
On the Diagram of Thought

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September 15th, 2024

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, refinements, and verifications 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, refined, or verified, enabling the LLM to iteratively improve its reasoning through natural language feedback. By leveraging auto-regressive next-token prediction with role-specific tokens, DoT facilitates seamless transitions between proposing ideas and critically evaluating them, providing richer feedback than binary signals. Furthermore, we formalize the DoT framework using *Topos Theory*, providing a mathematical foundation that ensures logical consistency and soundness in the reasoning process. 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, robust reasoning capabilities, and theoretical grounding¹.

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) represent reasoning as linear sequences of intermediate steps, enabling models to “think aloud.” While effective for some tasks, this linear structure may not capture the complexities of human reasoning, which often involves revisiting and refining ideas.

Extensions such as Tree-of-Thought (ToT) (Yao et al., 2023) and Graph-of-Thought (GoT) (Besta et al., 2024) introduce branching structures to explore 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 multiple models, 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 natural language critiques, offering richer, more informative feedback than binary signals. This allows the

¹The code is available at <https://github.com/diagram-of-thought/diagram-of-thought>.

model to receive detailed explanations of errors, facilitating deeper understanding and more effective refinement of propositions.

By embedding the entire reasoning process within one model and leveraging auto-regressive next-token prediction with special tokens (e.g., <proposer>, <critic>, <summarizer>), DoT eliminates the need for multi-LLM collaboration or external control mechanisms. This simplification not only streamlines deployment but also aligns closely with standard training paradigms for LLMs, making it easier to integrate into existing workflows.

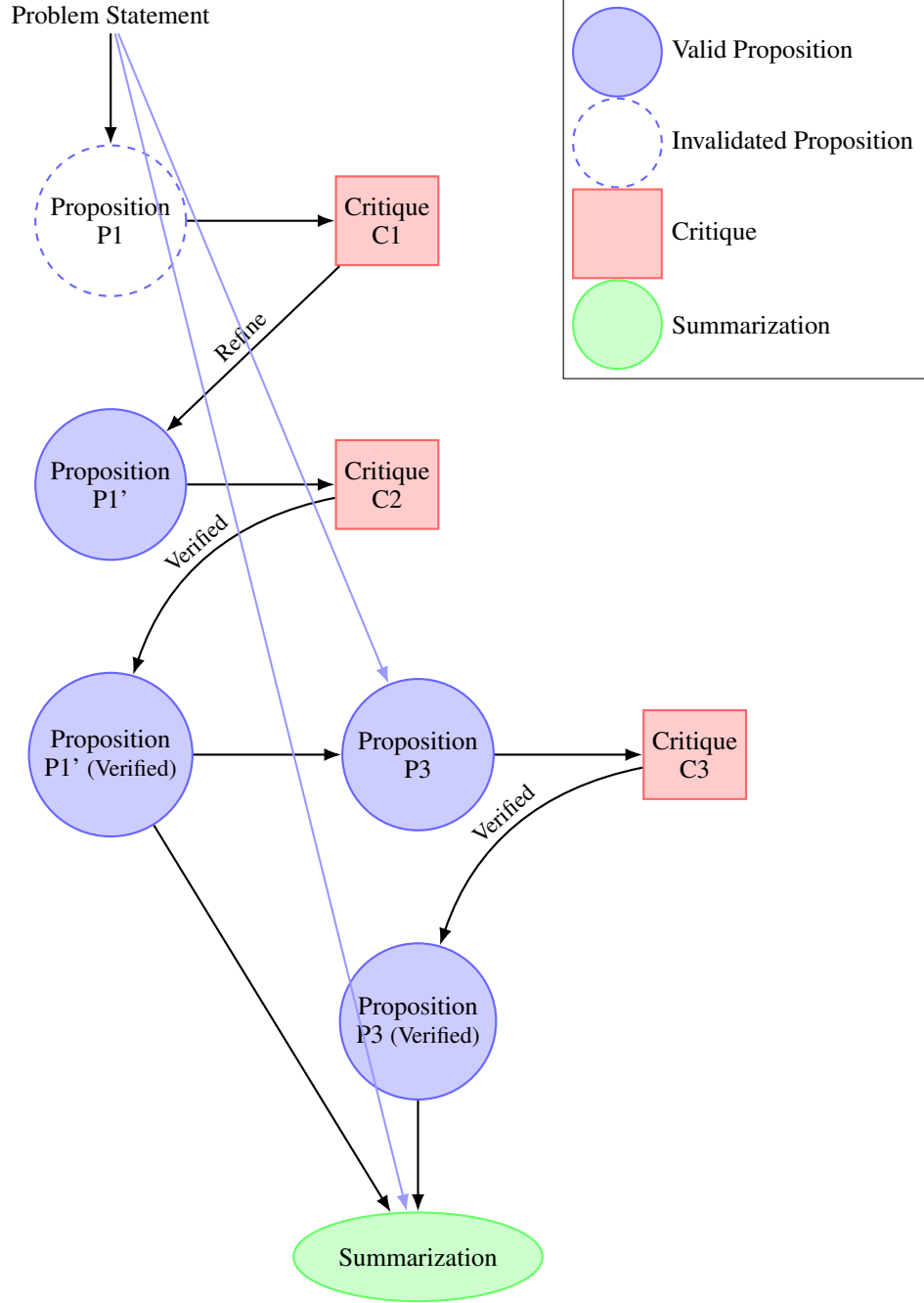



Figure 1: Diagram of Thought: Directed Acyclic Graph of Iterative Reasoning

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, critiques, refinements, and verifications.
2. We demonstrate how leveraging auto-regressive next-token prediction with role-specific tokens allows the model to seamlessly transition between proposing ideas and critically evaluating them, enriching the feedback loop without external intervention.
3. We provide a theoretical foundation by formalizing DoT within Topos theory, clarifying the relationship between DoT and categorical logic, and ensuring logical consistency and soundness in the reasoning process.

Which one is larger, 9.11 or 9.8?

 <proposer> To determine which number is larger between 9.11 and 9.8, we can compare their decimal places.

- The first digits before the decimal point are the same: 9.
- After the decimal point, we compare the numbers digit by digit.
 - In 9.11, the first digit after the decimal is 1.
 - In 9.8, the first digit after the decimal is 8.

Since 8 is greater than 1, we can conclude that 9.8 is larger than 9.11.

Therefore, 9.8 is larger. </proposer>


<critic> The proposer's comparison process is mostly correct, but a slight clarification is necessary. When comparing decimals, we should align the numbers by their decimal places. So instead of directly comparing 9.11 with 9.8, we should think of 9.8 as 9.80. This way, it becomes clear that 9.80 (9.8) is greater than 9.11.

The final conclusion remains correct: 9.8 is larger than 9.11, but it's better to write 9.80 for clarity during comparison. </critic>

<summarizer> When comparing 9.11 and 9.8 (or 9.80 for easier comparison), we find that 9.80 is larger than 9.11. Therefore, the correct answer is that 9.8 is larger than 9.11. </summarizer>

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

How many 'r's in the word 'strawberry'?

 <proposer> To determine how many 'r's are in the word "strawberry," we can simply count the occurrences of the letter 'r' in the word.

- The word "strawberry" contains 10 letters.
- By examining each letter: s, t, r, a, w, b, e, r, r, y
 - We find three occurrences of the letter 'r'.

Thus, there are 3 'r's in the word "strawberry." </proposer>

<critic> The proposer's approach is correct. The letters in "strawberry" are accurately listed, and the count of 'r's is correct. There are indeed 3 'r's in the word. </critic> <summarizer> The word "strawberry" contains 3 occurrences of the letter 'r.' </summarizer>

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 iterative aspects of human reasoning.

Tree-of-Thought (ToT) (Yao et al., 2023) extends CoT by allowing the exploration of multiple reasoning paths in a tree structure, accommodating branching possibilities and enabling backtracking. 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. These approaches, while flexible, often require managing multiple reasoning trajectories, which can be computationally intensive and challenging to implement within a single LLM framework. 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 but adds complexity by involving multiple models and external orchestration.

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 iterative aspects of logical deduction while maintaining computational efficiency. 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, critiques, refinements, and verifications, 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 with role-specific tokens:

- **Proposer** (<proposer>): Generates propositions or reasoning steps, contributing new nodes to the DAG.
- **Critic** (<critic>): Evaluates propositions, identifying errors, inconsistencies, or logical fallacies, and adds critique nodes.
- **Summarizer** (<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. 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. Based on the critique, the **Proposer** generates a refined proposition, represented as a new node in the DAG.

4. This cycle repeats, with propositions being refined until they are verified.
5. Once sufficient valid propositions have been established, the **Summarizer** synthesizes the reasoning, performing a topological sort on the DAG to produce a coherent chain-of-thought.

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.

Figure 1 illustrates the DoT framework. Each proposition and its refinements are represented as nodes, with critiques leading to new nodes rather than cycles. This maintains the acyclic nature of the graph, allowing for a topological sort to produce the final chain-of-thought.

3.3 Training and Inference

Training the model within the DoT framework involves incorporating training examples formatted with the DoT structure, including role-specific tokens and DAG representations. The model learns to recognize and generate content appropriate for each role based on contextual cues.

During inference, the model generates propositions, critiques, and summaries by predicting the next token, guided by the role-specific tokens. This allows for seamless transitions between roles and the construction of the reasoning DAG within a single model.

4 Topos-Theoretic Formalization of DoT

The Diagram of Thought (DoT) framework can be formalized using *Topos Theory*, a branch of category theory that provides a unifying framework for mathematics and logic (MacLane & Moerdijk, 2012). By leveraging the structures of toposes and PreNet categories, we can represent the reasoning processes in DoT, ensuring logical consistency and soundness.

4.1 Mathematical Foundations

A *topos* \mathcal{E} is a category that behaves like 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 Ω , which encapsulates the notion of truth values within the internal logic (Lambek & Scott, 1988).

In the DoT framework, propositions, inferences, and critiques are represented within the internal language of a topos \mathcal{E} . Each proposition is modeled as a subobject $P \hookrightarrow 1_{\mathcal{E}}$ of the terminal object, representing the conditions under which the proposition holds true. Logical relationships and inferences between propositions are depicted as morphisms in \mathcal{E} . An edge from proposition P to proposition Q corresponds to a morphism $f : P \rightarrow Q$, indicating that P logically entails Q within the internal logic.

Critiques are represented as morphisms to the subobject classifier, $c_P : P \rightarrow \Omega$, assigning truth values to propositions and evaluating their validity. Refinements of propositions based on critiques are modeled by morphisms $r : P \rightarrow P'$, representing the transformation or correction of the original proposition.

4.2 Iterative Reasoning, Colimits, and PreNet Categories

The cumulative and dynamic nature of iterative reasoning in DoT is captured using the concepts of colimits and PreNet Categories from category theory. A diagram in a topos \mathcal{E} , represented as a functor $D : \mathcal{J} \rightarrow \mathcal{E}$, models the reasoning DAG constructed during the reasoning process, where \mathcal{J} is an index category reflecting the structure of the DAG.

The colimit of the diagram D , denoted $\varinjlim D$, aggregates all propositions, critiques, refinements, and inferences into a single coherent object within \mathcal{E} . This aggregation corresponds to the cumulative reasoning process in DoT, ensuring that all valid reasoning steps are incorporated into the final conclusion. The role of the **Summarizer** (<summarizer>) in the DoT framework is analogous to taking the colimit in category theory. Just as the summarizer synthesizes verified propositions into

a coherent chain-of-thought, the colimit combines all objects and morphisms in the diagram into a unified result, respecting the logical relationships specified by the diagram.

To model the dynamic aspects of reasoning, we incorporate PreNet Categories, which generalize Petri nets and allow the 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 of PreNets is equivalent to a presheaf category and is itself a topos (Baez et al., 2021).*

By modeling the reasoning process within a PreNet category, we can represent the DAG of propositions and inferences, where the index category \mathcal{J} corresponds to the structure of the DAG. The colimit $\varinjlim D$ 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, while also modeling concurrent reasoning pathways. The PreNet structure captures both the sequential and parallel aspects of the reasoning process, reflecting the flexibility and depth of the DoT framework.

4.3 Ensuring Logical Consistency and Soundness

The topos-theoretic formalization, combined with PreNet categories, ensures that the reasoning process in DoT is logically consistent and sound. The internal logic of the topos allows for precise manipulation of logical propositions, with morphisms representing valid logical inferences. The acyclic structure of the DAG, reflected in the diagram D , prevents circular dependencies, aligning with the requirement for well-founded logical deductions.

By aggregating propositions and inferences via colimits in the context of PreNet categories, we coherently assemble the cumulative reasoning process, incorporating all valid inferences without contradictions. This formalism guarantees that the final reasoning output is logically consistent and derived through valid inferences, even when concurrent reasoning paths are considered.

4.4 Implications for the DoT Framework

Formalizing the DoT framework within Topos theory and PreNet categories provides a robust mathematical foundation for the reasoning processes modeled by DoT, ensuring precision and rigor in the representation of logical deductions. By integrating critiques as morphisms to the subobject classifier and modeling concurrent reasoning paths with PreNet categories, the feedback mechanism and dynamic aspects of reasoning are embedded directly into the logical framework.

This formalism ensures 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. The correspondence between the colimit and the summarizer role highlights how category theory can inform the design of reasoning mechanisms in LLMs, bridging the gap between theoretical concepts and practical implementation.

Example. 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 $f : P \rightarrow Q$. A critique of P is a morphism $c_P : P \rightarrow \Omega$, indicating that P may not universally hold.

Based on the critique, P is refined to P' , with a morphism $r : P \rightarrow P'$ representing the refinement process. A new inference from P' to Q is established, represented by a morphism $f' : P' \rightarrow Q$. The diagram formed by these objects and morphisms represents the reasoning process, and its colimit $\varinjlim D$ aggregates these into a coherent conclusion.

In the DoT framework, the summarizer corresponds to taking this colimit, synthesizing the refined and verified propositions from concurrent reasoning pathways into a final chain-of-thought that represents the comprehensive solution to the problem.

5 Conclusion

In this paper, we presented the *Diagram of Thought* (DoT) 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, refinements, and verifications 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 with role-specific tokens to manage role transitions seamlessly, enabling the model to generate detailed reasoning processes without external intervention.

We further provided a *topos-theoretic* formalization of the DoT framework, offering a mathematical foundation that clarifies the relationship between the reasoning processes and categorical logic. By representing propositions, inferences, and critiques within the structures of a topos, we ensured logical consistency and soundness in the reasoning process. This theoretical grounding validates the efficacy of DoT in enhancing the reasoning capabilities of large language models and bridges the gap between practical implementation and mathematical rigor.

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