

IMPLICIT CHAIN OF THOUGHT REASONING VIA KNOWLEDGE DISTILLATION

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ABSTRACT

To augment language models with the ability to reason, researchers usually prompt or finetune them to produce chain of thought reasoning steps before producing the final answer. However, although people use natural language to reason effectively, it may be that LMs could reason more effectively with some intermediate computation that is not in natural language. In this work, we explore an alternative reasoning approach: instead of explicitly producing the chain of thought reasoning steps, we use the language model’s internal hidden states to perform implicit reasoning. The implicit reasoning steps are distilled from a teacher model trained on explicit chain-of-thought reasoning, and instead of doing reasoning “horizontally” by producing intermediate words one-by-one, we distill it such that the reasoning happens “vertically” among the hidden states in different layers. We conduct experiments on a multi-digit multiplication task and a grade school math problem dataset and find that this approach enables solving tasks previously not solvable without explicit chain-of-thought, at a speed comparable to no chain-of-thought.

1 INTRODUCTION

Large language models have demonstrated significant capabilities in tasks that demand both language understanding and reasoning, such as multi-hop question answering (Yang et al., 2018; Yao et al., 2023b) and solving math problems (Hendrycks et al., 2021; Cobbe et al., 2021; Welleck et al., 2022; Wei et al., 2022b; Kojima et al., 2022; Chen et al., 2022; Yue et al., 2023; Chern et al., 2023). To elicit their reasoning abilities, a prevalent paradigm has been the chain-of-thought reasoning approach (Nye et al., 2021; Wei et al., 2022b; Kojima et al., 2022). Under this paradigm, models are trained or prompted to articulate intermediate steps before producing the final answer.

Although this approach aligns with human problem-solving strategies, it might not fully leverage the computational potential of these language models. Consider the transformer architecture (Vaswani et al., 2017), which can manifest computation both “horizontally” by generating words in sequence and “vertically” by processing through its many layers of internal hidden states. With models like GPT-3 having as many as 96 layers (Brown et al., 2020), one might wonder: Why not let these models reason internally, “vertically” through their layers, and present the solution without necessarily articulating every intermediate step? Such an approach would not only save the significant time cost of autoregressively generating the chain-of-thought: it may also allow models to develop more efficient, if less human-interpretable, methods of reasoning, unconstrained by human conventions.

While chain-of-thought (CoT) methods have achieved impressive successes, generating the CoT itself delays the production of the desired ultimate answer, and it is worth investigating whether insights from CoT methods can be exploited in models that directly produce the answer. Drawing

^{*}Work primarily conducted at Harvard University.

inspiration from how the human brain compiles (Anderson, 2005) explicit, conscious, deliberate reasoning (System 2) to more implicit, automatic, intuitive thinking (System 1) (Kahneman, 2011), we seek a method to compile explicit CoT reasoning into a model that directly produces the final answer. We call this the *implicit chain-of-thought* approach. We take the internal states across transformer layers produced when generating the CoT in a teacher model trained to do so, and train an emulator model to predict a compressed encoding of this sequence of states: the predicted sequence is then used as additional information at inference time for a student model that directly generates only the final answer. In this sense, we compile the internal states that would be autoregressively generated horizontally in an explicit CoT model into the predicted vertical sequence of internal states which is used to generate the answer directly. This replaces (horizontal) reasoning across an explicit CoT with implicit (vertical) reasoning from layer to layer.

Standard CoT training uses ‘teacher forcing’ to require the model to explicitly generate the CoT, but the new method uses a teacher model (which explicitly generates the CoT) to train another model to predict the teacher’s internal states when generating the CoT: ‘teacher teaching’ rather than teacher forcing.

With this as our base, we propose a three-step strategy:

1. Mind-Reading the Teacher: We train a student model to “read” the teacher’s “thought process”—the continuous hidden states during intermediate reasoning step generation. The student model, rather than replicating these steps, uses some of the teacher’s hidden states to produce the answer.
2. Thought Emulation: We then employ knowledge distillation (Hinton et al., 2015; Kim & Rush, 2016) to train an emulator that predicts the teacher’s hidden states from the input “vertically”, across layers, eliminating the need for “horizontal” explicit reasoning steps.
3. Couple and Optimize: Finally, we combine the emulator, which predicts the teacher’s thought process, with the mind-reading student, which produces the final answer from the emulated teacher’s thought process. This combined system is then optimized end-to-end, allowing the student model to develop its own reasoning methods that might differ from the teacher’s approach.

Our experiments show the potential of implicit chain-of-thought reasoning. On a synthetic multi-digit multiplication task, we found that while standard training cannot yield the final answer without explicit reasoning (even GPT-4 struggles with five-digit by five-digit multiplication), our method, applied to a GPT-2 Medium model, is able to provide direct answers for up to five-digit by five-digit multiplications. Moreover, when dealing with real-world tasks like grade school math problems, our method achieves a 22% accuracy on GSM8k (Cobbe et al., 2021) without the need for explicitly generating the intermediate steps.

The contributions of our work are as follows: First, we show the benefits of shifting from teacher-forcing to teacher-teaching by enabling faster generation. Second, we show the effectiveness of distilling explicit reasoning in a teacher to implicit reasoning in a student. Third, we demonstrate the improved performance on directly generating responses to math problems that results from chaining together the first two contributions. Our code, data, and pretrained models are available at https://github.com/da03/implicit_chain_of_thought/.

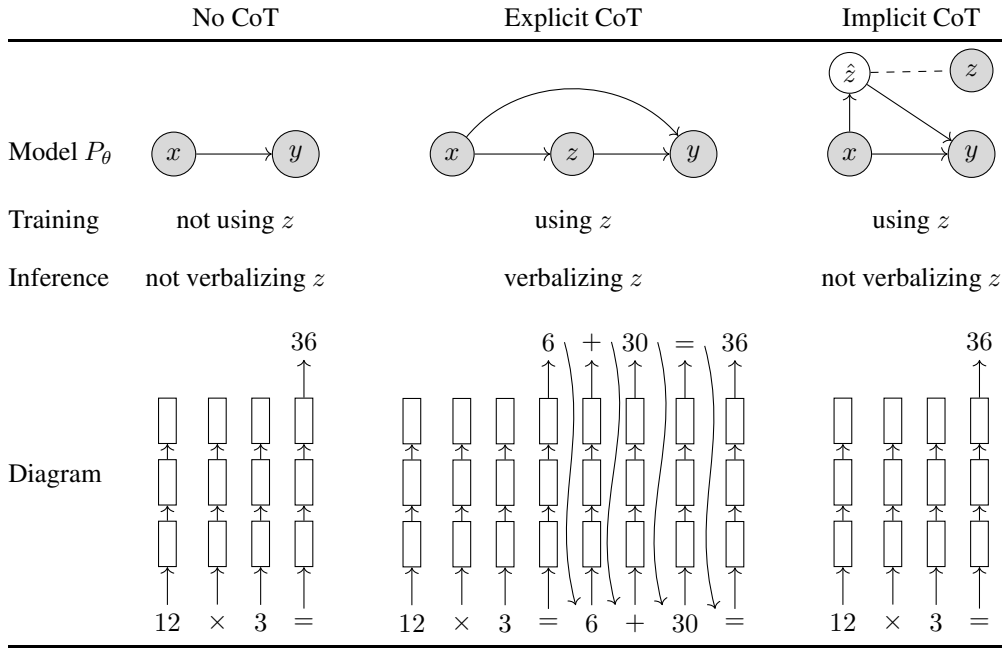
2 EXPLICIT, IMPLICIT, AND NO CHAIN-OF-THOUGHT REASONING

Consider a task that requires multi-step reasoning. Let x be the input, z the intermediate reasoning steps, and y the output. As an example, for the multiplication problem $12 \times 3 = ?$, x is 12×3 , z might be $6 + 30$ (making explicit the intermediate partial products), and y is 36. The objective of a model trained for this task is to determine the conditional distribution $P(y | x)$. We distinguish three approaches for solving this task: no chain-of-thought reasoning (No CoT), explicit chain-of-thought reasoning (Explicit CoT), and implicit chain-of-thought reasoning (Implicit CoT).

2.1 NO CHAIN-OF-THOUGHT REASONING

In this approach, models are trained to generate the final output y using the input x , with the intermediate steps z left out. Mathematically, we directly parameterize the mapping from input to output using a model $P_\theta(y | x)$ and train it with input-output pairs (x, y) . Using the 12×3 multiplication example, the model directly infers the answer 36, as illustrated in the “No CoT” column of Table 1.

Table 1: Comparison between three methods of reasoning: no chain-of-thought (No CoT), explicit chain-of-thought (Explicit CoT), and implicit chain-of-thought (Implicit CoT). The reasoning process is illustrated using a multi-digit multiplication example: $12 \times 3 = 6 + 30 = 36$. Here, x denotes the input ' 12×3 ', y denotes the output 36, and z denotes the intermediate steps $6 + 30$. For the model P_θ , observed variables are shaded. In No CoT, the model is trained to predict the output directly from the input. Explicit CoT predicts the intermediate steps before the final output. Implicit CoT is trained to reason internally using its hidden states and subsequently predict the output.



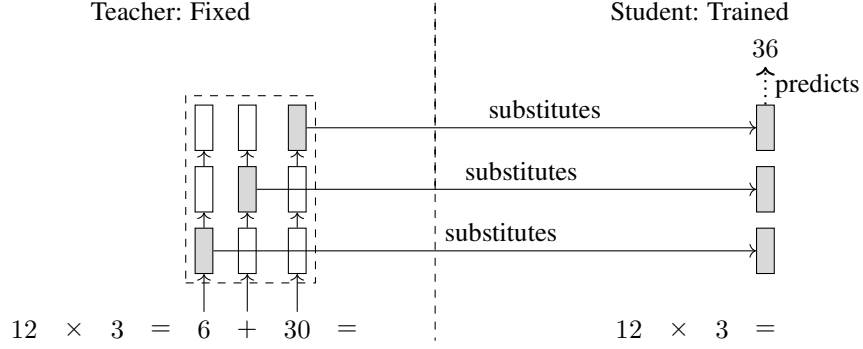
This method can work well for simple tasks, but expecting models to deduce answers for more complex tasks without intermediary guidance can be daunting, analogous to teaching multi-digit multiplication to students without showing the intermediate calculations.

2.2 EXPLICIT CHAIN-OF-THOUGHT REASONING

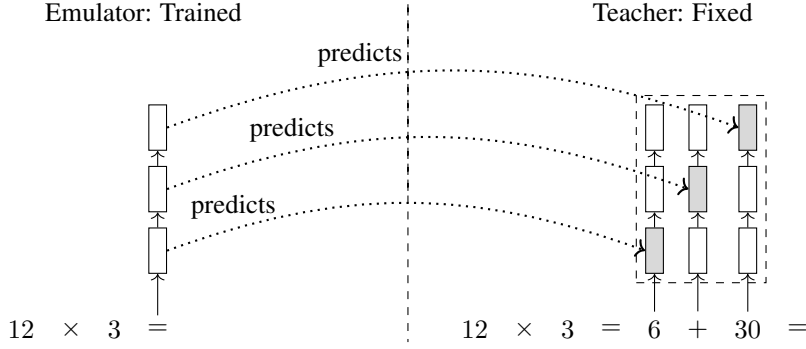
In explicit chain-of-thought reasoning (Nye et al., 2021; Wei et al., 2022b), models are trained to produce the intermediate steps z before the final output y . Instead of only modeling $P(y|x)$, the model looks at the joint distribution $P(y, z|x)$ and breaks it down to $P_\theta(z|x)P_\theta(y|x, z)$. During training, both components $P_\theta(z|x)$ and $P_\theta(y|x, z)$ are trained in a supervised way. At test time, the model first predicts the reasoning steps from the input, then the final output. For the multiplication 12×3 , the model predicts $6 + 30$ first and then 36, as shown in the ‘‘Explicit CoT’’ column of Table 1. While this method breaks down the task into simpler steps, it can be verbose; as we’ll see in later experiments, even a five-digit multiplication needs to generate seventy intermediate tokens.

2.3 IMPLICIT CHAIN-OF-THOUGHT REASONING

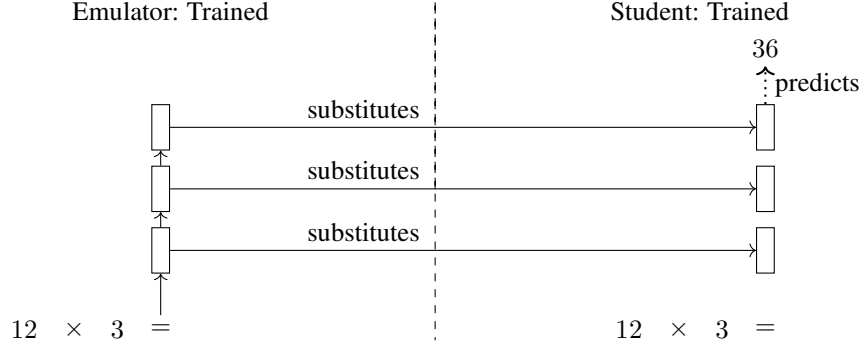
Implicit chain-of-thought reasoning is a middle ground between the two methods above. During training, the model sees intermediate steps z , but during testing, it doesn’t explicitly produce them. Instead, it processes these steps in its internal states, labeled as \hat{z} , to produce the final output y . Formally, $P(y|x) \approx \int_{\hat{z}} P_\theta(\hat{z}|x)P_\theta(y|x, \hat{z})$. This mirrors how humans, once they’ve internalized a concept thoroughly, often bypass explicit reasoning, directly leaping to conclusions. Referring back to our multiplication example, the model directly predicts 36 for $x = 12 \times 3$, having computed the steps internally. The inference diagram for this is the same as the no chain-of-thought reasoning, as seen in Table 1 under ‘‘Implicit CoT’’.



(a) Mind-Reading the Teacher



(b) Thought Emulation



(c) Couple and Optimize

Figure 1: The three-step strategy for implicit chain-of-thought reasoning.. (a) Mind-Reading the Teacher: A student model “reads” the teacher’s continuous hidden states (internal reasoning process) and uses them to produce the output solution. (b) Thought Emulation: An emulator is trained to predict the teacher’s hidden states based on the given input, thus mimicking the internal reasoning process of the teacher without generating explicit horizontal reasoning steps. (c) Couple and Optimize: Integration of the emulator and the mind-reading student forms a combined system. This system is then finetuned end-to-end, enabling the student model’s development of its own reasoning trajectories, possibly deviating from the teacher’s method.

3 APPROACH TO IMPLICIT CHAIN OF THOUGHT REASONING

As a first step toward achieving implicit chain-of-thought reasoning, we outline a three-step strategy based on a teacher model trained for horizontal explicit chain-of-thought reasoning. First, we train a student model to generate the answer using the hidden states of the teacher model, which hold information about the intermediate reasoning steps. This allows the student to produce the final answer directly from the input and teacher states without needing the explicit reasoning steps. We call this “Mind-Reading the Teacher”. Next, we apply knowledge distillation to train an emulator that can predict the teacher’s hidden states from the input by reasoning vertically, a step we term “Thought Emulation”. Finally, we combine the student and emulator. Here, the student uses the teacher states predicted by the thought emulator to predict the final output from the input. We then finetune this combined model end-to-end to improve the internal reasoning process, a step we name “Couple and Optimize”. All these phases are illustrated in Figure 1.

Having outlined the general methodology, we now delve into the implementation specifics when employing the transformer architecture (Vaswani et al., 2017) for our teacher, student, and emulator models. Transformer’s layer-wise processing offers a natural platform to leverage the vertical reasoning concept.

3.1 MIND-READING THE TEACHER

As the teacher processes the input, the intermediate reasoning steps, and the output, its hidden states capture token-related information. Specifically, for a transformer model with L layers running on T intermediate tokens, the hidden states can be expressed in a 2D matrix \mathbf{z} of dimensions $L \times T$, with each element \mathbf{z}_{lt} representing the hidden state at layer l for intermediate token t .

Information Extraction For simplicity first assume $T = L$. While the matrix holds $L \times T$ vectors, we start by selecting L vectors, allowing an emulator with an equal number of layers to predict just one vector per layer. Through experimentation, we found that simply taking the matrix’s diagonal elements was effective. The intuition is that predicting \mathbf{z}_{11} is easy for the emulator since only one intermediate token is introduced¹. Progressing diagonally, from \mathbf{z}_{11} to \mathbf{z}_{LL} , we gradually add more intermediate tokens and layers, ensuring a gradient of increasing difficulty for the emulator, until \mathbf{z}_{LL} , which ideally has enough information to let the teacher start producing the output².

Variable Length Chain-of-Thought Real-world scenarios may present a variable number of intermediate tokens, resulting in a variable number of columns T . To handle this, we introduce a hyper-parameter Δ and take evenly-spaced columns (about one every Δ columns) while still selecting one vector per row. The selected l -th vector is \mathbf{z}_{l,t_l} , determined by:

$$t_l = \min(\lfloor 1 + \Delta(l - 1) \rfloor, T).$$

In our experiments, we search over both fixed Δ values, and also a dynamic Δ value $\frac{T-1}{L-1}$ which adapts to the number of intermediate tokens T in each example, based on validation performance.

Student Training We use a student with the same number of layers as the teacher. Following the extraction of L vectors, these vectors substitute the corresponding hidden states of the student right after input. Refer to Figure 1a for a visual illustration. The student model is then trained to predict the final answer, with the teacher model fixed.

3.2 THOUGHT EMULATION

At test time, the student cannot rely on the L selected vectors $\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_L$ (we abuse notation and omit the second index in \mathbf{z}) from the teacher, so we need to train an emulator to predict those L vectors directly from the input. We use an emulator with the same number of layers as the teacher,

¹In our experiments the first intermediate token is always a special token separating input and reasoning.

²For predicting the first answer token, only the top teacher state is used; lower-layer states \mathbf{z}_{ll} ($l < L$) are only accessible to the second answer token and onward via attention. This is not an issue because we can prepend a special token to the answer, separating reasoning and output.

such that after the input it only needs to predict one vector $\hat{\mathbf{z}}_l$ per layer, as shown in Figure 1b. We train this emulator by minimizing mean squared loss:

$$\min_{\hat{\mathbf{z}}_l} \sum_{l=1}^L \|\mathbf{z}_l - \hat{\mathbf{z}}_l\|_2^2. \quad (1)$$

Multiple Reasoning Pathways When there exist multiple possible reasoning pathways, trying to match the teacher’s state using a mean squared loss can lead to poor predictions. This is akin to employing a single Gaussian distribution to fit a mixture-of-Gaussians distribution, which merely identifies its center. For instance, consider a grade school math problem: *Asumi has 30 books on history, 25 books on literature. How many books does Asumi have in total?* The possible intermediate steps could be either (1) $30 + 25$ or (2) $25 + 30$, corresponding to two possible hidden states $\mathbf{z}_l^{(1)}$ and $\mathbf{z}_l^{(2)}$. Using Equation (1), the optimal solution would be $\hat{\mathbf{z}}_l = (\mathbf{z}_l^{(1)} + \mathbf{z}_l^{(2)})/2$, which doesn’t correspond to any valid reasoning path³.

To account for multiple reasoning pathways, instead of predicting one $\hat{\mathbf{z}}_l$ per layer, we predict a *mixture* of components $P(\hat{\mathbf{z}}_l) = \sum_{c_l} P(\hat{\mathbf{z}}_l^{c_l} | c_l) P(c_l)$, such that each mixture component c_l captures a different mode of the distribution of teacher states.

To parameterize this distribution, at layer l , assume the hidden state of the emulator is \mathbf{h}_l . We parameterize the distribution of each mixture component $P(\hat{\mathbf{z}}_l^{c_l} | c_l)$ as a Gaussian $\mathcal{N}(f(\mathbf{h}_l, c_l); 1)$ and the distribution over mixture components $P(c_l)$ as a categorical distribution $g(\mathbf{h}_l, c_l)$.

Empirically, we found that directly fitting this mixture is prone to mode collapsing (He et al., 2019), where only a few mixture components get used. To alleviate this issue, we leverage the intermediate token z_{t_l} ⁴ at position t_l and supervise c_l to be the same as this token. The final objective is

$$\min_{\mathbf{h}_l} \sum_{l=1}^L \frac{\|\mathbf{z}_l - f(\mathbf{h}_l, c_l)\|_2^2}{2} - \log P(c_l = z_{t_l}). \quad (2)$$

Taking the above example, at the first layer ($l = 1$ and $t_l = 1$), in case (1) we would supervise the mixture component c_1 to be “30” and fit $\hat{\mathbf{z}}^{30}$ to $\mathbf{z}_l^{(1)}$; in case (2) we would supervise c_1 to be “25” and fit $\hat{\mathbf{z}}^{25}$ to $\mathbf{z}_l^{(2)}$, hence the two cases are fit with different mixture components.

3.3 COUPLE AND OPTIMIZE

We can now feed the emulator’s predicted teacher states $\hat{\mathbf{z}}_l$ to the mind-reading student and optimize the entire system end-to-end by maximizing the probability of the final output. Importantly, as the combined system learns, the internal reasoning process might diverge from the teacher’s approach. Note also that this step doesn’t require training data with intermediate reasoning steps.

For the mixture model, ideally we want to use the most probable reasoning pathway by taking the argmax of $P(c_l)$, but that operation is not fully differentiable. Instead, we approximate argmax using a softmax with a low temperature, which is fully differentiable. See Appendix D for more details.

4 EXPERIMENTAL SETUP

4.1 DATA

We conduct experiments on two tasks: we first consider the multi-digit multiplication task from the BIG-bench benchmark (bench authors, 2023; Suzgun et al., 2023), which is the most challenging among arithmetic tasks (Yang et al., 2023). In particular, we use the four-digit (4×4) and five-digit (5×5) multiplication problems, since these two tasks prove very challenging to solve under no CoT. The second task we use is grade school math problems, which requires both language understanding and mathematical reasoning. In particular, we use the GSM8K dataset (Cobbe et al., 2021).

³The emulator cannot distinguish the two cases because it only gets access to the input x .

⁴we use unbolded z to represent the intermediate tokens.

Table 2: Dataset Statistics. Sizes refer to the training set. The number of input, output, and intermediate tokens are median values on the validation set. The number of tokens are based on the GPT-2 tokenizer, and a special ending symbol is counted for both intermediate tokens and output tokens.

Dataset	Orig Size	Aug Size	#Input Tokens	#Intermediate Tokens	#Output tokens
4×4 Mult	0	808k	9	47	9
5×5 Mult	0	808k	11	75	11
GSM8K-Aug	7k	378k	51	59	2

Intermediate Reasoning Steps For the multiplication task, we break down the problem by multiplying the multiplicand by each digit of the multiplier and keep track of partial products and partial sums. On GSM8K, following Wei et al. (2022b) we use the natural language intermediate steps for explicit CoT. For training the teacher of implicit CoT, to minimize the gap between the number of transformer layers and the number of intermediate steps, we only keep the equations.

Data Augmentation In our preliminary experiments, we found that our proposed approach to implicit CoT requires a large training set, potentially due to its different mode of training compared to the pretrained language models we base on. Therefore, we generate synthetic data for both tasks.

For the multi-digit multiplication tasks, we randomly sample equations that do not overlap with the BIG-bench dataset. For GSM8K, we used GPT-4 (OpenAI, 2023) to generate 400k additional mathematical problems with the same format as GSM8K. We then clean the dataset and name it GSM8K-Aug. Note that for both tasks we do not change the original test sets. The statistics of the augmented datasets are shown in Table 2, which show that with explicit CoT the number of generated tokens rise by 5- to 30-fold. More data details can be found in Appendix A.

4.2 BASELINES

We compare our approach to both no CoT and explicit CoT. We compare to GPT-2 Small, GPT-2 Medium, GPT-2 Large, finetuned on the augmented training datasets. We also compare to ChatGPT and GPT-4 under few-shot prompting settings in Appendix C.

4.3 MODELS

For implicit CoT, we finetune GPT-2 Small and GPT-2 Medium. For the diagonal teacher states, we normalize them to be zero-mean with standard deviation one to stabilize emulator training⁵. For the “Mind-Reading the Teacher” step, we add a trainable one-layer MLP on top of the teacher states before copying. For the “Thought Emulation” step, we add an LSTM network (Hochreiter & Schmidhuber, 1997) with self-attention to process the vertical hidden states before predicting the teacher states. For the mixture model, we add a linear projection on top of the emulator hidden states to predict the distribution over mixture components, and to compute $f(\mathbf{h}_l, c_l)$, we concatenate \mathbf{h}_l with the embedding of the mixture component c_l , and then process them with a one-layer MLP.

We used the mixture approach for GSM8K-Aug but not for multiplication, because the multiplication intermediate steps are unique given any input by construction. For the mixture approach we use a temperature of 0.05 during “Couple and Optimize”. See Appendix D for full model details.

5 RESULTS

Table 3 presents the main results. Compared to no CoT, our approach enables solving tasks previously not solvable without explicit CoT: for example, GPT-2 Medium only got 2% accuracy on 5×5 multiplication under the no CoT setting, but got 96% accuracy under the implicit CoT setting.

⁵We found that hidden states from higher layers tend to have larger norms. We applied this normalization to each hidden vector, same as applying layer normalization (Ba et al., 2016) without trainable parameters.

Table 3: Main results. Accuracy (Acc) measures the exact match accuracy of producing the final answer. Throughput measures the number of examples per second during inference using a batch size of 1, and is normalized by the throughput of the corresponding No CoT model.

Model	#Layers	4 × 4 Mult		5 × 5 Mult		GSM8K-Aug	
		Acc	Throughput	Acc	Throughput	Acc	Throughput
No CoT							
GPT-2 Small	12	0.29	1.00	0.01	1.00	0.13	1.00
GPT-2 Medium	24	0.76	1.00	0.02	1.00	0.17	1.00
GPT-2 Large	36	0.34	1.00	0.01	1.00	0.13	1.00
Implicit CoT							
GPT-2 Small	12	0.97	0.67	0.10	0.71	0.20	0.66
GPT-2 Medium	24	0.96	0.69	0.96	0.73	0.22	0.66
Explicit CoT							
GPT-2 Small	12	1.00	0.17	1.00	0.14	0.41	0.08
GPT-2 Medium	24	1.00	0.17	1.00	0.14	0.44	0.08
GPT-2 Large	36	1.00	0.17	0.99	0.15	0.45	0.08

Similarly, on GSM8K-Aug, implicit CoT enables directly producing the final answer with a 22% accuracy, whereas the best GPT-2 model with no CoT only achieves 17% accuracy.

Interestingly, GPT-2 Small performed well on 4×4 multiplication under implicit CoT, achieving 97%. However, its performance significantly dropped to 10% on 5×5 , whereas GPT-2 Medium achieved a 96% accuracy. This suggests that the effectiveness of implicit CoT might depend on having a sufficient number of layers for the required intermediate calculations.

Compared to explicit CoT, implicit CoT lags behind by a large margin, possibly due to two reasons: first, the base language models we used were all pretrained for horizontal reasoning; second, the number of layers we used in our experiments (24 for GPT-2 Medium) might not be sufficient for the number of reasoning steps needed. That being said, implicit CoT has a higher inference speed, especially for tasks with many intermediate steps such as GSM8K-Aug and 5×5 multiplication. For example, on 5×5 multiplication using GPT-2 Medium, implicit CoT is 73% as fast as no CoT, but explicit CoT is only 14% as fast. This is because implicit CoT generates the final answer right away, with the only overhead being the emulator, which can also be parallelized in theory (although not in our experiments).

6 ANALYSIS

Taking Different Subsets as Teacher’s Thought Process In our main experiments, we took the diagonal elements from the matrix of teacher hidden states. Several other methods of extracting a compressed encoding of these hidden states did not perform as well. On the 4×4 multiplication task using GPT-2 Small, when we use diagonal elements, the validation accuracy is 100.0%, and when we take the first column, we get 29.9%; using top row gets 84.4%; using bottom row gets 57.6%.

Mixture Due to the existence of multiple possible reasoning pathways, the mixture approach is crucial for GSM8K-Aug. Without the mixture approach, we achieve 11.2% validation accuracy on GSM8K-Aug (GPT-2 Small, $\Delta = 2$). With the mixture approach, this rises to 20.2%.

Coupling & Optimization The “Optimize” part is important as well. On GSM8K-Aug with GPT-2 Medium and $\Delta = 1$, coupling the emulator and the mind-reading student without further optimization only results in a validation accuracy of 9.4%, compared to 21.9% after further optimization. Allowing the model to develop its own reasoning pathway is also important: if we fix the emulator and only optimize the student, accuracy drops to 13.0%.

For the mixture approach, since we supervised mixture components to be the same as the current intermediate token, we can map back the predicted mixture components to words. Before the “Op-

timize” step, these mapped words look similar to the intermediate reasoning steps produced by the teacher when $\Delta = 1$, and if we directly use them for prediction, we can get an accuracy of 9.4%. However, after the “Optimize” step, the predicted mixture components are no longer interpretable, as shown in Table 5 in Appendix F,

7 RELATED WORK

Emergent Capabilities Research has shown that, under sufficient optimization, language models can solve basic arithmetic tasks (Power et al., 2022). Even for tasks that require multi-step reasoning, increasing both model and data size improves the model’s direct performance. For example, Wei et al. (2022a) observed that test accuracy on the GSM8K dataset (no CoT) rises from below 5% to around 7% as the training FLOPs increase from 10^{21} to 10^{24} . Concurrent to our work, Yang et al. (2023) trained a 2B language model to solve 5×5 multiplication with an accuracy of 89.9% through curriculum learning on 50M training examples. These findings demonstrate that sufficiently scaled models can internally reason over multiple steps. Our approach differs in its use of the teacher model’s thought process to more efficiently attain these models.

Knowledge Distillation Our “Thought Emulation” step is a type of knowledge distillation, where the teacher model transfers its knowledge to a student model (Hinton et al., 2015). Traditionally, this technique is used for model compression (Kim & Rush, 2016) or for non-autoregressive machine translation (Gu et al., 2018). In our approach, it’s used to distill the teacher model’s horizontal reasoning process into a vertical reasoning process in the emulator and the student model.

8 LIMITATIONS

Lack of Transparency and Interpretability One of the main advantages of explicit CoT is its inherent transparency: the intermediate steps allow for easy interpretation of the model’s reasoning process. In contrast, implicit CoT, by virtue of its internal processing within hidden states, lacks this transparency. While it achieves compactness and efficiency in generation, it sacrifices human interpretability, making it challenging to understand how the model arrives at its conclusions.

Reliance on the Teacher’s Thought Process Our current three-step strategy is, at a high level, trying to distill the teacher model’s horizontal reasoning process into the vertical reasoning process of the student and the emulator. While the ultimate goal of implicit reasoning is to allow models to develop their own unique trajectories of reasoning, our initial approach still relies heavily on the teacher’s thought processes for a starting point.

Performance Discrepancies Our current results of implicit CoT still lag behind the performance of explicit CoT. However, this work is just a first step towards building implicit CoT, and there exists ample room for further optimization.

9 CONCLUSION AND FUTURE WORK

In this work, we proposed the concept of implicit chain of thought reasoning for transformer-based language models, where reasoning is performed “vertically” among the transformer hidden states, instead of being performed “horizontally” in the form of generating intermediate tokens. This concept potentially enables the model to break away from the human-like reasoning process and develop its own internal reasoning process.

To operationalize this concept, we proposed a three-step approach—mind-reading the teacher, thought emulation, and coupling and optimization, where the high-level idea is to distill the knowledge of a teacher trained for horizontal reasoning into a student and an emulator trained for vertical reasoning. Experiments on an arithmetic multiplication task and a grade school math problem dataset show that, for the task of directly producing an answer, the proposed approach substantially improves the performance of transformer language models—although explicitly producing a chain-of-thought improves the accuracy of final answers further, by a large margin.

We see many exciting future directions that can be built on top of this work. For example, instead of the three-step strategy, one might explore a fully end-to-end joint training strategy using a variational auto encoder (Kingma & Welling, 2022) by treating the model’s internal reasoning process as an unobserved latent variable. Another direction would be using image modeling techniques that can model distributions with multiple modes such as diffusion (Sohl-Dickstein et al., 2015; Ho et al., 2020; Song et al., 2021) to train the thought emulator. One might also explore incorporating this approach into the pretraining process, such that a pretrained language model can both do horizontal explicit chain-of-thought reasoning, and also do vertical implicit chain-of-thought reasoning, as opposed to existing models whose performance gets much worse when not allowed to use explicit reasoning steps.

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REFERENCES

- John R Anderson. Human symbol manipulation within an integrated cognitive architecture. *Cognitive science*, 29(3):313–341, 2005.
- Jimmy Lei Ba, Jamie Ryan Kiros, and Geoffrey E. Hinton. Layer normalization, 2016.
- BIG bench authors. Beyond the imitation game: Quantifying and extrapolating the capabilities of language models. *Transactions on Machine Learning Research*, 2023. ISSN 2835-8856. URL <https://openreview.net/forum?id=uyTL5Bvosj>.
- Maciej Besta, Nils Blach, Ales Kubicek, Robert Gerstenberger, Lukas Gianinazzi, Joanna Gajda, Tomasz Lehmann, Michal Podstawski, Hubert Niewiadomski, Piotr Nyczyk, and Torsten Hoefer. Graph of thoughts: Solving elaborate problems with large language models, 2023.
- Tom B. Brown, Benjamin Mann, Nick Ryder, Melanie Subbiah, Jared Kaplan, Prafulla Dhariwal, Arvind Neelakantan, Pranav Shyam, Girish Sastry, Amanda Askell, Sandhini Agarwal, Ariel Herbert-Voss, Gretchen Krueger, Tom Henighan, Rewon Child, Aditya Ramesh, Daniel M. Ziegler, Jeffrey Wu, Clemens Winter, Christopher Hesse, Mark Chen, Eric Sigler, Mateusz Litwin, Scott Gray, Benjamin Chess, Jack Clark, Christopher Berner, Sam McCandlish, Alec Radford, Ilya Sutskever, and Dario Amodei. Language models are few-shot learners, 2020.
- Massimo Caccia, Lucas Caccia, William Fedus, Hugo Larochelle, Joelle Pineau, and Laurent Charlin. Language gans falling short, 2020.
- Wenhu Chen, Xueguang Ma, Xinyi Wang, and William W. Cohen. Program of thoughts prompting: Disentangling computation from reasoning for numerical reasoning tasks, 2022.
- Ethan Chern, Haoyang Zou, Xuefeng Li, Jiewen Hu, Kehua Feng, Junlong Li, and Pengfei Liu. Generative ai for math: Abel. <https://github.com/GAIR-NLP/abel>, 2023.
- Karl Cobbe, Vineet Kosaraju, Mohammad Bavarian, Mark Chen, Heewoo Jun, Lukasz Kaiser, Matthias Plappert, Jerry Tworek, Jacob Hilton, Reiichiro Nakano, Christopher Hesse, and John Schulman. Training verifiers to solve math word problems, 2021.
- Mingkai Deng, Jianyu Wang, Cheng-Ping Hsieh, Yihan Wang, Han Guo, Tianmin Shu, Meng Song, Eric Xing, and Zhiting Hu. RLPrompt: Optimizing discrete text prompts with reinforcement learning. In *Proceedings of the 2022 Conference on Empirical Methods in Natural Language Processing*, pp. 3369–3391, Abu Dhabi, United Arab Emirates, December 2022. Association for Computational Linguistics. doi: 10.18653/v1/2022.emnlp-main.222. URL <https://aclanthology.org/2022.emnlp-main.222>.
- Yao Fu, Hao Peng, Ashish Sabharwal, Peter Clark, and Tushar Khot. Complexity-based prompting for multi-step reasoning. In *The Eleventh International Conference on Learning Representations*, 2023. URL <https://openreview.net/forum?id=yflicZHC-l9>.

- Jiatao Gu, James Bradbury, Caiming Xiong, Victor O.K. Li, and Richard Socher. Non-autoregressive neural machine translation. In *International Conference on Learning Representations*, 2018. URL <https://openreview.net/forum?id=B1l8Bt1Cb>.
- Tanmay Gupta and Aniruddha Kembhavi. Visual programming: Compositional visual reasoning without training. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp. 14953–14962, 2023.
- Junxian He, Daniel Spokoyny, Graham Neubig, and Taylor Berg-Kirkpatrick. Lagging inference networks and posterior collapse in variational autoencoders. In *International Conference on Learning Representations*, 2019. URL <https://openreview.net/forum?id=rylDfnCqF7>.
- Dan Hendrycks, Collin Burns, Saurav Kadavath, Akul Arora, Steven Basart, Eric Tang, Dawn Song, and Jacob Steinhardt. Measuring mathematical problem solving with the MATH dataset. In *Thirty-fifth Conference on Neural Information Processing Systems Datasets and Benchmarks Track (Round 2)*, 2021. URL <https://openreview.net/forum?id=7Bywt2mQsCe>.
- Geoffrey Hinton, Oriol Vinyals, and Jeff Dean. Distilling the knowledge in a neural network, 2015.
- Jonathan Ho, Ajay Jain, and Pieter Abbeel. Denoising diffusion probabilistic models. *Advances in Neural Information Processing Systems*, 33:6840–6851, 2020.
- Sepp Hochreiter and Jürgen Schmidhuber. Long short-term memory. *Neural computation*, 9(8): 1735–1780, 1997.
- Eric Jang, Shixiang Gu, and Ben Poole. Categorical reparameterization with gumbel-softmax. In *International Conference on Learning Representations*, 2017. URL <https://openreview.net/forum?id=rkE3y85ee>.
- Daniel Kahneman. *Thinking, fast and slow*. macmillan, 2011.
- Yoon Kim and Alexander M. Rush. Sequence-level knowledge distillation. In *Proceedings of the 2016 Conference on Empirical Methods in Natural Language Processing*, pp. 1317–1327, Austin, Texas, November 2016. Association for Computational Linguistics. doi: 10.18653/v1/D16-1139. URL <https://aclanthology.org/D16-1139>.
- Diederik P. Kingma and Jimmy Ba. Adam: A method for stochastic optimization, 2017.
- Diederik P Kingma and Max Welling. Auto-encoding variational bayes, 2022.
- Takeshi Kojima, Shixiang Shane Gu, Machel Reid, Yutaka Matsuo, and Yusuke Iwasawa. Large language models are zero-shot reasoners. In Alice H. Oh, Alekh Agarwal, Danielle Belgrave, and Kyunghyun Cho (eds.), *Advances in Neural Information Processing Systems*, 2022. URL <https://openreview.net/forum?id=e2TbB5y0yFf>.
- Jieyi Long. Large language model guided tree-of-thought, 2023.
- Ilya Loshchilov and Frank Hutter. Decoupled weight decay regularization. In *International Conference on Learning Representations*, 2019. URL <https://openreview.net/forum?id=Bkg6RiCqY7>.
- Thang Luong, Hieu Pham, and Christopher D. Manning. Effective approaches to attention-based neural machine translation. In *Proceedings of the 2015 Conference on Empirical Methods in Natural Language Processing*, pp. 1412–1421, Lisbon, Portugal, September 2015. Association for Computational Linguistics. doi: 10.18653/v1/D15-1166. URL <https://aclanthology.org/D15-1166>.
- Chris J. Maddison, Andriy Mnih, and Yee Whye Teh. The concrete distribution: A continuous relaxation of discrete random variables. In *International Conference on Learning Representations*, 2017. URL <https://openreview.net/forum?id=S1jE5L5gl>.
- Maxwell Nye, Anders Johan Andreassen, Guy Gur-Ari, Henryk Michalewski, Jacob Austin, David Bieber, David Dohan, Aitor Lewkowycz, Maarten Bosma, David Luan, Charles Sutton, and Augustus Odena. Show your work: Scratchpads for intermediate computation with language models, 2021.

OpenAI. Gpt-4 technical report, 2023.

Long Ouyang, Jeffrey Wu, Xu Jiang, Diogo Almeida, Carroll Wainwright, Pamela Mishkin, Chong Zhang, Sandhini Agarwal, Katarina Slama, Alex Ray, John Schulman, Jacob Hilton, Fraser Kelton, Luke Miller, Maddie Simens, Amanda Askell, Peter Welinder, Paul F Christiano, Jan Leike, and Ryan Lowe. Training language models to follow instructions with human feedback. In S. Koyejo, S. Mohamed, A. Agarwal, D. Belgrave, K. Cho, and A. Oh (eds.), *Advances in Neural Information Processing Systems*, volume 35, pp. 27730–27744. Curran Associates, Inc., 2022. URL https://proceedings.neurips.cc/paper_files/paper/2022/file/blefde53be364a73914f5880

Alethea Power, Yuri Burda, Harri Edwards, Igor Babuschkin, and Vedant Misra. Grokking: Generalization beyond overfitting on small algorithmic datasets, 2022.

Rajkumar Ramamurthy, Prithviraj Ammanabrolu, Kianté Brantley, Jack Hessel, Rafet Sifa, Christian Bauckhage, Hannaneh Hajishirzi, and Yejin Choi. Is reinforcement learning (not) for natural language processing: Benchmarks, baselines, and building blocks for natural language policy optimization. In *The Eleventh International Conference on Learning Representations*, 2023. URL <https://openreview.net/forum?id=8aHzds2uUyB>.

Simas Sakenis and Stuart Shieber. Guiding transformers to process in steps, 2022. URL https://openreview.net/forum?id=lu_DAxnWsh.

Timo Schick, Jane Dwivedi-Yu, Roberto Dessì, Roberta Raileanu, Maria Lomeli, Luke Zettlemoyer, Nicola Cancedda, and Thomas Scialom. Toolformer: Language models can teach themselves to use tools, 2023.

John Schulman, Filip Wolski, Prafulla Dhariwal, Alec Radford, and Oleg Klimov. Proximal policy optimization algorithms, 2017.

Chandan Singh, John X. Morris, Jyoti Aneja, Alexander M. Rush, and Jianfeng Gao. Explaining patterns in data with language models via interpretable autoprompting, 2023.

Jascha Sohl-Dickstein, Eric Weiss, Niru Maheswaranathan, and Surya Ganguli. Deep unsupervised learning using nonequilibrium thermodynamics. In *International Conference on Machine Learning*, pp. 2256–2265. PMLR, 2015.

Yang Song, Jascha Sohl-Dickstein, Diederik P Kingma, Abhishek Kumar, Stefano Ermon, and Ben Poole. Score-based generative modeling through stochastic differential equations. In *International Conference on Learning Representations*, 2021. URL <https://openreview.net/forum?id=PxTIGl2RRHS>.

Nisan Stiennon, Long Ouyang, Jeffrey Wu, Daniel Ziegler, Ryan Lowe, Chelsea Voss, Alec Radford, Dario Amodei, and Paul F Christiano. Learning to summarize with human feedback. In H. Larochelle, M. Ranzato, R. Hadsell, M.F. Balcan, and H. Lin (eds.), *Advances in Neural Information Processing Systems*, volume 33, pp. 3008–3021. Curran Associates, Inc., 2020. URL https://proceedings.neurips.cc/paper_files/paper/2020/file/1f89885d556929e98d3ef9b8

Mirac Suzgun, Nathan Scales, Nathanael Schärli, Sebastian Gehrmann, Yi Tay, Hyung Won Chung, Aakanksha Chowdhery, Quoc Le, Ed Chi, Denny Zhou, and Jason Wei. Challenging BIG-bench tasks and whether chain-of-thought can solve them. In *Findings of the Association for Computational Linguistics: ACL 2023*, pp. 13003–13051, Toronto, Canada, July 2023. Association for Computational Linguistics. doi: 10.18653/v1/2023.findings-acl.824. URL <https://aclanthology.org/2023.findings-acl.824>.

Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin. Attention is all you need. In I. Guyon, U. Von Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett (eds.), *Advances in Neural Information Processing Systems*, volume 30. Curran Associates, Inc., 2017. URL https://proceedings.neurips.cc/paper_files/paper/2017/file/3f5ee243547dee91fbd053c1

- Xuezhi Wang, Jason Wei, Dale Schuurmans, Quoc V Le, Ed H. Chi, Sharan Narang, Aakanksha Chowdhery, and Denny Zhou. Self-consistency improves chain of thought reasoning in language models. In *The Eleventh International Conference on Learning Representations*, 2023. URL <https://openreview.net/forum?id=1PL1NIMMrw>.
- Jason Wei, Yi Tay, Rishi Bommasani, Colin Raffel, Barret Zoph, Sebastian Borgeaud, Dani Yogatama, Maarten Bosma, Denny Zhou, Donald Metzler, Ed H. Chi, Tatsunori Hashimoto, Oriol Vinyals, Percy Liang, Jeff Dean, and William Fedus. Emergent abilities of large language models. *Transactions on Machine Learning Research*, 2022a. ISSN 2835-8856. URL <https://openreview.net/forum?id=yzkSU5zdwD>. Survey Certification.
- Jason Wei, Xuezhi Wang, Dale Schuurmans, Maarten Bosma, brian ichter, Fei Xia, Ed H. Chi, Quoc V Le, and Denny Zhou. Chain of thought prompting elicits reasoning in large language models. In Alice H. Oh, Alekh Agarwal, Danielle Belgrave, and Kyunghyun Cho (eds.), *Advances in Neural Information Processing Systems*, 2022b. URL https://openreview.net/forum?id=_VjQlMeSB_J.
- Sean Welleck, Jiacheng Liu, Ximing Lu, Hannaneh Hajishirzi, and Yejin Choi. Naturalprover: Grounded mathematical proof generation with language models. In Alice H. Oh, Alekh Agarwal, Danielle Belgrave, and Kyunghyun Cho (eds.), *Advances in Neural Information Processing Systems*, 2022. URL <https://openreview.net/forum?id=rhdfTOiXBng>.
- Zhen Yang, Ming Ding, Qingsong Lv, Zhihuan Jiang, Zehai He, Yuyi Guo, Jinfeng Bai, and Jie Tang. Gpt can solve mathematical problems without a calculator, 2023.
- Zhilin Yang, Peng Qi, Saizheng Zhang, Yoshua Bengio, William Cohen, Ruslan Salakhutdinov, and Christopher D. Manning. HotpotQA: A dataset for diverse, explainable multi-hop question answering. In *Proceedings of the 2018 Conference on Empirical Methods in Natural Language Processing*, pp. 2369–2380, Brussels, Belgium, October-November 2018. Association for Computational Linguistics. doi: 10.18653/v1/D18-1259. URL <https://aclanthology.org/D18-1259>.
- Shunyu Yao, Dian Yu, Jeffrey Zhao, Izhak Shafran, Thomas L. Griffiths, Yuan Cao, and Karthik Narasimhan. Tree of thoughts: Deliberate problem solving with large language models, 2023a.
- Shunyu Yao, Jeffrey Zhao, Dian Yu, Nan Du, Izhak Shafran, Karthik R Narasimhan, and Yuan Cao. React: Synergizing reasoning and acting in language models. In *The Eleventh International Conference on Learning Representations*, 2023b. URL https://openreview.net/forum?id=WE_vluYUL-X.
- Xiang Yue, Xingwei Qu, Ge Zhang, Yao Fu, Wenhao Huang, Huan Sun, Yu Su, and Wenhui Chen. Mammoth: Building math generalist models through hybrid instruction tuning, 2023.
- Yongchao Zhou, Andrei Ioan Muresanu, Ziwen Han, Keiran Paster, Silviu Pitis, Harris Chan, and Jimmy Ba. Large language models are human-level prompt engineers. In *The Eleventh International Conference on Learning Representations*, 2023. URL <https://openreview.net/forum?id=92gvk82DE->.
- Andy Zou, Zifan Wang, J. Zico Kolter, and Matt Fredrikson. Universal and transferable adversarial attacks on aligned language models, 2023.

A DATA AUGMENTATION AND PROCESSING

A.1 MULTI-DIGIT MULTIPLICATION

For each multi-digit multiplication task, we randomly sampled two numbers and compute their product. We collected 808k training equations and 1k validation equations after removing duplicates. We used the BIG-bench data as our test set. To generate the intermediate steps, we broke down the problem by multiplying the multiplicand by each digit of the multiplier, and we kept track of both partial products and partial sums. To make the task easier, we reversed the order of the digits such that lower digits come first. For example, for 917×412 , the intermediate steps are

$$4\ 3\ 8\ 1 + 0\ 7\ 1\ 9\ 0\ (4\ 0\ 0\ 1\ 1) + 0\ 0\ 8\ 6\ 6\ 3,$$

where we broke down 917×412 into $917 * 2 + 917 * 10 + 917 * 400 = \underbrace{1834 + 09170}_{11004} + 366800$.

Note that the partial sum 11004 is reversed and written in the parentheses as $(4\ 0\ 0\ 1\ 1)$.

A.2 GRADE SCHOOL MATH PROBLEMS

We used the training set of GSM8K (Cobbe et al., 2021) as a seed dataset and generated similar examples by prompting GPT-4. We used the below prompt template and a temperature of 1 to improve the diversity of the generated dataset:

Create 5 new math word problems following the JSON format of the given examples.

Example math word problems:

1): {"question": "Meena bakes 5 dozen cookies for the school's bake sale. She sells 2 dozen cookies to her biology teacher, Mr. Stone. Her friend Brock buys 7 cookies, and her friend Katy buys twice as many as Brock. How many cookies does Meena have left?", "answer": "Meena bakes a total of $5 \times 12 = \langle\langle 5 \times 12 = 60 \rangle\rangle 60$ cookies. Mr. Stone buys $2 \times 12 = \langle\langle 2 \times 12 = 24 \rangle\rangle 24$ cookies. Brock buys 7 cookies, so Katy buys $2 \times 7 = \langle\langle 7 \times 2 = 14 \rangle\rangle 14$ cookies. Meena sells a total of $24 + 7 + 14 = \langle\langle 24 + 7 + 14 = 45 \rangle\rangle 45$ cookies. She has $60 - 45 = \langle\langle 60 - 45 = 15 \rangle\rangle 15$ cookies left. #### 15"}

2): [...]

3): [...]

4): [...]

5): [...]

Similar examples:

6):

Each time we prompted GPT-4, we took 5 random examples uniformly sampled from the training set of GSM8K. We prompted GPT-4 80k times, resulting in 400k generated examples. We then filtered out examples with invalid JSON format, or examples whose intermediate steps didn't lead to the same final answer (for example, in the above example, the last equation is $\langle\langle 60 - 45 = 15 \rangle\rangle$, which matches the final answer 15, so it is valid). After applying this filtering, we got a dataset of 379k examples, where we left out 1k for validation. We used the test set from GSM8K as our test set.

For training explicit CoT, we used the natural language intermediate steps, which was shown in Wei et al. (2022b) to perform better than using equations. For example, for the input *Tom bought his games for \$200. They tripled in value and he then sold 40% of them. How much did he sell the games for?*, the intermediate steps are *The value of the games increased to $200 \times 3 = \$600$ So he sold $600 \times .4 = \$240$ worth of games.* For training the implicit CoT teacher, we only used the equations as intermediate steps based on our finding that more intermediate steps generally need more layers for the implicit chain-of-thought approach. For the aforementioned example, the intermediate steps for implicit CoT would be $200 \times 3 = 600$ $600 \times .4 = 240$.

Table 4: Raw results. Accuracy (Acc) measures the exact match accuracy of producing the final answer. Throughput measures the number of examples per second during inference using a batch size of 1. [†]: few-shot prompting instead of finetuning, and throughput is measured based on API calls with a large variability across runs.

Model	#Layers	4 × 4 Mult		5 × 5 Mult		GSM8K-Aug	
		Acc	Throughput	Acc	Throughput	Acc	Throughput
No CoT							
GPT-2 Small	12	28.7%	13.2	1.2%	11.1	13.3%	24.7
GPT-2 Medium	24	76.2%	7.0	1.9%	5.9	17.0%	13.2
GPT-2 Large	36	33.6%	4.8	0.9%	4.0	12.7%	9.1
ChatGPT [†]	96	2.2%	1.0	0.0%	1.4	28.1%	1.8
GPT-4 [†]	-	4.0%	0.7	0.0%	0.8	43.8%	0.9
Implicit CoT							
GPT-2 Small	12	96.6%	8.9	9.5%	7.9	20.0%	16.4
GPT-2 Medium	24	96.1%	4.8	96.4%	4.3	21.9%	8.7
Explicit CoT							
GPT-2 Small	12	100.0%	2.3	100.0%	1.5	40.7%	2.0
GPT-2 Medium	24	100.0%	1.2	100.0%	0.8	43.9%	1.1
GPT-2 Large	36	100.0%	0.8	99.3%	0.6	44.8%	0.7
ChatGPT [†]	96	42.8%	0.1	4.5%	0.1	61.5%	0.2
GPT-4 [†]	-	77.0%	0.1	44.3%	0.1	90.9%	0.1

B RAW RESULTS

The raw results of our experiments are presented in Table 4. Surprisingly, GPT-4 with no CoT performs on par with GPT-2 Large finetuned with explicit CoT, which we suspect might be either due to data contamination or due to emergent capabilities at scale (Wei et al., 2022a).

C FEW-SHOT PROMPTING BASELINES

In Table 4, we used ChatGPT and GPT-4 as baselines. For those baselines, we used few-shot prompting with five examples and a temperature of 0 (greedy decoding). Each time we randomly sampled five example demonstrations from the training set. For the arithmetic multiplication datasets, we used the original numbers instead of using the reversed digits, and removed the whitespaces between digits.

For the no CoT setting, below shows an example prompt for 4×4 multiplication:

Answer the final question following the exact format of the given examples. Do not break the problem down, directly produce the answer.
 Example problems:
 Q: 5646 * 1576
 A: ##### 08898096
 [...]
 Q: 7560 * 3228
 A: ##### 24403680
 Question to answer:
 Q: 1668 * 4380

For explicit CoT, an example prompt for 4×4 multiplication is:

Answer the final question following the exact format of the given examples. Do not output anything else.
 Example problems:

Q: 5646 * 1576 A: 1): 6 * 5646 = 33876 (partial sum 0 + 33876 = 33876) 2): 70 * 5646 = 395220 (partial sum 33876 + 395220 = 429096) 3): 500 * 5646 = 2823000 (partial sum 429096 + 2823000 = 3252096) 4): 1000 * 5646 = 5646000 (partial sum 3252096 + 5646000 = 8898096) ##### 8898096

[...]

Question to answer:

Q: 1668 * 4380

D MODEL DETAILS

D.1 MIND-READING THE TEACHER

In this step, for each layer, we add a trainable one-layer MLP on top of the teacher state before using it to substitute the corresponding student state. This MLP first uses a linear layer to project the teacher state of size H to a vector of size $4H$, and then we apply ReLU before projecting it with another linear layer back to size H .

In experiments, we search over Δ values from $\{1, 2, 3\}$, and also the dynamic Δ value $\frac{T-1}{L-1}$. We found that the dynamic Δ value performs the best for the arithmetic tasks. For GSM8K, we found $\Delta = 2$ works the best for GPT-2 Small and $\Delta = 1$ works the best for GPT-2 Medium.

D.2 THOUGHT EMULATION

We discuss the more general mixture approach first. At each layer l , we first compute the corresponding column in the intermediate steps t_l based on Δ . Denote the emulator hidden state at this layer as \mathbf{h}_l , then we parameterize the mixture distribution $P(c_l)$ using a linear projection to the size of the vocabulary (since we supervised c_l to be the same as the corresponding word z_{t_l} in the intermediate steps), and then we use a softmax to get a valid probability distribution. Then in order to parameterize $f(\mathbf{h}_l, c_l)$, we embed $c_l = z_{t_l}$ into a vector of size H (H is the same as the transformer’s hidden size), and concatenate this vector with \mathbf{h}_l , and pass through a one-layer MLP. This MLP has the same architecture as the MLP described in “Mind-Reading the Teacher” but uses a separate set of parameters.

In the original transformer architecture (Vaswani et al., 2017), the hidden state at the current layer is directly used as input to the next layer. Here we cannot follow that formulation, as then it cannot account for which mixture component is being used (since \mathbf{h}_l doesn’t contain information about c_l). Therefore, we take $f(\mathbf{h}_l, c_l)$, which contains information about c_l , and use an LSTM (Hochreiter & Schmidhuber, 1997) with self-attention to process it, and take the output to feed to the next transformer layer. The LSTM with self-attention is implemented similar to Luong et al. (2015), where we first project $f(\mathbf{h}_{1:l}, c_{1:l})$ into keys and queries, and then we use $f(\mathbf{h}_l, c_l)$ as query to attend to $f(\mathbf{h}_{1:l-1}, c_{1:l-1})$ using dot attention, and compute a weighted sum of previous keys using attention weights. We then concatenate the resulting vector (typically termed the context vector) with the output of the RNN and use a linear projection to project it back to size H as the output of the LSTM. This context vector is also added to $f(\mathbf{h}_{l+1}, c_{l+1})$ as the input to the next step of LSTM. Finally, we feed in the output of the LSTM to the next transformer layer $l + 1$.

When not using the mixture approach, we simply set c_l to 1 in the above process.

D.3 COUPLE AND OPTIMIZE

The couple and optimize step is straightforward, with the exception of using the mixture approach. Ideally we want to take the argmax of the predicted mixture component at each layer, corresponding to committing to the most likely token at each reasoning step, but argmax is not directly differentiable. To make the computation fully differentiable, inspired by Gumbel-Softmax (Jang et al., 2017; Maddison et al., 2017) we use softmax with temperature to temper the distribution over mixture components c_l :

$$P(c_l; \text{temperature}) \propto P(c_l)^{1/\text{temperature}}.$$

Table 5: Visualizing the predicted mixture components. We used GPT-2 Medium with $\Delta = 1$, such that layer l 's mixture component was supervised to be the l -th token of the intermediate steps in the Thought Emulation step. Before "Couple and Optimize", the task accuracy is 11.2% on the validation set and afterwards it rises to 21.9%. If we use the mapped mixture components to derive the final answer, before "Couple and Optimize" we get 9.4% and after it we get 0%.

Ground Truth z	Predicted Before Couple & Opt	Predicted After Couple & Opt
4*2=8 8*4=32 40-32=8	4*2=8 4*8=32 32- initiated=14	rewrite HELPonialrunnerGreek 6 inscribedidget Store diversion – Speedileen grasped victimized648 setup official delinqu "# lawful HELPatin
10*2=20 10+20=30	10*2=20 10+20=30	rewrite HELPonialrunnerGreek 6 inscribedidget Store opens – solderileen graspedAccording648 PharaohPosarry HELP untneath floors
320+430=750 400+300=700 750+430+400+700=2280	320+230=550 340+440=780 300+310=780 384+960=RPG40	rewrite HELPonialrunnerGreek Thankfully inscribedidget Store diversion – victimizedileen MO- TAccordinglectedileenPos delinqu creat Tamil Rai conceptual
4/2=2 16/2=8 8*2=16 4*16=64	16/2=8 8*2=16 16/4=4	rewrite HELPonialrunnerGreek Thankfully inscribedidget Store diversion calib solderileen grasped RakousseAcc victimized valu- ableper565 HELP/

With this tempered distribution, we compute a weighted sum \bar{c}_l over the one-hot representation of c_l , and compute $f(\mathbf{h}_l, \bar{c}_l)$, where when this function computes embeddings of \bar{c}_l , it computes a weighted sum of all embeddings in the vocabulary using $P(c_l)^{1/\text{temperature}}$ as weights. This process is fully differentiable, and when the temperature goes to zero, we recover taking the argmax of $P(c_l)$. In our experiments, we fix the temperature to a small value 0.05.

For the arithmetic tasks, we finetune both the emulator and the student after coupling. But for GSM8K, we found the coupled model tends to overfit even with the augmented dataset, and fixing the student alleviates overfitting.

E OPTIMIZATION DETAILS

We use AdamW to optimize all our models (Kingma & Ba, 2017; Loshchilov & Hutter, 2019) with a batch size of 32 and a learning rate of $5e-5$. For 4×4 multiplication, we trained the baselines for 30 epochs and the student model in implicit CoT for 15 epochs. For 5×5 multiplication, we trained both the baselines and the student model in implicit CoT for 40 epochs. For GSM8K, we trained both the baselines and the student model in implicit CoT for 15 epochs. For thought emulation, we trained for 30 epochs. For couple and optimize, we trained for 10 epochs on 4×4 and 5×5 multiplication and 20 epochs for GSM8K.

F VISUALIZING THE INTERNAL REASONING PROCESS

Since we supervised the mixture components c_l using the intermediate tokens z_{t_l} , when $\Delta = 1$ we can map back the mixture components with highest probability into words in the vocabulary and visualize the reasoning process. As shown in Table 5, right after the Thought Emulation step but before the Couple and Optimize step, the mixture components look quite similar to the intermediate steps in data (which is not surprising given that's how we trained them). However, after further optimization of the coupled system, the mixture components no longer align with human-interpretable

reasoning steps, indicating that the model’s internal reasoning process might differ from that of human’s.

G MORE RELATED WORK

Chain-of-Thought Reasoning To enable language models to handle tasks that require multi-step reasoning, researchers have advocated training these models to explicitly generate intermediate computation steps (Nye et al., 2021; Sakenis & Shieber, 2022). With the rise of large pretrained models, methods that do not require training these models have emerged. For instance, Wei et al. (2022b) introduced chain-of-thought prompting using few-shot examples with intermediate steps. Similarly, Kojima et al. (2022) guided models to “think step-by-step” in a zero-shot setting. Further research has explored alternative prompting data structures (Yao et al., 2023a; Long, 2023; Besta et al., 2023), optimal CoT prompting techniques (Wang et al., 2023; Fu et al., 2023), applying CoT to generate programs (Chen et al., 2022), use APIs (Yao et al., 2023b; Schick et al., 2023), and even in vision domains (Gupta & Kembhavi, 2023). Yet, these methods all require explicit intermediate steps, while our work directly generates the final answer.

Reinforcement Learning for NLP In our work, continuous hidden states of the model are utilized for reasoning. Since this system is entirely differentiable, gradient descent is employed for optimization. Another avenue could involve letting models form their own symbolic reasoning pathways, potentially distinct from human reasoning, and fine-tuning the system through reinforcement learning (Schulman et al., 2017; Stiennon et al., 2020; Caccia et al., 2020; Ramamurthy et al., 2023; Ouyang et al., 2022). One could design a reward system based on the accuracy of the final answer and the efficiency of the reasoning pathway, akin to auto-prompting approaches (Zhou et al., 2023; Singh et al., 2023; Deng et al., 2022; Zou et al., 2023).