselines (success % of letters, words, and games). Comparison between ToT and THOUGHTSCULPT (MCTS) with 20 and 100 search steps

G Constrained Generation LLM Evaluation

To evaluate the preferred output based on concept coverage and appropriateness, we conduct an additional assessment using GPT-4. We prompt GPT-4 to select the output that is most preferred, considering both its coverage of relevant concepts and the appropriateness of how this coverage is utilized. Figure 6, which compares THOUGHTSCULPT with MCTS against THOUGHTSCULPT with DFS and a third baseline (which intuitively represents the case where neither version of THOUGHTSCULPT produces a satisfactory output), shows that THOUGHTSCULPT with MCTS is significantly favored.

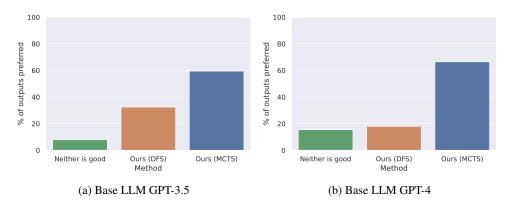


Figure 6: GPT-4's comprehensive preference based on concept coverage and appropriateness over the final outputs for Constrained Generation. THOUGHTSCULPT with MCTS is preferred by a wide margin.

H Game of 24

We additionally experiment with our method on the game of 24 using the same test set provided by (Yao et al., 2023a). Compared to (Yao et al., 2023a)'s prompts with detailed few-shot examples for this task, THOUGHTSCULPT uses a much more general prompt. As illustrated in Table 9, THOUGHTSCULPT still outperforms ToT in this comparison despite this setup that might be expected to favor ToT.

	Success %
CoT-SC (k=100) (Yao et al., 2023a)	9
IO - Refine (k=10) (Yao et al., 2023a)	27
ToT $(b = 1)$ (Yao et al., 2023a)	45
ToT $(b = 5)$ (Yao et al., 2023a)	74
ThoughtSculpt (MCTS) $(b = 5)$	79

Table 9: Game of 24 Result

H.1 Game of 24 Task prompts

```
TASK_DESCRIPTION = """\
Use the given four numbers and basic arithmetic operations (+ - \star /) to obtain 24.
You can use the numbers only once but you can use them in any order.
......
SOLUTION_OUTPUT_FORMAT = """ \
# Think step by step first. Then, please output the solution in the following format
                                             (in a Python code block).
```python
(1 + 2) * (2 * 4)
Your response.
REVISE_SOLUTIONS = """`\
Instruction
{instruction}
Current Solution
{solution}
Calculate the result of the current solution.
Do you think the solution is correct? If not, please provide feedback.
Output format
···json
}}
 "calculation": "step by step calculation of the current solution",
 "result: int,
"feedback": "Your feedback here",
 "correct" : true/false
}}
.....
```

# I Effectiveness of components

Our framework has two core components that use LLM: the thought evaluator, providing both numeric and language feedback for revision, and the thought generator, which generates subsequent nodes based on this feedback to improve outputs. Both are essential, as removing either makes the method non-functional. We conducted an additional ablation study by "weakening" these modules. We replaced GPT-4 with Llama3.1-8B-Instruct as the language model for either the thought evaluator or the thought generator in the Constrained Generation task. The results are summarized below:

Modules	% Coverage
ThoughtSculpt	99.0
ThoughtSculpt (weakened generator)	98.5
ThoughtSculpt (weakened evaluator)	96.3
ThoughtSculpt (weakened generator + evaluator)	90.7

Table 10: Coverage of Different ThoughtSculpt's Components

These results highlight the critical role of a strong evaluator in deep reasoning tasks, as it provides essential revision feedback that significantly enhances the generator's effectiveness.