# Mixture of Parrots: Mixtures of experts improve memorization more than reasoning

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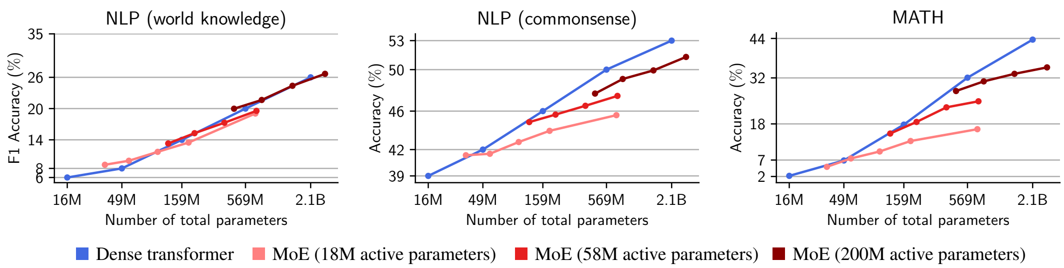
## Abstract

The Mixture-of-Experts (MoE) architecture enables a significant increase in the total number of model parameters with minimal computational overhead. However, it is not clear what performance tradeoffs, if any, exist between MoEs and standard dense transformers. In this paper, we show that as we increase the number of experts (while fixing the number of active parameters), the memorization performance consistently increases while the reasoning capabilities saturate. We begin by analyzing the theoretical limitations of MoEs at reasoning. We prove that there exist graph problems that cannot be solved by any number of experts of a certain width; however, the same task can be solved by a dense model with a slightly larger width. On the other hand, we find that on memory-intensive tasks, MoEs can effectively leverage a small number of active parameters with a large number of experts to memorize the data. To empirically validate our findings, we pre-train a series of MoEs and dense transformers and evaluate them on commonly used benchmarks in math and natural language. We find that increasing the number of experts helps solve knowledge-intensive tasks, but fails to yield the same benefits for reasoning tasks.

## 1 Introduction

The explosion in capabilities of large language models in recent years has largely been enabled by scaling their size, as measured by the number of parameters in the model. In the standard Transformer architecture, scaling the number of parameters entails a proportional increase in computational cost, e.g. doubling the number of parameters requires doubling the number of floating-point operations (FLOPs), making training and inference more computational intensive. Mixture-of-Experts (MoE) were introduced as a solution for this problem [66, 38, 21]. MoEs replace the single MLP in each Transformer block with multiple MLPs (called experts), where each token is routed to a few experts based on a linear routing function. The number of parameters in the MoE layer therefore increases with the total number of experts, while the compute increases only with the number of "active" experts (i.e., the number of experts to which the token is routed to). This offers a promising option for scaling models: increase the number of experts instead of the model dimension or its depth. For this reason, MoEs have become very popular, and many frontier models today are based on the MoE architecture [2, 17, 4, 16, 30, 79].

In this work we study whether MoE indeed offers a "free-lunch", enabling gains in performance with no computational cost. Interestingly, we find that the benefit from MoEs greatly depends on the task at hand. We show that for reasoning-based tasks, such as graph problems and mathematical reasoning, MoEs offer limited performance gains, and increasing the number of experts cannot compete with scaling the dimension (width) of the model. On the other hand, for memory-intensive tasks, we show that scaling the number of experts is competitive with scaling standard "dense" MLPs.




(a) Evaluation: world knowledge (b) Evaluation: commonsense (c) Evaluation: math

Figure 1: **(a) Evaluation: world knowledge.** We train a series of dense transformers and MoEs on 65B tokens from a corpus essentially made of Fineweb-edu, Cosmopedia and Wikipedia (see section 4 for details). We then evaluate the models on several world knowledge benchmarks (e.g., TriviaQA [33], Natural Questions [36]) and report the average F1 accuracy. Surprisingly, at a fixed number of total parameters, MoEs with substantially fewer active parameters approximately match the performance of dense models. This highlights the importance of experts in tasks that require memorization. **(b) Evaluation: commonsense.** Here we evaluate the aforementioned pre-trained models on natural language commonsense benchmarks (e.g., HellaSwag [83], WinoGrande [62]). On these reasoning tasks, we observe that MoEs perform worse than dense models and more significant benefits are obtained by increasing the number of active parameters. **(c) Evaluation: math.** Here we train a series of dense transformers and MoEs on 65B tokens from a corpus essentially made of Proof-Pile2 [7] (see section 4 for details). The results are consistent with the ones in (b): MoEs perform worse than dense models at equal number of total parameters.

To demonstrate these claims, we begin with a theoretical analysis of MoEs and dense models. We use communication-complexity lower bounds to show that a single-layer MoE requires a critical dimension to solve a simple graph connectivity problem, implying that MoEs offer no benefit for solving this problem and only consume unnecessary memory. On the other hand, we show that for a pure memorization task, where the model only needs to "remember" an arbitrary set of examples, scaling the number of experts is equivalent to scaling the number of parameters in dense transformers, implying a significant computational gain when fixing the number of active parameters (section 3).

Finally, we train dense transformers and MoEs on real datasets of mathematical reasoning and natural language, and perform intensive benchmarking of these models on a wide variety of downstream tasks. For memory-intensive tasks, MoEs surprisingly have a great advantage, where increasing the number of experts can match the performance of large dense models (Figure 1a). However, we show that for tasks that rely on reasoning, scaling the number of experts cannot compete with increasing the model dimension (Figures 1b-1c). Moreover, MoEs exhibit some memorization behaviors when trained on math problems (Figure 2). Taken together, our results show that the gains from using MoEs depend greatly on the nature of the training data and downstream task, and that while MoEs can improve performance in certain cases, sometimes increasing the effective size (width) of the model is unavoidable.

## 2 Related work

**Mixture of Experts.** Mixture-of-Experts (MoE) date back to the work of [28, 32]. [66, 21] were the first to scale this idea to deep learning and obtain state-of-the-art models in machine translation. Since then, several works have improved their routing algorithms [38, 39, 61, 13, 90, 5, 88], have improved their downstream performance after finetuning [19, 93] or made their training and inference more efficient [60, 22, 55, 72]. However, only a few papers have studied the science of MoEs and their comparison with dense transformers. [13, 35] establish scaling laws for MoEs. [11] design a specific classification problem where a model with multiple experts provably outperforms one with only one expert. [66, 38, 6, 39, 21, 19] show that given a fixed FLOP budget, MoEs are always better. However, these papers claim that on a per parameter basis, MoEs always seem comparatively worse than dense models. In this paper, we temper this claim by showing that it depends on the *nature of the task* at hand: on reasoning tasks, we validate this claim but on memory-intensive tasks, equally-sized MoEs perform as well as dense transformers.

**Language models and memorization.** Large language models (LLMs) store a considerable amount of knowledge in their parameters [59, 24]. They memorize useful knowledge such as facts and commonsense [87]. Many works studied how memorization occurs in LLMs by developing tools to locate the knowledge in the model [48, 3, 42] or by tracking the training dynamics [73, 68]. We draw inspiration from [3] and evaluate the memorization of our models by pre-training them on a mixture of datasets that includes Wikipedia, and at test time, evaluate them on world knowledge benchmarks, which are essentially question answering tasks on Wikipedia facts. With respect to theoretical findings, [34, 45, 44] provide upper bounds on the number of parameters needed for dense transformers to perform memorization tasks under various conditions.

**Language models and reasoning.** In recent years, transformer-based language models have displayed remarkable effectiveness in solving a broad range of reasoning tasks. Specifically, the reasoning capabilities of transformers have been studied in the context of arithmetic problems [29, 12, 26, 91, 47, 37], mathematical reasoning [84, 27, 76] graph problems [63, 20, 31, 75] and code challenges [67, 92]. Recently, state-of-the-art language models were used for solving complex math olympiad problems [18, 53, 54]. With respect to theoretical findings, various works study the reasoning capabilities of transformers, relating their expressive power to other complexity classes and formal languages [77, 89, 69]. Other works study how chain-of-thought can improve the reasoning capabilities of language models in terms of expressive power and learnability [1, 49, 46]. However, the reasoning capabilities of MoE language models compared to their dense counterparts have received comparatively less attention.

## 3 Theory: representational capacity

In this section, we analyze the capability of MoE transformers compared to standard (dense) models. We begin by studying a simple graph problem that requires scaling the hidden dimension of the transformer, showing that MoEs with small hidden dimension cannot solve this problem, regardless of the number of experts used. Then, we show that MoEs can effectively memorize random inputs, requiring significantly less computational resources (active parameters) compared to dense models.

Consider a one-layer transformer $f \in \text{Transformer}^N_{m,H,1}$ which takes as input a sequence of length $N$ and has logarithmic bit-precision. $f$ embeds the input into dimension $m$ via the function $\phi$. $f$ has $h \geq 1$ attention heads, whose outputs are combined via concatenation before we apply point-wise function $\psi$ [1]. $f$ is a *dense* transformer, if $\psi$ is an MLP, i.e. function of the form:

$$\psi(\boldsymbol{x}) = \boldsymbol{u}^\top \sigma(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}), \quad \text{for } \boldsymbol{W} \in \mathbb{R}^{m' \times m}, b \in \mathbb{R}^{m'}, \boldsymbol{u} \in \mathbb{R}^{m'}$$

where $\sigma$ is the ReLU activation function. $f \in \text{Transformer}^N_{m,H,1,K}$ is an MoE transformer with $K$ experts if $\psi$ is a function of the form:

$$\psi(\boldsymbol{x}) = \mathbf{u}_i^\top \sigma(\boldsymbol{W}_i \boldsymbol{x} + \boldsymbol{b}_i) \text{ for } i = \operatorname*{argmax}_j \mathbf{r}_j^\top \boldsymbol{x}$$

where $\boldsymbol{W}_1, \dots, \boldsymbol{W}_k \in \mathbb{R}^{m' \times m}$, $\boldsymbol{b}_1, \dots, \boldsymbol{b}_k \in \mathbb{R}^{m'}$, $\mathbf{u}_1, \dots, \mathbf{u}_k \in \mathbb{R}^{m'}$ are the parameters of each expert and $r_1, \dots, r_k$ define the routing function (we use top-1 routing).

Define the parameters as $Q_h, V_h, K_h \in \mathbb{R}^{m \times m}$, $\phi : \mathcal{X} \to \mathbb{R}^m$, $\psi : \mathbb{R}^m \to \mathbb{R}$. The output of $f$ is:

$$f(\boldsymbol{x}_1, \dots, \boldsymbol{x}_N) = \psi\Big(\big[\text{softmax}\big(\phi(x_N)^\top Q_h K_h^\top \phi(X)\big)\phi(X) V_h\big]_{h \in [H]}\Big).$$

### 3.1 MoEs require a critical hidden size to solve graph reasoning tasks

We begin by showing a lower-bound on the width for a depth-1 mixture of expert model for the length-2 path problem. This lower bound implies a lower bound for search and retrieval tasks such as graph connectivity, shortest path, and cycle detection.

[1] In multi-layer Transformers, each layer outputs a vector of size $m$. However, since our focus in this section will be on binary classification problems, we will let the transformer output a single scalar, and we interpret the output of the final token as the prediction for the classification task.

**Theorem 3.1** (Length-2 path lower-bound on sparse transformers)**.** *For some input sequence $G = (V, E)$, fix two disjoint subsets $A, B \subset [N-1]$, and consider a single-layer transformer $f \in \text{Transformer}^N_{m,H,1,K}$ with $O(\log N)$-bit precision that solves length-2 path for any input $X$ where $X_A$ is a function of edges with the source $s$, $X_B$ is a function of edges with the destination $d$. Then, $f$ has width satisfying $mH = \Omega(|V|/\log N)$.*

The proof follows almost identically from the proof in [63] for the class $\text{Transformer}^N_{m,H,1}$. The original proof does not place constraints on the function $\psi$ and is based on a communication-complexity argument. As such we may design $\psi$ so that it first routes and then chooses which expert to apply. We give a complete proof in Appendix A. As such, the result of [63] can also be extended to the class $\text{Transformer}^N_{m,H,1,K}$.

**Upper bound on width of depth-1 dense transformer for reasoning.** In this section we give an upper bound for the width required for a dense model to solve the length-2 path problem.

**Theorem 3.2** (Length-2 path width upper bound for transformer)**.** *There exists a transformer of width $|V|$ and $O(\log N)$-bit precision that solves length-2 path problem for any input.*

The proof relies on an encoding of the inputs where the output values only exceed a certain threshold when $u$ and $v$, the source and destination vertices, have edges with a common vertex. We defer the proof to Appendix A.

**Parameter-matched comparison of dense and sparse depth-1 transformers.** Using the lower-bound on width required for a sparse transformer (Theorem 3.1) and the upper-bound on width required for a dense transformer (Theorem 3.2), we compare dense and sparse transformers when they have the same number of total parameters. We find that when the number of experts exceeds $(\log N)^2$, the sparse model is unable to solve the same task as the dense model.

**Corollary 3.3.** *Consider a sparse transformer (with $K$ experts) and a dense transformer with the same number of parameters. There exists a number of experts $K$ so that the the sparse model is not able to solve the reasoning task, but the dense transformer solves the task.*

*Proof.* Suppose we have two depth-1 transformers, where one is a dense model and the other is a mixture of experts with $K$ experts. Let the width of the dense model be $m_d$, and the width of the sparse model be $m_s$. The number of parameters in the dense model is $O(m_d^2)$ and the number of parameters in the sparse model is $O(Km_s^2)$. In order to match the number of parameters, it must be the case that $m_s = \frac{m_d}{\sqrt{K}}$. Suppose we let $m_d = |V|$, as this is sufficient to solve the above problems. For any $K \geq \Omega\big((\log N)^2\big)$, the sparse model is not sufficiently wide to solve the problem. □

### 3.2 MoEs use their experts to solve memory-intensive tasks

In this section, we provide an upper-bound on the number of parameters necessary for a sparse transformer to solve memorization tasks, followed by a lower-bound on the number of parameters needed for a dense transformer to solve the same task. We use these results to compare the memorization capabilities of dense and sparse transformers with the same number of active parameters. We find that with enough experts, the sparse transformer is able to solve memorization tasks with less active parameters than the dense transformer. In both bounds we assume that transformer has logarithmic number of bits to encode each parameter.

We consider sequences $\{(X^i, y_i)\}_{i=1}^n$ where $X^i \in \mathbb{R}^{N \times m}$ are input sequences of length $N$ in dimension $m$ such that $X^i[j]$ is sampled from a Gaussian distribution $\mathcal{N}(0, I_m)$. We assume $y_1, \ldots, y_N \in \{\pm \mathbf{1}\}$ are arbitrary labels for the $n$ sequences. The objective is for a transformer to memorize these sequences, i.e. map each input $X^i$ to a label $y_i$. The classification is determined by the sign of the last token output.

**Upper-bound on MoE for memorization.** We begin by showing that, with high probability over the choice of the inputs, the MoE architecture can memorize (i.e., arbitrarily label the examples), with a small number of active parameters.

**Theorem 3.4.** *With probability at least $0.99$, there exists a one-layer MoE transformer with $K$ experts, using $O\left(\frac{mn}{K} + mK\right)$ active parameters and $O(mn + mK)$ total parameters that, when applied* *to each sequence $X^i$, outputs at the last token a value whose sign matches $y_i$, i.e.,* $\mathrm{sign}(f(X_i)) = y_i$ *for all* $i = 1, \ldots, n$.

Specifically, if we choose $K = \sqrt{n}$ we get that an MoE architecture can solve the memorization problem with $O(m\sqrt{n})$ active parameters. . To prove this result, we show that for a random linear routing function, the number of examples routed to each expert is approximately $n/K$. Then, we show that an expert with $O(n/K)$ neurons can memorize a sample of size $O(n/K)$. We present the full proof in Appendix A.

**Lower bound on memorization with dense Transformer.** Next, we give a lower-bound on the number of parameters for a dense transformer to perform memorization.

**Theorem 3.5** (Lower bound for dense model)**.** *Given the same task as above, a dense Transformer requires $\tilde{\Omega}(n)$ parameters to solve the memorization task.*

This bound follows from the fact that there are $2^n$ possible labels for any fixed set of $n$ inputs, and at most $2^{cW}$ functions with $W$ parameters and $c$ bit per parameters.

**Separation between MoEs and Dense Models.** Observe that the previous results on memorization imply a separation between MoEs and dense models in terms of the number of active parameters. Namely, we showed that an MoE with $O(m\sqrt{n})$ active parameters can memorize, while a dense model requires $\tilde{\Omega}(n)$ parameters. So, for large enough $n$ (i.e. when $n \gg m^2$), MoEs are significantly more efficient. Comparing the number of total parameters, MoEs require $O(mn)$ parameters (assuming $K \leq n$), so both MoE and dense models have linear dependence on $n$ in the total parameter count.

# 4 Pre-trained models

In this section, we pre-train dense transformers and MoEs and compare their performance on standard math and natural language benchmarks. We break the downstream tasks into those that require more memorization and those that require more reasoning. The memorization-intensive tasks test for "world knowledge" and consist of benchmarks like TriviaQA [33]. We break the reasoning-intensive tasks into two subcategories: one for natural language reasoning tasks like WinoGrande [62] and another for mathematical reasoning tasks like Hendrycks-MATH [25]. Descriptions of the architecture, hyperparameters, pre-training dataset, and evaluation are in Appendix B.

## 4.1 Results

**Experts improve memorization more than reasoning.** We observe that our theoretical results from section 3 hold when pre-training and evaluating language models on natural language and math. In Figure 1a, we report the accuracy of our models with respect to the number of *total* parameters. All the lines in the plot approximately coincide which implies that regardless of the number of active parameters, MoEs can effectively use their routing to leverage all of their parameters to solve memory-intensive tasks. On the other hand, on commonsense and math benchmarks (Figures 1b,1c) we find that MoEs do not reach the performance of dense models with the same number of total parameters. This indicates that for these reasoning tasks, increasing the dense model width is more effective that adding experts.

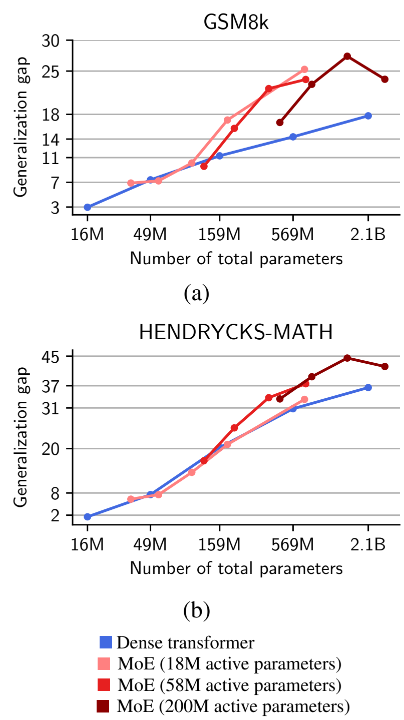



Figure 2: Generalization gap i.e., difference between the training and test accuracies, when the test set is GSM8k (a) and Hendrycks-MATH (b).

**On mathematics tasks, MoEs display a higher train-test gap than dense models, suggestive of memorization.** We provide additional evidence that memorization occurs in pre-trained MoEs by considering the generalization gap. In Figure 2 we select 6,319 random problems from the

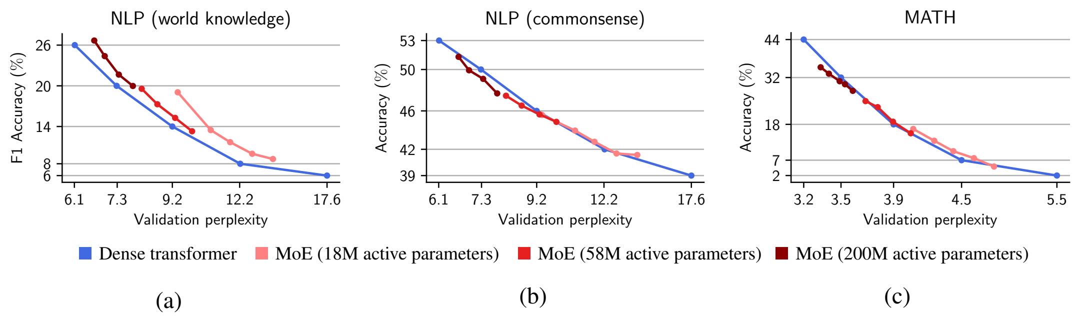



Figure 3: (a) On world knowledge benchmarks, MoEs consistently outperform dense transformers in downstream performance when fixing the validation perplexity. (b-c) In reasoning benchmarks, dense transformers perform about the same as MoEs at a fixed validation perplexity. MoEs can achieve these perplexities with less active parameters, but may require substantially more total parameters.

OpenMathInstruct dataset, which is part of the training mixture data. More precisely, we pick 5,000 Hendrycks-MATH like examples and 1,319 GSM8k-like examples to ensure that the number of training examples matches with the corresponding number of examples in GSM8k and Hendrycks-MATH test sets. We then report the *generalization gap*, which is the gap between the accuracy on training examples and test examples. Despite making a *single* pass on the OpenMathInstruct dataset, Figure 2 shows that at scales beyond 159M parameters, MoEs suffer from a more significant generalization gap than dense transformers. This is suggestive that MoEs are more liable to memorize training data than dense models.

**MoE models excel at world knowledge tasks but match dense models in reasoning when perplexity is fixed.** Finally, we focus on the relationship between validation perplexity and downstream performance in Figure 3. Rather than comparing models by their parameter count, we can compare them based on how well they fit the training distribution as measured by validation perplexity. Even though two models may have the same perplexity, they will have learned different functions. The question is then if we can see any high level patterns in which types of functions a particular model class is more likely to learn. Figure 3a shows that at a fixed perplexity, the MoE models outperform the dense models on world knowledge tasks. This suggests that MoEs do have a bias towards learning functions that memorize training data. On the other hand, Figures 3b and 3c show that MoEs and dense models perform about the same on the reasoning tasks at fixed validation perplexity. We can square this with the results from Figure 1 by noting that at equal total number of parameters an MoE has worse validation perplexity than the corresponding dense model. This suggests that while MoEs do not change the relationship between perplexity and downstream accuracy on reasoning tasks relative to dense models, they may struggle to learn the reasoning parts of the training distribution as well.

Overall, our main findings in Figure 1 and supplementary experiments in Figures 2 and 3 corroborate the hypothesis that MoEs can effectively use more experts to increase their memory capacity, but not necessarily their capability to reason.

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# A Proofs

## A.1 Reasoning proofs

**Definition A.1** (Set-disjointness task)**.** Set disjointness is the following task: given two inputs $A, B \in \{0,1\}^r$ for some $r \in \mathbb{N}$, compute $\max_i A_i B_i$.

Set-disjointness can be thought of as follows: Alice and Bob are given sets $A$ and $B$ respectively. Their objective is to determine whether they have any overlapping items in their sets.

**Lemma A.2** (Equivalence of set-disjointness and length-2 path)**.** *The set-disjointness task is equivalent to the length-2 path task.*

*Proof.* ($\implies$): Given an instance of set-disjointness, we can encode it into a length-2 path problem. Denote every item $i$ as a vertex. Denote two extra vertices as $A$, $B$, corresponding to Alice and Bob. For every element $i$ that Alice has, draw an edge between $A$ and $i$. For every element $i$ that Bob has, draw an edge between $B$ to $i$. If and only if there are any overlapping elements, then there is a length-2 path from $A$ to $B$. The number of elements because the number of vertices that do not belong to Alice or Bob.

($\impliedby$): Consider an instance $G = (V, E), s, d$ of length-2 path, where $s$ is the source vertex and $d$ is the sink vertex. For all vertices with an edge with $s$, put this element into Alice's set of elements. For all vertices with an edge with $d$, put this element into Bobs's set of elements. If and only if there is a length-2 path, then Alice and Bob's sets are overlapping. Then, $r$ is the number of vertices. □

**Lemma A.3** (Communication complexity lower-bound on concatenated outputs)**.** *For some sequence length, fix two disjoint subsets $A, B \subset [N-1]$, and consider a single-layer transformer $f \in \mathit{Transformer}^N_{m,H,1}$ with $O(\log N)$-bit precision that solves set disjointness for any input $X$ where $X_A$ is a function of Alice's input $a \in \{0,1\}^r$, $X_B$ is a function of Bob's input $b \in \{0,1\}^r$, and $X_{[N]\setminus(A\cup B)}$ is fixed regardless of $a, b$. Then, $f$ has width satisfying $mH = \Omega(r/\log N)$.*

*Proof.* By re-writing the following, the remainder of the proof from [63] still holds.

$$\mathrm{DISJ}(a,b) = \psi\Big(\big[\mathrm{softmax}\big(\phi(x_N)^\top Q_h K_h^\top \phi(X)\big)\phi(X)v_h\big]_{h\in[H]}\Big).$$

This is because we may still use the same definition for $Z_{h,S}, L_{h,S}$ as in the proof. Hence, this concludes the proof. □

### A.1.1 Proof of Theorem 3.1

We restate the corollary.

**Theorem A.4** (Theorem 3.1)**.** *For some input sequence $G = (V, E)$, fix two disjoint subsets $A, B \subset [N-1]$, and consider a single-layer transformer $f \in \mathit{Transformer}^N_{m,H,1,K}$ with $O(\log N)$-bit precision that solves length-2 path for any input $X$ where $X_A$ is a function of edges with the source $s$, $X_B$ is a function of edges with the destination $d$. Then, $f$ has width satisfying $mH = \Omega(|V|/\log N)$.*

*Proof.* The proof outline is as follows:

1. Adapt Lemma 39 [63] to support concatenation instead of addition from different attention heads.

2. The lower bound with concatenation holds for length-2 path because set-disjointness and length-2 path are equivalent.

3. Extend the result to sparse transformers.

We complete the first step with Lemma A.3. We complete the second set due to Lemma A.2. It remains to show that a router function also yields the same lower bound. We show that Lemma 39 of [63] can be generalized to the case in which $\psi$ is applied according to a routing function. Specifically, consider a top-1 routing function $r : \mathbb{R}^m \to [K]$, and $K$ element-wise functions $\psi_1, \ldots, \psi_K : \mathbb{R}^m \to \mathbb{R}$. For shorthand, define:

$$Y(X_N) = \left[\text{softmax}\left(\phi(x_N)^\top Q_h K_h^\top \phi(X)\right)\phi(X)v_h\right]_{h\in[H]},$$

which is the output of the attention head prior to applying the element-wise transformation. Next, we define $f(X_N)$ as the output when the router function $r$ is used to select $\psi_i$.

$$f(X_N) = \sum_{i\in K} \mathbf{I}\{r(Y(X_N)) = i\}\psi_i(Y(X_N)).$$

Because the lower bound does not place any restrictions on the function $\psi$ and rather argues a communication-complexity lower bound due to information from $Y(X_N)$, the lower bound also holds for a routing function. $\square$

#### A.1.2 Proof of Theorem 3.2

We re-state Theorem 3.2 and give its proof.

**Theorem A.5** (Theorem 3.2)**.** *For sequence length $N$, $f \in \text{Transformer}^N_{m,H,1}$ with $O(\log N)$-bit precision that solves length-2 path for any input $X$. Then, there exists a dense transformer with width $|V|$ which solves the problem.*

*Proof.* Tokens are elements in $\mathcal{V} = V \cup \{0\} \times V \cup \{0\}$. The input is as follows: for vertex $i$, if the source shares an edge with that vertex, then the $i$'th input value is $(s, i)$. Otherwise, it is $(s, 0)$. The first $|V|$ tokens we see correspond to edges possibly shared with the source vertex. Then, the last $|V|$ input tokens correspond to edges possibly shared with the destination vertex and share the same format as the first $r$ tokens. In between, we can have arbitrary edges $(u, v)$. We define an embedding function where $\mathbf{e}_i$ is the $i$'th standard basis vector in dimension $r$.

$$\begin{aligned} \phi &: \mathcal{V} \to \mathbb{R}^{|V|} \\ (u, v) &\mapsto \begin{cases} \mathbf{e}_i & \text{if } i > 0 \text{ and } u = s \text{ or } u = v \\ \mathbf{0} & \text{if } i = 0. \end{cases} \end{aligned}$$

Next, we define $V_h \in \mathbb{R}^{|V|\times|V|}$ to be the identity matrix, and $Q_h, V_h \in \mathbb{R}^{|V|\times|V|}$ both to have 0 everywhere. Consequently, the attention matrix is given by:

$$\left(\begin{bmatrix} 1/|V| & \ldots & 1/|V| \\ \vdots & \ddots & \\ 1/|V| & & 1/|V| \end{bmatrix} \phi(X)\right)_{j,i} = \begin{cases} 2/|V| & \text{if there is a path through } ii \\ 1/|V| & \text{if one target vertex shares an edge with } i \\ 0 & \text{otherwise.} \end{cases}$$

For any entry that exceeds $\frac{1}{|V|}$, the correct answer is there is a length-2 path. Hence, any thresholding function which achieves this separation suffices. $\square$

#### A.1.3 Proof of Corollary ??

**Corollary A.6.** *Consider a sparse transformer (with $K$ experts) and a dense transformer with the same number of parameters. There exists a number of experts $K$ so that the the sparse model is not able to solve the reasoning task, but the dense transformer solves the task.*

*Proof.* Suppose we have two depth-1 transformers, where one is a dense model and the other is a mixture of experts with $K$ experts. Let the width of the dense model be $m_d$, and the width of the sparse model be $m_s$. The number of parameters in the dense model is $O(m_d^2)$ and the number of parameters in the sparse model is $O(Km_s^2)$. In order to match the number of parameters, it must be the case that $m_s = \frac{m_d}{\sqrt{K}}$. Suppose we let $m_d = |V|$, as this is sufficient to solve the above problems. For any $K \geq \Omega\big((\log N)^2\big)$, the sparse model is not sufficiently wide to solve the problem. $\square$

### A.2 Memorization Proofs

In this section, we use $d$ to denote the input dimension, $N$ to denote the number of examples and $n$ to denote the sequence length.

**Lemma A.7.** *Let $x_1, x_2, \ldots, x_N \in \mathbb{R}^d$ be independently sampled from the multivariate normal distribution $\mathcal{N}(0, \sigma^2 I_d)$, where $\sigma > 0$ and $I_d$ is the $d \times d$ identity matrix. For any $\delta \in (0,1)$, with probability at least $1-\delta$, every pair of distinct vectors $x_i$ and $x_j$ satisfies*

$$|x_i^\top x_j| \leq \sigma^2 \sqrt{2d\left(2\ln N + \ln \frac{2}{\delta}\right)}.$$

*Proof.* We aim to bound the inner product $x_i^\top x_j$ for each pair $(i,j)$ with $i \neq j$. Since the vectors are sampled independently from $\mathcal{N}(0, \sigma^2 I_d)$, each component $x_{ik}$ and $x_{jk}$ is independently distributed as $\mathcal{N}(0, \sigma^2)$.

For fixed $i \neq j$, the inner product $S_{ij} = x_i^\top x_j = \sum_{k=1}^d x_{ik} x_{jk}$ is the sum of $d$ independent random variables. Each term $x_{ik}x_{jk}$ has:

- **Mean:**
$$\mathbb{E}[x_{ik}x_{jk}] = \mathbb{E}[x_{ik}]\mathbb{E}[x_{jk}] = 0.$$
- **Variance:**
$$\mathrm{Var}[x_{ik}x_{jk}] = \mathbb{E}[x_{ik}^2]\mathbb{E}[x_{jk}^2] = \sigma^4.$$

Since $S_{ij}$ is a sum of independent, zero-mean random variables with variance $\sigma^4$, the variance of $S_{ij}$ is:

$$\mathrm{Var}[S_{ij}] = d\sigma^4.$$

We use the fact that $S_{ij}$ is approximately normally distributed due to the Central Limit Theorem. For a normal distribution $Z \sim \mathcal{N}(0, \sigma_Z^2)$, the tail probability satisfies:

$$\mathbb{P}(|Z| \geq t) \leq 2\exp\left(-\frac{t^2}{2\sigma_Z^2}\right).$$

Applying this to $S_{ij}$, we have:

$$\mathbb{P}\left(|x_i^\top x_j| \geq t\right) \leq 2\exp\left(-\frac{t^2}{2d\sigma^4}\right).$$

There are $\binom{N}{2} \leq \dfrac{N^2}{2}$ pairs of distinct vectors. Applying the union bound over all pairs:

$$\mathbb{P}\left(\exists\, i \neq j : |x_i^\top x_j| \geq t\right) \leq N^2 \exp\left(-\frac{t^2}{2d\sigma^4}\right).$$

To ensure that this probability is at most $\delta$, set:

$$N^2 \exp\left(-\frac{t^2}{2d\sigma^4}\right) \leq \delta.$$

Taking the natural logarithm:

$$-\frac{t^2}{2d\sigma^4} + 2\ln N \leq \ln \delta.$$

Rewriting:

$$\frac{t^2}{2d\sigma^4} \geq 2\ln N - \ln\delta.$$

Noting that $-\ln\delta = \ln\frac{1}{\delta}$, we have:

$$\frac{t^2}{2d\sigma^4} \geq 2\ln N + \ln\frac{1}{\delta}.$$

Including the factor from the inequality, adjust as:

$$\frac{t^2}{2d\sigma^4} \geq 2\ln N + \ln\frac{2}{\delta}.$$

Thus,

$$t \geq \sigma^2\sqrt{2d\left(2\ln N + \ln\frac{2}{\delta}\right)}.$$

Therefore, with probability at least $1-\delta$, every pair of distinct vectors satisfies:

$$|x_i^\top x_j| \leq \sigma^2\sqrt{2d\left(2\ln N + \ln\frac{2}{\delta}\right)}.$$

□

**Lemma A.8.** *Let $x_1, x_2, \ldots, x_N \in \mathbb{R}^d$ be independently sampled from the multivariate normal distribution $\mathcal{N}(0, \sigma^2 I_d)$. For any $\delta \in (0,1)$, with probability at least $1-\delta$, every vector $x_i$ satisfies*

$$\|x_i\|_\infty \leq \sigma\sqrt{2\ln\left(\frac{2Nd}{\delta}\right)}.$$

*Proof.* Each component $x_{ik}$ is independently distributed as $\mathcal{N}(0,\sigma^2)$. For a Gaussian random variable $X \sim \mathcal{N}(0,\sigma^2)$, the tail probability is:

$$\mathbb{P}(|X| \geq t) \leq 2\exp\left(-\frac{t^2}{2\sigma^2}\right).$$

For a fixed vector $x_i$, the probability that its $L_\infty$ norm exceeds $t$ is:

$$\mathbb{P}\left(\|x_i\|_\infty \geq t\right) \leq 2d\exp\left(-\frac{t^2}{2\sigma^2}\right).$$

Applying the union bound over all $N$ vectors:

$$\mathbb{P}\left(\exists\, i : \|x_i\|_\infty \geq t\right) \leq 2Nd\exp\left(-\frac{t^2}{2\sigma^2}\right).$$

To ensure this probability is at most $\delta$, set:

$$2Nd\exp\left(-\frac{t^2}{2\sigma^2}\right) \leq \delta.$$

Taking logarithms:

$$-\frac{t^2}{2\sigma^2} + \ln(2Nd) \leq \ln\delta.$$

Rewriting:

$$\frac{t^2}{2\sigma^2} \geq \ln\frac{2Nd}{\delta}.$$

Solving for $t$:

$$t \geq \sigma\sqrt{2\ln\left(\frac{2Nd}{\delta}\right)}.$$

Therefore, with probability at least $1-\delta$, every vector $x_i$ satisfies:

$$\|x_i\|_\infty \leq \sigma\sqrt{2\ln\left(\frac{2Nd}{\delta}\right)}.$$

□

**Lemma A.9.** *Let $x_1, x_2, \ldots, x_N \in \mathbb{R}^d$ be independently sampled from the multivariate normal distribution $\mathcal{N}(0, \sigma^2 I_d)$. For any $\delta \in (0,1)$, with probability at least $1-\delta$, every vector $x_i$ satisfies*

$$\|x_i\|_2 \geq \sigma\sqrt{d}\left(1 - \sqrt{\frac{2\ln\left(\frac{N}{\delta}\right)}{d}}\right).$$

*Proof.* Each vector $x_i$ has components that are independent $\mathcal{N}(0,\sigma^2)$ random variables. Thus, $\|x_i\|_2^2 = \sum_{k=1}^d x_{ik}^2$ is distributed as $\sigma^2\chi_d^2$, where $\chi_d^2$ denotes the chi-squared distribution with $d$ degrees of freedom.

Using concentration inequalities for chi-squared distributions, for any $\varepsilon \in (0,1)$:

$$\mathbb{P}\left(\|x_i\|_2^2 \leq \sigma^2 d(1-\varepsilon)\right) \leq \exp\left(-\frac{d\varepsilon^2}{4}\right).$$

Applying the union bound over all $N$ vectors:

$$\mathbb{P}\left(\exists\, i : \|x_i\|_2^2 \leq \sigma^2 d(1-\varepsilon)\right) \leq N\exp\left(-\frac{d\varepsilon^2}{4}\right).$$

To ensure this probability is at most $\delta$, set:

$$N\exp\left(-\frac{d\varepsilon^2}{4}\right) \leq \delta.$$

Taking logarithms:

$$-\frac{d\varepsilon^2}{4} + \ln N \leq \ln\delta.$$

Rewriting:

$$\frac{d\varepsilon^2}{4} \geq \ln\frac{N}{\delta}.$$

Solving for $\varepsilon$:

$$\varepsilon \geq 2\sqrt{\frac{\ln\left(\frac{N}{\delta}\right)}{d}}.$$

Since $\varepsilon \in (0,1)$, we can use the inequality $\sqrt{1-\varepsilon} \geq 1-\frac{\varepsilon}{2}$ for $\varepsilon \in (0,1)$. Therefore, with probability at least $1-\delta$, every vector $x_i$ satisfies:

$$\begin{aligned}\|x_i\|_2 &\geq \sigma\sqrt{d(1-\varepsilon)} \\ &\geq \sigma\sqrt{d}\left(1-\frac{\varepsilon}{2}\right) \\ &\geq \sigma\sqrt{d}\left(1-\sqrt{\frac{2\ln\left(\frac{N}{\delta}\right)}{d}}\right).\end{aligned}$$

$\square$

**Theorem A.10.** *Let $x_1, x_2, \ldots, x_N \in \mathbb{R}^d$ be independently sampled from the multivariate normal distribution $\mathcal{N}(0, \sigma^2 I_d)$, and let $y_1, y_2, \ldots, y_N \in \{\pm 1\}$ be arbitrary labels. Then, with probability at least $1-\delta$, there exists a one-hidden-layer ReLU neural network with $N$ neurons that correctly classifies the points $x_i$ according to their labels $y_i$, i.e.,*

$$\operatorname{sign}(f(x_i)) = y_i \quad \textit{for all } i = 1, \ldots, N,$$

*where $f$ is the function computed by the network. Furthermore, the $L_\infty$-norms of the weights and biases are bounded as follows:*

- *Input weights:* $\|w_i\|_\infty \leq \sigma\sqrt{2\ln\left(\frac{2Nd}{\delta}\right)}$.
- *Biases:* $|b_i| \leq \sigma^2 d\left(1+\sqrt{\frac{2\ln\left(\frac{N}{\delta}\right)}{d}}\right)$.
- *Output weights:* $|\alpha_i| = 1$.

*Proof.* We will construct a one-hidden-layer ReLU network that correctly classifies the points $x_i$ with the specified labels $y_i$. The network has the following structure:

- **Hidden layer:** Consists of $N$ neurons with weights $w_i \in \mathbb{R}^d$ and biases $b_i$.
- **Output layer:** Computes the function $f(x) = \sum_{i=1}^N \alpha_i \operatorname{ReLU}(w_i^\top x + b_i)$, where $\alpha_i = y_i$.

**Step 1: High-Probability Bounds**

From Lemmas A.7, A.8, and A.9, with probability at least $1-\delta$, the following hold simultaneously for all $i \neq j$:

1. **Bound on** $\|x_i\|_\infty$ (Lemma A.8):

$$\|x_i\|_\infty \leq \sigma\sqrt{2\ln\left(\frac{2Nd}{\delta}\right)}.$$

2. **Lower bound on** $\|x_i\|_2$ (Lemma A.9):

$$\|x_i\|_2 \geq \sigma\sqrt{d}\left(1-\sqrt{\frac{2\ln\left(\frac{N}{\delta}\right)}{d}}\right).$$

3. **Bound on** $|x_i^\top x_j|$ (Lemma A.7):

$$|x_i^\top x_j| \leq \sigma^2 \sqrt{2d\left(2\ln N + \ln\frac{2}{\delta}\right)}.$$

**Step 2: Constructing the Network**

We define the weights and biases as follows:

- **Input weights:** $w_i = x_i$.
- **Biases:** $b_i = -x_i^\top x_i + s$, where $s = \dfrac{\sigma^2 d}{2}$.
- **Output weights:** $\alpha_i = y_i$.

**Step 3: Network Output on Training Points**

For each training point $x_j$, the pre-activation of the $i$-th hidden neuron is:

$$z_{ij} = w_i^\top x_j + b_i = x_i^\top x_j - x_i^\top x_i + s.$$

We consider two cases:

**Case 1:** $i = j$

$$z_{jj} = x_j^\top x_j - x_j^\top x_j + s = s > 0.$$

Therefore,

$$\mathrm{ReLU}(z_{jj}) = s.$$

**Case 2:** $i \neq j$

Using the bounds from Step 1:

$$\begin{aligned} z_{ij} &= x_i^\top x_j - x_i^\top x_i + s \\ &\leq |x_i^\top x_j| - \|x_i\|_2^2 + s \\ &\leq \sigma^2 \sqrt{2d\left(2\ln N + \ln\frac{2}{\delta}\right)} - \sigma^2 d \left(1 - \sqrt{\frac{2\ln\left(\frac{N}{\delta}\right)}{d}}\right)^2 + s. \end{aligned}$$

Simplify the expression (assuming $d$ is large enough that terms involving $\dfrac{\ln N}{d}$ are small):

Let $\varepsilon = \sqrt{\dfrac{2\ln\left(\frac{N}{\delta}\right)}{d}}$, and $\gamma = \sqrt{\dfrac{2\left(2\ln N + \ln\frac{2}{\delta}\right)}{d}}$.

Then:

$$z_{ij} \leq \sigma^2 d\left(\gamma - (1-\varepsilon)^2\right) + s.$$

Note that:

$$(1-\varepsilon)^2 = 1 - 2\varepsilon + \varepsilon^2.$$

Therefore,

$$z_{ij} \leq \sigma^2 d\left(\gamma - 1 + 2\varepsilon - \varepsilon^2\right) + s.$$

Assuming $\varepsilon$ and $\varepsilon^2$ are small, and $\gamma$ is small compared to 1 (since $d$ is large), we have:

$$z_{ij} \leq -c\sigma^2 d,$$

for some positive constant $c > 0$. Therefore,

$$\mathrm{ReLU}(z_{ij}) = 0.$$

**Step 4: Final Output**

The network output for $x_j$ is:

$$f(x_j) = \sum_{i=1}^{N} \alpha_i \,\mathrm{ReLU}(z_{ij}) = y_j s + \sum_{i \neq j} y_i \cdot 0 = y_j s.$$

Since $s > 0$, the sign of $f(x_j)$ matches $y_j$:

$$\mathrm{sign}(f(x_j)) = \mathrm{sign}(y_j s) = y_j.$$

**Step 5: Bounding the Weights and Biases**

- **Input Weights:** From Lemma A.8:

$$\|w_i\|_\infty = \|x_i\|_\infty \leq \sigma \sqrt{2 \ln\left(\frac{2Nd}{\delta}\right)}.$$

- **Biases:** Using the bound on $\|x_i\|_2$ from Lemma A.9:

$$\begin{aligned}
|b_i| &= \left|-x_i^\top x_i + s\right| \\
&\leq \|x_i\|_2^2 + s \\
&\leq \left(\sigma\sqrt{d}\,(1-\varepsilon)\right)^2 + \frac{\sigma^2 d}{2} \\
&= \sigma^2 d \left((1-\varepsilon)^2 + \frac{1}{2}\right) \\
&= \sigma^2 d \left(1 - 2\varepsilon + \varepsilon^2 + \frac{1}{2}\right) \\
&\leq \sigma^2 d \left(\frac{3}{2} - 2\varepsilon\right).
\end{aligned}$$

- **Output Weights:** $|\alpha_i| = |y_i| = 1$.

$\square$

**Theorem A.11.** *Let $X_1, X_2, \ldots, X_N \in \mathbb{R}^{n \times d}$ be $N$ sequences of length $n$, where each token $X_{ik} \in \mathbb{R}^d$ is independently sampled from the multivariate normal distribution $\mathcal{N}(0, I_d)$. Let $y_1, y_2, \ldots, y_N \in \{\pm 1\}$ be arbitrary labels. Then, with probability at least $1 - \delta$, there exists a one-layer transformer with inner dimension $N$ should probably use a different variable that, when applied to each sequence $X_i$, outputs at the last token a value whose sign matches $y_i$, i.e.,*

$$\mathrm{sign}(f(X_i)) = y_i \quad \text{for all } i = 1, \ldots, N,$$

*where $f$ is the function computed by the transformer. Furthermore, the $L_\infty$-norms of the weights and biases of the transformer are explicitly bounded as follows:*

- *The $L_\infty$-norm of all weights in the attention mechanism is at most 1.*
- *The $L_\infty$-norm of the feed-forward weights is at most*

$$\|W_{\mathit{ff}}\|_\infty \leq \frac{1}{\sqrt{n}} \sqrt{2 \ln\left(\frac{2Nd}{\delta}\right)}.$$

- *The $L_\infty$-norm of the feed-forward biases is at most*

$$\|b_{\mathit{ff}}\|_\infty \le \frac{d}{n}\left(1+\sqrt{\frac{2\ln\left(\frac{N}{\delta}\right)}{d}}\right).$$

- *The output weights satisfy $|\alpha_i| = 1$ for all $i$.*

*Proof.* We will construct a one-layer transformer with inner dimension $N$ that correctly classifies the sequences $X_i$ according to their labels $y_i$. The transformer consists of:

- **Self-Attention Layer:** Configured to compute the average of the input tokens at the last position.
- **Feed-Forward Network:** Applied at the last token to classify the averaged input.

**Step 1: Configure Self-Attention to Compute Token Averages**

Our goal is to compute the average of the input tokens $X_{i1}, X_{i2}, \ldots, X_{in}$ at the last token position. To achieve uniform attention, we set the query and key matrices to zero:

- $W^Q = 0 \in \mathbb{R}^{d\times d_k}$
- $W^K = 0 \in \mathbb{R}^{d\times d_k}$

Since $Q_t = W^Q X_{it} = 0$ and $K_{t'} = W^K X_{it'} = 0$ for all tokens $t, t'$, the attention scores become:

$$\text{AttentionScore}_{t,t'} = \frac{Q_t^\top K_{t'}}{\sqrt{d_k}} = 0.$$

The softmax of a vector of zeros yields uniform attention weights:

$$\alpha_{t,t'} = \frac{1}{n}.$$

We set the value matrix $W^V = I_d$ (the identity matrix), so the output of the attention layer at the last token $t = n$ is:

$$h_n = \sum_{t'=1}^{n} \alpha_{n,t'} V_{t'} = \frac{1}{n}\sum_{t'=1}^{n} X_{it'} = S_i,$$

where $S_i \in \mathbb{R}^d$ is the average of the input tokens for sequence $X_i$:

$$S_i = \frac{1}{n}\sum_{k=1}^{n} X_{ik}.$$

**Step 2: Distribution of $S_i$**

Since each $X_{ik}$ is independently sampled from $\mathcal{N}(0, I_d)$, the average $S_i$ is distributed as:

$$S_i \sim \mathcal{N}\left(0, \frac{1}{n} I_d\right).$$

**Step 3: Apply the Feed-Forward Network Theorem**

We now apply the previous theorem (Theorem A.10) to the vectors $S_i$. Specifically, since $S_i$ are independently sampled from $\mathcal{N}\left(0, \frac{1}{n} I_d\right)$, we set $\sigma = \frac{1}{\sqrt{n}}$ in Theorem A.10. The theorem guarantees that, with probability at least $1-\delta$, there exists a one-hidden-layer ReLU neural network with $N$ neurons that correctly classifies the vectors $S_i$ according to their labels $y_i$, i.e.,

$$\operatorname{sign}(f(S_i)) = y_i \quad \text{for all } i = 1, \ldots, N,$$

where

$$f(S) = \sum_{i=1}^{N} \alpha_i \operatorname{ReLU}(w_i^\top S + b_i),$$

with $\alpha_i = y_i$.

**Step 4: Bounding the Weights and Biases**

From Theorem A.10, with $\sigma = \dfrac{1}{\sqrt{n}}$, the $L_\infty$-norms of the weights and biases are bounded as follows:

- **Input Weights:**
$$\|w_i\|_\infty \leq \frac{1}{\sqrt{n}} \sqrt{2 \ln \left( \frac{2Nd}{\delta} \right)}.$$

- **Biases:**
$$|b_i| \leq \frac{1}{n} d \left( 1 + \sqrt{\frac{2 \ln \left( \frac{N}{\delta} \right)}{d}} \right).$$

- **Output Weights:** $|\alpha_i| = |y_i| = 1$.

**Step 5: Mapping to Transformer Architecture**

We design the feed-forward network at the last token to simulate the ReLU network operating on $S_i$:

- **Feed-Forward Network at Last Token:** Consists of weights $W_{\text{ff}} \in \mathbb{R}^{d \times N}$ and biases $b_{\text{ff}} \in \mathbb{R}^N$, where the $i$-th column of $W_{\text{ff}}$ is $w_i$, and the $i$-th element of $b_{\text{ff}}$ is $b_i$.
- **Output Layer:** Computes $f(X_i) = \alpha^\top \operatorname{ReLU}(W_{\text{ff}}^\top S_i + b_{\text{ff}})$, where $\alpha_i = y_i$.

**Step 6: Bounding the Transformer Weights**

The $L_\infty$-norms of the transformer weights and biases are explicitly bounded:

- **Attention Weights:** Since $W^Q = 0$ and $W^K = 0$, their $L_\infty$-norms are zero. The value matrix $W^V = I_d$ has $L_\infty$-norm equal to 1.
- **Feed-Forward Weights:**
$$\|W_{\text{ff}}\|_\infty = \max_{i,k} |w_{ik}| \leq \frac{1}{\sqrt{n}} \sqrt{2 \ln \left( \frac{2Nd}{\delta} \right)}.$$

- **Feed-Forward Biases:**
$$\|b_{\text{ff}}\|_\infty = \max_i |b_i| \leq \frac{d}{n} \left( 1 + \sqrt{\frac{2 \ln \left( \frac{N}{\delta} \right)}{d}} \right).$$

- **Output Weights:** $|\alpha_i| = 1$.

**Step 7: Network Output on Sequences**

For each sequence $X_i$, the transformer computes:

1. **Attention Layer:** Outputs $S_i$ at the last token.

2. **Feed-Forward Network:** Computes

$$h_i = \mathrm{ReLU}(W_{\text{ff}}^\top S_i + b_{\text{ff}}) \in \mathbb{R}^N.$$

3. **Final Output:**

$$f(X_i) = \alpha^\top h_i = \sum_{j=1}^{N} y_j \,\mathrm{ReLU}(w_j^\top S_i + b_j).$$

Since the feed-forward network at the last token simulates the ReLU network from Step 3, we have:

$$\mathrm{sign}(f(X_i)) = \mathrm{sign}(f(S_i)) = y_i.$$

**Conclusion**

With the constructed transformer, all sequences $X_i$ are correctly classified according to their labels $y_i$, and the $L_\infty$-norms of the weights and biases are explicitly bounded as specified.

$\square$

**Theorem A.12.** *Let $X_1, X_2, \ldots, X_N \in \mathbb{R}^{n\times d}$ be $N$ sequences of length $n$, where each token $X_{ik} \in \mathbb{R}^d$ is independently sampled from the multivariate normal distribution $\mathcal{N}(0, I_d)$. Let $y_1, y_2, \ldots, y_N \in \{\pm 1\}$ be arbitrary labels. Then, with probability at least $1-\delta$, there exists a one-layer Mixture-of-Experts (MoE) transformer with $K$ experts, each having $O\left(\frac{N}{K}\right)$ neurons, that, when applied to each sequence $X_i$, outputs at the last token a value whose sign matches $y_i$, i.e.,*

$$\mathrm{sign}(f(X_i)) = y_i \quad \textit{for all } i = 1, \ldots, N.$$

*Furthermore, the $L_\infty$-norms of the weights and biases of the transformer are explicitly bounded, and the bit-complexity (number of bits per parameter) is*

$$O\left(\log(nd) + \log\ln\left(\frac{NK}{\delta}\right)\right).$$

*Proof.* We construct a one-layer MoE transformer with $K$ experts to classify the sequences $X_i$ according to their labels $y_i$. The transformer operates as follows:

1. **Self-Attention Layer:** Configured to compute the average of the input tokens at the last position.
2. **Routing Function:** Assigns each sequence to one of the $K$ experts based on a routing decision.
3. **Expert Networks:** Each expert processes its assigned sequences using a feed-forward network.

**Step 1: Configure Self-Attention to Compute Token Averages**

As in the previous theorem, we set the query and key matrices to zero to achieve uniform attention weights:

- $W^Q = 0 \in \mathbb{R}^{d\times d_k}$
- $W^K = 0 \in \mathbb{R}^{d\times d_k}$

The output at the last token $t = n$ is the average of the input tokens:

$$h_n = \frac{1}{n}\sum_{k=1}^{n} X_{ik} = S_i,$$

where $S_i \sim \mathcal{N}\left(0, \frac{1}{n} I_d\right)$.

**Step 2: Define Routing Vectors and Assign Inputs to Experts**

We define routing vectors $r_1, r_2, \dots, r_K \in \mathbb{R}^d$, where each $r_j$ is independently sampled from $\mathcal{N}(0, I_d)$. For each sequence $X_i$, we compute routing scores:

$$s_{ij} = r_j^\top S_i, \quad \text{for } j = 1, \dots, K.$$

The sequence $X_i$ is assigned to expert $j^*$ where:

$$j^* = \arg \max_{1 \le j \le K} s_{ij}.$$

Since $S_i \sim \mathcal{N}\left(0, \frac{1}{n} I_d\right)$ and $r_j \sim \mathcal{N}(0, I_d)$, the routing scores $s_{ij}$ are independent and distributed as $\mathcal{N}\left(0, \frac{1}{n}\right)$.

**Step 3: Balance Inputs Among Experts**

For each input $S_i$, the probability that it is assigned to expert $j$ is:

$$\mathbb{P}(X_i \text{ assigned to expert } j) = \frac{1}{K}.$$

Let $N_j$ denote the number of inputs assigned to expert $j$. Since assignments are independent, $N_j$ follows a binomial distribution Binomial$(N, \frac{1}{K})$.

Using Hoeffding's inequality, for any $\varepsilon > 0$:

$$\mathbb{P}\left(\left|N_j - \frac{N}{K}\right| \ge \varepsilon N\right) \le 2 \exp\left(-2\varepsilon^2 N\right).$$

Set $\varepsilon = \sqrt{\frac{\ln(2K/\delta)}{2N}}$. Then,

$$\mathbb{P}\left(\left|N_j - \frac{N}{K}\right| \ge \varepsilon N\right) \le \frac{\delta}{K}.$$

Applying the union bound over all experts:

$$\mathbb{P}\left(\exists j : \left|N_j - \frac{N}{K}\right| \ge \varepsilon N\right) \le \delta.$$

Therefore, with probability at least $1 - \delta$, each expert receives at most

$$N_j \le \frac{N}{K} + \varepsilon N = \frac{N}{K} + N\sqrt{\frac{\ln(2K/\delta)}{2N}} = \frac{N}{K} + \sqrt{\frac{N \ln(2K/\delta)}{2}}.$$

Since $N$ is large, $N_j = O\left(\frac{N}{K}\right)$.

**Step 4: Apply the Feed-Forward Network Theorem to Each Expert**

Within each expert $j$, we have $N_j$ inputs $S_i$ assigned to it. We apply Theorem A.10 (from the previous result) to construct a feed-forward ReLU network that correctly classifies these inputs. Specifically:

- Inputs: The vectors $S_i$ assigned to expert $j$, each sampled from $\mathcal{N}\left(0, \frac{1}{n} I_d\right)$.
- Labels: The corresponding $y_i$ for these inputs.
- Network Size: The network uses $N_j$ neurons.

From Theorem A.10 (with $\sigma = \frac{1}{\sqrt{n}}$ and $N$ replaced by $N_j$), with probability at least $1 - \frac{\delta}{K}$, the network correctly classifies all inputs assigned to expert $j$. Applying the union bound over all experts, with probability at least $1 - \delta$, all experts correctly classify their assigned inputs.

**Step 5: Bounding the Weights and Biases**

From Theorem A.10, the $L_\infty$-norms of the weights and biases in each expert are bounded:

- **Input Weights:**

$$\|w_i\|_\infty \leq \frac{1}{\sqrt{n}}\sqrt{2\ln\left(\frac{2N_j d}{\delta/K}\right)} \leq \frac{1}{\sqrt{n}}\sqrt{2\ln\left(\frac{2NdK}{\delta}\right)}.$$

- **Biases:**

$$|b_i| \leq \frac{d}{n}\left(1+\sqrt{\frac{2\ln\left(\frac{N_j}{\delta/K}\right)}{d}}\right) \leq \frac{d}{n}\left(1+\sqrt{\frac{2\ln\left(\frac{NK}{\delta}\right)}{d}}\right).$$

- **Output Weights:** $|\alpha_i| = 1$.

**Step 6: Bounding the Bit-Complexity**

To determine the bit-complexity per parameter, we need to calculate the number of bits required to represent the weights and biases with sufficient precision.

Let $\epsilon$ be the desired precision for representing each parameter.

**Weights:**

The maximum absolute value of the weights is:

$$M_w = \frac{1}{\sqrt{n}}\sqrt{2\ln\left(\frac{2NdK}{\delta}\right)}.$$

The number of bits required per weight parameter is:

$$\begin{aligned}
\text{Bits}_w &= O\left(\log\left(\frac{M_w}{\epsilon}\right)\right) \\
&= O\left(\log\left(\frac{1}{\sqrt{n}}\sqrt{2\ln\left(\frac{2NdK}{\delta}\right)}\frac{1}{\epsilon}\right)\right) \\
&= O\left(\log\left(\frac{1}{\sqrt{n}}\right) + \frac{1}{2}\log\left(2\ln\left(\frac{2NdK}{\delta}\right)\right) + \log\left(\frac{1}{\epsilon}\right)\right) \\
&= O\left(\left(-\frac{1}{2}\log n\right) + \frac{1}{2}\log\ln\left(\frac{NK}{\delta}\right) + \frac{1}{2}\log\left(2\ln d\right) + \log\left(\frac{1}{\epsilon}\right)\right).
\end{aligned}$$

Simplifying, we have:

$$\text{Bits}_w = O\left(\log n + \log d + \log\ln\left(\frac{NK}{\delta}\right) + \log\left(\frac{1}{\epsilon}\right)\right).$$

Note that the negative term $-\frac{1}{2}\log n$ becomes negligible in the overall $O$ notation, as we are concerned with the total number of bits required.

**Biases:**

The maximum absolute value of the biases is:

$$M_b = \frac{d}{n}\left(1+\sqrt{\frac{2\ln\left(\frac{NK}{\delta}\right)}{d}}\right) \leq \frac{d}{n}\left(1+\sqrt{\frac{2\ln\left(\frac{NK}{\delta}\right)}{d}}\right).$$

Since $\sqrt{\frac{2\ln\left(\frac{NK}{\delta}\right)}{d}}$ is small for large $d$, we can approximate $M_b \approx \frac{d}{n}$. The number of bits required per bias parameter is:

$$\begin{aligned}\text{Bits}_b &= O\left(\log\left(\frac{M_b}{\epsilon}\right)\right) \\ &= O\left(\log\left(\frac{d}{n\epsilon}\right)\right) \\ &= O\left(\log d + \log n + \log\left(\frac{1}{\epsilon}\right)\right).\end{aligned}$$

**Total Bit-Complexity per Parameter:**

Combining the bits required for weights and biases, the bit-complexity per parameter is:

$$\text{Bits} = O\left(\log n + \log d + \log\ln\left(\frac{NK}{\delta}\right) + \log\left(\frac{1}{\epsilon}\right)\right).$$

Since $\epsilon$ is a constant precision (e.g., machine epsilon), we can omit $\log\left(\frac{1}{\epsilon}\right)$ in the $O$ notation. Therefore, the bit-complexity per parameter depends logarithmically on $n$ and $d$, and logarithmically on the logarithm of $N$, $K$, and $1/\delta$. This means that $n$ and $d$ are inside a single logarithm, while $N$, $K$, and $1/\delta$ are inside a double logarithm.

**Step 7: Final Transformer Architecture**

The MoE transformer consists of:

- **Attention Layer:** Computes $S_i = \frac{1}{n}\sum_{k=1}^{n} X_{ik}$ at the last token.
- **Routing Function:** Assigns $S_i$ to expert $j^* = \arg\max_j r_j^\top S_i$.
- **Experts:** Each expert $j$ has its own feed-forward network with weights and biases as constructed in Step 4.
- **Output:** For each $X_i$, the transformer outputs $f(X_i) = f_j(S_i)$ where $f_j$ is the function computed by expert $j$.

**Conclusion**

With the constructed MoE transformer, all sequences $X_i$ are correctly classified according to their labels $y_i$. The total number of neurons across all experts is:

$$\sum_{j=1}^{K} N_j = N,$$

since each input is assigned to exactly one expert. The $L_\infty$-norms of the weights and biases are explicitly bounded, and the bit-complexity per parameter is

$$O\left(\log(nd) + \log\ln\left(\frac{NK}{\delta}\right)\right).$$

This completes the proof.

□

*Proof of Theorem 3.5.* Let $c$ be the number of bits used for encoding each parameters (and we assume that $c$ is logarithmic in the problem parameters). Denote by $\mathcal{H}$ the class of all transformers with $W$ parameters and $c$ bits per parameters. Since $\mathcal{H}$ is a finite class, where each function in the class can be encoded with $cW$ bits, we have $|\mathcal{H}| \leq 2^{cW}$. Let $X^1, \dots, X^N \in \mathbb{R}^{n\times d}$ be the $N$ input points.

Assume a $\mathcal{H}$ can solve the memorization task. Then, for every choice of $y_1, \ldots, y_N \in \{\pm 1\}$, there exists a transformer $f \in \mathcal{H}$ s.t. $f(X_i) = y_i$ for all $i \in [N]$. There are $2^N$ possible assignments for $y_1, \ldots y_N$ and therefore there are at least $2^N$ different functions in $\mathcal{H}$. So, we get $2^N \leq |\mathcal{H}| \leq 2^{cW}$ and therefore $W \geq N/c$. $\square$

# B Training details

**Architecture.** We train dense transformers and MoEs using the OLMoE codebase [52]. We set the number of layers $L = 20$ and vary the width $d \in \{256, 512, 1024, 2048, 4096\}$ for dense transformers and $d \in \{256, 512, 1024\}$. Similarly to [52], we consistently set the intermediate dimension in the FFN/MoE blocks to be equal to $d$ (and not $4d$). For MoEs, we vary the number of experts $E \in \{8, 16, 32, 64\}$. For the specific case of width 256, we also train a MoE with 256 experts because its parameter count approximately matches the one of a width-2048 dense model and thus, we can compare the downstream performance of the two models. We use top-2 token-choice routing, without token dropping which is implemented in the dMoE function from the Megablocks package [22].

**Training hyperparameters.** We use the AdamW optimizer [43] with a weight decay equal to 0.1. We set the learning rate to 0.001, train on 63B tokens (60k steps) with batch size 512 and sequence length of 2048. We use warmup during the 20% first training steps and a linear decay scheduler. We train our models using FSDP [86].

**Pre-training datasets.** We train two collections of models, one series on natural language and another one on math. The "natural language" dataset is a mixture constituted of FineWeb-edu [58], Cosmopedia [8], Wikipedia and the training sets of the downstream tasks we evaluate on. The "math" dataset is a mixture made of Proof-Pile 2 [7] and instruction datasets such as OpenMathInstruct [74] and MetaMathQA [81]. A precise description of the training mixtures can be found in subsection B.1.

**Evaluation.** We measure the validation perplexity on 5,000 held-out sequences sampled from the training distribution. And we evaluate our models on a series of natural language and math benchmarks. Explicitly, we divide them into three categories:

- World-knowledge tasks: TriviaQA [33], Natural Questions [36], HotpotQA [80], WebQuestions [9], ComplexWebQuestions [70].
- Commonsense tasks: ARC-C and ARC-E [14], CommonsenseQA [71], HellaSwag [83], OpenbookQA [50], PIQA [10], SciQ [78], SIQA [64], WinoGrande [62].
- Math benchmarks: SVAMP [57], GSM8k [15], GSM-Hard [23], Hendrycks-MATH [25] and Minerva-MATH [40].

In all our experiments, we plot the average accuracy for each of these three categories.

## B.1 Details on pre-training datasets

In section 4, we pretrain two collections of models, one on "natural language" and the other on "math". Here, we give a precise breakdown of our training mixtures. We start with the "natural language" training mixture that totals 64B tokens:

- 37B tokens from Fineweb-edu dedup [58].
- 14B tokens from Cosmopedia [8].
- 12B tokens from Wikipedia (we loop over Wikipedia 3 times).
- 1B tokens from the training set of the downstream tasks we test on. We create 3 copies of each of these to increase their presence in the mixture. The presence of these datasets is pretty important as argued in [3] so that the model is familiar with the downstream tasks at test time.
  * ComplexWebQuestions training set [70]
  * HotPotQA training set [80]
  * Natural Questions training set [36]

    * TriviaQA training set [33]
    * WebQuestions training set [9]
    * ARC-Easy and ARC-Challenge training sets [14]
    * Hellaswag training set [83]
    * OpenBookQA training set [50]
    * PIQA training set [10]
    * SciQ training set [78]
    * SIQA training set [64]
    * Winogrande training set [62]

Our “math" training mixture that totals 66B tokens gathers:

- 55B tokens from Proof-Pile 2 [7] that contain AlgebraicStack (11B), OpenWebMath [56] and ArXiv (29B).
- 2B tokens from OpenMathInstruct-1: we select the instances with a correct answer from the training set [74]
- 7B tokens from DeepMind math [65]
- 2B tokens from the following instruction-like datasets:
    * Math-Orca [51]
    * TinyGSM [41] (we only select 1 million examples from there).
    * StackMathQA [85]
    * MAmmoTH2 [82] (we only select the mathstackexchange subset).
    * NuminaMath-CoT [53] (duplicated 3 times)
    * MetaMathQA [81] (duplicated 3 times)