TRAINING LARGE LANGUAGE MODELS TO REASON IN A CONTINUOUS LATENT SPACE

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ABSTRACT

Large language models (LLMs) are restricted to reason in the "language space", where they typically express the reasoning process with a chain-of-thought (CoT) to solve a complex reasoning problem. However, we argue that language space may not always be optimal for reasoning. For example, some critical tokens require complex planning, making them difficult to compute in a single forward pass, while many other tokens contribute little to the actual reasoning process. To explore the potential of LLM reasoning in an unrestricted latent space instead of using natural language, we introduce a new paradigm COCONUT (Chain of Continuous Thought). We utilize the last hidden state of the LLM as a representation of the reasoning state (termed "continuous thought"). Rather than decoding this into a word token, we feed it back to the LLM as the subsequent input embedding directly in the continuous space. This novel latent reasoning paradigm leads to emergent advanced reasoning patterns: the continuous thought can encode multiple alternative next reasoning steps, allowing the model to perform a breadth-first search (BFS) to solve the problem, rather than prematurely committing to a single deterministic path like CoT. COCONUT outperforms CoT in certain logical reasoning tasks that require substantial backtracking during planning, with fewer thinking tokens during inference. These findings demonstrate the promise of latent reasoning and offer valuable insights for future research.

1 INTRODUCTION

Large language models (LLMs) have demonstrated remarkable reasoning abilities, emerging from extensive pretraining on human languages (Dubey et al., 2024; Achiam et al., 2023). While next token prediction is an effective training objective, it imposes a fundamental constraint on the LLM as a reasoning machine: the explicit reasoning process of LLMs must be generated in word tokens. For example, a prevalent approach, known as chain-of-thought (CoT) reasoning (Wei et al., 2022), involves prompting or training LLMs to generate solutions step-by-step using natural language. However, this is in stark contrast to certain human cognition results. Neuroimaging studies have consistently shown that the language network – a set of brain regions responsible for language comprehension and production – remains largely inactive during various reasoning tasks (Amalric & Dehaene, 2019; Monti et al., 2012; 2007; 2009; Fedorenko et al., 2011). Further evidence indicates that human language is optimized for communication rather than reasoning (Fedorenko et al., 2024).

A significant issue arises when LLMs use language for reasoning: the amount of reasoning required for each particular token varies greatly, yet current LLM architectures allocate nearly the same computing budget for predicting every token. Some critical tokens require complex planning and is challenging to compute in a single forward pass, while most other tokens in a reasoning chain are generated solely for fluency, contributing little to the actual reasoning process. While previous work has attempted to fix these problems by performing additional reasoning before generating some critical tokens (Zelikman et al., 2024) or prompting LLMs to generate succinct reasoning chains (Madaan & Yazdanbakhsh, 2022), these solutions remain constrained within the language space and do not solve the fundamental problems. On the contrary, it would be ideal for LLMs to

[*]Work done at Meta

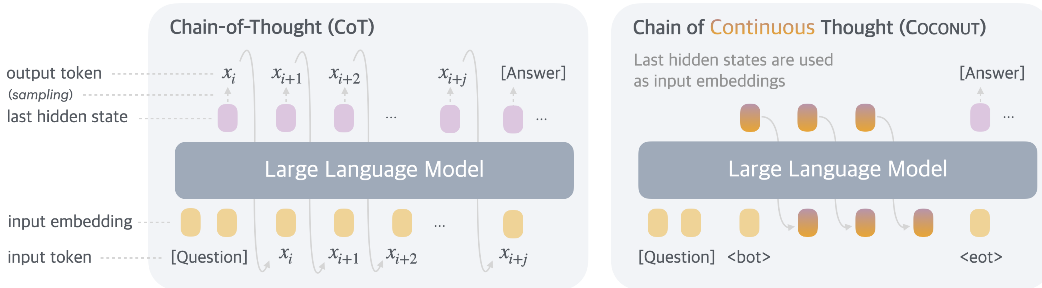

Figure 1: A comparison of Chain of Continuous Thought (COCONUT) with Chain-of-Thought (CoT). In CoT, the model generates the reasoning process as a word token sequence (e.g., $[x_i, x_{i+1}, ..., x_{i+j}]$ in the figure). COCONUT regards the last hidden state as a representation of the reasoning state (termed "continuous thought"), and directly uses it as the next input embedding. This allows the LLM to reason in an unrestricted latent space instead of a language space.

have the freedom to reason without any language constraints, and then translate their findings into language only when necessary.

In this work we instead explore LLM reasoning in a latent space by introducing a novel paradigm, COCONUT (Chain of Continuous Thought). It involves a simple modification to the traditional CoT process: instead of mapping between hidden states and language tokens using the language model head and embedding layer, COCONUT directly feeds the last hidden state (a continuous thought) as the input embedding for the next token (Figure 1). This modification frees the reasoning from being within the language space, and the system can be optimized end-to-end by gradient descent. To enhance the training of latent reasoning, we employ a multi-stage training strategy inspired by Deng et al. (2024), which effectively utilizes language reasoning chains to guide the training process.

COCONUT exhibits a novel reasoning patterns, and shows the potential to enhance the planning ability of LLM. It outperforms CoT on ProsQA, our new dataset that requires the model to perform essential search and planning. Analysis reveals that, rather than prematurely committing to a single deterministic path like CoT, continuous thoughts in COCONUT can encode multiple potential next steps simultaneously, allowing for a reasoning process akin to breadth-first search (BFS). While the model may not initially make the correct decision, it can maintain many possible options within the continuous thoughts and progressively eliminate incorrect paths through reasoning, guided by some implicit value functions.

We further validate the feasibility of latent reasoning through more analysis on three datasets. Notably, augmenting LLM with 6 continuous thoughts doubles the performance on math reasoning (GSM8k, Cobbe et al., 2021). Though the performance is not yet on par with generating a complete language CoT, we show that it provides a better trade-off in reasoning efficiency. On other planning-intense tasks like ProsQA and ProntoQA (Saparov & He, 2022), COCONUT is able to outperform CoT while generating fewer tokens during inference. We believe that these findings underscore the potential of latent reasoning and could provide valuable insights for future research.

2 RELATED WORK

Chain-of-thought (CoT) reasoning. We use the term chain-of-thought broadly to refer to methods that generate an intermediate reasoning process in language before outputting the final answer. This includes prompting LLMs (Wei et al., 2022; Khot et al., 2022; Zhou et al., 2022), or training LLMs to generate reasoning chains, either with supervised finetuning (Yue et al., 2023; Yu et al., 2023) or reinforcement learning (Wang et al., 2024; Havrilla et al., 2024; Shao et al., 2024; Yu et al., 2024a). Madaan & Yazdanbakhsh (2022) classified the tokens in CoT into symbols, patterns, and text, and proposed to guide the LLM to generate concise CoT based on analysis of their roles. Recent theoretical analyses have demonstrated the usefulness of CoT from the perspective of model expressivity (Feng et al., 2023; Merrill & Sabharwal, 2023; Li et al., 2024). By employing CoT, the effective depth of the transformer increases because the generated outputs are looped back to the input (Feng et al., 2023). These analyses, combined with the established effectiveness of CoT, motivated our design that feeds the continuous thoughts back to the LLM as the next input embedding. While CoT has proven effective for certain tasks, its autoregressive generation nature makes it challenging to mimic human reasoning on more complex problems (LeCun, 2022; Hao et al., 2023), which typically require planning and search. There are works that equip LLMs with explicit tree

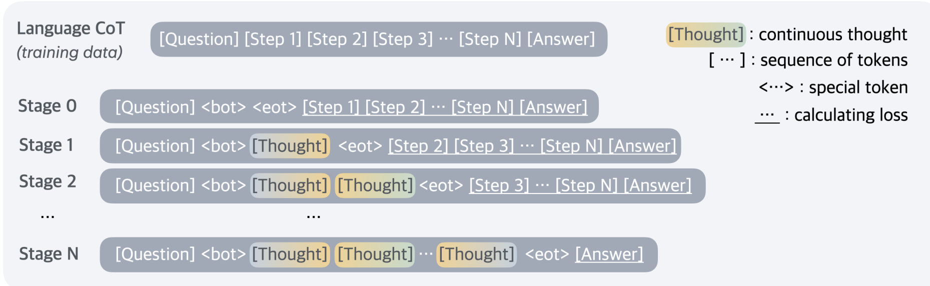

Figure 2: Training procedure of Chain of Continuous Thought (COCONUT). Given training data with language reasoning steps, at each training stage we integrate c additional continuous thoughts ($c = 1$ in this example), and remove one language reasoning step. The cross-entropy loss is then used on the remaining tokens after continuous thoughts.

search algorithms (Xie et al., 2023; Yao et al., 2023; Hao et al., 2024), or train the LLM on search dynamics and trajectories (Lehnert et al., 2024; Gandhi et al., 2024; Su et al., 2024). In our analysis, we find that after removing the constraint of a language space, a new reasoning pattern similar to BFS emerges, even though the model is not explicitly trained in this way.

Latent reasoning in LLMs. Previous works mostly define latent reasoning in LLMs as the hidden computation in transformers (Yang et al., 2024; Biran et al., 2024). Yang et al. (2024) constructed a dataset of two-hop reasoning problems and discovered that it is possible to recover the intermediate variable from the hidden representations. Biran et al. (2024) further proposed to intervene the latent reasoning by "back-patching" the hidden representation. Shalev et al. (2024) discovered parallel latent reasoning paths in LLMs. Another line of work has discovered that, even if the model generates a CoT to reason, the model may actually utilize a different latent reasoning process. This phenomenon is known as the unfaithfulness of CoT reasoning (Wang et al., 2022; Turpin et al., 2024). To enhance the latent reasoning of LLM, previous research proposed to augment it with additional tokens. Goyal et al. (2023) pretrained the model by randomly inserting a learnable `<pause>` tokens to the training corpus. This improves LLM's performance on a variety of tasks, especially when followed by supervised finetuning with `<pause>` tokens. On the other hand, Pfau et al. (2024) further explored the usage of filler tokens, e.g., "**. . .**", and concluded that they work well for highly parallelizable problems. However, Pfau et al. (2024) mentioned these methods do not extend the expressivity of the LLM like CoT; hence, they may not scale to more general and complex reasoning problems. Wang et al. (2023) proposed to predict a planning token as a discrete latent variable before generating the next reasoning step. Recently, it has also been found that one can "internalize" the CoT reasoning into latent reasoning in the transformer with knowledge distillation (Deng et al., 2023) or a special training curriculum which gradually shortens CoT (Deng et al., 2024). Yu et al. (2024b) also proposed to distill a model that can reason latently from data generated with complex reasoning algorithms. These training methods can be combined to our framework, and specifically, we find that breaking down the learning of continuous thoughts into multiple stages, inspired by iCoT (Deng et al., 2024), is very beneficial for the training. Looped architectures (Bai et al., 2019; Giannou et al., 2023; Fan et al., 2024) have some similarities to the computing process of continuous thoughts, but we focus on common reasoning tasks and aim at investigating latent reasoning in comparison to language space. Pham et al. (2023) explored the idea of multi-agent communication in a continuous embedding space rather than language.

3 COCONUT: CHAIN OF CONTINUOUS THOUGHT

In this section, we introduce our new paradigm COCONUT (Chain of Continuous Thought) for reasoning in an unconstrained latent space. We begin by introducing the background and notation we use for language models. For an input sequence $x = (x_1, ..., x_T)$, the standard large language model $\mathcal{M}$ can be described as:

$$H_t = \text{Transformer}(E_t)$$

$$\mathcal{M}(x_{t+1} \mid x_{\leq t}) = \text{softmax}(Wh_t)$$

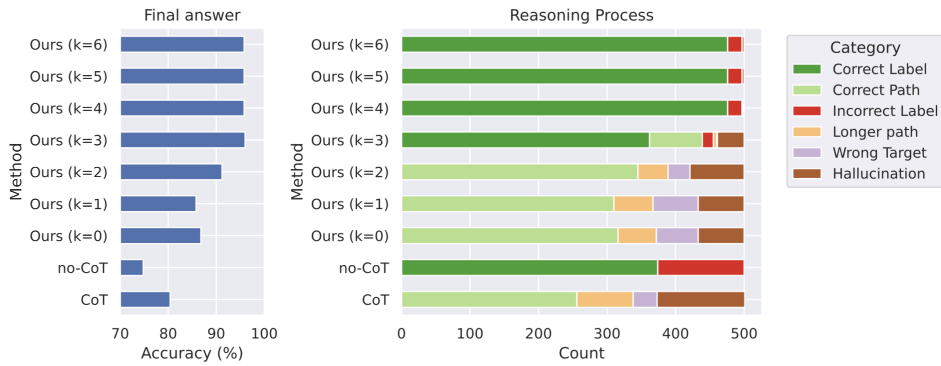

Figure 3: The accuracy of final answer (left) and reasoning process (right) of multiple variants of COCONUT and baselines on ProsQA.

where $E_t = [e(x_1), e(x_2), ..., e(x_t)]$ is the sequence of token embeddings up to position t; $H_t \in \mathbb{R}^{t \times d}$ is the matrix of the last hidden states for all tokens up to position t; h_t is the last hidden state of position t, i.e., $h_t = H_t[t, :]$; $e(\cdot)$ is the token embedding function; W is the parameter of the language model head.

Method Overview. In the proposed COCONUT method, the LLM switches between the "language mode" and "latent mode" (Figure 1). In language mode, the model operates as a standard language model, autoregressively generating the next token. In latent mode, it directly utilizes the last hidden state as the next input embedding. This last hidden state represents the current reasoning state, termed as a "continuous thought".

Special tokens <bot> and <eot> are employed to mark the beginning and end of the latent thought mode, respectively. As an example, we assume latent reasoning occurs between positions i and j, i.e., $x_i =$ <bot> and $x_j =$ <eot>. When the model is in the latent mode ($i < t < j$), we use the last hidden state from the previous token to replace the input embedding, i.e., $E_t = [e(x_1), e(x_2), ..., e(x_i), h_i, h_{i+1}, ..., h_{t-1}]$. After the latent mode finishes ($t \geq j$), the input reverts to using the token embedding, i.e., $E_t = [e(x_1), e(x_2), ..., e(x_i), h_i, h_{i+1}, ..., h_{j-1}, e(x_j), ..., e(x_t)]$. It is worth noting that the last hidden states have been processed by the final normalization layer, so they are not too large in magnitude. $\mathcal{M}(x_{t+1} \mid x_{\leq t})$ is not defined when $i < t < j$, since the latent thought is not intended to be mapped back to language space. However, $\text{softmax}(Wh_t)$ can still be calculated for probing purposes (see Section 5).

Training Procedure. In this work, we focus on a problem-solving setting where the model receives a question as input and is expected to generate an answer through a reasoning process. We leverage language CoT data to supervise continuous thought by implementing a multi-stage training curriculum inspired by Deng et al. (2024). As shown in Figure 2, in the initial stage, the model is trained on regular CoT instances. Assume the total number of training stage (excluding the initial stage) is set to N ($N = 6$ in this example). In the subsequent stages, at the k-th stage, the first k reasoning steps in the CoT are replaced with $k \times c$ continuous thoughts[1], where c is a hyperparameter controlling the number of latent thoughts replacing a single language reasoning step. Following Deng et al. (2024), we also reset the optimizer state when training stages switch. We insert <bot> and <eot> tokens (which are not counted towards c) to encapsulate the continuous thoughts.

During the training process, we optimize the normal negative log-likelihood loss, but mask the loss on questions and latent thoughts. It is important to note that the objective does **not** encourage the continuous thought to *compress the removed language thought*, but rather to *facilitate the prediction of future reasoning*. Therefore, it's possible for the LLM to learn more effective representations of reasoning steps compared to human language.

Training Details. Our proposed continuous thoughts are fully differentiable and allow for back-propagation. We perform $n + 1$ forward passes when n latent thoughts are scheduled in the current training stage, computing a new latent thought with each pass and finally conducting an additional forward pass to obtain a loss on the remaining text sequence. While we can save any repetitive computing by using a KV cache, the sequential computation of COCONUT poses challenges on

[1]If a language reasoning chain is shorter than k steps, then all the language thoughts will be removed.

parallelism for existing training infrastructure. Further optimizing the training efficiency of COCONUT remains an important direction for future research.

Inference Process. The inference process for COCONUT is analogous to standard language model decoding, except that in latent mode, we directly feed the last hidden state as the next input embedding. A challenge lies in determining when to switch between latent and language modes. As we focus on the problem-solving setting, we insert a `<bot>` token immediately following the question tokens. For `<eot>`, we consider two potential strategies: a) train a binary classifier on latent thoughts to enable the model to autonomously decide when to terminate the latent reasoning, or b) always pad the latent thoughts to a constant length. We found that both approaches work comparably well. Therefore, we use the second option in our experiment for simplicity, unless specified otherwise.

4 CONTINUOUS SPACE ENABLES LATENT TREE SEARCH

In this section, we provide a proof of concept on the advantage of continuous latent space reasoning. On ProsQA, a new dataset that requires extensive planning ability, COCONUT outperforms language space CoT reasoning. Interestingly, our analysis indicates that the continuous representation of reasoning can encode multiple alternative next reasoning steps. This allows the model to perform a breadth-first search (BFS) to solve the problem, instead of prematurely committing to a single deterministic path like language CoT.

We start by introducing the experimental setup (Section 4.1). By leveraging COCONUT's ability to switch between language and latent space reasoning, we are able to control the model to interpolate between fully latent reasoning and fully language reasoning and test their performance (Section 4.2). This enables us to interpret the latent reasoning process as tree search (Section 4.3). Based on this perspective, we explain why latent reasoning can make the decision easier for LLMs (Section 4.4).

4.1 EXPERIMENTAL SETUP

Dataset. We introduce ProsQA (Proof with Search Question-Answering), a new logical reasoning dataset. A visualized example is shown in Figure 4. Each instance in ProsQA consists of a directed acyclic graph (DAG) of logical relationships between concepts, presented as natural language statements. The task requires models to determine logical relationships by finding valid paths through this graph, demanding sophisticated planning and search strategies. Unlike previous logical reasoning datasets like ProntoQA (Saparov & He, 2022), ProsQA's DAG structure introduces complex exploration paths, making it particularly challenging for models to identify the correct reasoning chain. More comprehensive details about the dataset construction and characteristics can be found in Appendix A.

Experimental Setup. We use a pre-trained GPT-2 model as the base model for all experiments. The learning rate is set to 1×10^{-4} while the effective batch size is 128. As reference, we report the performance of (1) *CoT*: the model is trained with CoT data, and during inference, the model will generate a complete reasoning chain to solve the problem. (2) *no-CoT*: the model is trained with only the question and answer pairs, without any reasoning steps. During inference, the model will output the final answer directly.

Method. We train a COCONUT model following the training procedure in Section 3. Since the maximum reasoning steps in ProsQA is 6, we set the number of training stages to $N = 6$ in the training procedure. In each stage, we train the model for 5 epochs, and stay in the last stage until the 50 epochs. The checkpoint with the best accuracy in the last stage is used for evaluation.

To understand the properties of latent and language reasoning space, *we manipulate the model to switch between fully latent reasoning and fully language reasoning*. The design of COCONUT allows us to control the number of latent thoughts by manually setting the position of the `<eot>` token during inference. When we enforce COCONUT to use k continuous thoughts, the model is expected to output the remaining reasoning chain in language, starting from the $k + 1$ step. In our experiments, we test variants of COCONUT on ProsQA with $k \in \{0, 1, 2, 3, 4, 5, 6\}$. Note that all these variants only differ in inference time while sharing the same model weights.

Metrics. We apply two sets of evaluation metrics. One of them is based on the correctness of the *final answer*, regardless of the reasoning process. It is the metric used in the main experimental results above (Section 5.3). To enable fine-grained analysis, we define another metric on the *reasoning process*. Assuming we have a complete language reasoning chain which specifies a path in the graph, we can classify it into (1) **Correct Path**: The output is one of the shortest paths to the correct answer. (2) **Longer Path**: A valid path that correctly answers the question but is longer than the shortest path. (3) **Hallucination**: The path includes nonexistent edges or is disconnected. (4) **Wrong Target**: A valid path in the graph, but the destination node is not the one being asked. These four categories naturally apply to the output from COCONUT ($k = 0$) and *CoT*, which generate the full path. For COCONUT with $k > 0$ that outputs only partial paths in language (with the initial steps in continuous reasoning), we classify the reasoning as a Correct Path *if a valid explanation can complete it*. Also, we define Longer Path and Wrong Target for partial paths similarly. If no valid explanation completes the path, it's classified as hallucination. In *no-CoT* and COCONUT with larger k, the model may only output the final answer without any partial path, and it falls into (5) **Correct Label** or (6) **Incorrect Label**. These six categories cover all cases without overlap.

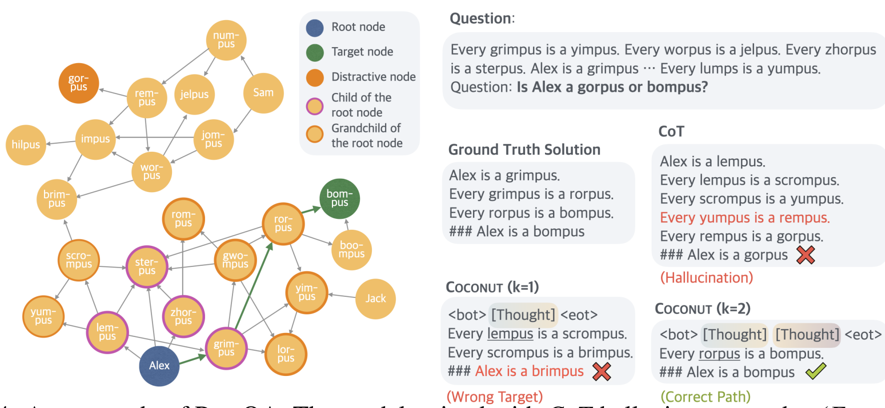

Figure 4: A case study of ProsQA. The model trained with *CoT* hallucinates an edge (*Every yumpus is a rempus*) after getting stuck in a dead end. COCONUT (k=1) outputs a path that ends with an irrelevant node. COCONUT (k=2) solves the problem correctly.

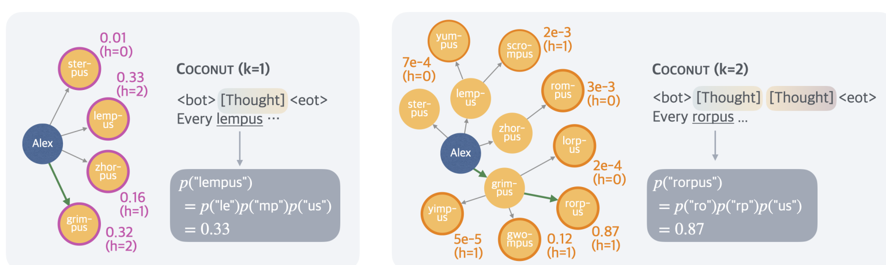

Figure 5: An illustration of the latent search trees. The example is the same test case as in Figure 4. The height of a node (denoted as h in the figure) is defined as the longest distance to any leaf nodes in the graph. We show the probability of the first concept predicted by the model following latent thoughts (e.g., "lempus" in the left figure). It is calculated as the multiplication of the probability of all tokens within the concept conditioned on previous context (omitted in the figure for brevity). This metric can be interpreted as an implicit value function estimated by the model, assessing the potential of each node leading to the correct answer.

4.2 EXPERIMENTAL RESULTS

Figure 3 shows a comparative analysis of different reasoning methods on ProsQA. (1) COCONUT ($k = 6$), which reasons fully with continuous thoughts, achieves higher final answer accuracy than using *CoT*. As shown in the right plot, the model trained with *CoT* often hallucinates edges that don't exist, or output a path leading to a wrong target. That's because when generating the reasoning chain automatically, it's hard to immediately determine which edge to choose, without delibrate planning. (2) As more reasoning is done with continuous thoughts in COCONUT (increasing k), both final answer accuracy (Figure 3, left) and the rate of correct reasoning processes ("Correct Label" and "Correct Path" in Figure 3, right) improve. Additionally, the rate of "Hallucination" and "Wrong

Target" decrease, which typically occur when the model makes a wrong move earlier. This also indicates the better planning ability when more reasoning happens in the latent space.

A case study is shown in Figure 4, where *CoT* hallucinates an nonexistent edge, COCONUT ($k = 1$) leads to a wrong target, but COCONUT ($k = 2$) successfully solves the problem. In this example, the model cannot accurately determine which edge to choose at the earlier step. However, as latent reasoning can avoid making a hard choice upfront, the model can progressively eliminate incorrect options in subsequent steps and achieves higher accuracy at the end of reasoning. We show more evidence and details of this reasoning process in Section 4.3. The comparison between *CoT* and COCONUT ($k = 0$) reveals another interesting observation, which we discuss in Appendix B.1.

4.3 INTERPRETING THE LATENT SEARCH TREE

Given the intuition that continuous thoughts can encode multiple potential next steps, the latent reasoning can be interpreted as a search tree, rather than merely a reasoning "chain". Taking the case of Figure 4 as a concrete example, the first step could be selecting one of the children of *Alex*, i.e., *{lempus, sterpus, zhorpus, grimpus}*. We depict all possible branches in the left part of Figure 5. Similarly, in the second step, the frontier nodes will be the grandchildren of *Alex* (Figure 5, right).

Unlike a standard breadth-first search (BFS), which explores all frontier nodes uniformly, the model demonstrates the ability to prioritize promising nodes while pruning less relevant ones. To uncover the model's preferences, we analyze its subsequent outputs in language space. For instance, if the model is forced to switch back to language space after a single latent thought ($k = 1$), it predicts the next step in a structured format, such as "every [Concept A] is a [Concept B]." By examining the probability distribution over potential fillers for [Concept A], we can derive numeric values for the children of the root node *Alex* (Figure 5, left). Similarly, when $k = 2$, the prediction probabilities for all frontier nodes—the grandchildren of *Alex*—are obtained (Figure 5, right).

The probability distribution can be viewed as the model's implicit *value function*, estimating each node's potential to reach the target. As shown in the figure, "lempus", "zhorpus", "grimpus", and "sterpus" have a value of 0.33, 0.16, 0.32, and 0.01, respectively. This indicates that in the first continuous thought, the model has mostly ruled out "sterpus" as an option but remains uncertain about the correct choice among the other three. In the second thought, however, the model has mostly ruled out other options but focused on "rorpus". With the statistics on the test set in Appendix B.2, we can see that the model effectively make use of the latent space to explore multiple paths in parallel, and this ability is more pronounced in the early stages of the exploration.

4.4 WHY IS A LATENT SPACE BETTER FOR PLANNING?

In this section, we explore why latent reasoning is advantageous for planning, drawing on the search tree perspective and the value function defined earlier. Referring to our illustrative example, a key distinction between *"sterpus"* and the other three options lies in the structure of the search tree: *"sterpus"* is a leaf node (Figure 4). This makes it immediately identifiable as an incorrect choice, as it cannot lead to the target node *"bompus"*. In contrast, the other nodes have more descendants to explore, making their evaluation more challenging.

To quantify a node's exploratory potential, we measure its height in the tree, defined as the shortest distance to any leaf node. Based on this notion, we hypothesize that *nodes with lower heights are easier to evaluate accurately*, as their exploratory potential is limited. Consistent with this hypothesis, in our example, the model exhibits greater uncertainty between *"grimpus"* and *"lempus"*, both of which have a height of 2—higher than the other candidates.

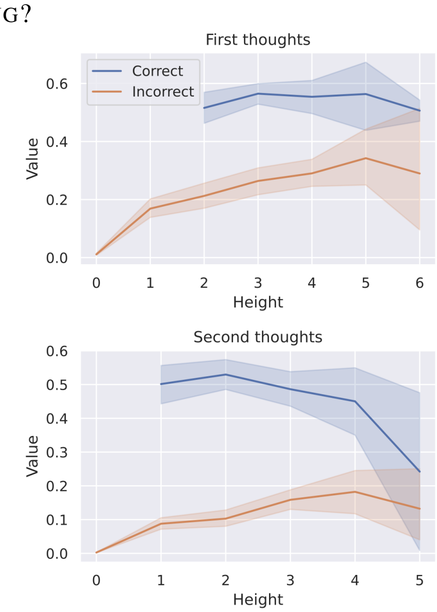

Figure 6: Accuracy on GSM8k with different number of continuous thoughts.

To test this hypothesis more rigorously, we analyze the correlation between the model's prediction probabilities

Method	GSM8k		ProntoQA		ProsQA	
	Acc. (%)	# Tokens	Acc. (%)	# Tokens	Acc. (%)	# Tokens
CoT	42.9 ±0.2	25.0	98.8 ±0.8	92.5	77.5 ±1.9	49.4
No-CoT	16.5 ±0.5	2.2	93.8 ±0.7	3.0	76.7 ±1.0	8.2
iCoT	30.0*	2.2	99.8 ±0.3	3.0	98.2 ±0.3	8.2
Pause Token	16.4 ±1.8	2.2	77.7 ±21.0	3.0	75.9 ±0.7	8.2
COCONUT (Ours)	34.1 ±1.5	8.2	99.8 ±0.2	9.0	97.0 ±0.3	14.2
- *w/o curriculum*	14.4 ±0.8	8.2	52.4 ±0.4	9.0	76.1 ±0.2	14.2
- *w/o thought*	21.6 ±0.5	2.3	99.9 ±0.1	3.0	95.5 ±1.1	8.2
- *pause as thought*	24.1 ±0.7	2.2	100.0 ±0.1	3.0	96.6 ±0.8	8.2

Table 1: Results on three datasets. Higher accuracy indicates stronger reasoning ability, while generating fewer tokens indicates better efficiency. *The result of *iCoT* is from Deng et al. (2024).

and node heights during the first and second latent reasoning steps across the test set. Figure 6 reveals a clear pattern: the model successfully assigns lower values to incorrect nodes and higher values to correct nodes when their heights are low. However, as node heights increase, this distinction becomes less pronounced, indicating greater difficulty in accurate evaluation.

In conclusion, these findings highlight the benefits of leveraging latent space for planning. By delaying definite decisions and expanding the latent reasoning process, the model pushes its exploration closer to the search tree's terminal states, making it easier to distinguish correct nodes from incorrect ones.

5 Empirical Results with Coconut

After analyzing the properties of latent reasoning, we validate the feasibility of LLM reasoning in a continuous latent space through more comprehensive experiments, highlighting the reasoning efficiency over language space.

5.1 Experimental Setup

Math Reasoning. We use GSM8k (Cobbe et al., 2021) as the dataset for math reasoning. It consists of grade school-level math problems. To train the model, we use a synthetic dataset generated by Deng et al. (2023). We use two continuous thoughts for each reasoning step (i.e., $c = 2$), and set the number of training stages to 3.

Logical Reasoning. Logical reasoning involves the proper application of known conditions to prove or disprove a conclusion using logical rules. We use the ProntoQA (Saparov & He, 2022) dataset, and our newly proposed ProsQA dataset, which more challenging due to more distracting branches. We use one continuous thought for each reasoning step (i.e., $c = 1$), and set the number of training stages to 6.

More details of datasets and training settings are described in Appendix A and Appendix B.3.

5.2 Baselines and Variants of Coconut

We consider the following baselines: (1) *CoT*, and (2) *No-CoT*, which were introduced in Section 4. (3) *iCoT* (Deng et al., 2024): The model is trained with language reasoning chains and follows a carefully designed schedule that "internalizes" CoT. As the training goes on, tokens at the beginning of the reasoning chain are gradually removed until only the answer remains. During inference, the model directly predicts the answer. (4) *Pause token* (Goyal et al., 2023): The model is trained using only the question and answer, without a reasoning chain. However, different from *No-CoT*, special `<pause>` tokens are inserted between the question and answer, which provides the model with additional computational capacity to derive the answer. The number of `<pause>` tokens is set the same as continuous thoughts in COCONUT. We also evaluate some variants of COCONUT: (1) *w/o curriculum*, which directly trains the model in the last stage. The model uses continuous thoughts to solve the whole problem. (2) *w/o thought*: We keep the multi-stage training, but don't add any continuous latent thoughts. While this is similar to *iCoT* in the high-level idea, the exact training schedule is set to be consistent with COCONUT, instead of *iCoT*, for a strict comparison. (3) *Pause as* *thought*: We use special <pause> tokens to replace the continuous thoughts, and apply the same multi-stage training curriculum as COCONUT.

5.3 Results and Discussion

We show the overall results on all datasets in Table 1. Using continuous thoughts effectively enhance LLM reasoning over the No-CoT baseline. For example, by using 6 continuous thoughts, COCONUT achieves 34.1% accuracy on GSM8k, which significantly outperforms *No-CoT* (16.5%). We list several key conclusions from the experiments as follows. More discussions are in Appendix B.6.

Continuous representations are efficient representations of reasoning. Compared to CoT, COCONUT generates fewer tokens and achieves higher accuracy on ProntoQA and ProsQA. Though it does not outperform *CoT* on GSM8k, we show that it provides a better trade-off between reasoning efficiency and accuracy (Figure 7, I): We interpolate between fully continuous thoughts and fully language reasoning steps with COCONUT, and noted the results as "continuous". As a comparison, we train a series of *CoT* models which skip the first $m = 1, 2, 3$ reasoning steps, along with complete *CoT* and *no-CoT*, as denoted as "language" in the figure. As shown in the figure, using continuous thoughts effectively alleviates the performance drop as the the model generates fewer tokens. Another interesting observation is that, when we decode the first continuous thought, it often corresponds to possible intermediate variables in the calculation (Figure 9). This also suggests that the continuous thoughts are more efficient representations of reasoning.

"Chaining" continuous thoughts enhances reasoning. In conventional CoT, the output token serves as the next input, which proves to increase the effective depth of LLMs and enhance their expressiveness (Feng et al., 2023). In our experiments, we found that COCONUT also exhibits a chaining effect in the continuous latent space.

COCONUT outperformed other architectures trained with similar strategies, surpassing the latest baseline, *iCoT* (Deng et al., 2024), and significantly outperforming COCONUT (*pause as thought*). This shows the effectiveness of continuous thoughts over pause tokens. Furthermore, we test with different numbers of continuous thoughts for one language reasoning step c (Figure 7, II). As we increased c from 0 to 1 to 2, the models uses 0, 3, 6 continuous thoughts in total to solve the problem (without generating any language). Consequently, the model's performance steadily improved.[2] This suggests that a chaining effect similar to CoT can be observed in the latent space.

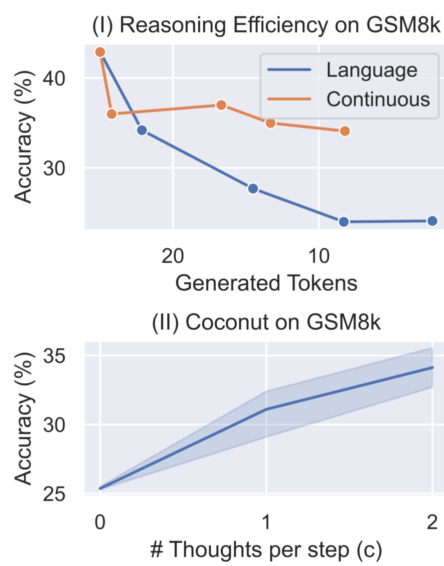

Figure 7: Accuracy on GSM8k with different number of continuous thoughts.

In two other synthetic tasks, we found that the variants of COCONUT (*w/o thoughts* or *pause as thought*), and the *iCoT* baseline also achieve impressive accuracy. This indicates that the model's computational capacity may not be the bottleneck in these tasks. In contrast, GSM8k, being an open-domain question-answering task, likely involves more complex contextual understanding and modeling, placing higher demands on computational capability.

6 Conclusion

We propose a new reasoning paradigm COCONUT. We show its interesting tree search pattern, and its efficiency in several reasoning tasks. We anticipate that our findings will inspire further research into latent reasoning, contributing to the development of more advanced machine reasoning systems.

[2] We discuss the case of larger c in Appendix B.7.

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A Datasets

A.1 Examples

We provide some examples of the questions and CoT solutions for the datasets used in our experiments.

GSM8k

```
Question = "John cuts his grass to 2 inches.  It grows .5
inches per month.  When it gets to 4 inches he cuts it back
down to 2 inches.  It cost $100 to get his grass cut.  How
much does he pay per year?"
Steps = ["«4-2=2»", "«2/.5=4»", "«12/4=3»", "«100*3=300»"]
Answer = "300"
```

ProntoQA

```
Question = "Brimpuses are not luminous.  Shumpuses are
amenable.  Each yumpus is a lorpus.  Gorpuses are shumpuses.
Each zumpus is a grimpus.  Gorpuses are rompuses.  Dumpuses
are not floral.  Lempuses are cold.  Brimpuses are impuses.
Every lorpus is floral.  Every rompus is transparent.
Grimpuses are muffled.  Rompuses are yumpuses.  Rompuses
are wumpuses.  Zumpuses are fast.  Wumpuses are bitter.
Every sterpus is orange.  Each lorpus is a vumpus.  Yumpuses
are feisty.  Each yumpus is a lempus.  Gorpuses are snowy.
Zumpuses are gorpuses.  Every lorpus is a sterpus.  Stella
is a brimpus.  Stella is a zumpus.  True or false:  Stella is
not floral."
Steps = ["Stella is a zumpus.  Zumpuses are gorpuses.",
"Stella is a gorpus.  Gorpuses are rompuses.", "Stella is a
rompus.  Rompuses are yumpuses.", "Stella is a yumpus.  Each
yumpus is a lorpus.", "Stella is a lorpus.  Every lorpus is
floral.", "Stella is floral."]
Answer = "False"
```

ProsQA

```
Question = "Every shumpus is a rempus.  Every shumpus is a
yimpus.  Every terpus is a fompus.  Every terpus is a gerpus.
Every gerpus is a brimpus.  Alex is a rempus.  Every rorpus
is a scrompus.  Every rorpus is a yimpus.  Every terpus is a
brimpus.  Every brimpus is a lempus.  Tom is a terpus.  Every
shumpus is a timpus.  Every yimpus is a boompus.  Davis is
a shumpus.  Every gerpus is a lorpus.  Davis is a fompus.
Every shumpus is a boompus.  Every shumpus is a rorpus.
Every terpus is a lorpus.  Every boompus is a timpus.  Every
fompus is a yerpus.  Tom is a dumpus.  Every rempus is a
rorpus.  Is Tom a lempus or scrompus?"
Steps = ["Tom is a terpus.", "Every terpus is a brimpus.",
"Every brimpus is a lempus."]
Answer = "Tom is a lempus."
```

A.2 CONSTRUCTION OF PROSQA

To construct the dataset, we first compile a set of typical entity names, such as "Alex" and "Jack," along with fictional concept names like "lorpus" and "rorpus," following the setting of ProntoQA (Saparov & He, 2022). Each problem is structured as a binary question: "Is [Entity] a [Concept A] or [Concept B]?" Assuming [Concept A] is the correct answer, we build a directed acyclic graph (DAG) where each node represents an entity or a concept. The graph is constructed such that a path exists from [Entity] to [Concept A] but not to [Concept B].

Algorithm 1 describes the graph construction process. The DAG is incrementally built by adding nodes and randomly connecting them with edges. To preserve the validity of the binary choice, with

# Nodes	# Edges	Len. of Shortest Path	# Shortest Paths
23.0	36.0	3.8	1.6

Table 2: Statistics of the graph structure in ProsQA.

some probability, we enforce that the new node cannot simultaneously serve as a descendant to both node 0 and 1. This separation maintains distinct families of nodes and balances their sizes to prevent model shortcuts.

After the graph is constructed, nodes without parents are assigned entity names, while other nodes receive concept names. To formulate a question of the form "Is [Entity] a [Concept A] or [Concept B]?"", we designate node 0 in the graph as [Entity], a leaf node labeled 1 as [Concept A], and a leaf node labeled 2 as [Concept B]. This setup ensures a path from [Entity] to [Concept A] without any connection to [Concept B], introducing a moderately complex reasoning path. Finally, to avoid positional biases, [Concept A] and [Concept B] are randomly permuted in each question.

Algorithm 1 Graph Construction for ProsQA

```
edges ← {}
nodes ← {0, 1}
labels ← {0 : 1, 1 : 2}
        ▷ Labels: 1 (descendant of node 0), 2 (descendant of node 1), 3 (both), 0 (neither).
groups ← {0 : {}, 1 : {0}, 2 : {1}, 3 : {}}
idx ← 2
while idx < N do
        ▷ For each new node, randomly add edges from existing nodes
    n_in_nodes ← poisson(1.5)
    rand ← random()
    if rand ≤ 0.35 then
        candidates ← groups[0] ∪ groups[1]        ▷ Cannot be a descendant of node 1.
    else if rand ≤ 0.7 then
        candidates ← groups[0] ∪ groups[2]        ▷ Cannot be a descendant of node 0.
    else
        candidates ← nodes
    end if
    n_in_nodes ← min(len(candidates), n_in_nodes)
    weights ← [depth_to_root(c) · 1.5 + 1 ∀c ∈ candidates]
        ▷ Define sampling weights to prioritize deeper nodes.
        ▷ This way, the solution reasoning chain is expected to be longer.
    in_nodes ← random_choice(candidates, n_in_nodes, prob = weights/sum(weights))
    cur_label ← 0
    for in_idx ∈ in_nodes do
        cur_label ← cur_label | labels[in_idx]        ▷ Update label using bitwise OR.
        edges.append((in_idx, idx))
    end for
    groups[cur_label].append(idx)
    labels[idx] ← cur_label
    nodes ← nodes ∪ {idx}
    idx ← idx + 1
end while
```

A.3 Statistics

We show the size of all datasets in Table 3.

Dataset	Training	Validation	Test
GSM8k	385,620	500	1319
ProntoQA	9,000	200	800
ProsQA	17,886	300	500

Table 3: Statistics of the datasets.

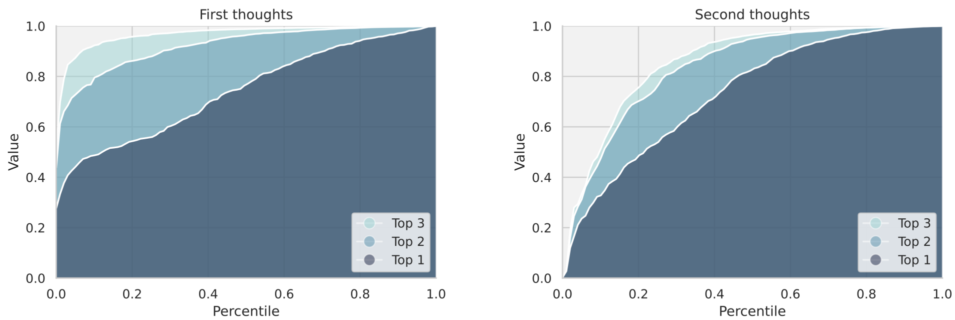

Figure 8: Analysis of parallelism in latent tree search. The left plot depicts the cumulative value of the top-1, top-2, and top-3 candidate nodes for the first thoughts, calculated across test cases and ranked by percentile. The significant gaps between the lines reflect the model's ability to explore alternative latent thoughts in parallel. The right plot shows the corresponding analysis for the second thoughts, where the gaps between lines are narrower, indicating reduced parallelism and increased certainty in reasoning as the search tree develops. This shift highlights the model's transition toward more focused exploration in later stages.

B More Discussion on Empirical Results

B.1 Coconut Generates Better Reasoning Chains

As shown in Figure 3, even when Coconut is forced to generate a complete reasoning chain, the accuracy of the answers is still higher than *CoT*. The generated reasoning paths are also more accurate with less hallucination. From this, we can infer that the training method of mixing different stages improves the model's ability to plan ahead. The training objective of *CoT* always concentrates on the generation of the immediate next step, making the model "shortsighted". In later stages of Coconut training, the first few steps are hidden, allowing the model to focus more on future steps. This is related to the findings of Gloeckle et al. (2024), where they propose multi-token prediction as a new pretraining objective to improve the LLM's ability to plan ahead.

B.2 Analysis of Parallelism in Latent Tree Search

We present an analysis of the model's ability to explore alternative latent thoughts in parallel. As shown in Figure 8, the model makes use of the latent space to explore multiple paths in parallel, and this ability is more pronounced in the early stages of the search.

B.3 Training Details

Math Reasoning. By default, we use 2 latent thoughts (i.e., $c = 2$) for each reasoning step. We analyze the correlation between performance and c in Section 5.3. The model goes through 3 stages besides the initial stage. Then, we have an additional stage, where we still use $3 \times c$ continuous thoughts as in the penultimate stage, but remove all the remaining language reasoning chain. This handles the long-tail distribution of reasoning chains longer than 3 steps. We train the model for 6 epochs in the initial stage, and 3 epochs in each remaining stage.

Logical Reasoning. We use one continuous thought for every reasoning step (i.e., $c = 1$). The model goes through 6 training stages in addition to the initial stage, because the maximum number of

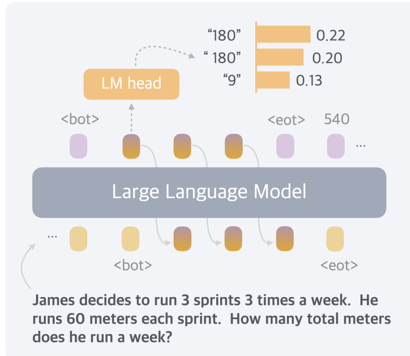

Figure 9: A case study where we decode the continuous thought into language tokens.

reasoning steps is 6 in these two datasets. The model then fully reasons with continuous thoughts to solve the problems in the last stage. We train the model for 5 epochs per stage.

For all datasets, after the standard schedule, the model stays in the final training stage, until the 50th epoch. We select the checkpoint based on the accuracy on the validation set. For inference, we manually set the number of continuous thoughts to be consistent with their final training stage. We use greedy decoding for all experiments.

B.4 Clock-Time Reasoning Efficiency Metric

We present a clock-time comparison to evaluate reasoning efficiency. The reported values represent the average inference time per test case (in seconds), with a batch size of 1, measured on an Nvidia A100 GPU. For the no-CoT and CoT baselines, we employ the standard generate method from the `transformers`[3] library. Our results show that clock time is generally proportional to the number of newly generated tokens, as detailed in Table 1.

Method	GSM8k	ProntoQA	ProsQA
No-CoT	0.03	0.03	0.08
CoT	0.26	0.85	0.47
Coconut	0.09	0.11	0.15

Table 4: Inference time (in seconds) comparison across tasks and methods.

B.5 Interpretation of Continuous Thoughts

In Figure 9, we show a case study where we decode the continuous thought into language tokens. The first continuous thought can be decoded into tokens like "180", " 180" (with a space), and "9". Note that, the reasoning trace for this problem should be $3 \times 3 \times 60 = 9 \times 60 = 540$, or $3 \times 3 \times 60 = 3 \times 180 = 540$. The interpretations of the first thought happen to be the first intermediate variables in the calculation. Moreover, it encodes a distribution of different traces into the continuous thoughts. This is consistent to the analysis in Section 4.3.

B.6 More Discussions on Empirical Results

Performance Differences among Different Datasets. We discuss the performance differences among different datasets, to understand which tasks benefit more from latent reasoning.

- Real-World vs. Synthetic Domains: GSM8k represents a real-world, open-domain question-answering task. Unlike the synthetic datasets used in our study, it demands more complex contextual understanding and modeling, which can place greater demands on computational

[3] `https://github.com/huggingface/transformers`

capabilities. This hypothesis is supported by the observation that COCONUT outperforms all other latent reasoning methods, and its accuracy steadily improves as the number of thoughts per step (c) increases from 0 to 2. Additionally, GSM8k requires diverse commonsense and world knowledge. This may give CoT an advantage, as it aligns closely with the pretraining objectives of the underlying language model, enabling it to better leverage its knowledge compared to COCONUT.

- Planning Requirements: Complex reasoning tasks often require the model to "look ahead" to determine whether a particular step is optimal (also known as planning). Among the datasets in our experiments, GSM8k involves grade-school-level math word problems that allow for intuitive judgment of the next reasoning step. Similarly, ProntoQA includes distracting branches of limited size, making it relatively straightforward to identify the correct next step. In contrast, ProsQA, based on a randomly generated Directed Acyclic Graph (DAG) structure, presents a significant challenge to the model's planning abilities. Our experimental results suggest that tasks requiring extensive planning benefit more from latent space reasoning (including COCONUT, some of its variants, and *iCoT*) than from reasoning using language tokens (*CoT*).

The LLM still needs guidance to learn continuous thoughts. In the ideal case, the model should learn the most effective continuous thoughts automatically through gradient descent on questions and answers (i.e., COCONUT *w/o curriculum*). However, from the experimental results, we found the models trained this way do not perform any better than *no-CoT*. With the multi-stage curriculum which decomposes the training into easier objectives, COCONUT is able to achieve top performance across various tasks. The multi-stage training also integrates well with pause tokens (COCONUT-*pause as thought*). Despite using the same architecture and similar multistage training objectives, we observed a small gap between the performance of *iCoT* and COCONUT *(w/o thoughts)*. The finer-grained removal schedule (token by token) and a few other tricks in *iCoT* may ease the training process. We leave combining *iCoT* and COCONUT as a future work. While the multi-stage training used for COCONUT has proven effective further research is definitely needed to develop better and more general strategies for learning reasoning in latent space, especially without the supervision from language reasoning chains

B.7 USING MORE CONTINUOUS THOUGHTS

In Figure 7 (II), we present the performance of COCONUT on GSM8k using $c \in \{0, 1, 2\}$. When experimenting with $c = 3$, we observe a slight performance drop accompanied by increased variance. Analysis of the training logs indicates that adding three continuous thoughts at once – particularly during the final stage transition – leads to a sharp spike in training loss, causing instability. Future work will explore finer-grained schedules, such as incrementally adding continuous thoughts one at a time while removing fewer language tokens, as in iCoT (Deng et al., 2024). Additionally, combining language and latent reasoning—e.g., generating the reasoning skeleton in language and completing the reasoning process in latent space—could provide a promising direction for improving performance and stability.