

Multi-Step Reasoning with Large Language Models, a Survey

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Language models with billions of parameters exhibit in-context learning abilities, enabling few-shot learning on tasks that the model was not specifically trained for. Traditional models achieve breakthrough performance on language tasks, but do not perform well on basic reasoning benchmarks. However, a new in-context learning approach, Chain-of-thought, has demonstrated strong multi-step reasoning abilities on these benchmarks.

The research on LLM reasoning abilities started with the question whether LLMs can solve grade school math word problems, and has expanded to other tasks in the past few years. This paper reviews the field of multi-step reasoning with LLMs. We propose a taxonomy that identifies different ways to generate, evaluate, and control multi-step reasoning. We provide an in-depth coverage of core approaches and open problems, and we propose a research agenda for the near future.

We find that multi-step reasoning approaches have progressed beyond math word problems, and can now successfully solve challenges in logic, combinatorial games, and robotics, sometimes by first generating code that is then executed by external tools. Many studies in multi-step methods are using reinforcement learning for finetuning, external optimization loops, in context reinforcement learning, and self-reflection.

CCS Concepts: • Computing methodologies → Natural language processing.

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1 INTRODUCTION

Transformer-based Large Language Models (LLMs) that are trained on large datasets have achieved breakthrough performance at text generation tasks that directly build on next token prediction [115, 152, 163]; they are good at natural language understanding (GLUE, SQuAD, Xsum) [99, 119, 155, 156], translation [73, 106, 130], question answering [143], and other language generation tasks. The success of models such as ChatGPT [102] is impressive.

Transformer-based generative language models whose size is beyond hundreds of billions parameters are not only good at language generation, they also enable a new type of machine learning, called *in-context learning* [15]. In-context learning, also known as prompt-based learning, is an emergent ability that occurs in LLMs beyond a certain size (hundreds of billions of parameters—less, with judicious prompting) that have been finetuned for conversational responses [163]. In-context learning is inference-time, prompt-based, few-shot learning with instructions. As opposed to finetuning, model parameters are not adapted by in-context learning.

Language generation tasks are solved well by LLMs with prompt-based learning. On the other hand tasks that require reasoning, such as grade school math word problems, are more difficult for LLMs [30]. Spurred-on by the impressive

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performance on language tasks, much research has focused on understanding the reason for the poor performance of LLMs on reasoning tasks, and how it can be improved. Among this research, the Chain-of-thought paper by Wei et al. [164] stands out. This work, and later work by Kojima et al. [74], showed that adding a simple instruction to the prompt, *Let's think step by step*, can provoke an LLM to perform the required intermediate reasoning steps to answer difficult problems in a multi-step approach. Subsequently, performance on math word benchmarks has increased markedly. Much of the performance increase of models such as OpenAI o1, o3 [61] and DeepSeek R1 [49, 131] is attributed to multi-step reasoning methods as reviewed here, with reinforcement learning playing an increasingly important role, both for in-context learning and finetuning [25, 37, 168, 173].

The line of research into multi-step LLM-reasoning was started with grade school math word problems, with the GSM8K benchmark [30]. Soon, other reasoning domains were included, such as reasoning about advanced math problems, computer code, robotic movement, and games. Many works have been published that build on Chain-of-thought [27]. In this paper, we survey the literature using a straightforward taxonomy. We discuss papers based on several reasoning benchmarks, as well as directly-related follow up work.

Having started with basic math word problems, multi-step LLM reasoning approaches now perform logic reasoning, planning, combinatorial games, and robotic actions, amongst others. Some approaches do so by prompting the LLM to generate code that is then interpreted by external tools. Many studies in multi-step methods are using reinforcement learning, for finetuning, in context reinforcement learning, external optimization loops, and self-reflection. The main contributions of this paper are: (1) we provide a survey of relevant approaches in multi-step reasoning with LLMs, (2) we propose a taxonomy based on the reasoning literature (step generation, step evaluation, and control of reasoning steps), and (3) we formulate a research agenda for reasoning with LLMs.

This survey is organized as follows. Section 2.1 provides background information on the most relevant developments in LLMs, including in-context learning and finetuning. Of great importance are the benchmarks that are used in this field (Section 2.4). Next, in Section 3 we provide a taxonomy of the field, where we discuss the main approaches in detail. Then, in Section 4 we discuss our findings in a broader perspective. We also discuss the relation between multi-step reasoning and work on self-reflection and metacognition. This section concludes with an agenda for future research. Finally, Section 5 concludes the survey.

2 BACKGROUND, SCOPE AND SELECTION OF PAPERS

Reasoning has a long and active history in AI, in logical inference, and in other fields, such as commonsense and analogical reasoning [81, 97]. Indeed, some of the early criticism on LLMs was that they could not reason, and that they made obvious and basic reasoning errors, showing a lack of understanding. Berglund et al. [10] provide the example of a model that is trained to report that “Valentina Tereshkova was the first woman to travel to space,” but is not able to answer the question, “Who was the first woman to travel to space?” pointing indeed to a lack of semantic understanding. Other work suggests that results are less generalizable and transferable than often assumed, showing how base-10 arithmetic skills do not transfer to base-9 arithmetic problems [169]. Different kinds of reasoning have played an important role in LLM research.

2.1 Scope

The interest in Chain-of-thought has stimulated more research into language and logic. Logic-LM combines LLMs with symbolic logic solvers in an agentic way, where the symbolic solver is called by the LLM as a tool [104]. Xu et al. [174] use a similar approach. Relevant logic-reasoning benchmarks are PrOntoQA [126], ProofWriter [141], FOLIO [50], Manuscript submitted to ACM

LogicalDeduction [138], and AR-LSAT [188]. The logic-LLM approaches often combine Chain-of-thought and symbolic solvers in an agentic-LLM approach [112], or transform the problem in an intermediate formal language. The use of LLMs for generating formal languages is further discussed in section 4.4.

More recently, LLMs are also shown to struggle with analogies and analogical reasoning [81, 97], a topic that is related to self-reflection (see Sections 3.3.3 and 4.3.3).

The question whether LLMs can reason prompted the development of the GSM8k benchmark [30] in 2021, a benchmark of some of easy reasoning problems (of the type: “Question: Natalia sold clips to 48 of her friends in April, and then she sold half as many clips in May. How many clips did Natalia sell altogether in April and May? Answer: 72”). This benchmark was specifically designed to test if LLMs can answer basic mathematical multi-step reasoning questions, or if they can not reason at all. Initially, performance was poor, but a year later Wei et al. [164] showed that by providing multi-step examples in the prompt—a *chain of thought*—much better performance was possible. Many works followed, and reasoning in language models has become an active area of study. In this survey, we focus on prompt-based multi-step reasoning algorithms. After starting with math word problems, work has more recently been extended to combinatorial games, puzzles, robotics, logic, and other fields of reasoning. At the end of this survey, we discuss connections to other fields, such as self-reflection and in-context reinforcement learning.

Before we discuss the works on reasoning, this section reviews background terminology on LLMs. Our overview is brief. Excellent recent general surveys on LLMs are, for example, Minaee et al. [96] and Zhao et al. [185]. Other works focus on the nature of reasoning and its definition [26, 58, 180], on evaluating logical reasoning in LLMs [88, 98, 104], on reinforcement learning in reasoning [173], on reasoning in language [180], or on Chain-of-thought itself [27].

The papers in this survey were selected as follows. We started by selecting papers on the ability to solve math word benchmarks (as a proxy for reasoning ability), that contained the search terms *reasoning* and *large language model* in their title or abstract, with a focus on papers that reference the Chain-of-thought paper. Although multi-step reasoning with LLMs initially was aimed at solving math world problems, it is now wider, including benchmarks and approaches for computer code, game play, puzzles, robot movement, and webpage navigation (see Table 2). We selected recent papers (two years prior to the writing of the survey) that show experimental results on selected benchmark datasets.

We focus on prompt-based, in-context learning, methods based on Chain-of-thought, that are used in reasoning LLMs such as OpenAI o1 and o3 [61, 168, 173]. We also include papers that work with external algorithms, finetuning or supervised learning that have contributed to the approaches.

We discuss the generic training pipeline for LLMs, we discuss how in-context learning works, and we discuss commonly used benchmarks. We start with the generic language model training pipeline.

2.2 Language Model Training Pipeline

LLMs are typically constructed in a sequence of stages, from data preparation, through training, to inference. The training pipeline for most LLMs is quite elaborate. We will now list a brief pipeline of the most commonly used stages, based on the survey by Minaee et al. [96].

In training an LLM, the first stage is to *acquire* a large, general, unlabeled, high-quality text corpus. Some considerations on the selection of the texts are discussed in Brown et al. [15]. The next stage is *pretraining* the transformer model [152] on this large corpus. This stage yields a generative language model. Pretraining is done using self-supervised autoregressive training on the unlabeled dataset (text corpus). Then the general model is *finetuned* to a specific (narrow) task. This can be done using supervised learning with a new labeled dataset consisting of prompts and answers (supervised finetuning, SFT, for example with low-rank optimization [56, 96, 163], or reinforcement learning [25, 140],

specific for the task at hand. A small number of the surveyed papers also address the finetuning stage. A specific form of finetuning is *instruction tuning*, to improve instruction following for a certain task. Instruction tuning is supervised by a labeled dataset of instruction prompts and corresponding outputs. Depending on the purpose of the model the next step is *alignment* of the finetuned model with user expectations (preference alignment). Alignment is usually performed to ensure that the model produces more ethically and socially acceptable answers, preventing, for example, hate speech. The machine learning method that is commonly used in this stage Reinforcement Learning with Human Feedback [102] or Direct Preference Optimization [117]. Optionally, model training can be *optimized* to improve cost-effectiveness, for example, mixed precision training [95], quantization [64], or knowledge distillation [48, 175].

Once the model has been trained in the steps described above, it can be used further in the *inference* stage. Here, the model is used to provide an answer to the prompt. The inference-time stage is post-training, no model parameters are changed anymore [15, 36]; *in-context learning*, or *prompt-learning*, takes place in this stage. Due to its low barrier of entry, without the need for expensive training or finetuning, this form of advanced prompt engineering has become a popular training method. This is the stage on which most of the surveyed papers focus, using prompts for the LLM to perform a complex multi-step reasoning task. The following section provides a brief introduction to in-context learning.

2.3 In-Context Learning

In large models, beyond hundreds of billions of parameters, a new kind of learning has emerged, that has been called *in-context learning* or *prompt-learning* [15]. It occurs not when the model is trained, but when it is used, at inference time. Since no parameters are changed in this stage, it is not a *model training* stage; in-context-learning “learns” inside the context, or prompt, using information that is already encoded in the trained model parameters and the prompt, not by training the model anymore. In-context learning is often able to give good results with few examples, so-called *few-shot* learning, learning from the few examples in combination with the knowledge of the model. The large size of the model, containing rich and general knowledge, is enabling the few-shot learning (see Dong et al. [36] for a survey).

In in-context learning, a prompt, consisting of a piece of demonstration context, is concatenated with a query question, and is given to the language model, for text generation [89]. For example, when the task is emotion recognition in a social media post, “I missed the bus today,” can be followed by “I felt so [____]”, and the model could answer with “bad”. Alternatively, for translation, we could follow “I missed the bus today,” by “French: [____]” to request a translation [89]. The prompt contains background information that is recognized by the model, selecting the desired model context. In-context learning works when language models contain enough knowledge, allowing them to generalize on the (few) examples provided in the prompt.

Contexts that contain a few examples are said to perform few-shot learning. Contexts that contain only instructions with zero examples are said to perform zero-shot learning. In-context learning takes place at inference time, after the computationally intensive training stages where parameters have been pretrained and finetuned, when the model is queried by the user to provide answers. No parameters are changed anymore with in-context learning. This is quite different from the common approach in supervised deep learning—or self-supervised deep learning—where large datasets are used during training to update model parameters with backward propagation in lengthy and costly training epochs [47]. Indeed, in-context learning takes place fully at inference time, no parameters are trained, instead, *learning* now refers to adjusting the answers to the examples in the prompt and the internal knowledge acquired during training. Common approaches to few-shot learning, such as metalearning, do include training and finetuning of parameters to achieve generalization, and are computationally expensive (see, for example, [41] or [55, 62] for a survey). In-context learning, in comparison, is computationally cheap, and it has become a popular research approach..

Benchmark	GPT-3 175B	Chain-of-thought [164]
GSM8K	15.6	46.9
ASDiv	70.3	71.3
MAWPS	72.7	87.1
SVAMP	65.7	68.9
AQuA	24.8	35.8

Table 1. Accuracy of GPT-3 and Chain-of-thought on popular Math Word Problems benchmarks [164]

Prompts provide a user-friendly interface to LLMs. The success of in-context learning tends to be quite sensitive to the way a prompt is formulated; a new field called *prompt engineering* has emerged to help human users learn how to make LLMs do what we want them to do [46, 115, 125, 163]. The current survey thus discusses advanced prompt engineering methods.

2.4 Multi-step Reasoning Benchmarks

Progress in artificial intelligence is measured by benchmarks. Benchmarks define the goal that researchers aim to achieve in their experiments. In natural language processing, a wide array of benchmarks exist to measure progress, such as on question answering (for example, CommonsenseQA [142]), word prediction (for example, LAMBADA [105]), translation (for example, WMT’22 [73]), language understanding (for example, GLUE [155, 156]), and text summarization (for example, Xsum [99]).

The field of LLMs is quite active. We will mention relevant benchmarks for testing the multi-step reasoning abilities of LLMs. The research on reasoning with LLMs started with math word problem benchmarks. The benchmark that is most frequently associated with multi-step reasoning with LLMs is the dataset of grade school math word problems GSM8K [30]. GSM8K was created with the aim of providing high quality, high diversity, moderate difficulty, problems and solutions in natural language. It consists of 8500 human-written math problems. Language models struggled to achieve good performance on this dataset before Chain-of-thought was introduced. An example of a math word task follows. *Problem:* Beth bakes 4 trays with two dozen batches of cookies in a week. If these cookies are shared amongst 16 people equally, how many cookies does each person consume? *Answer:* $4 \times 2 \times 12 / 16 = 6$.

Other benchmarks of similar math word problems are the SVAMP varying structures benchmarks [107], the ASDiv dataset of diverse math problems [94], the AQuA dataset of algebraic word problems [85], and the MAWPS benchmark [75]. Table 1 summarizes the accuracy of Chain-of-thought on these basic math word problems, against the baseline of GPT-3 175B as LLM [164], as percentage of benchmark questions answered correctly. We see that Chain-of-thought performs well against the baseline of GPT-3 on some benchmarks, but there is certainly room for further improvement on others.

In addition to the initial set of math word benchmarks, further reasoning approaches have been introduced that test performance in other fields of reasoning. Benchmarks have been developed on Advanced mathematical questions [31], Computer code comprehension (Human evaluation, Spider [181], Transcoder [122]), Robotic movement (Alfworld [136], Kitchen [2]), Puzzle solving (Game24 [179]), Creative writing [179]), Gaming (Checkmate problems[176], MineCraft [39]), and Webpage navigation (WebShop [177]). These benchmarks are used by other approaches in our survey, as we will see in more detail in Section 3.

The scope of this survey is limited to multi-step reasoning approaches. Other studies have published more challenging benchmarks, to study the performance of Chain-of-thought and self-reflection in LLMs in puzzles and (logic) games [103, 123, 166].

It can be difficult to directly compare different benchmarking results, since there may be differences in the way the experiments were conducted. Kamoi et al. [69] provide a critical analysis of benchmarking problems in LLM reasoning. Despite these challenges, general conclusions can be drawn. Section 4.1 provides guidance on how to choose reasoning approaches for different problem types.

3 STEP GENERATION, EVALUATION AND CONTROL

This survey examines how LLMs based on the transformer architecture can be prompted to solve multi-step reasoning tasks. The Chain-of-thought paper shows how a simple command could prompt an LLM to perform reasoning steps, yielding much better performance in math word problems. Since then much research has further explored this approach, trying to build stronger general problem solvers for other types of reasoning problems.

A typical approach to solve a complex problem is to subdivide it into smaller steps and to solve those. This approach is related to classical divide and conquer [6]. It consists of three stages. New steps are (1) *generated*, (2) *evaluated*, and the search of the generated steps is (3) *controlled* in some way. The in-context reasoning approaches that we survey follow a general three-stage pipeline [92]:

- (1) **Generate:** prompt the model for the generation of steps,
- (2) **Evaluate:** prompt for evaluation of the generated steps,
- (3) **Control:** prompt for control of the number of steps that are generated and how deep ahead the reasoning process will look.

This three-stage pipeline is the basis of our taxonomy. We will now discuss the three stages more deeply; for ease of reference they are numbered according to the Subsection in which they are described in more detail (3.1, 3.2, 3.3). Please also refer to Figure 1, or Table 2, for a diagram of the categories and subcategories of different approaches for the generation, evaluation, and control of reasoning steps.¹

(3.1) *Generation.* The first stage is to create a prompt that instructs the LLM to generate reasoning steps. The problem must be split into substeps. This can be achieved with a problem-specific prompt that contains elements of the problem, such as: “First calculate how many marbles Mary had originally, then how many her friend had, and finally how many they had together.” In general, it is possible to prompt an LLM to fill in the blanks in a step-by-step fashion. In the papers that we discuss, there are three main approaches for generating the step-by-step prompt, numbered with the Subsection in which the approaches are described. First, the prompt may be handcrafted for the problem by the researchers: (3.1.1) *hand-written prompt*. Second, the prompt or prompts may come from a source that is external to the model, such as another model or dataset: (3.1.2) *external knowledge-based prompt*. Third, the model itself can be prompted to generate a (series of) prompt(s) to analyze the problem (3.1.3) *model-generated prompt*. As we will see, all three approaches have their advantages and disadvantages.

Generating the subproblem-steps is the first stage that is necessary for in-context learning to perform reasoning. Each paper in our survey performs at least this stage of the reasoning pipeline. In some of the early papers (around 2022) it is the only stage of the pipeline that is performed.

¹We show the approaches in the Figure in their main category only. Some approaches show innovations in two categories, and are shown twice. (Since all approaches have a generation, an evaluation, and a control aspect, all could in principle occur three times, and all three columns can be found in Table 2).

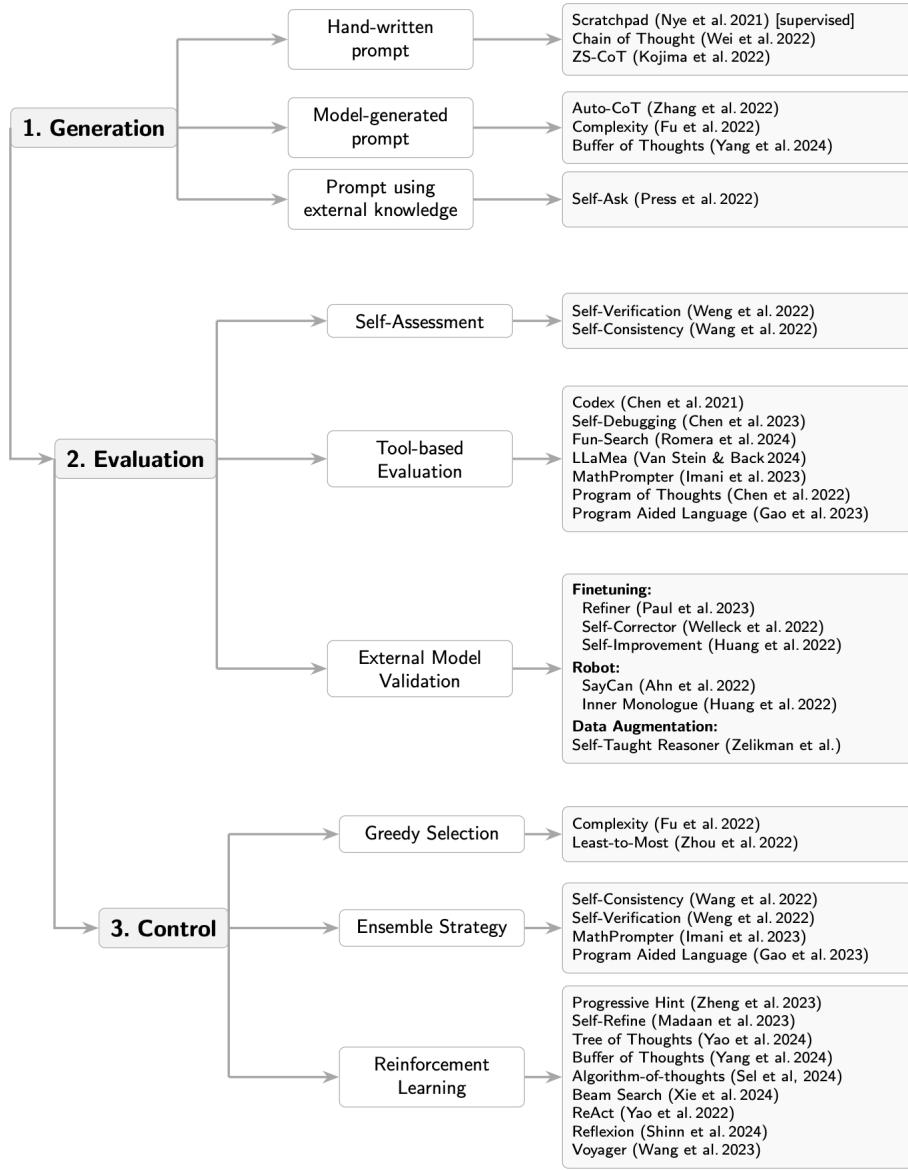


Fig. 1. Taxonomy of LLM-Reasoning Approaches: Prompt Generation, Evaluation, and Control

(3.2) *Evaluation.* After the prompt has been generated and the model has answered it, the next stage is to evaluate the quality of this answer. Such evaluation is often necessary to improve and perform well on the benchmark. Again, we see three main approaches for substep evaluation. First, the steps may be evaluated by the model itself: (3.2.1) *self-assessment*. Second, an external program can be used to evaluate the steps. For example, when the steps are expressed as computer code, an external interpreter or compiler can be used to check the validity and the outcome: (3.2.2) *tool-based evaluation*.

Finally, an external model can be used, LLM or otherwise. For example, in robotics, an external physics model can determine if certain actions are physically possible: (3.2.3) *external model validation*.

(3.3) *Control*. The third stage is control. A reasoning process that consists of multiple steps is a sequential decision process [86]. When a single chain of reasoning steps is generated, the control flow of the reasoning process is simple: greedily evaluate the first step and then the next one, if present. The control flow of the reasoning process may also be more intricate. Some reasoning problems can be divided into multiple subproblems. To execute, evaluate and combine the results of all substeps, a separate controller may be needed. This controller can be a prompt or an external algorithm.

Again, we distinguish three approaches. Most papers use a (3.3.1) *greedy selection* approach: a single prompt with a single chain of steps is generated, and these steps are directly executed and followed. The second approach is to generate an (3.3.2) *ensemble strategy* of reasoning steps, evaluate them, combine the individual results, and present them as the result of the ensemble. Finally, a full tree-search or a (3.3.3) *reinforcement learning* (RL) algorithm can be used as scaffolding. In this case, when a step is followed and evaluated, the LLM can roll back and try a different reasoning step [110]. Going further, a full reinforcement learning approach can be used [111, 140] to find an optimal policy for the sequential decision process. In general a Markov Decision Process of state, action, transition, and reward function can be specified, and step control can become a process where prompts are generated dynamically under the control of an external RL algorithm, or as in-context reinforcement learning (ICRL) [80].

Taxonomy Table. Table 2 lists the main papers of this survey. We show the domain they work on, the type of prompt generation, the evaluation of the result, and the control method. These three categories of approaches—indicated by their Sections (3.1) generation, (3.2) evaluation, (3.3) control—are shown in the table as groups divided by horizontal lines. The first group in the Table, from Scratchpad to Self-ask, focuses on creating a prompt that *generates* the reasoning steps. The entries in the cells of this column are shown in bold, highlighting the focus of the approaches. The approaches in this group are the start of the field of LLM-reasoning. The Chain-of-thought approach is especially an inspiration for many works. The prompts are often written manually by the researchers for each problem; the steps are encoded in one prompt, and step control is greedy. There is no specific evaluation of the steps, other than comparing results to the benchmark. The Scratchpad approach is special in that it uses supervised learning, not prompt-learning; the work showed that LLMs can generate internal reasoning steps by supervised learning, paving the way for in-context works.

The second group, from Self-verification to Self-taught-reasoner, focuses on *evaluation* of the reasoning steps in the prompt. This column is shown in bold in the table. The approaches in this group aim to improve the Chain-of-thought results by reducing error accumulation that occurs when multiple steps are taken in a reasoning chain. A variety of step control methods is used by these approaches, which is discussed in more detail later. Note that not all approaches use natural language problems. For example, the subgroup of Codex to Program-aided-language focuses on formal languages. They generate code or math equations, typically in Python, to formalize the steps of the reasoning problem, or as result of the task. LLMs are quite good at code generation [17], and these approaches typically achieve good performance. The use of code also allows the approaches to call external programs such as interpreters and debuggers to evaluate the correctness of the reasoning steps that are generated.

There is also a special subgroup, Refiner to Self-improvement, that uses finetuning in addition to prompt learning. Here, new data is generated based on reasoning exemplars, which is then used to further train the model. The extra data is often generated as a separate dataset, sometimes called *critic* or *corrector*.

Table 2. Taxonomy of approaches: Generation, Evaluation, and Control. Reported benchmark results: '=' is absolute score, '+' is improvement to a baseline

Approach	Domain	(3.1) Step generation	(3.2) Step evaluation	(3.3) Step control	Result
Scratchpad [101]	math word	hand-wr/superv	-	greedy/1prompt	PolyEval +19%, Python +21%
Chain-of-thought [164]	math word	hand-written	-	greedy/1prompt	GSM8K +39%, SVAMP +10%, ASDiv +2%, AQuA +11%, MAWPS +14%, CSQA +1.8%, StrategyQA +0.2%
ZS-CoT [74]	math word	hand-written	-	greedy/1prompt	MultiArith -89%, GSM8K =70%
Auto-CoT [184]	math word	model-generated	-	clustering	MultiArith +0.3%, GSM8K +1%, AddSub +3.5%, AQuA +0.7%, SingleEq +0.4%, SVAMP +0.6%, CSQA +1%, StrategyQA +0%, Letter +0.7%, Coin +2.7%
Complexity [43]	math word	hand-written	self-consistency	greedy/1prompt	GSM8K +7%, MultiArith +3%, Penguins +3%
Self-ask [113]	math word	ext knowledge	LLM	multi-hop q.	Bamboogle =60%, 2Wiki =40%, Musique =15%
Self-verification [167]	math word	hand-written	back-verify	ensemble	GSM8K +4%, SingleEq +2%, AddSub +4%, MultiArith +3%, AQuA +3%, SVAMP +1%
Self-consistency [161]	math word	hand-written	majority	ensemble	GSM8K +18%, SVAMP +11%, AQuA +12%, StrategyQA +6%, ARC-c +4%
Codex [17]	code	-	tool-based	-	HumanEval =70%
Self-debugging [21]	code	hand-written	tool-based	greedy	Spider +9%, MBPP +12%, TransCoder +12%
Fun-search [120]	code	hand-written	tool-based	evolutionary alg	cap set 8 =512
LLaMEA [150]	code	hand-written	tool-based	evolutionary alg	BBOP +11%
MathPrompter [63]	math	hand-written	tool-based	ensemble	MultiArith =92%
Program-of-thoughts [18]	math word	hand-wr, Codex	Python+Consist.	split reason/cmput	GSM8K =71%, SVAMP =85%, ASDIV =85%, AddSub =92%, MultiArith =99%
Program-aided-lang [44]	math word	hand-wr, Codex	NLP/Python	ensemble	GSM8K =72%, SVAMP =79%, ASDIV =79%, SingleEq =96%, SingleOP =94%, AddSub = 92%, MultiArith = 99%, Penguins = 93%
Refiner [108]	math word	finetune	critic model	gen/crit feedback	SVAMP =72%, GSM8K =78%
Self-correction [165]	math word	finetune	corrector model	gen/corr feedback	MathProgSynth +24%, LexConstrGen =98%, ToxicityControl =0.0%
Self-improvement [57]	math word	finetune	self-assessment	CoT/consistency	GSM8K =82%, DROP =83%, ARC-c =90%, OpenBookQA =94%, ANLI-A3 =68%
Say-can [2]	robot	model-generated	external model	greedy	Kitchen =31%
Inner-monologue [60]	robot	hand-written	various	greedy	TableTop =90%, Kitchen =60%
Self-taught-reasoner [182]	math word	finetune	augmentation	feedback	CommonsenseQA =72%
Least-to-most [189]	math word	hand-written	self-assessment	curriculum	SCAN =99%
Progressive-hint [186]	math word	model-generated	self-assessment	stable prompt	AddSub +2%, MultiArith +0%, SingleEq +2%, SVAMP +3%, GSM8K +5%, AQuA +1%
Self-refine [92]	math word	model-generated	self-assessment	greedy/feedback	Sentiment +32%, Dialog +49%, CodeOptim +8%, CodeRead +28%, MathReason +0%, AcronymGen +25%, ConstrainedGen +30%
Tree-of-thoughts [179]	puzzles	model-generated	self-assessment	BFS/DFS	Game24 +74%, CreativeWriting , Crossword
Buffer-of-thoughts [176]	math word	thought template	self-assessment	buffer manager	Game24 +11%, GeoShapes +20%, Checkmate +51%
Algorithm-of-thoughts [129]	puzzles	model-generated	self-assessment	in-context RL	GSM8K =89%, StrategyQA =84%, Crossword
Beam-search [172]	math word	model-generated	self-assessment	Beam Search	GSM8K +6%, AQuA +9%, StrategyQA +5%
ReAct [178]	action	external knowledge	self-assessment	reinf learning	ALFWorld =34%, WebShop =10%
Reflexion [135]	decision	model-generated	ext model	reinf learning	HumanEval =91%
Voyager [158]	Minecraft	model-generated	Minecraft	reinf learning	15 x faster

There are two approaches, Say-can and Inner-monologue, whose application domain is control of robot movement. Robotic movement is constrained by the laws of physics (both in the body of the robot as in aspects of its environment). The laws of physics are learned and used to ground the reasoning steps in reality (to reduce hallucination).

The third group, Least-to-most to Voyager, addresses step *control* (shown in bold in this column). Whereas in the previous approaches the reasoning steps are written in a single, static, prompt, these approaches generate the steps in multiple, dynamic, prompts. This allows control of the space of reasoning steps. Various search control approaches are used, all in the form of an external algorithm that performs calls to the LLM with different prompts. The control methods range from simple greedy and depth-first search to elaborate beam search and reinforcement learning schemes.

The last column of the Table summarizes reported benchmark results. The '=' symbol indicates absolute scores on the benchmarks, while '+' indicates relative improvement in percentage points over a baseline LLM, typically GPT-3.5. Results vary strongly, both between approaches and within a single approach between benchmarks. Also, different LLMs were used, from early stage to more mature models, open and commercial, and the baselines differ. For some benchmarks, such as the Creative Writing benchmark in Tree-of-thoughts, results are best reported qualitatively. The

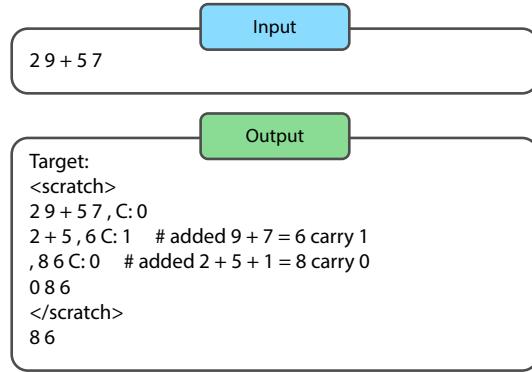


Fig. 2. Example of input and target for supervised learning on a *long addition* problem of adding two numbers. The carry is recorded in the C: digit. Comments (after #) are not part of the learning target (adapted from [101])

source papers provide more measurement details, Section 4.1 discusses when to which approach to use for different applications.

In conclusion, we see a diverse array of methods that often achieve high performance in reasoning on their respective domains. To better understand the approaches, we discuss them in more detail, starting with the generation of steps.

3.1 Generation of Steps

Originally, LLMs performed poorly on math word problems such as GSM8K [30]. Different approaches were tried unsuccessfully, for example scaling up the size of the LLM [116]. The LLM architecture, based on transformers, is designed to produce a single token. When we prompt such an architecture to produce an answer, it does so. What we should do instead, is to prompt it to follow intermediate steps, answer those, and thus work towards the final answer, just as a student is taught to break down a complex problem into smaller steps. We should guide the model to explicitly produce intermediate steps, and combine the intermediate results. This idea was used by Nye et al. [101] in Scratchpads, a transformer model that performs multi-step computations by asking it to emit intermediate computation steps into a *scratchpad*. They train the model by supervised learning (not prompt-based in-context learning). Figure 2 shows an example. On experiments with addition, polynomial evaluation, and Python code execution, versions that produced the intermediate steps on a scratchpad performed considerably better than versions that did not, going from 35% to 95%, from 32% to 51%, and from 30% to 42% accuracy, respectively.

If supervised learning can produce intermediate steps, would prompt learning be able to do so too?

3.1.1 Hand-written Prompt. This question was studied by Wei et al. [164], amongst others. A basic way to instruct an LLM to generate steps by prompt-learning is to manually write a prompt for the large language model to follow the reasoning steps. When the LLM is prompted to rephrase information from the question as intermediate reasoning steps in its answer, the LLM performed much better than when it was prompted to answer a math problem directly, without reproducing information from the question in its answer in multiple steps. The example from the Chain-of-thought paper is shown in Figure 3. Table 1 shows that the largest accuracy increase is on GSM8K, from 16% to 47%.

The idea that an LLM can be made to follow step-by-step instructions, and the performance improvement by Chain-of-thought have caused much excitement and have opened up further research on reasoning with LLMs. In the Manuscript submitted to ACM

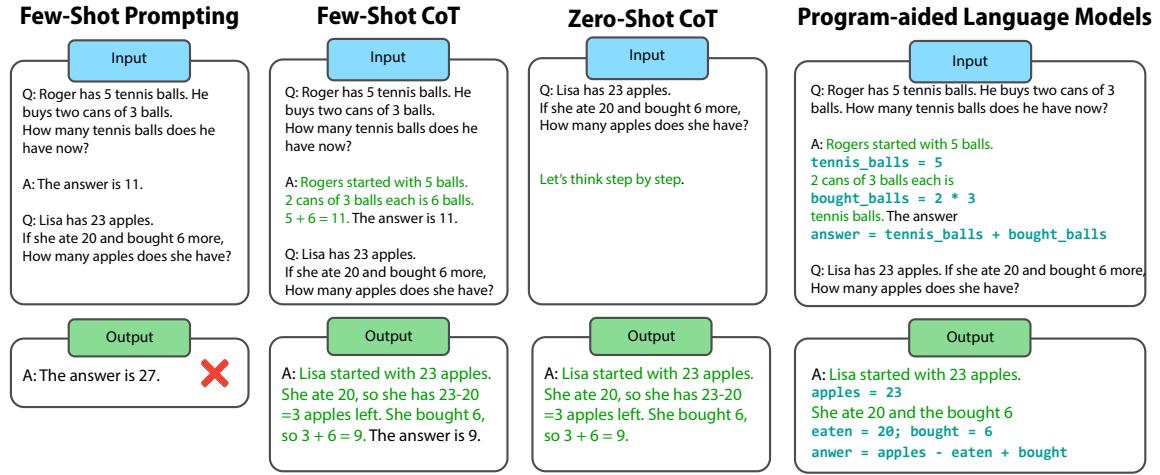


Fig. 3. Different chain-of-thought (CoT) prompting techniques. At the top the prompts, at the bottom the answers. When shown the longer example prompt, the LLM follows the longer example when answering the question (Few-Shot CoT [164]). Without example answer and using *Let's think step by step* results in similar answers (Zero-Shot CoT [74]). With Program-aided-language models [44] similar reasoning can be achieved.

original paper the prompts were handwritten by the researchers for the individual types of problems, and evaluations are conducted with benchmarks (not by an LLM).² In a later work the prompts were generated automatically by the LLM [184], and evaluated.

Kojima et al. [74] go a step further. They show that the addition of a single text to the prompt (*Let's think step by step*) significantly improves performance. Since this text does not contain problem-related elements, it is as a form of zero-shot learning. Figure 3 (third column) compares the approaches. Experiments further show that with this addition to the prompt significant performance gains are also achieved on other reasoning benchmarks, including arithmetic, symbolic, and logical reasoning (achieving 70% accuracy on GSM8K/PaLM when Self-consistency is also included).

The Chain-of-thought idea itself is inspired by earlier work where natural language steps are generated for arithmetic reasoning [30, 85], and the use of formal languages for reasoning [3, 20, 22, 121].

3.1.2 Prompt using External Knowledge. Chain-of-thought prompts are written manually, by the researchers, an approach that does not scale. We can also use external information about the problem to improve the prompt. Press et al. [113] study how subproblems are related to the main problem, which they call *compositional reasoning*. They study how often a model is able to answer the subproblems, but not the overall problem. This difference is called the compositionality gap. They find that in GPT-3, as model size increases, the single-hop question-answering performance improves faster than the multi-hop performance: while more powerful models memorize and recall more factual knowledge, no improvement in their compositional reasoning occurs. The ability to reason does not depend on the size of the model.

Subsequently, a method called *Self-ask* is proposed, that asks elicitive follow-up questions (like Chain-of-thought, but with the *follow up*: prompt), that the model then answers. Self-ask can also use an external search engine to answer

²The Chain-of-thought idea is about prompt generation, not about the evaluation or the search control of the reasoning steps. Hence, in Table 2 Chain-of-thought is labeled as *greedy* without an evaluation.

intermediate prompts, instead of the model. The initial subquestion is fed into the search engine, and the answer is processed by the model, which generates another subquestion, and so on, until it produces the final answer. Self-ask was tested on three benchmarks that were specifically designed for multi-hop questions. Although it performs only a few percentage points better than vanilla Chain-of-thought, it showed how external knowledge can be used in a reasoning setting.

3.1.3 Model-Generated Prompt. In addition to manually writing prompts or using external information, we can also let the LLM itself study the problem to write the best reasoning-prompt. An example of such self-improvement is Auto-chain-of-thought [184]. This approach builds on the observation by Kojima et al. [74] that large language models are zero-shot reasoners. First, Auto-chain generates specific questions for a given dataset and partitions them into clusters. Then an external algorithm uses the model to generate examples that are sampled for diversity. The constructed demonstrations augment the in-context prompt. This approach also performed a few percentage points better than hand-written Chain-of-thought prompts, on ten benchmarks, using GPT-3 (see Table 2).

Fu et al. [43] introduce Complexity-based prompting. Inspired by Chain-of-thought and Self-consistency, their work specifically studies the impact of the complexity of the reasoning chain (the number of steps), and introduces a related reasoning approach (Complexity-based prompting). They find that prompts with the largest complexity perform best, and also that answers with the highest complexity are the best. Complexity-based prompting achieves somewhat higher performance on three math reasoning benchmarks: GSM8K improves 7 points, MathQA 6 points, and the Penguins benchmark from Big Bench Hard improve 3 percentage points.

We see that the initial approaches showed larger improvements than the later approaches. It is time to look at another category of approaches, that focus on the evaluation of reasoning steps.

3.2 Evaluation of Steps

After discussing prompts for the generation of reasoning steps, the next stage in the generation/evaluation/control pipeline is *evaluation* of the results of the steps. This stage focuses on reducing error accumulation of multi-step reasoning chains. We will start with approaches where the same model performs step-generation and step-evaluation.

3.2.1 Self-Assessment. When LLMs are prompted to perform reasoning steps, they perform a sequence of steps and predict multiple tokens. Performing a sequence of steps makes them sensitive to mistakes and vulnerable to error accumulation (logical, factual, ethical, or otherwise) [167, 170]. Several methods have been developed to prevent error accumulation. One approach is to create a new model to separately evaluate the results. Shen et al. [132] and Li et al. [84] train an external verifier to check results. In contrast, Weng et al. [167] propose an automated approach using evaluation by the same LLM, called Self-verification. They note that human reasoning also suffers from the problem of accumulating errors, and that in human reasoning we frequently revisit our thought process to verify the accuracy of our reasoning steps. The LLM is prompted to use the conclusion of the Chain-of-thought reasoning chain as a condition for solving the original problem and then compare the answer, going back to the original question. The LLM is given variations of its own conclusion and is instructed to choose the one with the highest similarity to the original question. (Note that there can be feedback issues using an LLM to evaluate itself, for a discussion see Zheng et al. [187].) Experiments are reported on GPT-3 [17] and on Instruct-GPT [102]. The accuracy of Chain-of-thought was improved by a few percentage points on arithmetic and general reasoning tasks (GSM8K 65%, AQuA 48%, SVAMP 77%).

A popular related approach is Self-consistency [161]. Self-consistency is a straightforward ensemble approach (a well-known machine learning technique to make a strong learner out of multiple weaker learners [13, 124]). Greedy Manuscript submitted to ACM

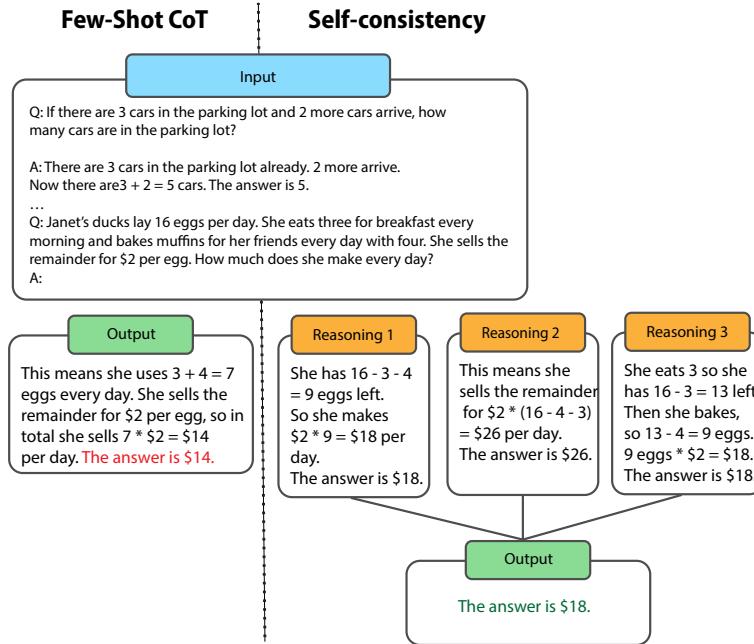


Fig. 4. Self-Consistency (Adapted from [161]), showing majority voting

single-path decoding is replaced by sampling diverse reasoning paths, evaluating them, and selecting the most consistent answer. Self-consistency asks the LLM to simply perform the same query multiple times, and takes the majority-vote of the answers, or decoding paths. Self-consistency works since complex reasoning problems typically allow different reasoning paths that lead to the correct answer. Figure 4 summarizes the approach. Self-consistency has been evaluated on arithmetic reasoning, commonsense reasoning and symbolic reasoning, on a variety of LLMs, including GPT-3 [15, 24, 144, 145]. Self-consistency further improves the performance of Chain-of-thought by 10-20 percentage points, and has been used as a baseline in many of the other approaches in this survey.

3.2.2 Tool-based Validation. Another approach to improve the accuracy of evaluating the reasoning steps is to switch from a natural to a formal language. The advantage of a formal language is that it is less ambiguous than a natural language. Examples are computer languages, such as Python, or mathematical equations. Using a formal language for reasoning is a popular approach, and we discuss seven papers. Many approaches generate the steps in Python, and the code can then be evaluated by a formal evaluator, such as a compiler, debugger, or interpreter.

LLMs have been quite successful in generating computer code from natural language prompts. Chen et al. [17] introduced Codex, a GPT model that was trained on publicly available code in the repository GitHub. A production version of this work was introduced under the name GitHub Copilot. Codex is able to generate correct programs from descriptions in natural language, such as commentary strings.

The work on Codex is used as a basis for further research on reasoning in LLMs. Human programmers, when writing code, typically follow a cycle of writing some code, executing it to look for errors, and then using the feedback to improve the code. This step-by-step approach is followed in Self-debugging [21]. It follows the same steps of code generation,

code execution, and code explanation. Self-debugging is able to identify mistakes in its own code by investigating the execution results, and can also provide an explanation of the generated code, in natural language. It achieves strong performance: the text-to-SQL Spider benchmark improves 9 points, and the C++ to Python Transcoder benchmark improves by 12 percentage points.

Several works generate working code tuned for solving specific problems automatically, without human feedback. Romera-Paredes et al. [120] introduced FunSearch, an approach that integrates formal methods and LLMs to enhance mathematical reasoning and code generation. FunSearch uses a genetic approach with multiple populations of candidate solutions (programs), which are evaluated using a function depending on the problem specification. In addition to the evaluation function, also an initial program is given to the LLM in the first prompt. After evaluating a number of generated programs from the starting prompt, a new prompt is created, in an iterative fashion, combining a selection of sampled programs sorted according to their evaluation score, and the LLM is requested to generate a new program. Another work leverages evolutionary computation methods to generate and optimize evolutionary algorithms [150]. This approach, LLaMEA (Large Language Model Evolutionary Algorithm), utilizes LLMs to design and optimize evolutionary algorithms. The approach uses LLMs to generate initial algorithmic structures, which are then refined through mutation and selection. This enhances the efficiency of algorithm design, particularly in fields requiring innovative and adaptive solutions, improving accuracy on the *Black-Box Optimization Benchmark* [51] (*BBOB*) suite by 11 percentage points. A key difference between FunSearch and LLaMEA is that LLaMEA uses a sample-efficient elitism strategy by iteratively improving the best-so-far solution, requiring significantly fewer prompt evaluations than the large-population strategy proposed in FunSearch. Evolutionary approaches let the LLM discover new algorithms, solving existing problems in new ways, or solving entirely new problems. Another method, Evolution-of-heuristics [87], was proposed for evolving code snippets for guided local search to solve combinatorial optimization problems, such as the Traveling Salesperson Problem.

To improve prompt-based reasoning, Codex is used in an ensemble approach named MathPrompter [63]. This approach generates multiple algebraic expressions or Python functions, which then solve the same math problem. The results are compared, just like in Self-consistency and Self-verification, raising the confidence level in the results. MathPrompter achieved state-of-the-art accuracy on the MultiArith dataset (78.7% → 92.5%), evaluated on GPT-3 175B.

Two other approaches that use a formal language are Program-of-thought [18] and Program-aided-language [44]. Both approaches use the LLM to generate Python and then use an interpreter to evaluate the result. The approaches are similar although Program-aided-language uses generic prompts, and has been tested on more benchmarks. Figure 3 (fourth column) illustrates the Program-aided-language approach. When the evaluation of the reasoning steps is offloaded to the Python interpreter, decomposing the natural language problem into executable code-steps remains the only task for the LLM. (Earlier work in math word problems showed how to decompose a problem and reach an answer [85].) Gao et al. [44] provide extensive experimental evidence about the synergy between the neural LLM and the symbolic interpreter. Experiments are performed on 13 mathematical, symbolic, and algorithmic reasoning tasks, achieving more accurate results than much larger models (for example, Program-aided-language reported 72% on GSM8K and 93% on Penguins).

3.2.3 External Model Validation. We have seen many examples of successful prompt-based in-context reasoning and evaluation (at inference time—where no parameters were changed). We will now look at reasoning approaches that follow a more traditional parameter training approach. All approaches evaluate the output of the model and generate corrective data. That data is then added to the training pipeline, and the model is subsequently finetuned.

Finetuning. The Refiner approach [108] uses a generator model and a critic model that provide fine-grained feedback on reasoning errors. The generator generates multiple reasoning hypotheses, and the critic evaluates results by randomly selecting a hypothesis for feedback. The generator model is then finetuned based on its reasoning errors. A small supervised model is used to overcome the cold-start problem. The approach achieves 78% accuracy on GSM8K and also works well on related problems.

Welleck et al. [165] follow a similar approach which they call Self-correction. Here, the corrector is a separate model specialized in refining the outputs of the generator. Unlike Refiner, where the generator is finetuned based on the critic, Self-correction finetunes the corrector to rectify errors in the hypotheses produced by the generator. Self-corrector is not applied to math word problems, but to program synthesis, where a small corrector reduces toxicity to 0%.

A third finetuning approach is Self-improvement [57]. Here, too, the base model data is augmented by LLM-generated rationales, and then finetuned. They achieve 82% accuracy on GSM8K and similarly high scores on question answering and adversarial benchmarks. Noteworthy in all three finetuning approaches is that LLMs are capable of improving themselves by training on their own generated output, and that stability problems from feedback loops are overcome.

Dataset Augmentation. The final finetuning approach that we discuss uses dataset augmentation. In Self-taught-reasoner [182], an intermediate reasoning is generated, called a *rationale*. Rationales are shown to be valuable across diverse tasks such as mathematical and commonsense reasoning, code evaluation, social bias inference, and natural language inference. First an augmentation dataset is created by attempting to solve the original dataset. Next, the dataset is augmented using rationalizations and ground-truth answers to problems the model failed to solve. Finally, the model is finetuned on the combined dataset. Self-taught-reasoner performs comparably (72%) to finetuning a 30 times larger model on CommonsenseQA.

Reasoning about Robot Behavior. In addition to math word problems, computer code, and common sense, prompt-based reasoning has also been used to improve robot behavior. Language models contain a large amount of information about the real world [2]. In theory, this should allow them to reason realistically about robotic behavior. However, the models do not have knowledge about specific embodied aspects of a particular robot. If we could compare a Scratchpad-like list of intermediate reasoning steps with a list of possible movements of the robot in its environment, then we could prevent the model from suggesting impossible joint movements and actions, and prevent failures.

Say-can [2] learns a value function [67] of the behavior of a robot and its environment using temporal difference reinforcement learning [139]. This value function is combined with prompt-based reasoning by the language model, to constrain it from suggesting impossible actions. The goal of Say-can is to ground language in robotic affordances. In contrast to Scratchpad, which used supervised learning, the affordance model is learned interactively by reinforcement learning, and then applied using prompt-based learning on the LLM. The language model has high-level semantic knowledge about the task (Say). The learned affordance function (Can) provides an environment-grounding on what is possible. Say-can achieves a 31% success rate on 101 real-world robotic kitchen tasks.

Where Say-can learns affordances as a separate function, Inner-monologue [60] formulates robotic planning directly as part of the language prompt, internally. The input consists of many elements: textual descriptions from InstructGPT [15] for multi-step planning, scripted modules for object recognition, success detection, task-progress scene description, and language-conditioned pick-and-place primitives, similar to CLIPort [137]. The language feedback that is thus generated significantly improves performance on three benchmarks, achieving 90% accuracy on simulated and real table top rearrangement tasks and 60% on the kitchen environment. There are many other studies into robotic behavior.

An approach related to Inner-monologue is Chain-of-tools, which proposes a plan-execute-observe pipeline to ground reasoning about tool behavior [133, 134].

This concludes our discussion of the second stage of the reasoning pipeline, *evaluation* of the reasoning steps.

3.3 Control of Steps

The third stage is *control*. This stage controls how many sub-steps are generated, and how deep into the future the reasoning chain is generated. There are three main approaches: (3.3.1) *greedy selection*, which generates a step and then follows it, (3.3.2) *ensemble strategy*, which generates a set of possible next steps, and (3.3.3) a (*reinforcement learning*) search which generates multiple options for the steps, traversing a search tree with backtracking, controlling an exponential search space [173].

3.3.1 Greedy Selection. Most earlier works on prompt-based reasoning follow the greedy approach: generate a single prompt with a single sequence of steps and follow them. Among the greedy reasoners are Chain-of-thought, Auto-CoT, and Zero-shot CoT. Inner Monologue and Say-Can also use greedy reasoning.

In Least-to-most prompting [189], the key idea is to break down a complex problem into simpler subproblems and then solve these in sequence, explicitly encoding them in the prompt, related to Complexity-based prompting. In Least-to-most the answers to previously solved subproblems help in finding the answer, as a curriculum [8]. On symbolic manipulation, compositional generalization, and math reasoning, Least-to-most prompting generalizes well, achieving 99% accuracy on a compositional generalization benchmark.

3.3.2 Ensemble Strategy. The second kind of reasoning control is based on an ensemble of (sequences of) reasoning steps. For most problems, multiple different options exist for the next step. When all or some of these are generated and evaluated, then the consensus result can be reported as the outcome of an ensemble of steps. Self-consistency [161] and Self-verification [167] (in Section 3.2.1) are popular ensemble approaches to evaluate the results of reasoning steps, in which greedy single-path decoding used in Chain-of-thought prompting is replaced by a diverse set of paths. Taking this further, Chain-of-experts uses a mixture-of-experts ensemble for complex combinatorial problems [171]. PAL and MathPrompter also use the ensemble approach. The ensemble approach is popular in reasoning with LLM.

3.3.3 Reinforcement Learning. In reasoning, often multiple valid steps are possible, but pursuing all possibilities over multiple trajectories may lead to an infeasible number of possibilities. The third kind of reasoning control is to use a full-fledged controller that can traverse a tree, or perform reinforcement learning to do so [67, 111, 140]. When decomposing the problem, multiple alternative steps are generated that can be searched multiple steps into the future. Then, backtracking can be performed, allowing alternative steps to be tried.

Where greedy and ensemble processes can be controlled with a prompt by the LLM, this third category is more complex, and an external algorithm is used to control the reasoning process. The external algorithms call the LLM as a subroutine prompting it to perform requested tasks. The external algorithm allows more complex reasoning control, but we are now beyond prompt-based self-reasoning: control has been given to an algorithm that is external to the LLM and external to prompt-learning.

We start our discussion of control strategies with depth-first and breadth-first search, then go to beam search, and then to full reinforcement learning. A complex reasoning space can be traversed with a search algorithm. Tree-of-thoughts [179] uses breadth-first or depth-first search to dynamically follow different reasoning steps. The evaluation part in Tree-of-thoughts is performed with a prompt to the LLM. Together, the trio of generation, evaluation, and control allow

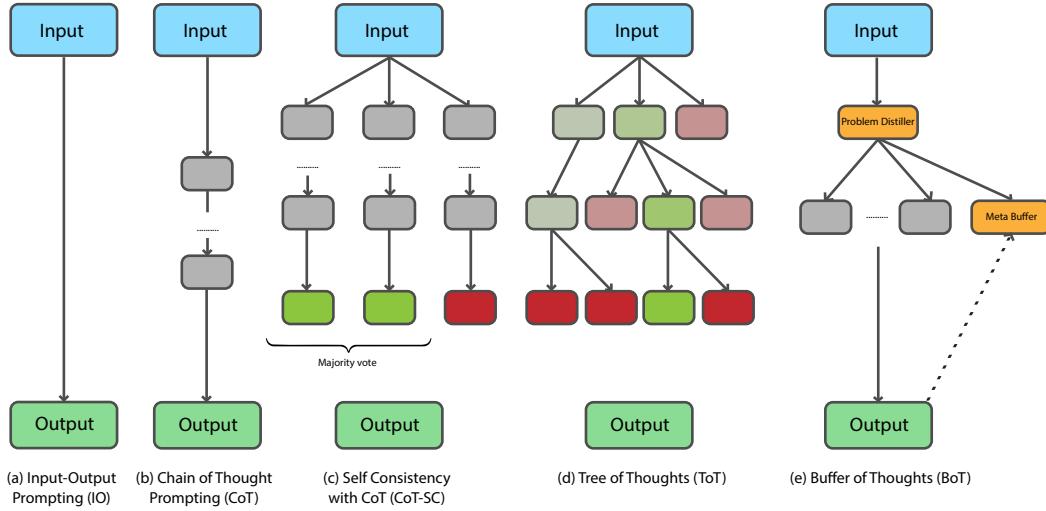


Fig. 5. Reasoning structure of Chain-of-Thought (b), Self-Consistency (c), Tree-of-Thoughts (d) and Buffer of Thoughts (e)

systematic exploration of the space of reasoning steps with look-ahead and backtracking. The authors compare their approach to Chain-of-thought and Self-consistency on the Game of 24, Creative writing, and Mini crossword, achieving an accuracy of 74% on a Game of 24 task. The other tasks are evaluated qualitatively. Figure 5 illustrates the different reasoning structures.³

Another approach, Buffer-of-thoughts [176], goes a step towards metareasoning [45]. It introduces a meta-buffer that stores high-level *thought-templates*. These thought-templates are derived from a variety of tasks. Figure 5 compares the Buffer-of-thoughts approach to other approaches such as Chain-of-thought and Tree-of-thoughts. Buffer-of-thoughts outperforms other methods in puzzles such as Game of 24 (by 11%) and checkmating (by 51%). Thought templates are related to metacognition (thinking about thinking), which is further discussed in Section 4.3.3.

A related search method is Beam-search-for-reasoning [172]. When the space of possible reasoning paths is large, Beam-search searches a promising part of this space. It uses self-evaluation to control exploration and to evaluate (decode) reasoning steps. Beam search uses Program-aided-language models for math word problems [44]. Using a Codex backbone [17], it surpasses the few-shot baselines by 6.34%, 9.56%, and 5.46% on the GSM8K, AQuA, and StrategyQA benchmarks, respectively.

Reinforcement learning is another step in the sophistication of optimization algorithms. It learns by interactive sampling, improving its policy based on rewards from the environment [140]. To use reinforcement learning, the reasoning problem is formulated as a Markov Decision Process: the agent-algorithm creates a prompt (an *action*), to sample a step (*t*) and get an answer (*state, reward*) from the environment-model. The answer can then be used to improve the prompt (next action), using the rewards to improve its policy of best actions for each state. The approaches that use reinforcement learning also do so in the form of an external algorithm.

Progressive-hint-prompting (PHP) uses reinforcement learning to interactively improve prompts [186]. PHP calls the LLM with dynamic prompts, using previously generated answers as hints, to progressively prompt the LLM towards

³A similarly named approach is Graph-of-thoughts [11]. Graph-of-thoughts allows more general reasoning graphs, providing a formal framework, where the different elements can then be specified manually.

the correct answers. It works as follows: (1) given a question (prompt), the LLM provides a base answer, and (2) by combining the question and answer, the LLM is queried and obtains a subsequent answer. We (3) repeat operation (2) until the answer becomes stable, as a regular policy-optimizing reinforcement learning algorithm. The authors have combined PHP with Chain-of-thought and with Self-consistency. Using GPT-4, state-of-the-art performance was achieved on grade school math questions (95%), simple math word problems (91%) and algebraic question answering (79%).

Another approach that is motivated by improving answers from feedback, is Self-refine [92]. Like PHP, the LLM generates an initial output and provides feedback for its answer, using the LLM to refine itself, iteratively. Self-refine prompts the LLM in three ways: (1) for initial generation, (2) for feedback, and (3) for refinement, following a greedy reasoning chain. Self-refine has been used with GPT-3.5 and GPT-4 as base LLMs, and has been benchmarked beyond math word problems on dialogue response generation [4], code optimization, code readability improvement, math reasoning, sentiment reversal, acronym generation, and constrained generation, showing substantial improvements over the base models (typically around 30 percentage points, see Table 2).

Another approach that combines reinforcement learning and LLMs is ReAct [178]. Most works focus on reasoning by the LLM, not on actions by an agent. The goal of ReAct is to combine progress in reasoning with action plan generation. (Or, to put it differently, other approaches use RL to improve LLM-reasoning, ReAct uses LLMs to improve RL agent policies.) ReAct uses Chain-of-thought prompt-learning as part of an RL framework that also uses external knowledge sources (Wikipedia) and finetuning; for error reduction, grounding, and for reducing hallucination. The framework allows hand-written prompts. On two interactive decision making benchmarks (Alfworld and WebShop), ReAct outperforms imitation and reinforcement learning methods by an absolute success rate of 34% and 10% respectively.

The ReAct work has been developed further. Reflexion [135] creates AI agents that learn by reflecting on failures and enhance their results, much like humans do. Reflexion uses three language models: actor, evaluator, and reflector. It works as follows: (1) an actor generates text and actions, (2) an evaluator model scores the outputs produced by the actor, and (3) a self-reflection model generates verbal reinforcement cues to assist the actor to self-improve (see Figure 6). For the actor, Chain-of-thought and ReAct can be used. Reflexion is evaluated on decision-making, reasoning, and coding tasks. Improvements of 10-20 percentage points are reported.

The reinforcement learning approaches that we discussed so far—React, Self-refine, Tree-of-thoughts, Buffer-of-thoughts, Reflexion—use external algorithms to manage state for the prompt improvement loop. A more elegant solution would be to perform reinforcement learning fully in-context, within-prompt. Indeed, Krishnamurthy et al. [77] explicitly asked the question whether LLMs can explore in context. This is the goal of the Algorithm-of-thoughts (AoT) approach [129]. Following work by Demircan et al. [34], Lee et al. [80], Wang et al. [160] that showed that transformer architectures can be pretrained and finetuned to perform in-context reinforcement learning, AoT aims to do so in general LLMs such as GPT-4, Claude and Gemini 1.5. They achieve results comparable to Tree-of thoughts on GSM8K, StrategyQA, and Crosswords. Achieving these results with in-context RL is a promising result for in-context learning. Other search-like in-context algorithms are studied by Schultz et al. [127] and Kempinski et al. [71] (Game-of-thoughts). Further work in games finds that LLMs struggle with the knowing-doing gap and the difference between using and mentioning game concepts [29, 103, 151].

To conclude this overview of reinforcement learning approaches, we discuss an application in the games domain. Voyager [158] is an agent for the game of Minecraft that uses an iterative prompting mechanism that generates code for embodied control. The agent includes self-verification and a skill library to maximize exploration. The goal of is to

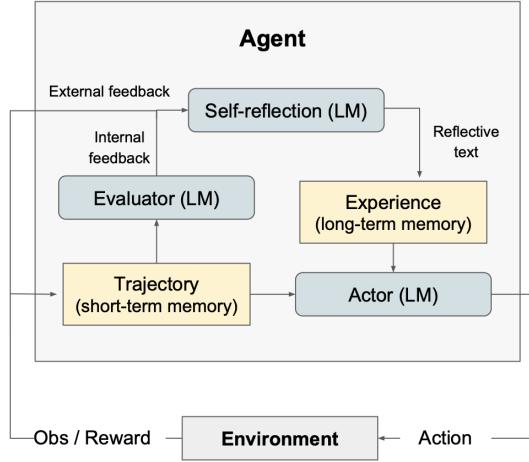


Fig. 6. Architecture of Reflexion [135], showing a close resemblance to the agent/environment structure of reinforcement learning

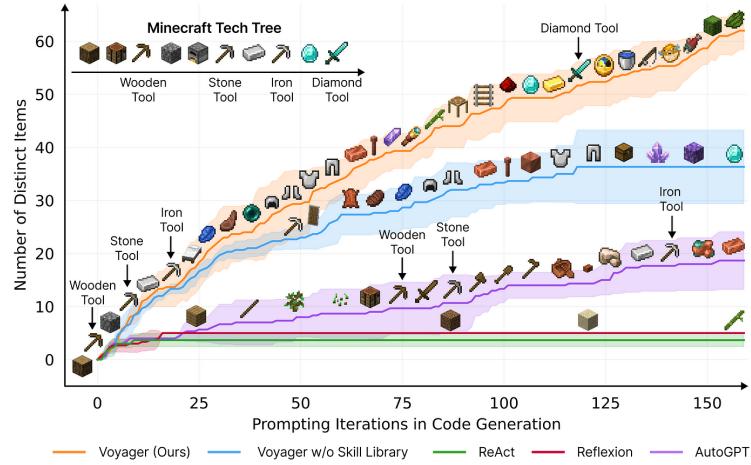


Fig. 7. Performance of Voyager in Minecraft [158]; Voyager performs well, reaching high scores by acquiring many tools

discover diverse items in Minecraft, a form of novelty search [38]. Voyager performs well, reaching high scores by acquiring many tools (see Figure 7) 15 times faster than the baseline.

The applications of reinforcement learning in LLM reasoning are many, and the connections run deep [114]. Wang et al. [159] use the similarity between RL timesteps and LLM reasoning steps to jointly train a value function together with the LLM policy by optimizing the soft Bellman equation, achieving 85% accuracy on GSM8K and 81% on Alfworld. Du et al. [37], Guo et al. [49] replace supervised finetuning by reinforcement learning, integrating it with reasoning, achieving large efficiency gains in the training pipeline in the DeepSeek r1 and Kimi models.

4 DISCUSSION

We have reviewed many reasoning approaches. It is now time to reflect on the approaches, to discuss limitations, and to look for promising areas of future work. First we discuss how to choose an approach for an application. Next, we discuss issues concerning hallucination, faithful reasoning, and scaling. Then we discuss what LLMs can and cannot do. Then, we highlight connections with sequential decision processes, metacognition, and programming languages, and we end with a research agenda.

4.1 Matching Methods and Applications

This survey has discussed different approaches, applications, and benchmarks. It is often difficult to directly compare benchmark results between individual papers, due to differences in measurement setup. For example, Kamoi et al. [69] critically compare self-reflection studies. We can provide, however, general guidance on what approach to use for different types of applications.

For *simple reasoning situations*, that require a single sequence of reasoning steps, Chain-of-thought is typically used. When the error rate is high, verification methods such as Self-consistency are popular. Indeed, this combination is used in many modern reasoning LLMs.

For *combinatorial puzzles and games* that would traditionally require backtracking, tree-search or reinforcement learning, solution methods need to be able to keep track of the enumeration state. However, an LLM without an external algorithm often fails to keep track of this state correctly between calls to the model. An approach such as Tree-of-thoughts, or ReAct, should be considered. Here, the state is managed externally, and the LLM is called for application-dependent functional processing. Various in-context reinforcement learning methods are being developed where state is managed by the LLM, as in, for example, Algorithm-of-thoughts. When performance is not sufficient, finetuning or pretraining for the domain at hand can be used.

For *complex problems*, where a sequence of steps or external control fail to perform well, other reasoning approaches are needed. We note that LLMs are good at generating computer code for many known problems [17]. Hence, when the preceding approaches do not work, the LLM can be asked to generate a program for the problem. In this approach, the LLM acts as a coding agent for its user. The LLM generates a program or a sequence of commands, which are then executed by an external tool, such as an interpreter, a robot, a planner, or a logic solver. In robotics, vision-language-action models have achieved impressive results [72], but also strong results in logistics [12], finance and medicine are reported [112].

4.2 Hallucination, Faithfulness and Scaling

Reasoning by LLMs is not error-free, and many studies aim to provide deeper insight into the reasoning processes in language models. Saparov and He [126] introduce a synthetic question/answer dataset designed to evaluate the reasoning abilities of LLMs. The work showed that LLMs are capable of reasoning to a certain degree, but that Chain-of-thought struggles with proof trees with a wide branching factor. In another study, Wang et al. [157] aim to increase our understanding of how Chain-of-thought works. The authors find that the order of the reasoning steps is important. Prompts should be relevant to the question, and coherent (steps should be in the correct order). Jin et al. [65] also study the impact of reasoning step length on LLMs, again finding a strong positive correlation between the length of the

prompt and reasoning abilities. Next, we discuss works on errors in the Chain-of-thought approach, studying whether the reasoning of the LLM is faithful, or that it gives the right answer for the wrong reason.

4.2.1 Faithfulness. Chain-of-thought approaches prompt a language model to take certain steps to solve the problem that the prompt specifies. One can ask the question, whether those steps are indeed the steps that the model has followed (faithful reasoning) or whether it took another road to arrive at the same answer (unfaithful reasoning). A few studies measure the faithfulness of reasoning with LLMs. Lanham et al. [78] notes that just like organic reasoners, a model’s reasoning may be post-hoc, it may be constructed after a certain conclusion has been found. By deliberately adding mistakes to the chain of thought, the authors measure the faithfulness of the model. They find a wide variation of post-hoc reasoning, with a tendency of larger models to be less faithful. Like regular LLMs, when not properly grounded, (Chain-of-thought) reasoning suffers from hallucination [59].

Another study adds deliberate bias to the prompt. For example, in a multiple-choice setting, they always make answer (A) the correct answer [147]. They find that a bias towards wrong answers can cause significant drops in accuracy, and that models frequently generate Chain-of-thought explanations rationalizing wrong answers. To address issues of faithfulness, Lyu et al. [91], Xu et al. [174] propose Faithful-chain-of-thought. This approach involves two stages. First, the natural language query is translated into a formal symbolic language. Second, the problem-solving stage processes the formal language, and can explain the reasoning steps it has thus taken. For the symbolic language, Python, Datalog, or PDDL is suggested. Another approach, mechanistic interpretability, studies methods to target individual representations inside the LLM, to see if the expected behavior occurs in practice [9, 19, 118].

Faithfulness studies tell us more about how models reason. Further surveys on this topic are Chuang et al. [28], Luo et al. [90], Mondorf and Plank [98], Paul et al. [109],

4.2.2 Scaling. The emergent abilities of LLMs have prompted research into the nature of scaling and reasoning with LLMs, and, specifically, how reasoning capabilities can be transferred to smaller language models. Scaling laws of LLMs are an active area of study, see for example [53, 54, 70]. Distillation of reasoning to smaller models can work surprisingly well in situations with more explicit instructions, and given the computational cost of training LLMs, there is much interest in transferring knowledge to small language models. Comprehensive surveys on knowledge distillation are Gu et al. [48], Xu et al. [175]. For reasoning specifically, Magister et al. [93] have studied reasoning in small language models, using a student model that learns from a teacher model, by finetuning. Other works focus on prompt distillation for retrieval [33], recommendation [82], embodied agents [23], and LLM graph reasoning [183].

Another study related to Self-taught-reasoner focuses on explanation in small language models, also achieving good results of knowledge transfer [83].

4.3 Limitations: What LLMs Can and Cannot do

The capabilities of LLMs are impressive. LLMs can be seen as large text-based surrogate models of the world (or the world how we describe it on the internet), and thus allow reasoning about a large variety of contexts and problems. Reasoning, such as in math word problems, were one of the capabilities that LLMs could not achieve, until recently. Let us look more closely at what language models currently can and cannot do.

4.3.1 What Can LLMs Do? With the right prompt, LLMs are able to solve many of the problems in grade school math word benchmarks and beyond. Prompt-based learning is able to perform reasoning tasks such as math word problems, robotic movement gaming, and Python code generation, at inference time, without expensive parameter training.

A taxonomy of generate-evaluate-control is able to describe the structure of the current LLM reasoning literature. Furthermore, the accuracy of the reasoning chains can be improved with ensemble methods, and self-verification. Hallucination can be reduced by grounding the model with external models, such as for robotic affordances, and information retrieval from search engines and Wikipedia. Going a step further, using external control algorithms as scaffolding (such as search or reinforcement learning), dynamic prompts can use the LLMs to perform complex and dynamic reasoning patterns. Note that the reasoning control is now two layers away from the core LLM: an external control algorithm, on top of in-context-learning, dynamically generating prompts for the LLM. This is reasoning *with* prompts *with* LLMs, not *by*.

At this point, it is interesting to note the confluence of the two schools of classical artificial intelligence, symbolic and connectionist.⁴ Search and reinforcement learning are rooted in the symbolic tradition, while LLMs are rooted in the connectionist tradition. The literature in this survey combines the two traditions. High performance reasoning is created with a (symbolic) searcher/learner on top of a (connectionist) LLM. In other fields similar combinations can be seen (for example, AlphaFold [16, 66] and retrosynthesis of molecules [128]). The LLM helps ground symbolic reasoning methods in language; symbolic methods help create prompts that let the LLM perform dynamic reasoning.

We note that benchmarks such as GSM8K have been central for the progress of the field, and that while reasoning started with math word problems, the field has extended to robotics, autonomous agents, games, and most emphatically computer code. Formal languages play an important role in the intermediate multi-step reasoning chains.

4.3.2 What Can LLMs Not Do? Now that grade school math word problems are largely solvable, harder reasoning benchmarks in other domains are appearing [1]. Most of the reasoning capabilities exhibited by LLMs are due to the representational powers of the transformer architecture, and how in-context learning is able to harness them. Prompt engineering and prompt control play a crucial role in the kind of reasoning that we have seen in the papers. Models can be instructed to write their own reasoning prompts; however, such Auto-GPT or Auto-CoT prompts need careful evaluation, verification, and grounding in the real world, to prevent degeneration into a hallucinatory world of their own. Models can also be instructed to interact with the world, and become the tool of external scaffolding that evaluates, controls and improves the prompts [112]. Some of what we experience as reasoning *by* the LLM, is controlled by the prompt or the scaffolding algorithm. Studies into in-context reinforcement learning aim to answer the question if prompt learning is able get the LLM to create a prompt to exhibit dynamic reasoning by itself [34, 80, 103, 127].

Some studies on symbolic planning are critical on the abilities of LLMs [148], and show examples of planning failures, arguing that LLMs are better used to improve heuristic elements of traditional planners, such as PDDL [68], to strengthen traditional symbolic planning approaches.

Other works study the dangers of the size of LLMs. Bender et al. [7] mention the environmental risks associated with the large computational training demands, as well as the difficulty of understanding the training data, for example in the context of bias. Furthermore, there are ethical, legal, and copyright concerns regarding the data that LLMs are trained on. Finally, to prevent putting too much trust in the outcome of LLMs, we should understand their failure modes better, such as the well-publicized problems of hallucination (inventing facts that look right but are not). Here, mechanistic interpretability can be used to explore LLM representations and understand where they go wrong [9, 19, 118].

⁴Reasoning and planning have been studied since the start of artificial intelligence, starting with logic and reasoning [100], search algorithms in puzzles and board games [76, 110], robot planning [40], classical machine learning such as decision trees and support vector machines [13, 32, 42], through knowledge representation and the semantic web [149]. Ever since the success of the connectionist approach [47, 79] (deep learning, including LLMs) researchers have tried to join the two approaches.

Some of the names of the approaches surveyed in this paper are suggestive of self-awareness and self-reflective capabilities. True (human) self-reflection, or metacognition, is still largely outside the capabilities of current LLMs. LLMs can be prompted to reason, to take small steps, to self-evaluate, and their search process can be controlled by an external algorithm. The self-reflective type of “intelligence” is written into the prompt by the prompt engineer or the control algorithm. We are unaware of any LLM that has been made to reflect on, or even control, its reasoning processes, controlling how many reasoning steps it should take, or limiting its reasoning once the answer had become good enough. True self-reflection remains future work, although some steps have been taken, as we will discuss next.

4.3.3 Reasoning towards Metacognition. Human thought exhibits the ability to reason about self, we are able to think about our own thinking processes. Metacognition studies this phenomenon [153]. Prompted by the success of Chain-of-thought and related works, metacognition has also been studied in the context of LLMs [146].

Many reasoning approaches highlight self-reflective aspects in their names and in how they work. The prompts that prompt the models to reason are being improved with the outcome of the reasoning process, and in Buffer-of-thoughts thought-templates are used that are derived from other reasoning processes. Wang and Zhao [162] study Metacognitive-prompting. Inspired by Chain-of-thought and Self-consistency, they create manually designed prompts to increase the understanding of language models. Another work, again inspired by Chain-of-thought and Self-consistency, connects psychology and LLMs. Didolkar et al. [35] study metacognitive capabilities of LLMs in mathematical problem solving, both on GSM8K and on the harder MATH problems [52]. First, the model is prompted to find a skill name for each problem instance in the dataset. For 7000 instances of GSM8K, 500 skill names were found by the model. Next, these 500 names are clustered down to 22 skills. They find that by using the names of these 22 skills in Chain-of-thought-like prompts, more problems are solved than with standard Chain-of-Thought/Self-consistency/PAL prompts. Examples of the 22 skill names are *multiplication-and-addition*, *basic-arithmetic*, *subtraction*, and *algebra*. Interestingly, the authors find that the skill exemplar repository that is trained on a strong model (GPT-4), also down-translates to a weak model (GPT-3). The performance of the weaker model benefits from the skill-name-enhanced prompts. Begus et al. [5] propose a program for the study of metalinguistic abilities of LLMs. LLMs struggle with analogies [81, 97] and analogical reasoning. Metacognitive reasoning with LLMs is still in its early stages.

4.4 LLMs that Generate Computer code

A persistent thread in the results in this survey is that LLMs are good at generating formal languages, such as PDDL, logic, math equations, and Python. The agentic approach in which LLMs are combined with external tools such as interpreters or debuggers often yields good performance [112]. LLMs can be used in different modes, which we will now discuss.

When LLMs are used in *direct* mode, a prompt is provided with an instruction, and an answer. This is the mode in which most casual users use an LLM.

LLMs can also be used in *algorithmic* mode, or Chain-of-thought mode, where an extra element is added to the prompt that gives an example of which steps to take to arrive at the answer [129]. Lee et al. [80], Schultz et al. [127], Wang et al. [160] show that the transformer architecture can be trained such that search and reinforcement learning algorithms can be executed in-context. (LLMs pretrained on natural language are typically not good at in-context reinforcement learning [103, 123]).

We have seen that LLMs are not good at preserving state between calls [71]. External algorithms can be added to manage the state, that call the LLM in an *external* mode [178, 179]. Tree-of-thoughts, and similar approaches, use the LLM in a stateless functional way, with the prompt containing the instructions, not unlike a natural language variant of a functional programming language such as LISP or Haskell.

Finally, an LLM can be used in *code generation* mode. The prompt specifies a problem, and the LLM is asked to generate computer code (such as Python or PDDL). The code may contain variables that manage the state correctly. The code can be executed directly, or first be checked and improved by a programmer. We expect that the use LLMs as code generators, and prompt-engineering as natural-language-programming, will continue to grow.

4.5 Research Agenda

At the end of this discussion, we list promising topics for future work. Reasoning with LLMs is an active field of research. It brings together elements of symbolic reasoning, connectionism, natural language, autonomous agents, affective reasoning [14] and metacognition. First we discuss current topics for the field of LLM-reasoning itself, then we discuss more general machine learning topics that are important for progress in LLM-reasoning, and finally we discuss more longer term, fundamental topics.

- *In Context Reinforcement Learning*—Search control beyond greedy search is often implemented as an external reinforcement learning algorithm. Is it possible to incorporate the control stage of the reasoning pipeline into one static prompt, as in-context reinforcement learning (ICRL)? Studies indicate that models can be trained for decision making [34, 80], but general LLMs have not yet been shown to perform ICRL well [103, 123, 127, 151].
- *Code*—Progress in reasoning using formal languages and computer code has been quite promising. GitHub Copilot is a success. Further integration of LLM-reasoning with software engineering tools is a promising area of research that can have a large practical impact on how software is written.
- *Grounding*—Reasoning in LLMs has been successfully applied in autonomous agents, robotics, and games. A challenge is the grounding of the reasoning process in the environment. Retrieval augmented generative methods (RAG) can help LLMs to actively find new information when the reasoning outcome is uncertain. RAG, search, and agentic LLMs, are also active areas of research [33, 112, 154].

Generic topics in machine learning that also influence prompt-based reasoning research are:

- *Benchmarks*—Progress in LLMs depends on the availability of the right benchmarks. As the field has progressed beyond math word problems, other benchmarks become prevalent, with more difficult and diverse tasks.
- *Faithfulness*—Our theoretical understanding of prompt-based reasoning with LLMs is incomplete. The research on faithfulness highlights one example of our lack of understanding. In general, more insight into the working of multi-step in-context learning in LLMs is dearly needed.
- *Smaller language models*—Efficiency is an important element for wide adoption of language models. Smaller models have many advantages over larger models: a smaller environmental footprint, more accessible to people and organizations with fewer computational resources, and the possibility to finetune them. Models may have fewer parameters, or the parameters may be quantized with fewer bits. Unfortunately, with a smaller number of parameters, the models also have less reasoning power. It is important for future work to investigate this trade-off. Solutions to compensate the limited capabilities of smaller models are distillation of reasoning to small language models and reinforcement learning approaches [131] to improve the efficiency of the finetuning/reasoning pipeline [37, 49].

For longer term future work, the following more fundamental questions are important:

- *Symbolic and Connectionist Computation*—How can we further improve LLM-reasoning: how can LLMs benefit from reasoning prompts based on the symbolic AI literature, and how can LLMs help ground symbolic reasoning in language?
- *Multimodal World-Models with Embodied Grounding*—How can an LLM maintain a unified, continually updated representation that integrates text, vision, audio, and sensorimotor feedback, enabling it to reason over events across modalities, and refine its world-model through closed perception–action loops in real-world environments?
- *Norm-Sensitive and Value-Aligned Reasoning*—How do we represent, adapt, and audit diverse cultural norms and ethical values within the reasoning process, ensuring that each step of an LLM’s chain-of-thought respects context-dependent moral constraints while remaining transparent and verifiable?
- *Reasoning in other languages than English*—The majority of the research into LLM reasoning is for English. Although there are efforts in creating benchmarks to test LLM capabilities in other languages⁵, these contain mainly NLP tasks such as question answering (QA) and natural language inference (NLI). In addition, challenges related to low-resource languages (languages for which very limited training data is available) have not been addressed yet.
- *Reasoning in specialized domains*—In an effort to guide development and evaluation of new methods, research in AI has a strong focus on benchmarking: standardized datasets with a limited set of problems that are realistic to evaluate. In the real world, however, reasoning problems also occur in more challenging contexts. A few examples are: legal reasoning for the interpretation of case law or writing contracts; scientific reasoning for advancing scientific fields; and medical reasoning for AI-assisted diagnostics.

5 CONCLUSION

Prompt-based in-context learning is an efficient machine learning method, requiring no parameter updates to the LLM. While achieving good performance on language tasks, performance on reasoning tasks was lacking originally. Reasoning tasks, such as math word problems, are typically solved in a step-by-step fashion. Recently prompts have been developed that guide an LLM to “think step by step” (Chain-of-thought), and to evaluate and verify the step results. The performance of multi-step reasoning with LLMs has improved greatly, and the field has progressed beyond math word problems. Together, the surveyed methods allow the LLM to follow high-quality multi-step reasoning chains. Python code or other formal languages have been used successfully to reduce the error in reasoning steps. Also, in the field of autonomous agents and robotic action, good performance has been achieved by grounding reasoning answers in the environment and the physical constraints of robotic movement.

For complex reasoning tasks a large number of reasoning steps may be generated. To control the size of the multi-step reasoning space dynamically, external scaffolding algorithms can be used. Often, variations on search algorithms are used, and especially reinforcement learning. The symbolic and connectionist AI traditions come together in reasoning prompts and search algorithms that help LLM neural networks solve natural language math word and related problems. Inference-time reasoning results can be used to augment finetuning, in a feedback loop.

LLMs hallucinate and suffer from bias, and their use poses different ethical dangers. In multi-step reasoning methods, self-verification methods have been developed to reduce error-accumulation, yet ethical dangers may remain, especially

⁵<https://github.com/NaiveNeuron/awesome-multilingual-llm-benchmarks>

since reflection is not error-free. Additionally, retrieval augmentation methods ground LLM output directly in sources such as Wikipedia.

Among the most popular reasoning benchmarks in this survey is GSM8K, which contains 8500 grade school math word problems. With older LLMs such as GPT-3, reasoning approaches show an improvement of 20-50% points over standard prompting methods, and some even more. Many current LLMs have since adopted the reasoning approaches. The success of reasoning with LLMs has attracted more applications, and with them, benchmarks are diverging.

The field of reasoning with LLMs is quite new, and theoretical understanding is lacking in important areas, such as faithful reasoning (models may sometimes find the right answer using an incorrect reasoning chain). There may be more opportunities for efficiency gains by integrating the training of reasoning models, using reinforcement learning, both in training and in context. Although prompt-based learning allows few-shot learning at inference time, the computational needs of LLM pretraining and finetuning are still high, hence the interest in small language models. Reasoning skills that work in large models can often be distilled to small models.

Human thought is capable of metacognition, we can think about our thinking process. Many of the names of the approaches in this survey suggest a link to metacognition (Reflexion, Self-refine, Self-improvement, Inner-monologue). The first preliminary experiments of language models that reason about their reasoning skills have appeared.

LLM-reasoning is an active field of research that shows great progress. Based on current limitations and open questions we provide a research agenda highlighting opportunities for further progress with reinforcement learning (for finetuning, in context reinforcement learning and self-reflection), for LLMs that generate code for external tools, for multimodal world models, for value-aligned reasoning, and for small language models, among others.

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