# A Survey of Chain of Thought Reasoning: Advances, Frontiers and Future

Zheng Chu<sup>1</sup>\*, Jingchang Chen<sup>1</sup>\*, Qianglong Chen<sup>2</sup>\*, Weijiang Yu<sup>2</sup>, Tao He<sup>1</sup> Haotian Wang<sup>1</sup>, Weihua Peng<sup>2</sup>, Ming Liu<sup>1†</sup>, Bing Qin<sup>1</sup>, Ting Liu<sup>1</sup>

<sup>1</sup>Harbin Institute of Technology, Harbin, China <sup>2</sup>Huawei Inc., Shenzhen, China

{zchu, jcchen, the, mliu<sup>†</sup>, qinb, tliu}@ir.hit.edu.cn {chenqianglong.ai, wanght1998, weijiangyu8, pengwh.hit}@gmail.com

# **Abstract**

Chain-of-thought reasoning, a cognitive process fundamental to human intelligence, has garnered significant attention in the realm of artificial intelligence and natural language processing. However, there still remains a lack of a comprehensive survey for this arena. To this end, we take the first step and present a thorough survey of this research field carefully and widely. We use X-of-Thought to refer to Chain-of-Thought in a broad sense. In detail, we systematically organize the current research according to the taxonomies of methods, including XoT construction, XoT structure variants, and enhanced XoT. Additionally, we describe XoT with frontier applications, covering planning, tool use, and distillation. Furthermore, we address challenges and discuss some future directions, including faithfulness, multi-modal, and theory. We hope this survey serves as a valuable resource for researchers seeking to innovate within the domain of chain-of-thought reasoning<sup>1</sup>.

# 1 Introduction

Pre-trained language models (PLMs) can automatically learn general representations from unlabeled text and achieve excellent performance through fine-tuning on downstream tasks. (Devlin et al., 2019; Raffel et al., 2020; Radford and Narasimhan, 2018). Recently, scaling up language models significantly improves performance and brings many surprises, such as emergent abilities (Wei et al., 2022a; Schaeffer et al., 2023). Therefore, the paradigm of natural language processing is shifting from pretraining with fine-tuning to pre-training with incontext learning. However, as of now, large-scale language models (LLMs) still have considerable room for improvement on complex reasoning tasks,

such as mathematical reasoning (Cobbe et al., 2021; Patel et al., 2021), commonsense reasoning (Talmor et al., 2021; Mihaylov et al., 2018), etc.

To leverage LLMs for addressing complex reasoning tasks, Wei et al. (2022b) extends in-context learning with step-by-step reasoning processes, first introducing the concept of chain-of-thought (CoT) prompting. Kojima et al. (2022) finds that simply adding a magic phrase *Let's think step by step* in prompts enables LLMs to perform zero-shot chain-of-thought reasoning without any human annotation. These studies have highlighted the significance of chain-of-thought in enhancing the model's capability for complex reasoning and improving its reasoning and planning abilities.

Subsequently, a substantial of works about X-of-thought (XoT) emerges like mushrooms after the rain in the NLP community, such as automatic XoT construction (Kojima et al., 2022; Zhang et al., 2023f; Xu et al., 2023), XoT structural variants (Chen et al., 2022a; Ning et al., 2023; Lei et al., 2023a; Yao et al., 2023b), etc. Note that to distinguish it from primitive CoT, we use XoT to refer to CoT in a broad sense, which is a collective term for the use of step-by-step reasoning methods.

However, these methods and datasets have not yet undergone systematic review and analysis. To fill this gap, we propose this work to conduct a comprehensive and detailed analysis of the XoT family. Even though there have been some surveys discussing chain-of-thought, they are limited to specific aspects, such as LLM reasoning with prompts (Qiao et al., 2023) and chain-of-thought prompt strategies (Yu et al., 2023c). In contrast, our survey not only provides a more thorough and comprehensive discussion of the topics they've already covered, but also includes additional topics and discussions, such as XoT construction, XoT structural variants and frontier application, etc. Concretely, in this paper, we first introduce the relevant background and preliminary (§2). Furthermore,

Equal Contribution.

<sup>†</sup> Corresponding Author.

<sup>&</sup>lt;sup>1</sup>Resources are available at https://github.com/ zchuz/CoT-Reasoning-Survey

we carefully classify the XoT series of work from multiple perspectives and complete an in-depth analysis (§4), including XoT construction methods (§4.1), XoT structure variants (§4.2) and XoT enhancement methods (§4.3). Then, we provide practical applications of the XoT in the frontier fields (§5). In order to inspire the follow-up work of XoT, we offer insights into potential avenues for future research in this area (§6). Finally, we compare and discuss existing methods (§7).

# **Background and Preliminary**

## Background

In recent years, with the continuous expansion of computing power, large-scale language models have sprung up (Brown et al., 2020; OpenAI, 2023; Touvron et al., 2023a; Scao et al., 2022; Touvron et al., 2023b; Zhao et al., 2023b), and as the model size continues to grow, many new capabilities have emerged, such as in-context learning and chain-ofthought reasoning (Brown et al., 2020; Wei et al., 2022b,a; Schaeffer et al., 2023).

Brown et al. (2020) finds that large-scale language models have excellent in-context learning (ICL) ability. ICL incorporates input-output demonstrations into the prompt text. With ICL, off-the-shelf LLMs can be employed without additional fine-tuning while achieving comparable performance. Nevertheless, this end-to-end approach tends to underperform when faced with complex reasoning tasks.

Wei et al. (2022b) finds that the reasoning ability of LLMs can be improved by adding step-by-step reasoning processes to the demonstration, which is known as chain-of-thought prompting. CoT prompting enables the model to gain a more precise understanding of both the question's intricacies and the reasoning process. Furthermore, the model generates a sequence of reasoning steps, which grants us a transparent view of the model's cognitive process, further enhancing interpretability.

## 2.2 Preliminary

In this section, we introduce the preliminary chainof-thought reasoning with LLMs, and we refer to the formula definition in (Qiao et al., 2023). Suppose there is a question Q, a prompt T and a probabilistic language model  $P_{LM}$ . The model takes the question and prompt as inputs to give the rationale  $\mathcal{R}$  and answer  $\mathcal{A}$ . We first consider in-context scenarios where the demonstrations do not contain

reasoning chains. We need to maximize the likelihood of Answer A, as shown in Equ (1,2).

$$p(\mathcal{A} \mid \mathcal{T}, \mathcal{Q}) = \prod_{i=1}^{|\mathcal{A}|} p_{LM}(a_i \mid \mathcal{T}, \mathcal{Q}, a_{< i})$$
 (1)  
$$\mathcal{T}_{ICL} = \{I, (x_1, y_1), \cdots, (x_n, y_n)\}$$
 (2)

$$\mathcal{T}_{ICL} = \{I, (x_1, y_1), \cdots, (x_n, y_n)\}$$
 (2)

In the chain-of-thought reasoning scenario, where the demonstrations contain reasoning process, we need to maximize the likelihood of Answer  $\mathcal{A}$  and rationale  $\mathcal{R}$ , as shown in Equ (3,4,5,6).

$$p(\mathcal{A} \mid \mathcal{T}, \mathcal{Q}) = p(\mathcal{A} \mid \mathcal{T}, \mathcal{Q}, \mathcal{R}) p(\mathcal{R} \mid \mathcal{T}, \mathcal{Q}) \quad (3)$$

$$p(\mathcal{R} \mid \mathcal{T}, \mathcal{Q}) = \prod_{i=1}^{|\mathcal{R}|} p_{LM}(r_i \mid \mathcal{T}, \mathcal{Q}, r_{< i})$$
 (4)

$$p(\mathcal{A} \mid \mathcal{T}, \mathcal{Q}) = \prod_{i=1}^{|\mathcal{R}|} p_{LM}(r_i \mid \mathcal{T}, \mathcal{Q}, r_{< i})$$
(4)  
$$p(\mathcal{A} \mid \mathcal{T}, \mathcal{Q}, \mathcal{R}) = \prod_{j=1}^{|\mathcal{A}|} p_{LM}(a_i \mid \mathcal{T}, \mathcal{Q}, \mathcal{R}, a_{< j})$$
(5)

$$\mathcal{T}_{\text{CoT}} = \{I, (x_1, e_1, y_1), \cdots, (x_n, e_n, y_n)\}$$
 (6)

## 3 Benchmarks

# 3.1 Mathematical Reasoning

Mathematical reasoning is often used to measure the reasoning power of a model. Early benchmarks contain simple arithmetic operations (Hosseini et al., 2014; Koncel-Kedziorski et al., 2015; Roy and Roth, 2015; Koncel-Kedziorski et al., 2016). Ling et al. (2017) labels the reasoning process in natural language form, and Amini et al. (2019) builds on AQUA by labeling the reasoning process in program form. Later benchmarks (Miao et al., 2020; Patel et al., 2021; Cobbe et al., 2021; Gao et al., 2023) contain more complex and diverse questions. (Zhu et al., 2021; Chen et al., 2021, 2022b) require reasoning based on the table content. There are also general benchmarks (Hendrycks et al., 2021; Mishra et al., 2022a,b) and reading comprehension form benchmarks (Dua et al., 2019; Chen et al., 2023). Recently, (Yu et al., 2021a) endowed pre-trained model with the ability of mathematical reasoning by using hierarchical reasoning and knowledge.

# Commonsense Reasoning

Commonsense reasoning is the process of making inferences, judgments, and understandings based on knowledge that is generally known and commonly perceived in the everyday world. How to acquire and understand commonsense knowledge

Task	Dataset	Size	Input	Output	Rationale	Description
Mathematical Reasoning	AddSub (Hosseini et al., 2014)	395	Question	Number	Equation	Simple arithmetic
	SingleEq (Koncel-Kedziorski et al., 2015)	508	Question	Number	Equation	Simple arithmetic
	MultiArith (Roy and Roth, 2015)	600	Question	Number	Equation	Simple arithmetic
	MAWPS (Koncel-Kedziorski et al., 2016)	3320	Question	Number	Equation	Simple arithmetic
	AQUA-RAT (Ling et al., 2017)	100,000	Question	Option	Natural Language	Math reasoning with NL rationale
	ASDiv (Miao et al., 2020)	2305	Question	Number	Equation	Multi-step math reasoning
	SVAMP (Patel et al., 2021)	1,000	Question	Number	Equation	Multi-step math reasoning
	GSM8K (Cobbe et al., 2021)	8.792	Question	Number	Natural Language	Multi-step math reasoning
	GSM-Hard (Gao et al., 2023)	936	Question	Number	Natural Language	GSM8K with larger number
	MathQA (Amini et al., 2019)	37,297	Question	Number	Operation	Annotated based on AQUA
	DROP (Dua et al., 2019)	96,567	Question+Passage	Number+Span	Equation	Reading comprehension form
	TheoremQA (Chen et al., 2023)	800	Question+Theorem	Number	X	Answer based on theorems
	TAT-QA (Zhu et al., 2021)	16,552	Question+Table+Text	Number+Span	Operation	Answer based on tables
	FinQA (Chen et al., 2021)	8,281	Question+Table+Text	Number	Operation	Answer based on tables
	ConvFinQA (Chen et al., 2021)	3892	Question+Table+Dialog	Number	Operation	Multi-turn dialogs
	MATH (Hendrycks et al., 2021)	12500	Ouestion	Number	Natural Language	Challenging competition math problems
		101.835	Question Ouestion+Text		Naturai Language	Multi-task benchmark
	NumGLUE (Mishra et al., 2022b)			Number+Span		
	LILA (Mishra et al., 2022a)	133,815	Question+Text	Free-form	Program	Multi-task benchmark
Commonsense Reasoning	ARC (Bhakthavatsalam et al., 2021)	7787	Question	Option	×	From science exam
	OpenBookQA (Mihaylov et al., 2018)	5,957	Question+Context	Option	×	Open-book knowledges
	PIQA (Bisk et al., 2020)	21000	Goal+Solution	Option	X	Physical commonsense knowledge
	CommonsenseQA (Talmor et al., 2019)	12247	Question	Option	X	Derived from ConceptNet
	CommonsenseQA 2.0 (Talmor et al., 2021)	14343	Question	Yes/No	X	Gaming annotation with high quality
	Event2Mind (Rashkin et al., 2018)	25000	Event	Intent+Reaction	X	Intension commonsense reasoning
	McTaco (Zhou et al., 2019)	13225	Question	Option	X	Event temporal commonsense reasoning
	CosmosQA (Huang et al., 2019)	35588	Question+Paragraph	Option	×	Narrative commonsense reasoning
	ComValidation (Wang et al., 2019)	11997	Statement	Option	X	Commonsense verification
	ComExplanation (Wang et al., 2019)	11997	Statement	Option/Free-form	×	Commonsense explanation
	StrategyQA (Geva et al., 2021)	2,780	Question	Yes/No	×	Multi-hop commonsense reasoning
	Last Letter Concat. (Wei et al., 2022b)	-	Words	Letters	×	Rule-based
0 1 1	Coin Flip (Wei et al., 2022b)	-	Statement	Yes/No	X	Rule-based
Symbolic	Reverse List (Wei et al., 2022b)	-	List	Reversed List	X	Rule-based
Reasoning	BigBench (Srivastava et al., 2022)	-	-		X	Contains multiple symbolic reasoning datasets
	BigBench-Hard (Suzgun et al., 2023)	-	-	-	×	Contains multiple symbolic reasoning datasets
	ReClor (Yu et al., 2020)	6,138	Question+Context	Option	х	Questions from GMAT and LSAT
	LogiQA (Liu et al., 2020)	8,678	Question+Paragraph	Option	X	Questions from China Civil Service Exam
	ProofWriter (Tafjord et al., 2021)	20192	Ouestion+Rule	Answer+Proof	Entailment Tree	Reasoning process generation
Logical	FOLIO (Han et al., 2022)	1435	Conclusion+Premise	Yes/No	X	First-order logic
Reasoning	DEER (Yang et al., 2022)	1,200	Fact	Rule	x	Inductive reasoning
	PrOntoQA (Saparov and He, 2023)	1,200	Question+Context	Yes/No+Proccess	First-Order Logic	Deductive reasoning
Multimodal Reasoning	VCR (Zellers et al., 2019)	264,720	Question+Image	Option	Natural Language	Visual commonsense reasoning
	VisualCOMET (Park et al., 2020)	1,465,704	Image+Event	Action+Intent	×	Visual commonsense reasoning
	PMR (Dong et al., 2022)	15,360	Image+Background	Option	×	Premise-based multi-modal reasoning
	ScienceQA (Lu et al., 2022)	21,208	Q+Image+Context	Option	Natural Language	Multi-modal reasoning with NL rationales
	VLEP (Lei et al., 2020)	28,726	Premise+Video	Option	X	Video event prediction
	CLEVRER (Yi et al., 2020)	305,280	Question+Video	Option/Free-form	Program	Video temporal and causal reasoning
	STAR (Wu et al., 2021)	600,000	Question+Video	Option	×	Video situated reasoning
	NEXT-QA (Xiao et al., 2021)	47,692	Question+Video	Option	×	Video temporal,causal,commonsense reasoning
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	Causal-VidQA (Li et al., 2022a)	107,600	Question+Video	Free-form	Natural Language	Video causal and commonsense reasoning

Table 1: An overview of benchmarks and tasks on reasoning.

is a major impediment to models facing commonsense reasoning. Many benchmarks and tasks are proposed focusing on commonsense understanding (Talmor et al., 2019, 2021; Bhakthavatsalam et al., 2021; Mihaylov et al., 2018; Geva et al., 2021; Huang et al., 2019; Bisk et al., 2020), event temporal commonsense reasoning (Rashkin et al., 2018; Zhou et al., 2019), and commonsense verification (Wang et al., 2019).

## 3.3 Symbolic Reasoning

Symbolic reasoning here refers specifically to the simulation of some simple operations, which are simple for humans yet challenging for LLMs. Last letter concatenation, coin flip, and reverse list (Wei et al., 2022b) are the most commonly used symbolic reasoning tasks. In addition, the collaborative benchmark BigBench (Srivastava et al., 2022) and BigBench-Hard (Suzgun et al., 2023) also contain several symbolic reasoning datasets, such as state tracking and object counting.

# 3.4 Logical Reasoning

Logical reasoning is divided into deductive reasoning, inductive reasoning, and abductive reasoning (Yu et al., 2023a). Deductive reasoning derives conclusions from general premises (Liu et al., 2020; Yu et al., 2020; Tafjord et al., 2021; Han et al., 2022). Inductive reasoning derives general conclusions from special cases (Yang et al., 2022). Abductive reasoning gives rational explanations for observed phenomena (Saparov and He, 2023).

## 3.5 Multi-modal Reasoning

In the real world, reasoning also involves information in modalities other than text, with visual modalities being the most prevalent. To this end, many benchmarks for visual multi-modal reasoning are proposed (Zellers et al., 2019; Park et al., 2020; Dong et al., 2022; Lu et al., 2022), and among them, ScienceQA (Lu et al., 2022) annotates reasoning process and is the most commonly used visual multi-modal reasoning benchmark. Video multi-modal reasoning (Lei et al., 2020; Yi et al.,

2020; Wu et al., 2021; Xiao et al., 2021; Li et al., 2022a; Gupta and Gupta, 2022) is more challenging as it introduces additional temporal information compared to visual multi-modal reasoning.

#### 3.6 Metrics

**Accuracy** Accuracy is used to assess a model's ability on classification tasks and is commonly used for multi-choice (Ling et al., 2017; Mihaylov et al., 2018; Liu et al., 2020; Lu et al., 2022) and yes/no (Talmor et al., 2021; Geva et al., 2021; Han et al., 2022) tasks.

$$Accuracy = \frac{N_{correct}}{N_{total}}$$
 (7)

EM and F1 EM and F1 are metrics used to evaluate free form (Mishra et al., 2022a; Wang et al., 2019; Yi et al., 2020) and span extraction (Dua et al., 2019; Zhu et al., 2021; Mishra et al., 2022b) tasks. Both are calculated at the token level.

$$F1 = \frac{2 \cdot P \cdot R}{P + R} \tag{8}$$

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$$EM = \frac{\sum \mathbb{I}[A = A']}{N_{\text{total}}}$$
(8)

where P and R stand for precision and recall, and EM calculates the proportion of predictions and answers that are exactly the same.

# **Methods**

In this section, we explore X-of-thought reasoning through three different categorizations: the construction of X-of-thought (§4.1), the structural variants of X-of-thought (§4.2), and the enhanced methods of X-of-thought (§4.3).

## 4.1 Construction Approach

After thorough analysis, we divide the construction of X-of-thought into three categories: 1) Manual XoT, 2) Automatic XoT, and 3) Semi-automatic XoT, described as follows.

## 4.1.1 Manual XoT

While large language models perform few-shot incontext learning via prompting, they are still limited in reasoning tasks. In order to explore the potential reasoning ability of large language models, one standard approach is to provide different forms of thoughts in demonstrations.

Wei et al. (2022b) first propose chain-of-thought prompting (Few-shot CoT) by manually providing

natural language form rationales to the demonstrations. To further ensure certainty in the reasoning process and reduce inconsistencies between reasoning path and answers, PAL (Gao et al., 2023), PoT (Chen et al., 2022a) and NLEP (Zhang et al., 2023e) leverage programming language as annotated rationales, which transforms the problemsolving into an executable Python program. Meanwhile, to take both advantages of natural language and programming language and raise the confidence of reasoning output, MathPrompter (Imani et al., 2023) uses the zero-shot chain-of-thought prompting to generate multiple algebraic expressions or Python functions, which can verify each other and improve the reliability of results. Furthermore, since the reasoning complexity of samples in demonstrations, such as chains with more reasoning steps, results in performance improvement, Fu et al. (2023a) proposes complexity-based prompting, where voting among high-complexity rationales is performed to get the final answer.

Manually constructed X-of-thought methods expand on in-context learning by adding different types of step-by-step intermediate reasoning processes to demonstrations. They allow LLMs to mimic and generate reasoning paths. Although manual XoT methods provide greater interpretability as well as trustworthiness for human understanding and outperform on complex tasks, i.e., mathematical reasoning, commonsense reasoning, symbolic reasoning, etc., manual annotating of rationales entails significant costs and suffers from drawbacks such as difficulty in demonstration selection and task generalization. Specifically, different tasks require different ways of demonstrations. Therefore, other works attempt to construct the reasoning path automatically, as discussed in §4.1.2.

## 4.1.2 Automatic XoT

Chain-of-thought prompting (Wei et al., 2022b) elicits the complex reasoning ability of LLMs with task-specific exemplars in a few-shot setting, which limits the scalability and generalization. To reduce the cost of hand-crafted few-shot exemplars, Kojima et al. (2022) proposes zero-shot CoT by introducing a magic phrase Let's think step by step after question, which enables LLMs to generate reasoning chains in a zero-shot manner. However, zero-shot CoT suffers from poor-quality reasoning paths, coming with many mistakes. Since the diversity of demonstration plays a vital role in reasoning chains generation, Auto-CoT (Zhang et al.,

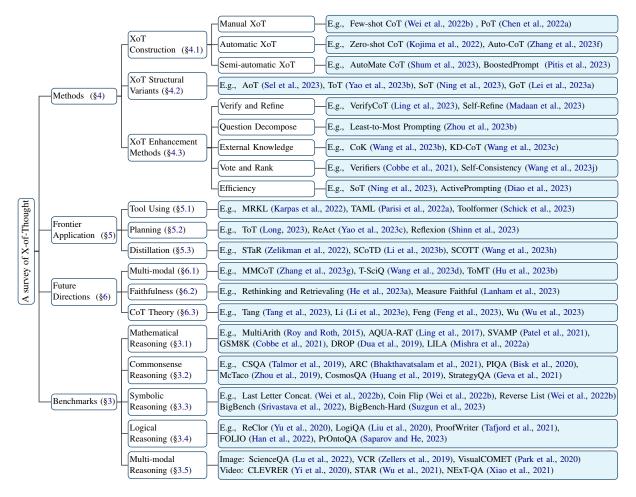


Figure 1: XoT Methods, Frontier Application, Future Direction, and Benchmarks.

2023f) generates the demonstrations automatically via clustering and representative exemplars selection, which improves the diversity and consistently matches or exceeds the performance of Few-shot CoT. COSP (Wan et al., 2023) introduces the outcome entropy of the question to aid demonstration selection. Xu et al. (2023) proposes Reprompting to find the effective CoT prompt by employing Gibbs sampling iteratively. Meanwhile, some mistakes in reasoning chains come from missing-step errors, Wang et al. (2023f) extend the zero-shot CoT into Plan-and-Solve (PS) Prompting via devising a plan to divide the entire task into smaller sub-tasks and carrying out the sub-tasks according to the plan with more detailed instructions. Logi-CoT (Zhao et al., 2023c) uses symbolic logic to validate the zero-shot reasoning process, thus reducing errors in reasoning. Besides, PoT (Chen et al., 2022a) also explore language models, such as Codex, to generate an executable Python program to solve math problems in zero-shot setting via adding Let's write a Python program step by step..., which mitigates errors in intermediate reasoning steps. Some work introduces agents to solve reasoning problems. For example, Agent Instruct (Crispino et al., 2023a) utilizes agents to generate task-related, informative instructions, which guides LLMs to perform zero-shot reasoning.

Unlike manual XoT, automatic XoT, using zeroshot prompt engineering or sampling, is scalable and can be generalized between domains without human intervention. However, due to the lack of human alignment, automatically generated chain-of-thought encounters challenges such as poor quality, hallucinations, and factual inconsistencies. Therefore, constructing XoT in a semi-automatic way is necessary, which is introduced in §4.1.3.

## 4.1.3 Semi-automatic XoT

Semi-automatic XoT methods integrate the advantages of both manual and automatic construction methods. Shao et al. (2023) proposes Synthetic Prompting, which leverages a few human-annotated examples to prompt models to generate more examples through an alternated forward-backward process and selects effective demonstrations to elicit better reasoning, alleviating the lack

of human alignment in AutoCoT. Although previous work solves the problem of manual annotating, demonstration selection can also significantly affect performance. Automate-CoT (Shum et al., 2023) employs reinforcement learning with a variance-reduced policy gradient strategy to estimate the significance of each example in a blackbox language model, eliciting better demonstration selection. Similarly, Lu et al. (2023b) proposes PromptPG, which utilizes policy gradient to learn to select demonstrations in tabular reasoning. Ye and Durrett (2023) initially uses two proxy metrics to evaluate each example and then searches over examples to find demonstrations that yield the best performance in a silver-labeled development set. Meanwhile, Pitis et al. (2023) proposes Boosted Prompting, a prompt ensembling way to improve the performance, which iteratively expands the examples when encountering the problem that the current demonstration is challenging to handle. Zou et al. (2023) introduce Meta-CoT, which automatically selects demonstrations based on the question category, eliminating the need for the task-specific prompt design.

The semi-automatic XoT methods reduce the workload of manual labeling while introducing human alignment signals and demonstration selection strategies to enhance the capability and stability of reasoning. Additionally, it enables cost-effective domain generalization. However, the demonstration selection problem has not been entirely resolved and requires more effort and research.

## 4.2 XoT Structural Variants

The most primitive chain-of-thought is a chain structure that describes intermediate reasoning steps in natural language. In this section, we introduce structural variants that modify the original chain structure, including chain structure variants, tree structure variants, and graph structure variants.

Chain Structure PAL (Gao et al., 2023) and PoT (Chen et al., 2022a) introduce programming languages to describe the reasoning process, thereby converting the reasoning problem into the implementation of an executable program to obtain the final answer. Since the program execution is deterministic and performs arithmetic computations accurately, this approach shows excellent performance in mathematical reasoning. Besides, symbol sequence is another type of thought representation. Chain-of-Symbol (Hu et al., 2023a) represents the

complex environments with condensed symbolic chain representations during planning, which reduces the complexity of the simulation environment. Chain structure variants are shown in Figure 2(c,d) Algorithm of Thought (Sel et al., 2023) injects algorithmic capabilities into the model, making the model's reasoning more logical by adding examples based on algorithms. Its absence of the huge search space of tree search (Long, 2023; Yao et al., 2023b) saves computational resources and achieves excellent performance.

Tree Structure The original chain structure inherently limits the scope of exploration. Through the incorporation of tree structures and tree search algorithms, models gain the capability to efficiently explore and backtrack during the reasoning process (Long, 2023; Yao et al., 2023b), as shown in Figure 2(e). Combined with self-assessment of intermediate thoughts, models can achieve global optimum solutions. The reasoning process of ToT involves uncertainty, which can potentially lead to cascading errors. TouT (Mo and Xin, 2023) introduces Monte Carlo Dropout in reasoning, taking into account the uncertainty. Yu et al. (2023b) delves into analogous problems, harnessing their solutions to elevate the intricate reasoning abilities of LLMs. These analogous problems exhibit a tree-like structure, ultimately converging to solve the main problem. However, the current tree-ofthought has considerable limitations on task selection and requires specific prompt designing for each task, which hinders its widespread application. SoT (Ning et al., 2023) is another variant of the tree structure, which decomposes a problem into subproblems that can be processed in parallel and solved simultaneously to speed up reasoning. However, its utility is restricted to parallel decomposable problems and is not suited for complex reasoning tasks.

Graph Structure Compared to trees, graphs introduce loops and rings, which bring more complex topological relationships and allow for modeling more complex reasoning, as shown in Figure 2(f). GoT (Besta et al., 2023; Lei et al., 2023a) regards intermediate thought as nodes within a graph, combining exploration and backtracking operations, and additionally introduces aggregation and refinement operations compared to tree-of-thought. The additional operations, aggregation and refinement elicit better reasoning in complex

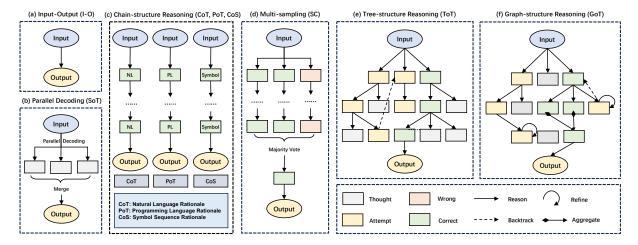


Figure 2: The evolution of reasoning, from direct I/O to chain structure, then to tree and graph structure.

tasks. Nevertheless, it faces the same dilemmas as the tree-of-thought, i.e., task limitations and poor generalizability. Besides, it has increased reasoning costs. Unlike GoT, which explicitly constructs a thought graph, ResPrompt (Jiang et al., 2023a) introduces residual connections between thoughts in the prompt text, allowing the reasoning of different steps to interact with each other.

As models transition from linear chains to hierarchical trees and intricate graphs, the interplay of thoughts becomes progressively more complex, thereby gradually enhancing the capacity to address intricate problems. However, as the complexity of the topology increases, associated methods impose more constraints on task selection, leading to a significant reduction in their generalizability and making their application difficult. Extending complex topology structure-based methods to general domains is a major challenge for future research.

## 4.3 XoT Enhancement Methods

In this section, we present the XoT enhancement methods. In total, we will provide an overview of five categories, which are adding verification and refinement (§4.3.1), question decomposition (§4.3.2), leveraging external knowledge (§4.3.3), voting and ranking (§4.3.4), and improving efficiency (§4.3.5).

# 4.3.1 Verify and Refine

Chain-of-thought reasoning often tends to be hallucinatory, producing incorrect reasoning steps. Errors in intermediate reasoning steps can, in turn, trigger a cascade of errors. Incorporating verification to obtain feedback and subsequently refining the reasoning process based on this feedback can

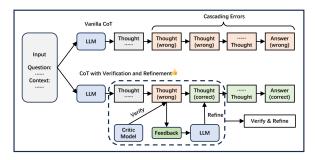


Figure 3: Verification and refinement reduce cascading errors in reasoning.

be a highly effective strategy for mitigating this phenomenon, which is similar to the process of human reflection. Figure 3 depicts the overview of verification and refinement.

VerifyCoT (Ling et al., 2023) devises a Natural Program, a deductive reasoning form, which allows models to produce accurate reasoning steps, with each subsequent step strictly based on the previous steps. DIVERSE (Li et al., 2022c) utilizes a voting mechanism to eliminate incorrect answers, followed by a fine-grained verification of each reasoning step independently. SCREWS(Shridhar et al., 2023) thinks that the post-modification result may not necessarily be superior to the origin, so it introduces a selection module to select a better result between the origin and modification. To facilitate knowledge-intensive tasks, Verify-and-Edit (Zhao et al., 2023a) incorporates external knowledge to re-reason uncertain examples, reducing factual mistakes in reasoning. Some research efforts attempt to unearth the internal knowledge of models. Some research efforts attempt to unearth the internal knowledge of models. To address factual errors, some

research attempts to unearth the intrinsic knowledge of LLMs. They acquire knowledge from the model before answering the questions (Dhuliawala et al., 2023; Zheng et al., 2023). Ji et al. (2023) further verifies the correctness of intrinsic knowledge, and Liu et al. (2023b) enhances the accuracy of intrinsic knowledge acquisition through reinforcement learning.

Inconsistency is another major challenge in reasoning, Dua et al. (2022) iteratively uses previous reasoning results as prompts until the model gives a consistent answer. Paul et al. (2023) trains a critic model to provide structured feedback on the reasoning process. Self-Refine (Madaan et al., 2023) performs iterative self-feedback and refinement to alleviate errors in reasoning. Compared with Self-Refine, Reflexion (Shinn et al., 2023) introduces reinforcement learning for reflection, which additionally brings decision-making capability. Meanwhile, some work introduces backward reasoning (Yu et al., 2023a) for verification. RCoT (Xue et al., 2023) reconstructs the question according to the reasoning chains, and its inconsistency with the original question exposes errors in the reasoning process. FOBAR (Jiang et al., 2023b) and Self Verification (Weng et al., 2022) perform verification by deducing the conditions in the question from the answer. FOBAR infers the variables in the question, and Self Verification infers the conditions in the question. However, Huang et al. (2023a) finds that LLMs struggle to self-correct without external feedback, and it could even lead to a performance decline.

LLM reasoning is an unsupervised process in which feedback signals from intermediate reasoning steps play a crucial role in improving reasoning. Guidance from feedback signals can effectively reduce the hallucination phenomena in reasoning. There is still significant research space for obtaining appropriate feedback and making accurate corrections based on that feedback.

# 4.3.2 Question Decomposition

The essence of X-of-thought reasoning lies in its step-by-step problem-solving. However, the original chain-of-thought reasoning approach does not explicitly strip out the step-by-step reasoning process and still uses one-stage generation. In this section, we discuss the question decomposition approach, which explicitly solves questions step-by-step. The overview is shown in Figure 4.

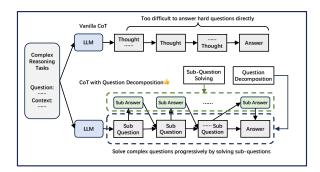


Figure 4: Question decomposition solves complex questions progressively by solving simple sub-questions.

Wang et al. (2022a) iteratively acquires knowledge from the model, making progress in multi-hop QA. Zhou et al. (2023b) proposes Least-to-Most Prompting, which initially breaks down the question into sub-questions in a top-down fashion, and subsequently, it solves a sub-question once at a time and leverages their solutions to facilitate subsequent sub-questions. Successive Prompting (Dua et al., 2022) takes a similar approach to Least-to-Most Prompting, and the difference is that it takes a decomposition with interleaved sub-questions and answers rather than two-stage decomposition. The above methods do not formulate tailored solutions for various sub-problems. Decomposed Prompting (Khot et al., 2023) designs a modular shared library, each dedicated to a class of subproblems, which can tailor more effective solutions to different classes of sub-problems. Apart from general tasks, some works focus on question decomposition on tabular reasoning. BINDER(Cheng et al., 2023) maps reasoning to a program in a neural-symbolic manner and obtains the final answer through a program executor such as Python or SQL. Ye et al. (2023) introduces DATER, which breaks down large tables into smaller ones and complex questions into simpler ones. The former reduces irrelevant information, while the latter reduces the complexity of reasoning.

Providing direct answers to complex questions can be challenging. By decomposing the question into simple sub-questions and solving them step-by-step, the difficulty is reduced. Moreover, each sub-question can be traced back to a specific reasoning step, making the reasoning process more transparent and explainable. Current work mostly uses top-down decomposition strategies, while bottom-up decomposition strategies based on backward reasoning remain to be explored in future work.

## 4.3.3 External Knowledge

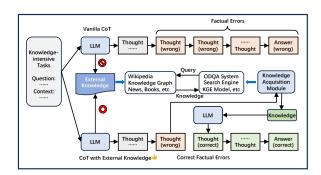


Figure 5: Introducing external knowledge reduces factual errors in reasoning.

The parameterized knowledge within models is limited and outdated. Thus, factual mistakes often occur when facing knowledge-intensive tasks. Introducing external knowledge can mitigate this phenomenon, as shown in Figure 5.

Lu et al. (2023a) introduces multilingual dictionaries in prompts to enhance machine translation. Li et al. (2023d) proposes chain-of-knowledge (CoK-Li), which obtains structured knowledge from a knowledge base via a query generator to perform knowledge-guided reasoning. Wang et al. (2023b) (CoK-Wang) also retrieves structured knowledge from KB. Moreover, it estimates the reasoning chains in terms of factuality and faithfulness and prompts models to rethink unreliable reasonings, which mitigates the knowledge retrieval errors in CoK-Li. KD-CoT (Wang et al., 2023c) addresses factual reasoning problems through a multi-turn QA approach. They design a feedbackaugmented retriever for retrieving relevant external knowledge in each round of QA to calibrate the reasoning process. Other studies use the model's own memory as external knowledge. For example, Memory-of-Thought (Li and Qiu, 2023) first performs pre-thinking to save the high-confidence thoughts into external memory, and during inference, it lets the LLM recall relevant memory to aid reasoning.

The parameterized knowledge in the model is fixed at the end of the pre-training, which leads to its shortcomings in terms of knowledge capacity and knowledge updating. While introducing external knowledge can alleviate this to some extent, it remains an imperfect solution. To fundamentally tackle this issue, continual learning (Lange et al., 2022; Wang et al., 2023g) stands as a promising avenue for future research endeavors.

## 4.3.4 Vote and Rank

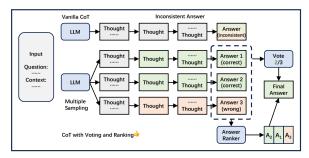


Figure 6: Voting and ranking reduce inconsistency by selecting final answers from multiple samplings.

Owing to the inherent stochasticity in the generation process, LLM reasoning exhibits an element of randomness and uncertainty. This problem can be effectively alleviated through multiple sampling strategies, as shown in Figure 6.

Some methods adopt ranking, such as (Cobbe et al., 2021), which trains a verifier to select high-confidence reasoning chains through ranking. Meanwhile, other methods select reasoning chains through a voting mechanism. Selfconsistency (Wang et al., 2023j) selects the most consistent answer by majority voting among sampled reasoning chains based on final answers. Furthermore, (Fu et al., 2023a) proposes Complex CoT, which utilizes a complexity-based voting strategy that leans towards selecting answers generated by more complex reasoning chains. However, answer-based voting mechanisms do not take into account the correctness of reasoning chains. Miao et al. (2023) takes the reasoning steps into account when voting, which can obtain both consistent answers and trustworthy reasoning processes simultaneously. Moreover, to consider the relations between intermediate steps across chains, Yoran et al. (2023) mixes information between reasoning chains and selects the most relevant facts to perform meta-reason over multiple reasoning chains. GRACE(Khalifa et al., 2023) trains a discriminator through contrastive learning and uses this discriminator to rank each intermediate reasoning step. Previous methods sample based on the probability distribution, while Diversity-of-Thought (Naik et al., 2023) obtains multiple reasoning paths by prompting with different instructions.

Drawing inspiration from ensemble learning, the practice of voting and ranking following with multiple sampling serves to diminish uncertainty. Furthermore, it has showcased substantial performance

improvements compared to the single-sample approach. Multiple sampling with voting has become a common technique in current X-of-thought studies. Integrating reasoning chains into voting remains a significant area of research for the future.

## 4.3.5 Efficiency

LLM reasoning and manually annotated reasoning chains impose expensive overheads. Aggarwal et al. (2023) improves self-consistency by dynamically adjusting the number of samples, which can significantly reduce inference costs with marginal performance degradation. Ning et al. (2023) decomposed the questions in parallel and handled them simultaneously, reducing the reasoning time overhead. But it cannot handle complex questions. Zhang et al. (2023b) accelerates the reasoning by selectively skipping some intermediate layers and then verifies the draft in another forward pass. Diao et al. (2023) borrows ideas from active learning to annotate examples with high uncertainty, reducing the human annotating cost.

Large-scale language models have showcased immense capabilities, but they also come with substantial overhead. Balancing the trade-off between performance and overhead may require significant attention in future research endeavors.

# 5 Frontier Application

## 5.1 Tool Use

Despite the extensive knowledge exhibited by LLMs, it is accompanied by several challenges. These encompass the incapacity to access upto-the-minute news, proclivity towards hallucinations when responding to queries involving out-of-domain knowledge, and the absence of sophisticated reasoning capacities like mathematical calculations or symbolic reasoning. By granting LLMs the ability to employ external tools, it becomes possible to augment the model's reasoning capabilities and assimilate external knowledge, enabling it to engage in information retrieval and environmental interaction.

MRKL (Karpas et al., 2022) introduces a novel framework comprising scalable modules (referred to as experts) and a router. These experts can take the form of neural networks or symbols. However, this study primarily focuses on conceptualization and training an LLM specifically for mathematical computation while not delving into implementing other module contents. TALM (Parisi et al.,

2022a) and Toolformer (Schick et al., 2023) integrate a text-centric methodology with supplementary tools to enhance the capabilities of language models. They employ a self-supervise mechanism to initiate performance enhancements, commencing with a limited set of tooltips. In a similar vein, HuggingGPT (Shen et al., 2023) leverages visual and speech models to process information from diverse modalities, thereby endowing LLMs with the capacity for multi-modal understanding and generation. Another question is how to select the appropriate tool. LATM (Cai et al., 2023) enables the tool-making ability of LLMs to make generalized API across different tasks, and GEAR (Lu et al., 2023c) considers the efficiency of tool-using by using smaller models to delegate tool grounding and execution.

However, converting a user request into API format is often not straightforward. The existing approaches mentioned above have limitations in facilitating multiple invocations of the tool and rectifying query errors. To tackle this problem, Re-Act (Yao et al., 2023c) integrates the strengths of reasoning and action to enhance and complement each other, augmenting problem-solving capability mutually. ART (Paranjape et al., 2023) uses a task library to select relevant tool usage and reasoning chains. MM-REACT (Yang et al., 2023) further utilizes vision experts to enable multi-modal reasoning and action.

The aforementioned research endeavors focus on designing tools (or APIs) to enhance the capabilities of LLMs in various domains. Combining XoT with tools effectively addresses the challenges faced by LLMs. X-of-thought reasoning enables models to effectively elicit, track, and update action plans while managing exceptions. Simultaneously, action operations facilitate the model's interaction with external sources, such as knowledge bases and environments, enabling it to gather additional information. To assess the proficiency of tools, API-Bank (Li et al., 2023c) and MetaTool (Huang et al., 2023c) introduce comprehensive benchmarks, providing a robust foundation to evaluate the performance and effectiveness of tool-augmented LLMs.

# 5.2 Planning

LLMs face challenges in providing accurate responses directly for intricate problems, necessitating the need to decompose them into sequential steps and sub-tasks. While CoT offers a straightfor-

ward approach to planning, it falls short in addressing highly complex problems and lacks the ability to evaluate and rectify errors through backtracking.

Numerous studies have extended the framework of chain-of-thought to various formats to enhance the capacity for planning further. Treeof-Thought (Yao et al., 2023b) enables LLMs to consider multiple reasoning paths in a tree and self-evaluate to determine the next course of action. In cases where global decisions are necessary, ToT allows forward or backward exploration through techniques like deep-first search or breadthfirst search. Reasoning via Planning (RAP) (Hao et al., 2023) also divides the problem into a tree and explores them by Monto Carlo tree search algorithm, using LLMs as both world-model and reasoning agent. Another method, Graph of Thought (GoT) (Yao et al., 2023d), employs graph nodes to represent individual thoughts and external Graph Neural Networks for organization. LLM+P (Liu et al., 2023a) and LLM+DP (Dagan et al., 2023) facilitate the generation of Planning Domain Definition Language (PDDL) (Gerevini, 2020) by LLMs. PDDL assists in decomposing complex problems and utilizing specialized models for planning before converting the results into natural language for LLM processing. However, it is essential to note that these methods use tree/graph/PDDL nodes to represent thoughts, which have limitations regarding their representation forms and can only handle specific planning problems.

Another technique is to improve the model's ability to correct errors and summarize historical experience. Self-Refine (Madaan et al., 2023) employs a unique approach where the output generated by the model is evaluated and provided with feedback using the same model. Reflexion (Shinn et al., 2023) enables the model to reflect on and rectify errors made in previous actions, resembles reinforcement learning in textual format, and involves dividing memory into long and short-term components. However, Reflexion cannot update the plan when an out-of-plan error occurs. AdaPlanner (Sun et al., 2023) introduces adaptive closed-loop plan refinement, which iterative refines the task plan based on the feedback of the environment. ISR-LLM (Zhou et al., 2023c) combines Self-Refine with PDDL to achieve a better success rate in longhorizon sequential tasks. Meanwhile, LATS (Zhou et al., 2023a) utilizes LM-based Monte Carlo Tree Search for a more flexible planning procedure.

Planning can be flexibly combined with tools (Ruan et al., 2023) or agents (Crispino et al., 2023b) to enrich reasoning ability. ToRA (Gou et al., 2023) designs mathematical specialized agents with external tools, and AutoUI (Zhang and Zhang, 2023) directly interacts with the multi-modal environment instead of converting visual inputs into text, which enhances the reasoning efficiency and reduces error propagation.

Planning augmented approaches have advanced conventional sequential planning by introducing search-based, graph-based, and definition language-based methods. On the other hand, some methods incorporate action, planning, reflection, or tools, aiming to enhance LLMs' long-term planning and error resilience capabilities.

### **5.3** CoT Distillation

LLM can be self-improved by distilling reasoning steps to solve complex problems. Huang et al. (2022) employs an LLM with self-consistency to generate reasoning chains from unlabeled data. These chains are subsequently utilized to fine-tune the model, enhancing its generalized reasoning capabilities. Zelikman et al. (2022) proposes STaR, a few-shot learning approach to improve LM's reasoning capabilities using a self-loop bootstrap strategy. SECToR (Zhang and Parkes, 2023) uses chain-of-thought to obtain arithmetic answers, then fine-tune the model to generate the answer without CoT directly.

Thought CoT is an emerging ability primarily observed in LLMs, with limited advancements in small models. However, enhancing small models' CoT ability is conceivable through techniques like distillation. Magister et al. (2023) demonstrates that fine-tuning T5 with reasoning chains generated by larger teacher models and utilizing an external calculator for answer resolution can substantially enhance task performance across diverse datasets. Ho et al. (2023) generates and filters multiple reasoning paths to enrich the diversity.

Numerous endeavors can be undertaken to reduce human costs using unannotated (or very few annotated) data by utilizing the self-consistency (Wang et al., 2023j). Hsieh et al. (2023) employs prompts to generate answers from much fewer labeled/unlabeled data, followed by the generation of rationales that prompt the language model to provide reasoning for the given answer. SCoTD (Li et al., 2023b) finds that sampling multi-

ple reasoning chains per instance from teachers is paramount for improving the capability of students. SCOTT (Wang et al., 2023h) utilizes contrastive decoding (Li et al., 2022b; O'Brien and Lewis, 2023) during rationale generation for teacher models. Furthermore, to tackle the shortcut problem, it employs a counterfactual reasoning objective while training student models. DialCoT (Han et al., 2023) decomposes reasoning steps into a multi-round dialog and selects the correct path using the PPO algorithm. Jie et al. (2023); Wang et al. (2023i) add special tokens for mathematic problems. This high-level information improves the consistency of reasoning steps.

The studies above adopt a shared paradigm wherein reasoning chains are generated through LLMs possessing superior reasoning capabilities. These reasoning chains are then distilled into smaller models. The effectiveness of the distillation process is improved by augmenting the sampling strategy from the larger model, for example, through the utilization of multiple sampling paths, consistency, or contrastive decoding, which leads to improved diversity and accuracy in the generated reasoning chains, ultimately benefiting the distillation process to smaller models. It's notable that language models have intricate tradeoffs and complex balances associated with multidimensional capabilities. Fu et al. (2023b) emphasizes that increasing task-specific chain-of-thought capabilities through distillation may also adversely impact the models' performance in solving generalized problems.

## **6 Future Directions**

While chain-of-thought reasoning has showcased remarkable performance on numerous tasks, some challenges still require further exploration. In this section, we provide a concise overview of three promising avenues for future research: multimodal X-of-thought reasoning (§6.1), faithful X-of-thought reasoning (§6.2), and X-of-thought reasoning theory (§6.3).

# 6.1 Multi-modal CoT

The shift from text unimodal to vision-text multimodal introduces richer information, meanwhile bringing more challenges. Some works have attempted to explore X-of-thought reasoning in multimodal scenarios by fine-tuning multi-modal models to generate a high-quality chain of thoughts.

Multimodal-CoT (Zhang et al., 2023g) firstly

fine-tunes multi-modal models to generate chainof-thoughts and then reasons over the rationales to obtain final answers. However, it suffers from the limitation of the linearity of the reasoning process and has difficulties in interacting between different modalities. To alleviate the challenges encountered by Multimodal-CoT, (Yao et al., 2023d) proposes Graph-of-Thought (GoT), which models the thought processes as a graph. It parses the reasoning chains into a thought graph, which enables a more realistic representation of thought processes by capturing non-sequential information interactions. This measure breaks the limitations of linear structure through graphical structures and further improves performance. Furthermore, Yao et al. (2023a) proposes Hypergraph-of-Thought (HoT), replacing thought graphs with hypergraphs, which enables models with better ability of highorder multi-hop reasoning and multi-modal comparative judgment. Meanwhile, some work takes an approach based on knowledge distillation. T-SciQ (Wang et al., 2023d) generates high-quality CoT rationales from LLMs as fine-tuning signals and introduces a novel data mixing strategy to produce effective samples for different questions.

The aforementioned studies explore multi-modal reasoning in small models and fine-tuning scenarios, which we regard as an initial endeavor in the realm of multi-modal chain-of-thought reasoning. We believe that video multi-modal reasoning combined with in-context learning should be the focus of future research. On the one hand, videos introduce additional temporal information with innate chaining relationships compared with images. Through chain-of-thought reasoning, the information in different frames can be naturally connected to explicitly model the temporal relationship, which is well-suited for video multi-modal reasoning. On the other hand, small models are capacity-limited and need fine-tuning to gain chainof-thought ability. Worse still, multi-modal reasoning chains are difficult to obtain, which further exacerbates the challenge. In comparison, contemporary vision-language foundation models (VLMs) (Alayrac et al., 2022; Li et al., 2023a; Wang et al., 2022b; Huang et al., 2023b; Peng et al., 2023; Yu et al., 2021b) have strong visionlanguage comprehension and are already capable of in-context learning with interleaved text and images. They provide a solid foundation for chain-ofthought reasoning with in-context learning. Utilizing chain-of-thought for video reasoning remains an unexplored territory with only a few studies. CoMT (Hu et al., 2023b) combines fast-thinking and slow-thinking in video reasoning and introduces a tree search strategy for planning, which firstly applies CoT in video multi-modal reasoning.

Although some works have started to utilize chain-of-thought reasoning and solve multi-modal reasoning tasks, previous works only focus on how to construct high-quality fine-tuned data, and there are still several challenges remaining:

- How to unify visual and language features to elicit better multi-modal understanding.
- How to use VLMs for chain-of-thought reasoning without fine-tuning.
- How to adapt image multi-modal reasoning into video multi-modal reasoning.

## 6.2 Faithfulness

Extensive research indicates that chain-of-thought reasoning can lead to hallucination phenomena, such as factual mistakes and contextual inconsistencies. Considering that language models fundamentally belong to statistical models, and due to factors such as data noise and knowledge forgetting, hallucination phenomena are unavoidable.

Some works focus on mitigating factual mistakes. He et al. (2023a) introduces external knowledge to evaluate reasoning chains and votes to filter out chains that contain factual mistakes but without correcting them Wang et al. (2023b) adopts a similar way, with the difference that it additionally introduces a reflection mechanism to correct low-scoring reasoning. Zhao et al. (2023a) filters out low-confidence reasoning by consistency and guides models to re-reasoning based on relevant external knowledge. While the aforementioned methods work well on knowledge-intensive tasks, they fall short in addressing the challenge of contextual inconsistencies. Zhang et al. (2023d) explores the hallucination snowballing phenomena during the reasoning process. Others aim to address the inconsistency issues. Radhakrishnan et al. (2023) observes that models are more faithful when dealing with simple questions. Thus, it improves faithfulness through question decomposition. Faithful CoT (Lyu et al., 2023) initially generates symbolic reasoning chains and later deterministically executes symbolic functions, mitigating reasoning inconsistencies. Lanham et al. (2023) explores the

factors that influence faithfulness, which provides an empirical perspective. It finds faithfulness varies on different tasks and decreases as the model size increases. CoNLI (Lei et al., 2023b) proposes a post-editing strategy to diminish the hallucinations. SynTra (Jones et al., 2023) performs prefix-tuning on a synthetic dataset designed to elicit hallucination easily, and then transfers this capability to real tasks.

Despite numerous efforts aimed at addressing the hallucination issues in large language models, these works have only mitigated the problem to some extent. There is still a long way to fully enhance the faithfulness of large language models. We summarize the future directions as follows:

- Improving the ability to recognize hallucination phenomena in the reasoning processes.
- Improving the accuracy of external knowledge retrieval and utilization to reduce factual mistakes.
- Improving the ability to recognize and correct contextual inconsistencies and logical mistakes, which is more challenging.
- How to fundamentally eliminate hallucination phenomena from alternative approaches, e.g. specific pre-training.

# 6.3 CoT Theory

Despite the impressive capability of chain-ofthought reasoning, the ability to generate chainof-thought following instructions still lacks a comprehensive explanation.

Some work addresses from an empirical perspective and can serve as a practical guide. Madaan and Yazdanbakhsh (2022) decomposes prompts into three components: symbols, patterns, and text, exploring the impact of CoT through counterfactual prompting. Wang et al. (2023a) analyzes the impact of demonstration selection. They find that the correctness of reasoning chains has a negligible effect, while the relevance to the question and correct reasoning order matters. Tang et al. (2023) explores the role of semantics. They find that chain-of-thought reasoning relies heavily on semantic knowledge introduced during pre-training and performs poorly in symbolic reasoning.

Others work analyze theoretically, exploring the underlying principles and internal mechanisms. Li et al. (2023e) deconstructs chain-of-thought reasoning as a multi-step combinatorial function. They

demonstrate that chain-of-thought reduces the complexity of in-context learning to tackle complex questions. Feng et al. (2023) theoretically proves that a fixed-size Transformer is sufficient for computational tasks and dynamic planning with chainof-thought. Merrill and Sabharwal (2023) observes that chain-of-thought can boost reasoning ability, with the extent of improvement increasing as the number of intermediate reasoning steps grows. Wu et al. (2023) leverages gradient-based feature attribution methods to explore the impact of chainof-thought on outputs. The results indicate that chain-of-thought exhibits robustness to perturbations and variations in the question. In addition, there are some claims suggesting that the chainof-thought ability stems from code data during the pre-training phase (Madaan et al., 2022; Zhang et al., 2023c), but there is currently no systematic work to substantiate this opinion.

Current research on chain-of-thought theory is still in its preliminary exploration stage. We summarize future research directions as follows:

- Explore the sources of chain-of-thought ability to achieve targeted improvements in CoT reasoning.
- Theoretically analyzing the advantages of chain-of-thought over in-context learning and exploring the boundaries of its capabilities.

# 7 Discussion

## 7.1 Comparison of XoT Construction

There are three main ways of constructing an X-of-thought for existing methods: (1) **Manual** labeling reasoning chains. (2) **Automatic** generating reasoning chains by models. (3) **Semi-automatic** generation with automatic expansion on a small number of manually labeled reasoning chains.

We observe that the manual construction methods (Wei et al., 2022b; Gao et al., 2023) face similar challenges to in-context learning, i.e., demonstration selection, instruction formatting, etc (Dong et al., 2023). This causes numerous difficulties in its application and hinders the transfer ability across different tasks. Automatic construction methods (Zhang et al., 2023f; Chen et al., 2022a; Xu et al., 2023) lack the guidance of high-quality annotations, resulting in performance deficiencies. Benefiting from the signals brought by manual annotations, semi-automatic methods (Shum et al., 2023; Shao et al., 2023) can generate high-quality

reasoning chains through self-bootstrapping and similar techniques, effectively addressing the challenges faced by previous approaches. While achieving excellent performance, it allows for easy transfer across different tasks.

# 7.2 Comparison between Verification/Refinement and Planning

Numerous parallels exist between planning methods and verification/refinement-based methods, as both rely on feedback from intermediate processes to adjust and refine behavior. The distinction lies in the fact that planning methods encompass decision-making, while verification/refinement-based methods solely address intermediate errors without delving into higher-level cognitive processes.

LLM reasoning processes are often hallucinatory, causing factual and logical mistakes. Verify and edit based methods (Ling et al., 2023; Zhao et al., 2023a; Madaan et al., 2023; Shinn et al., 2023) verify the correctness of the reasoning process and refine reasoning step that may cause hallucinatory. Through verification and refinement, cascading errors and hallucinatory phenomena in the reasoning process are significantly reduced.

The planning methods (Long, 2023; Yao et al., 2023b,c; Liu et al., 2023a; Shinn et al., 2023) introduce a decision-making process in the reasoning. They evaluate the intermediate reasoning steps to get feedback, and based on the feedback, they engage in exploration and backtracking to achieve superior solutions at a global level. Their specialization lies in handling complex problems, enabling them to achieve remarkable performance, especially when confronted with intricate multi-hop reasoning and planning tasks.

# 7.3 Compensate for Innate Weaknesses

LLMs have many inherent limitations when it comes to reasoning, such as the inability to access external information, arithmetic errors, and inconsistent reasoning. These issues can be cleverly circumvented by entrusting specific responsibilities to dedicated modules or models.

In response to the models' limitation in accessing external information, (Li et al., 2023d; Wang et al., 2023b; Lu et al., 2023a; Schick et al., 2023; Karpas et al., 2022; Yoran et al., 2023) utilizes external knowledge resources like knowledge base, search engines, and open-domain question-answering systems. Some work introduces a calculator to address arithmetic errors (Schick et al.,

2023; Karpas et al., 2022; Parisi et al., 2022b). Code execution is deterministic, and certain work enhances the consistency of the reasoning process by introducing code executor (Gao et al., 2023; Chen et al., 2022a; Bi et al., 2023; Imani et al., 2023). We believe that employing LLMs as an agent for central planning and reasoning, delegating specific sub-tasks to dedicated sub-models, is a potential avenue for applying large models in complex scenarios in the future (Wang et al., 2023e; Xi et al., 2023).

#### 7.4 Other Work

In this chapter, we will list other works that represent early attempts at chain-of-thought reasoning or are designed for specific domains.

Katz et al. (2022); Zhang et al. (2022) provide benchmarks and resources. Some work has empirically demonstrated the effectiveness of chainof-thought prompting (Lampinen et al., 2022; Ye and Durrett, 2022; Arora et al., 2023) and Shi et al. (2023) explores multi-lingual CoT reasoning. Other work focuses on specific domains, such as machine translation (He et al., 2023b), sentiment analysis (Fei et al., 2023), sentence embeddings (Zhang et al., 2023a), summarization (Wang et al., 2023k), arithmetic (Lee and Kim, 2023), and tabular reasoning (Chen, 2023; Jin and Lu, 2023), etc. Besides, some research utilizes specific pretraining to enhance certain capabilities, such as mathematical reasoning (Lewkowycz et al., 2022; Zhao et al., 2022).

# 8 Conclusion

In this paper, we conduct an extensive survey of existing research on X-of-thought reasoning, offering a comprehensive review of the field. We introduce the concept of generalized chain-of-thought (X-of-Thought) and examine advances in X-ofthought reasoning from various angles. Additionally, we investigate the applications of X-ofthought in cutting-edge domains. Furthermore, we spotlight the current challenges confronting this research and provide future prospects. To the best of our knowledge, this survey represents the first systematic exploration of chain-of-thought reasoning. Our objective is to furnish researchers interested in chain-of-thought reasoning with a thorough overview, with the hope that this survey will facilitate further research in this area.

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