Diagram of Thought: Iterative Reasoning via Next Token Prediction

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Abstract

We introduce *Diagram of Thought* (DoT), a framework that models iterative reasoning in large language models (LLMs) as the construction of a directed acyclic graph (DAG) within a single model. Unlike traditional approaches that represent reasoning as linear chains or trees, DoT organizes propositions, critiques, and validations into a cohesive DAG structure, allowing the model to explore complex reasoning pathways while maintaining logical consistency. Each node in the diagram corresponds to a proposition that has been proposed, critiqued, or refined, enabling the LLM to iteratively improve its reasoning through natural language feedback. By leveraging auto-regressive next-token prediction, DoT facilitates seamless transitions between proposing ideas and critically evaluating them, providing richer feedback than binary signals. This approach enhances both the training and inference processes within a single LLM, eliminating the need for multiple models or external control mechanisms. DoT offers a conceptual framework for designing next-generation reasoning-specialized models, emphasizing training efficiency and robust reasoning capabilities[1].

1 Introduction

The capabilities of large language models (LLMs) have expanded significantly, yet their proficiency in complex reasoning tasks remains limited. Traditional approaches like Chain-of-Thought (CoT) (Wei et al., 2022) have attempted to improve reasoning by prompting models to generate linear sequences of intermediate steps. Extensions such as Tree-of-Thought (ToT) (Yao et al., 2023) and Graph-of-Thought (GoT) (Besta et al., 2024) have introduced branching structures to capture multiple reasoning pathways. Cumulative Reasoning (CR) (Zhang et al., 2023) orchestrates an iterative process involving different specialized LLMs fulfilling roles such as proposer, verifier, and reporter. However, these methods often rely on external control mechanisms or manage multiple reasoning trajectories, complicating both training and deployment.

In this paper, we introduce *Diagram of Thought* (DoT), a framework that models logical deduction as the construction of a directed acyclic graph (DAG) within a single LLM. DoT incorporates critiques in natural language rather than binary signals, offering richer, more informative feedback that can be viewed as a form of "natural language rewards." This allows the model to receive detailed explanations of errors, facilitating deeper understanding and more effective refinement of propositions.

DoT is designed to be training-friendly, focusing on the auto-regressive next-token prediction capabilities of a single LLM. By embedding the entire reasoning process within one model, DoT eliminates the need for multi-LLM collaboration or external control mechanisms. This simplification not only

[1]Code is available at https://github.com/diagram-of-thought/diagram-of-thought.

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streamlines deployment but also aligns closely with standard training paradigms for LLMs, making it easier to integrate into existing workflows.

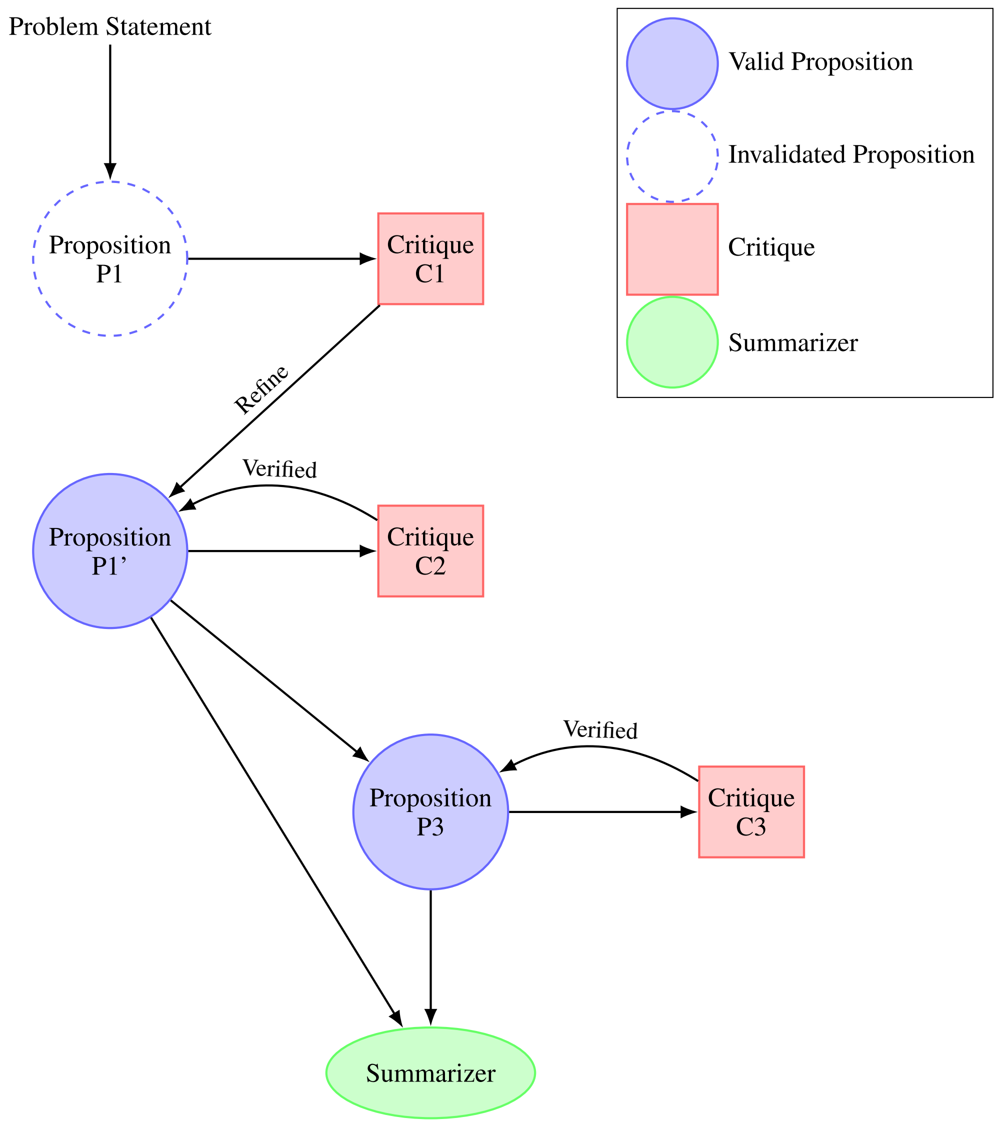

Figure 1: Diagram of Thought: Directed Acyclic Graph of Iterative Reasoning

Our contributions are as follows:

1. We present the Diagram of Thought (DoT) framework, modeling iterative reasoning as DAG construction within a single LLM, enhancing the reasoning process by integrating propositions and natural language critiques.
2. We demonstrate how leveraging auto-regressive next-token prediction with special tokens such as <proposer>, <critic>, and <summarizer> allows the model to seamlessly transition between proposing ideas and critically evaluating them, enriching the feedback loop without external intervention.
3. We provide a conceptual framework for next-generation reasoning-specialized model design, emphasizing the importance of training efficiency and robust inference capabilities within a single LLM.

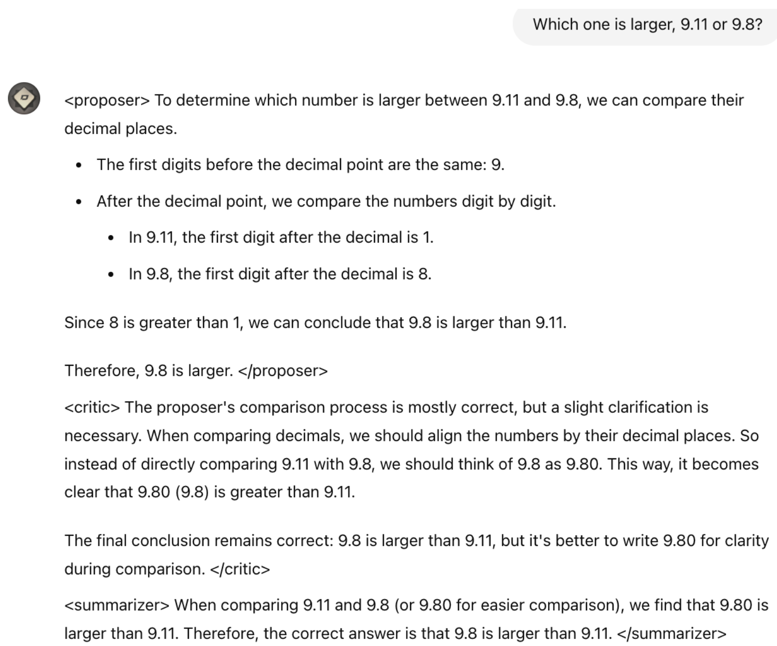

Figure 2: Asking LLM to answer the question: “Which one is larger, 9.11 or 9.8?”.

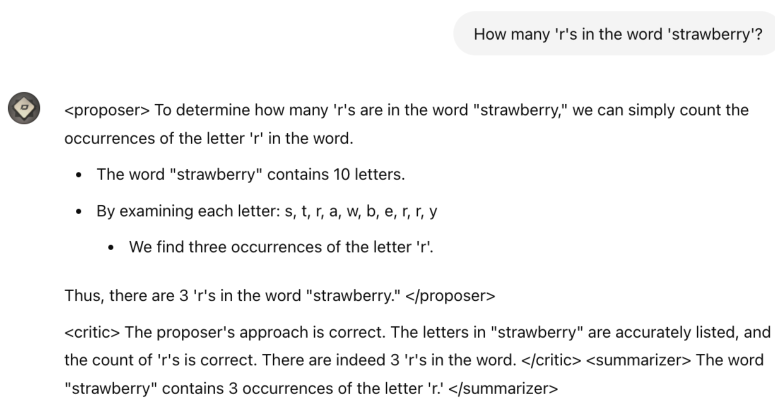

Figure 3: Asking LLM to answer the question: “How many ’r’s in the word ’strawberry’?”.

2 Related Work

Chain-of-Thought (CoT) (Wei et al., 2022) introduced the concept of enabling LLMs to generate intermediate reasoning steps, effectively allowing the model to ”think aloud.” This linear decomposition of reasoning tasks has been shown to improve performance on complex problem-solving tasks by making the latent reasoning process explicit. However, the linear nature of CoT may not adequately capture the non-linear and hierarchical structure inherent in complex reasoning.

Tree-of-Thought (ToT) (Yao et al., 2023) extends CoT by allowing the exploration of multiple reasoning paths in a tree structure, thus accommodating branching possibilities and enabling backtracking. Cumulative Reasoning (CR) (Zhang et al., 2023) introduces a collaborative reasoning process involving multiple specialized LLMs, each fulfilling a distinct role—proposer, verifier, and reporter. This framework mirrors human problem-solving by iteratively building upon previous propositions and validations. Graph-of-Thought (GoT) (Besta et al., 2024) further generalizes this idea by representing reasoning processes as graphs, capturing more complex relationships between reasoning steps.

While these approaches offer greater flexibility, they often require managing and traversing multiple reasoning trajectories, which can be computationally intensive and challenging to implement within a single LLM framework. Diagram of Thought (DoT) distinguishes itself by integrating the strengths of these approaches into a unified framework within a single LLM. By modeling reasoning as the construction of a DAG, DoT captures the non-linear and hierarchical aspects of logical deduction without necessitating multiple models or external control mechanisms. The use of auto-regressive next-token prediction enables the model to internally manage role transitions and reasoning steps, streamlining the reasoning process and simplifying implementation.

3 Diagram of Thought

The Diagram of Thought (DoT) framework models logical reasoning as the cumulative construction of a directed acyclic graph (DAG) within a single LLM. This DAG consists of nodes representing propositions and critiques, and edges denoting logical relationships or dependencies between them. The acyclic nature ensures the reasoning process progresses without circular dependencies, mirroring well-founded logical deduction.

3.1 Roles and Next-Token Prediction

Within the DoT framework, the LLM internally manages three roles using auto-regressive next-token prediction:

- **Proposer**: Generates propositions or reasoning steps, contributing new nodes to the DAG.
- **Critic**: Evaluates propositions, identifying errors, inconsistencies, or logical fallacies, and adds critique nodes.
- **Summarizer**: Synthesizes validated propositions into a coherent chain-of-thought, effectively performing a topological sort of the DAG to produce the final reasoning output.

These roles are delineated within the model's output through the use of special tokens (e.g., <proposer>, <critic>, <summarizer>). The LLM transitions between these roles seamlessly during generation, leveraging its auto-regressive capabilities to predict the next token based on the context.

3.2 Reasoning Process

The reasoning process unfolds as follows:

1. The **Proposer** introduces a proposition, adding a node to the DAG.
2. The **Critic** evaluates the proposition, either validating it or providing a critique. If a critique is provided, a new node is added, and an edge is established between the proposition and the critique.
3. This cycle repeats, with the proposer considering previous critiques and generating refined propositions.
4. Once sufficient valid propositions have been established, the **Summarizer** activates to synthesize the reasoning.

By exposing the model to both correct and incorrect reasoning, DoT allows the LLM to learn from its mistakes, refining its reasoning over time. This iterative process mirrors human problem-solving, where hypotheses are proposed, evaluated, and revised.

3.3 Training and Inference

Training the model within the DoT framework involves incorporating training examples formatted with the DoT structure, including role tags and DAG representations. We need to train the model to recognize and appropriately generate content for each role based on contextual cues and tags. Leveraging the model's auto-regressive nature to predict subsequent tokens, facilitating seamless role transitions and DAG construction.

This approach can be integrated into existing pre-training or fine-tuning pipelines with minimal adjustments. The reliance on a single LLM simplifies deployment, reducing computational overhead associated with managing multiple models or external reasoning modules.

4 Topos-Theoretic Perspectives

The Diagram of Thought (DoT) framework can be rigorously formalized using *Topos Theory*, a branch of category theory that unifies concepts from algebraic geometry, logic, and set theory (MacLane & Moerdijk, 2012). Topos theory provides a mathematical setting where logical reasoning and categorical structures coexist, offering a deep understanding of the reasoning processes modeled by DoT.

4.1 Mathematical Formulation

A *topos* $\mathcal{E}$ is a category that resembles the category of sets but with additional structure supporting internal logic. Specifically, a topos has all finite limits and colimits, exponentials, and a subobject classifier, making it suitable for modeling logical propositions and deductions (Lambek & Scott, 1988).

In the DoT framework, propositions, inferences, and critiques are formalized within the internal language of a topos $\mathcal{E}$. Each proposition or logical assertion is represented as a subobject of the terminal object $1_{\mathcal{E}}$. A subobject $P \hookrightarrow 1_{\mathcal{E}}$ functions as a generalized subset, indicating the conditions under which the proposition P holds true.

The topos $\mathcal{E}$ possesses a subobject classifier Ω, an object encapsulating the notion of truth values within the internal logic. Associated with each subobject $P \hookrightarrow 1_{\mathcal{E}}$ is a characteristic morphism $\chi_P : 1_{\mathcal{E}} \to \Omega$, which signifies the truth value of P.

Logical connectives and implications are represented within the internal logic of the topos. Conjunctions and disjunctions of propositions correspond to pullbacks and pushouts of subobjects, respectively. Negation is handled using the subobject classifier and the internal negation operation. An implication between propositions P and Q is represented by an exponential object Q^P, corresponding to the object of morphisms from P to Q within $\mathcal{E}$.

Inferential relationships between propositions are depicted as morphisms in $\mathcal{E}$. An edge from proposition P to proposition Q corresponds to a morphism $f : P \to Q$, indicating that P logically entails Q within the internal logic of the topos.

The reasoning process is captured as a Directed Acyclic Graph (DAG), where nodes represent propositions (subobjects of $1_{\mathcal{E}}$) or critiques, and edges represent inferential morphisms between them. The acyclic nature of the graph ensures the absence of circular dependencies, aligning with the requirement for well-founded logical deductions.

4.2 Cumulative Reasoning via Colimits

To model the dynamic and cumulative nature of reasoning in DoT, we employ the concepts of diagrams and colimits in category theory (MacLane & Moerdijk, 2012). A diagram in a category $\mathcal{E}$ is a functor $D : \mathcal{J} \to \mathcal{E}$, where $\mathcal{J}$ is an index category reflecting the structure of the DAG. In this context, $\mathcal{J}$ is a finite category corresponding to the finite DAG constructed during reasoning.

The colimit of the diagram D, denoted $\varinjlim D$, represents the aggregation of all propositions and inferences into a single coherent object within $\mathcal{E}$. This colimit effectively unifies the various propositions according to the inferential relationships specified by the morphisms in the diagram. By taking the colimit, we ensure that all valid reasoning steps are incorporated into the final conclusion. The categorical structure guarantees the existence of the colimit and that it faithfully represents the cumulative reasoning process, maintaining logical coherence and consistency.

Critiques play a crucial role in refining propositions within the DoT framework. In the topos-theoretic formalization, a critique of a proposition P is represented as a morphism $c_P : P \to \Omega$, where Ω is the subobject classifier. This morphism assigns to each element of P a truth value in Ω, effectively evaluating the validity of P. If a critique identifies issues with a proposition P, the refinement leads to a new proposition P'. This refinement is represented by a morphism $r : P \to P'$, indicating a transformation or correction of the original proposition. The process of refining propositions through critiques constructs a sequence of morphisms:

$$P_0 \xrightarrow{r_1} P_1 \xrightarrow{r_2} P_2 \xrightarrow{r_3} \cdots,$$

where each r_i represents the refinement informed by the critique at that step.

4.3 PreNet Categories and Dynamic Reasoning

To capture the dynamic aspects of the reasoning process, we incorporate *PreNet categories*, which generalize Petri nets and allow modeling of concurrent and sequential processes (Baez et al., 2021). A PreNet category $\mathcal{C}$ consists of objects representing states or propositions in the reasoning process and morphisms representing transitions or inference steps between propositions.

Proposition 4.1. *The category PreNet is equivalent to a presheaf category, and it is a topos (Baez et al., 2021).*

The reasoning DAG can be represented as a functor $F : \mathcal{J} \to \mathcal{C}$, where $\mathcal{J}$ is the index category reflecting the DAG's structure. This functor maps nodes and edges of the DAG to objects and morphisms in $\mathcal{C}$. The colimit $\varinjlim F$ in the PreNet category $\mathcal{C}$ represents the culmination of the reasoning process, aggregating all propositions and inferences into a final state. This approach aligns with the cumulative nature of reasoning in DoT, where each step builds upon the previous ones.

4.4 Logical Consistency and Soundness

The topos-theoretic framework ensures that the reasoning process modeled by DoT is logically consistent and sound. The internal logic supported by the topos $\mathcal{E}$ allows for precise manipulation of logical propositions, ensuring that all inferences are valid within higher-order logic. Morphisms between propositions represent valid logical inferences within $\mathcal{E}$. The acyclic nature of the DAG and the categorical structure prevent circular dependencies, ensuring well-founded reasoning. By aggregating propositions and inferences via colimits, the cumulative reasoning process is coherently assembled, incorporating all valid inferences without contradictions.

4.5 Implications for the DoT Framework

Formalizing the DoT framework within Topos Theory and PreNet categories yields several significant outcomes. The categorical formalism provides a solid mathematical foundation for the reasoning processes modeled by DoT, ensuring precision and rigor in the representation of logical deductions. The internal logic and categorical structures mirror the internal operations of a single LLM employing DoT. The LLM's generation of propositions, critiques, and summaries corresponds to the manipulation of objects and morphisms within the topos. Modeling higher-order logic within the topos allows DoT to handle complex reasoning tasks involving advanced logical constructs, enhancing the LLM's reasoning capabilities. By formalizing critiques as morphisms to the subobject classifier, the feedback mechanism is integrated directly into the logical framework, improving the effectiveness of the refinement process. The categorical structures ensure that the reasoning process is both consistent—free of contradictions—and complete, meaning all valid inferences are included, which is crucial for reliable reasoning in LLMs.

4.6 Example Illustration

To concretize these theoretical concepts, consider a simple example. Let P and Q be propositions represented as subobjects of $1_{\mathcal{E}}$. Suppose there is an inference from P to Q, represented by a morphism $f : P \to Q$. A critique of P is a morphism $c_P : P \to \Omega$, indicating that P may not universally hold. Based on the critique, P is refined to P', with a morphism $r : P \to P'$ representing the refinement process. A new inference from P' to Q is established, represented by a morphism $f' : P' \to Q$. The colimit of this diagram aggregates P', Q, and the inferences, resulting in a coherent reasoning chain that incorporates the critique and refinement.

5 Conclusion

We have presented the Diagram of Thought framework, which models iterative reasoning in large language models as the construction of a directed acyclic graph within a single LLM. By integrating propositions, critiques, and summaries into a unified DAG structure, DoT captures the complexities of logical deduction beyond linear or tree-based models. The framework leverages auto-regressive next-token prediction to manage role transitions seamlessly, enabling the model to generate detailed reasoning processes without external intervention.

The topos-theoretic formalization provides a rigorous mathematical foundation for DoT, ensuring logical consistency, soundness, and completeness in the reasoning process. By representing propositions, inferences, and critiques within the categorical structures of a topos and PreNet categories, we validate the efficacy of DoT in enhancing the reasoning capabilities of large language models. The framework's simplicity in training and deployment, combined with its ability to handle complex logical constructs, underscores its potential to advance the state of the art in reasoning-specialized LLMs.

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