

# Out-of-distribution generalization via composition: a lens through induction heads in Transformers

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## Abstract

Large language models (LLMs) such as GPT-4 sometimes appear to be creative, solving novel tasks often with a few demonstrations in the prompt. These tasks require the models to generalize on distributions different from those from training data—which is known as out-of-distribution (OOD) generalization. Despite the tremendous success of LLMs, how they approach OOD generalization remains an open and underexplored question. We examine OOD generalization in settings where instances are generated according to hidden rules, including in-context learning with symbolic reasoning. Models are required to infer the hidden rules behind input prompts without any fine-tuning.

We empirically examined the training dynamics of Transformers on a synthetic example and conducted extensive experiments on a variety of pretrained LLMs, focusing on a type of components known as induction heads. We found that OOD generalization and composition are tied together—models can learn rules by composing two self-attention layers, thereby achieving OOD generalization. Furthermore, a shared latent subspace in the embedding (or feature) space acts as a bridge for composition by aligning early layers and later layers, which we refer to as the *common bridge representation hypothesis*.

## 1 Introduction

Large language models (LLMs) are sometimes able to solve complex tasks that appear novel or require reasoning abilities. The appearance of creativity in task-solving has sparked recent discussions about artificial general intelligence [17, 44, 22, 13].

The classical notion of statistical generalization does not seem to account for the progress observed in LLMs. Traditionally, both training instances and test instances are drawn from the same distribution, and it is generally not expected that a model will generalize well on a different test distribution without explicit domain adaptation involving model updates.

The recent success of LLMs suggests a different story: if test data involve compositional structures, LLMs can generalize across different distributions with just a few demonstrations in the prompt (few-shot learning) or even without any demonstrations (zero-shot learning) [16] without updating the model parameters. Indeed, the apparent ability of models to infer rules from the context of a prompt—known as in-context learning (ICL)—is a hallmark of LLMs [21]. Moreover, a growing body of literature on chain-of-thought prompting explicitly exploits the compositional structures of reasoning tasks. For example, phrases like

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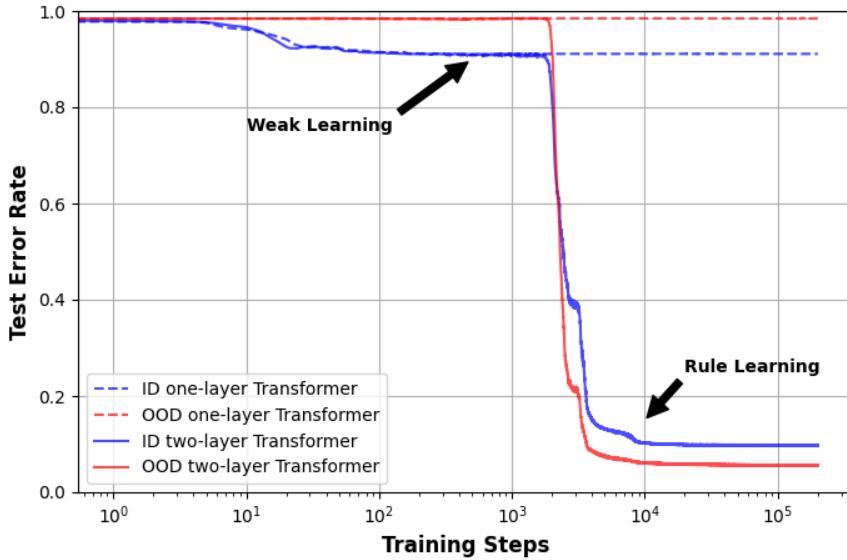


Figure 1: Training a two-layer Transformer (TF) and a one-layer TF for copying task using **fresh samples** of the format  $(*, s^\#, *, s^\#, *)$ . The models are evaluated on an in-distribution (**ID**) test dataset and an out-of-distribution (**OOD**) test dataset. **Weak learning phase:** the models rely on simple statistics of ID data and fail to generalize on OOD data; **Rule-learning phase:** two-layer TF learns the rule of copying from ID data and generalize well on ID/OOD data.

“let’s think step by step” are concatenated with input prompts to elicit reasoning [68, 41], and prompts with intermediate steps are used to improve accuracy on mathematical tasks [86].

The ability to generalize on distributions different from the training distribution—known as out-of-distribution (OOD) generalization—is well documented empirically, ranging from mathematical tasks that involve arithmetic or algebraic structures [40, 96, 1], to language reasoning problems requiring multistep inference [88, 70]. Yet, less is known about *when* a model achieves OOD generalization and *how* it solves a compositional task with OOD data.

Our empirical investigations are motivated by the pioneering work on the *induction head* [26, 58], which is a component within the Transformer architecture. Our main contributions are as follows.

1. On the synthetic task of copying sequences of arbitrary patterns, a 2-layer Transformer exhibits an abrupt emergence of subspace matching that accompanies OOD generalization between two Transformer layers, a phenomenon that echoes *emergent abilities* [86].
2. On language reasoning tasks where LLMs infer the meanings of planted symbols, including examples of in-context learning, OOD generalization requires a similar compositional structure. Extensive experiments on LLMs suggest the presence of a latent subspace for compositions in multilayer and multihead models, which we propose as the *common bridge representation hypothesis*.

## 1.1 An exemplar: copying

*Copying* is a simple yet nontrivial task that exemplifies OOD generalization. Briefly speaking, given a sequence that contains several consecutive tokens such as  $[A]$ ,  $[B]$ ,  $[C]$ , a model predicts the next token as

$[C]$  upon receiving  $[A], [B]$ :

$$\dots [A], [B], [C] \dots [A], [B] \xrightarrow{\text{next-token prediction}} \dots [A], [B], [C] \dots [A], [B], [\textcolor{blue}{C}]$$

Formally, consider a sequence of tokens  $\mathbf{s} = (s_1, \dots, s_T)$  where each  $s_t$  is in a discrete vocabulary set  $\mathcal{A}$ . Suppose that a segment of length  $L$  is repeated in this sequence:  $s_{T_0:(T_0+L-1)} = s_{(T-L+1):T}$  where  $L < (T - T_0)/2 + 1$ . Upon receiving the sequence  $\mathbf{s}_{1:(T-1)}$ , copying requires a model to output<sup>1</sup> token  $s_T$ .

Copying represents a primitive form of abstract reasoning. While humans can code the copying rule into a model, classical statistical models have difficulty learning this rule purely based on instances of such sequences. For instance, hidden Markov models and  $n$ -gram models [15] require estimating a large transition matrix or high-order conditional probability, which scales exponentially in  $L$ .

As a simple experiment, we fix  $|\mathcal{A}| = 64$  and consider a power law distribution  $\mathcal{P}$  on  $\mathcal{A}$ . We sample each sequence  $\mathbf{s}$  of length  $T_{\max} = 64$  independently by planting repeated segments in a “noisy background”:

1. Sample  $L$  uniformly from  $\{10, 11, \dots, 19\}$ , sample  $s_t^\#$  from  $\mathcal{P}$  independently for  $t = 1, \dots, L$ , and form a segment  $\mathbf{s}^\# = (s_1^\#, \dots, s_L^\#)$ ;
2. Denote  $r_L = T_{\max} - 2L$ . Sample two integers uniformly from  $\{1, 2, \dots, r_L\}$  and denote the smaller/larger ones by  $T_0, T_1$ ;
3. Form a sequence  $(*, \mathbf{s}^\#, *, \mathbf{s}^\#, *)$  where  $*$  is filled by random tokens of lengths  $T_0, T_1 - T_0, r_L - T_1$  respectively drawn from  $\mathcal{P}$  independently.

We train a 2-layer attention-only Transformer on batches of fresh samples, namely each training step uses independently drawn sequences. Model architecture and training follow the standard practice; see Section B for details. We report both in-distribution (ID) test errors and OOD test errors by computing the average token-wise prediction accuracy based on the second segment. Here the OOD error is evaluated on sequences of a similar format but  $\mathcal{P}$  is replaced by the uniform distribution  $\mathcal{P}_{\text{ood}}$ , and  $L$  is replaced by  $L_{\text{ood}} = 25$ . As a comparison, we train a 1-layer attention-only Transformer using the same data.

## 1.2 Compositional structure is integral to OOD generalization

In Figure 1, we observe that the 2-layer Transformer experiences two phases. (i) In the weak learning phase, the model learns the marginal token distribution  $\mathcal{P}$  and predicts the most probable token irrespective of the structure of the entire sequence  $\mathbf{s}$ . This results in a decrease of the ID error but not the OOD error. (ii) In the rule-learning phase, the model learns the copying rule and generalize reasonably well on both ID and OOD data. In contrast, one-layer Transformer only achieves weak learning. Note that the OOD error is smaller after training because the longer repetition segment means a larger signal strength.

Learning the copying rule requires the model to generalize on OOD instances in two aspects.

1. Generalize to a larger repetition length  $L_{\text{ood}}$  (aka length generalization).
2. Generalize to a different token distribution  $\mathcal{P}_{\text{ood}}$ .

Our analysis of training dynamics later suggests that the two layers of the Transformer play complementary roles: one layer specializes in processing positional information and another in token information. Composing the two layers yields OOD generalization.

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<sup>1</sup>Since Transformers output probabilities at test time, a predicted token  $s$  is the one that maximizes the conditional probability mass function  $p_T(s | \mathbf{s}_{1:(T-1)})$ .

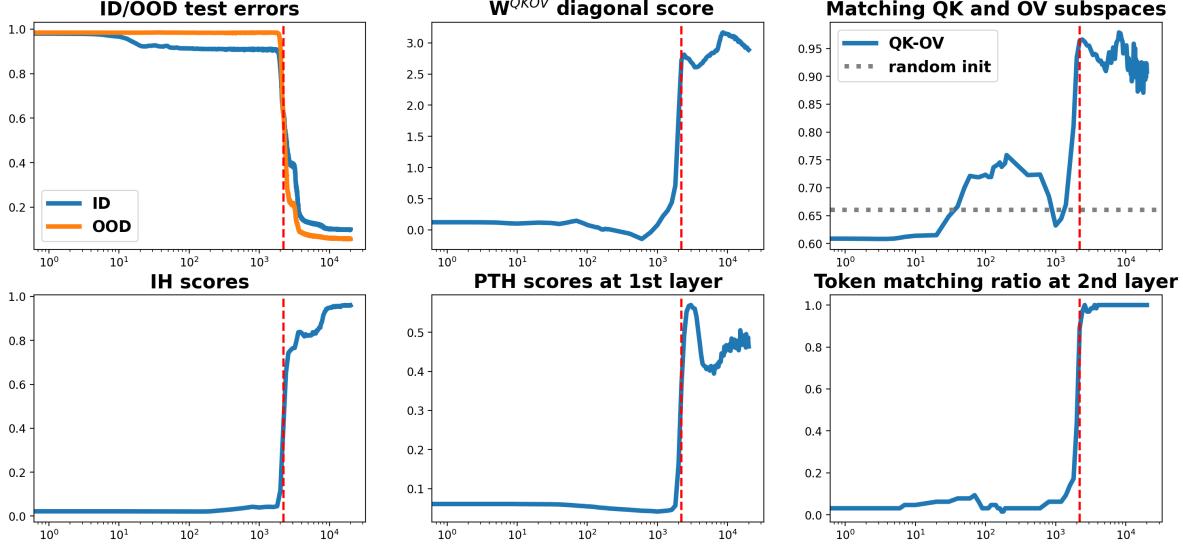


Figure 2: Measuring training dynamics for 2-layer 1-head Transformers on the copying synthetic data. **First row:** Test errors drop abruptly as structural matching occurs. Middle and right plots measure the matching between 1st-layer output circuit (OV) and 2nd-layer input circuit (QK). **Second row:** Model achieves OOD generalization by learning to compose two functionally distinct components (position matching vs. token matching). Left plot shows the formation of the IH on OOD data. Middle shows PTH scores on completely random tokens devoid of token info. Right shows token matching stripped of positional info.

## 2 Dissecting sharp transition in synthetic example

As in Section 1.1, we train a **minimally working** Transformer for the copying task as a clean synthetic example, though we find similar results on larger models. In particular, the model has 2 self-attention layers with a single head and no MLPs. The architecture and training are standard, including residual connection, LayerNorm, RoPE, dropout, autoregressive training with the AdamW optimizer, and weight decay. See Section A for a list of notations and Section B for experimental details.

**Model.** For analytical purposes, we introduce a basic form of Transformer from the circuits perspective [26]. Let  $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_T]^\top \in \mathbb{R}^{T \times d}$  be the initial embeddings or the hidden states representing a sequence of length  $T$  in  $d$  dimensions. A multihead self-attention (MSA) is a mapping  $\text{MSA}(\mathbf{X}; \mathbf{W}) : \mathbb{R}^{T \times d} \rightarrow \mathbb{R}^{T \times d}$  given by

$$\text{MSA}(\mathbf{X}; \mathbf{W}) := \underbrace{\mathbf{X}}_{\substack{\text{residual stream stores} \\ \text{info from previous layer}}} + \sum_{j=1}^H \underbrace{\text{Softmax} \left( \mathbf{X} \mathbf{W}_{\text{QK},j} \mathbf{X}^\top \right)}_{\substack{\text{attention matrix} \\ \text{QK circuit reads and} \\ \text{matches info from stream}}} \underbrace{\mathbf{X} \mathbf{W}_{\text{OV},j}^\top}_{\substack{\text{OV circuit writes and} \\ \text{adds info to stream}}} \quad (1)$$

where  $\mathbf{W}_{\text{QK},j}, \mathbf{W}_{\text{OV},j} \in \mathbb{R}^{d \times d}$  and  $\mathbf{W}$  is a collection of all such matrices. An (attention-only) Transformer is a composition of mappings  $\mathbf{X} \mapsto \text{MSA}(\mathbf{X}; \mathbf{W})$  where each layer has different trainable parameters  $\mathbf{W}$ . Section B.5 provides further details, interpretations, and comparison with practical model variants.

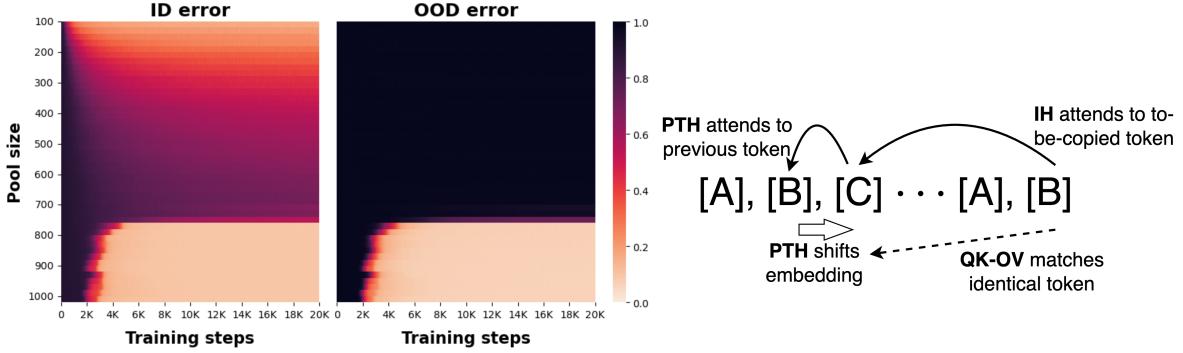


Figure 3: **Left:** Memorization vs. generalization: more varied repetition patterns help models to learn the copying rule. When the set  $\mathcal{S}$  of allowable  $s^\#$  during training has a size smaller than 740, models fail to learn the rule and generalize OOD under 20K steps, yet they can still memorize the patterns if the pool size is small. **Right:** Composition of two layers expresses the rule of copying. 1st-layer head shifts the embedding at [B] to [C]. Through the QK-OV circuits, the embedding at [C] then matches the last token [B] in the 2nd-layer attention calculation, resulting in attention to [C] and completes the copying task.

## 2.1 Progress measures

Under the circuits perspective in Eq. 1, each of the  $H$  attention head consists of a “reading” QK circuit, a “writing” OV circuit, and the softmax operation. Since  $H = 1$  in our experiment, our goal is to study how the 1st-layer attention head interact with the 2nd-layer head. To this end, we define several measurements.

1. Diagonal score. For 1st-layer  $\mathbf{W}_{\text{OV}}$  and 2nd-layer  $\mathbf{W}_{\text{QK}}$ , we calculate  $\mathbf{W}^{\text{QKOV}} = \mathbf{W}_{\text{QK}}\mathbf{W}_{\text{OV}} \in \mathbb{R}^{d \times d}$  and define  $z = z(\mathbf{W}_{\text{QK}}, \mathbf{W}_{\text{OV}})$  as

$$z = \frac{\text{Ave}\left((W_{ii}^{\text{QKOV}})_{i \leq d}\right) - \text{Ave}\left((W_{ij}^{\text{QKOV}})_{i,j \leq d}\right)}{\text{Std}\left((W_{ij}^{\text{QKOV}})_{i,j \leq d}\right)}$$

where Ave, Std mean taking average and standard deviation respectively.

This score measures the strength of diagonal entries. Roughly speaking,  $z$  is interpreted as the signal-to-noise ratio under the “ $\lambda \mathbf{I}_d + \text{noise}$ ” assumption on  $\mathbf{W}^{\text{QKOV}}$ .

2. Subspace matching score. Fix rank parameter  $r = 10$ . We calculate the top- $r$  right singular vectors  $\mathbf{U} \in \mathbb{R}^{d \times r}$  of 2nd-layer  $\mathbf{W}_{\text{QK}}$  and top- $r$  left singular vectors  $\mathbf{V} \in \mathbb{R}^{d \times r}$  of 1st-layer  $\mathbf{W}_{\text{OV}}$ . The column linear span  $\mathcal{P}_{\text{QK}} := \text{span}(\mathbf{U})$  (or similarly for  $\mathbf{V}$ ) represents the principal subspace for reading (or writing) information. We calculate a generalized cosine similarity between the two subspaces.

$$\text{sim}(\mathcal{P}_{\text{QK}}, \mathcal{P}_{\text{OV}}) := \sigma_{\max}(\mathbf{U}^\top \mathbf{V}), \quad (2)$$

where  $\sigma_{\max}$  denotes the largest singular value.

This score is equivalent to the regular cosine similarity between two optimally chosen unit vectors within the two subspaces. Results are analogous under a similar average similarity between  $\mathcal{P}_{\text{QK}}, \mathcal{P}_{\text{OV}}$ .

In Figure 2 (top row), we discovered simultaneous sharp transitions in generalization and also in the two scores. To investigate why the structural matching yields OOD generalization, we consider more measurements. An *attention matrix*  $\mathbf{A} = (A_{t,t'})_{t,t' \leq T}$  is the output of the softmax in Eq. 1. The weight  $A_{t,t'} \in [0, 1]$  represents the coefficient (aka attention) from position  $t$  to  $t'$  in a sequence and satisfies  $\sum_{t'} A_{t,t'} = 1$ .

3. PTH (previous-token head) and IH (induction-head) attention scores. Given an attention head and  $N$  input sequences, we first calculate the attention matrices  $(\mathbf{A}_i)_{i \leq N}$ . The PTH attention score measures the average attention to the previous adjacent token, and IH attention score measures the average attention to the to-be-copied token:

$$\text{score}^{\text{PTH}} = \text{Ave}_{i \leq N} \left( \frac{1}{T-1} \sum_{T \geq t \geq 2} (\mathbf{A}_i)_{t,t-1} \right), \quad (3)$$

$$\text{score}^{\text{IH}} = \text{Ave}_{i \leq N} \left( \frac{1}{|\mathcal{I}_i|} \sum_{t \in \mathcal{I}_i} (\mathbf{A}_i)_{t,t-L_i+1} \right). \quad (4)$$

where  $\mathcal{I}_i$  is the index set of repeating tokens (second segment  $s^\#$ ), and  $L_i$  is the relative distance between two segments.

To emphasize the OOD performance, we calculate IH scores by using the OOD dataset of format  $(*, s^\#, *, s^\#, *)$  described in Section 1.1. Moreover, PTH scores are based on random tokens uniformly drawn from the vocabulary as total removal of token-specific information.

4. Token matching ratio. Let  $e_j \in \mathbb{R}^d$  be the token embedding for the  $j$ -th token in the vocabulary.

$$\text{Matching ratio} = \text{Ave}_{j \in \mathcal{A}} \left[ \arg \max_{j' \leq j} (e_j^\top \mathbf{W}^{QKOV} e_{j'}) = j \right].$$

This ratio isolates pure token components  $e_j, e_{j'}$  from embeddings and examines whether functionally, an identical token maximally activates the 2nd-layer attention through the path of OV–QK circuits.

Additionally, we consider the same copying task with slightly generalized data generation: we restrict the repeating patterns  $s^\#$  to a subset  $\mathcal{S}$ . To be more specific, given length  $L$  and size  $S$ , first the subset  $\mathcal{S} \subset \mathcal{A}^L$  is determined by sampling the pattern  $S$  times independently according to Step 1 in Section 1.1; then each  $s^\#$  is drawn uniformly from  $\mathcal{S}$ . We call  $\mathcal{S}$  the *repetition pool*, and  $S = |\mathcal{S}|$  the *pool size*.

## 2.2 Results

**OOD generalization is accompanied by abrupt emergence of subspace matching.** The top row of Figure 2 shows that the sharp transition of generalization occurs at training steps around 2000. In the meantime, the weight matrices in the two layers of the model exhibit a sudden increase of alignment: a large diagonal component in  $\mathbf{W}^{QKOV}$  appears, and the two principal subspaces of  $\mathbf{W}_{\text{QK}}, \mathbf{W}_{\text{OV}}$  change from being relatively random (similar to random initialization) to highly synchronized.

The structure of  $\mathbf{W}^{QKOV}$  helps to match similar embeddings. Indeed, if we believe that  $\mathbf{W}_{\text{QK}} \mathbf{W}_{\text{OV}}$  has the “ $\lambda \mathbf{I}_d + \text{noise}$ ” structure, then the embedding  $\mathbf{x}_t$  at position  $t$  satisfies  $\mathbf{x}_t^\top \mathbf{W}_{\text{QK}} \mathbf{W}_{\text{OV}} \mathbf{y} \approx \mathbf{x}_t^\top \mathbf{y}$ . To maximize this inner product,  $\mathbf{y}$  of fixed length must be approximately aligned with  $\mathbf{x}_t$ , so embeddings similar to  $\mathbf{x}_t$  tend to receive large attentions in the 2nd layer. Further, subspace matching between QK and OV shows that aligning the embeddings depends on the low-dimensional principal subspaces.

**Two layers have complementary specialties: position shifting and token matching.** The bottom row of Figure 2 provides an explanation for OOD generalization. The 1st-layer attention head has a large PTH score after training, even for sequences of completely random tokens. The high PTH score indicates that the 1st-layer head specializes in position shifting. In fact, in the ideal case where  $A_{t,t-1} = 1$ , the map  $\mathbf{X} \mapsto \mathbf{AX}$  is simply the shifting operator. Complementarily, the 2nd-layer QK matches the OV circuit and serves as token matching. So upon accepting the shifted tokens as inputs, the 2nd-layer head attends to the next position after the repeated token. Collectively, they yield an IH head, attending correctly to the to-be-copied token; see Figure 3 (right).

**Memorization vs. generalization: pattern diversity matters.** Figure 3 shows that a smaller pool size  $S$  (decreasing from 1000 to 750) requires more training steps to achieve good generalization. Moreover, when  $S$  drops below 740, models fail to generalize well under 20K steps; instead, they may memorize the repetition patterns, yielding small ID errors especially for small  $S$ . We also find that memorizing models exhibit very different attention matrices (Section D.3), suggesting the failure of learning the copying rule.

### 3 Intervention experiments in LLMs

How is the synthetic example relevant to realistic reasoning tasks for LLMs? In this section we address this question by presenting two types of realistic scenarios: out-of-distribution (OOD) prompts (Section 3.1) and realistic compositional structures (Section 3.2). Through these examples, we aim to demonstrate two key points:

1. Prompts (natural language inputs) planted with arbitrarily chosen symbols can be inferred by LLMs in certain tasks without fine-tuning. This reasoning abilities depend crucially on IHs.
2. Subspace matching as the compositional mechanism takes a more general form in multilayer and multihead models, where a shared latent subspace matches many PTHs and IHs simultaneously.

**Pretrained LLMs.** We consider a variety of LLMs in our experiments: (1) Llama2-7B [80], (2) Llama3-8B [23], (3) Mistral-7B [38], (4) Falcon-7B [6], (5) Falcon2-11B [50], (6) OlMo-7B [30], (7) Gemma-7B [78], (8) Gemma2-8B [79]. See Appendix C.1 for details about models and implementations.

**Defining induction heads and previous-token heads.** We sample  $N = 100$  test prompts with a simple repetition pattern  $(s^\#, s^\#)$ : a block of 25 uniformly random tokens followed by a replica of the block, totaling  $T = 50$  tokens. For any layer  $\ell$  and head  $j$  of a Transformer, we denote by  $\mathbf{A}_i^{\ell,j} \in \mathbb{R}^{T \times T}$  the attention matrix defined in Eq. 1 on a test prompt  $i$ . By definition  $\sum_{t'} (\mathbf{A}_i)^{\ell,j}_{t,t'} = 1$ . This definition of IHs and PTHs only depend on the model, irrespective of downstream tasks.

For each model, we score all attention heads according to Eq. 3 and 4 based on the test prompts, yielding  $\text{score}_{\ell,j}^{\text{PTH}}$  and  $\text{score}_{\ell,j}^{\text{IH}}$ . Then we rank the PTH scores and IH scores in descending order respectively. For a pre-specified  $K$ , we define PTHs (or IHs) as the top- $K$  attention heads according to  $\text{score}_{\ell,j}^{\text{PTH}}$  (or  $\text{score}_{\ell,j}^{\text{IH}}$ ). Section E.2 provides lists of PTHs and IHs in each model.

#### 3.1 Symbolized language reasoning

In each task, we sample prompts based on a specified rule and use LLMs directly to predict next tokens. Tokens in blue are the target outputs for prediction. See appendix C.2 for a set of complete examples.

1. Fuzzy copying: [A], [B], [C] ... [A'], [B'], [C']

We consider conversion from lower-cased words to upper-cased words. For example, the correct completion of “bear snake fox poppy plate BEAR SNAKE FOX POPPY” is “PLATE”.

The IOI and ICL tasks below were proposed by [84] and [69], and recently analyzed by [87, 62, 2, 33, 73]. We extended the method in [69] to construct symbolized prompts.

2. Indirect object identification (IOI): [Subject] ... [Object] ... [Subject] ... [Object]

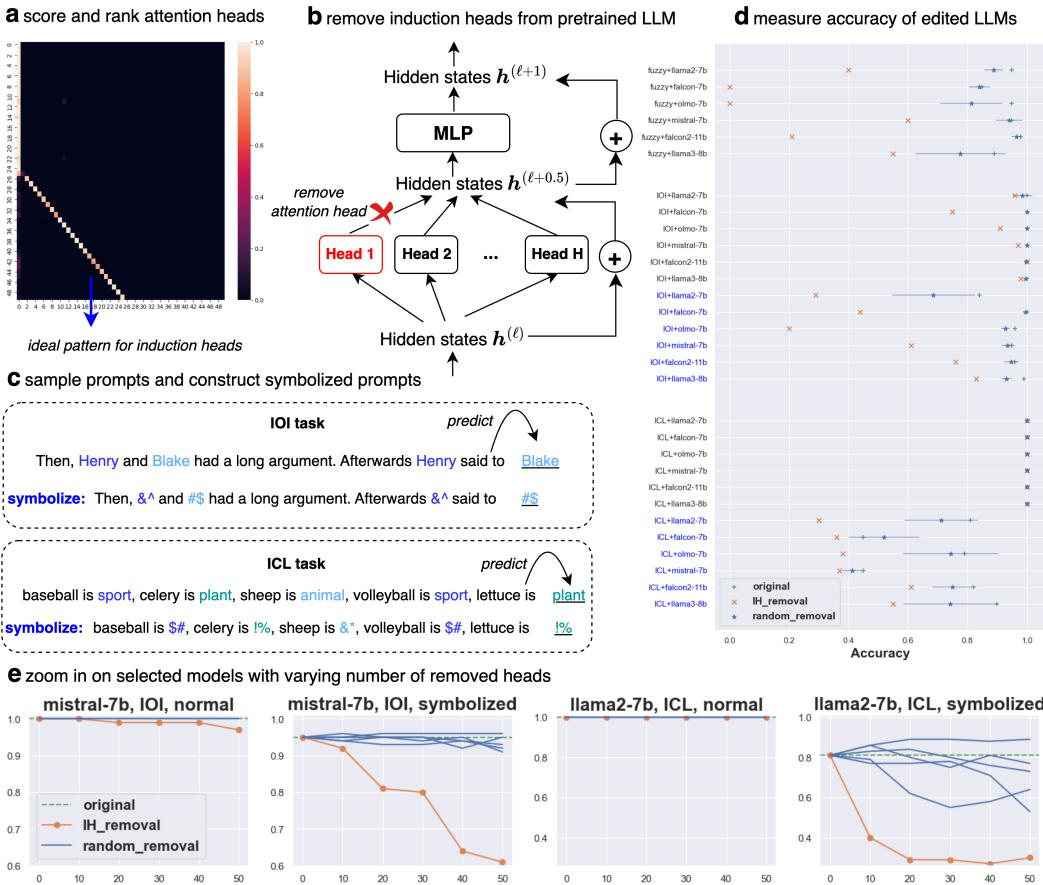


Figure 4: **LLMs depend on induction heads (IHs) for symbolized language reasoning.** (a) We rank attention heads and determine IHs as  $K = 50$  top-scoring heads. (b) We remove IHs by manually setting attention matrices to zero. (c) We sample instances according to the rule of each task and then construct OOD instances by symbolizing names/labels. (d) We measure the accuracy of various LLMs under IH removal. Symbolized tasks are indicated by blue names. We also report random baseline (deleting 50 randomly selected heads) using 5 random seeds, and report the variability using a segment showing  $\pm$  one standard deviation. (e) We show the accuracy vs. varying  $K$ , where a smaller  $K$  means deleting fewer heads.

We sample input prompts where [Subject] and [Object] are common English names; see Figure 4(c) for an example. Moreover, we consider a *symbolized* variant where the names of [Subject] and [Object] are replaced by arbitrary special symbols. We pick arbitrary symbols so that the prompt instances are unlikely seen during (thus OOD).

3. In-context learning (ICL): for  $f$  that maps an object to its category,

$$x_1, f(x_1), x_2, f(x_2) \dots x_n, \textcolor{blue}{f(x_n)}.$$

We consider mapping an object name  $x_i$  to one of the three categories  $\{\text{sport, plant, animal}\}$ . We concatenate instances that follow the format “object is category”; see Figure 4(c). Similarly, in the symbolized prompt, categories are replaced by special symbols. Again, the symbolized prompts are OOD because the three class labels are replaced by “unnatural” ones, requiring LLMs to infer their meanings at test time.

**Experiments with removal of IHs.** Given a prompt, we remove  $K = 50$  IHs from a pretrained LLM by manually setting its attention matrix  $A_i^{\ell,j}$  to a zero matrix. This effectively deletes the paths containing the targeted IHs from the architecture. As a baseline for comparison, we randomly select  $K$  pairs  $(\ell, j)$  from all possible attention heads for deletion, repeated on 5 random seeds.

We measure the prediction accuracy for IOI and ICL in the multiple-choice form, namely we pick the solution with the highest prediction probability among candidate solutions: [Subject] and [Object] for IOI, and the three categories for ICL. Accuracy by random guess is  $1/2$  and  $1/3$  respectively.

**Results: inferring from symbolized OOD prompts relies critically on IHs.** Symbolized IOI/ICL instances represent a form of language reasoning, as they require combining semantic understanding with an extra step of converting names/labels to symbols. A key finding from Figure 4(d)(e) is that while LLMs generalize reasonably well on OOD prompts, removal of IHs significantly reduces prediction accuracy compared with removal of random heads.

Interestingly, LLMs on normal IOI and ICL prompts are very robust to IH removal. One explanation for the discrepancy between ID and OOD is that LLMs rely on memorized facts for ID prompts, and use combined abilities (both memorized facts and IHs) to solve OOD prompts.

Additionally, on more sophisticated mathematical tasks, we find that chain-of-thought prompting is dependent on IHs (Section E.1).

### 3.2 Common bridge representation hypothesis

How do compositions work in LLMs beyond the synthetic example? With a microscopic analysis focusing on the copying task, we posit the following *Common Bridge Representation* (CBR) hypothesis.

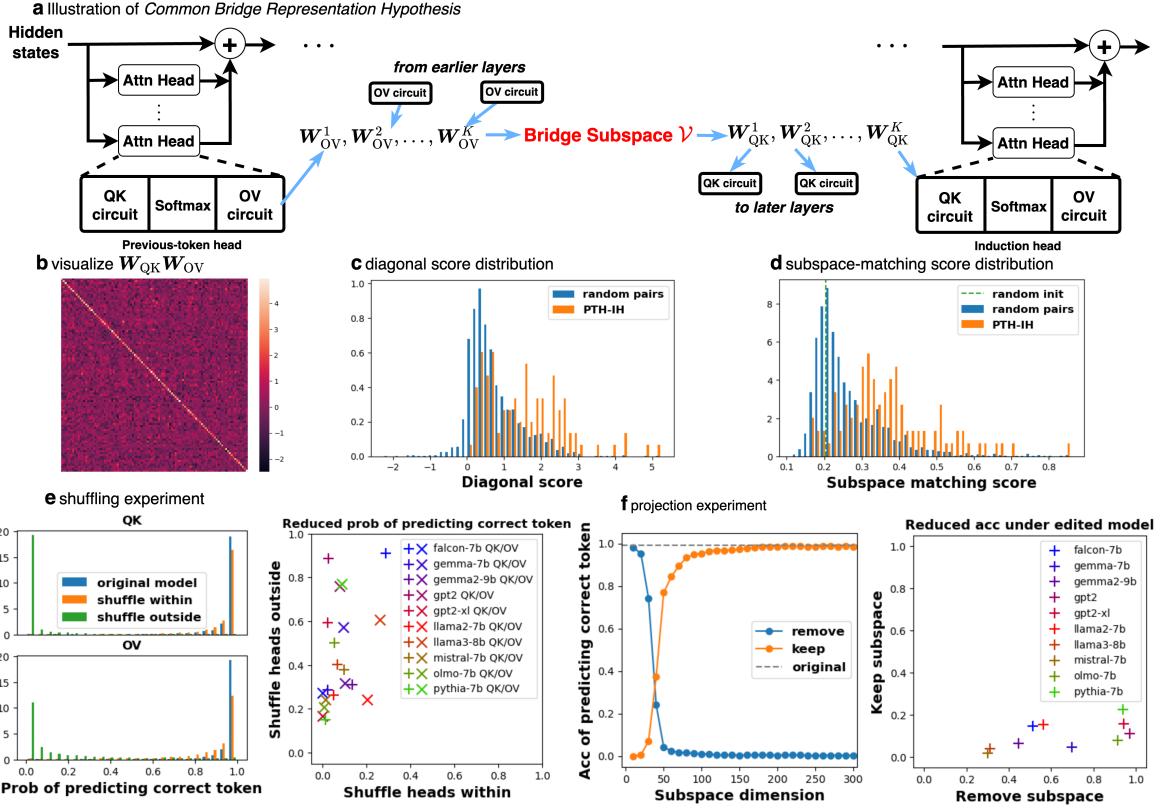
For compositional tasks, a latent subspace stores intermediate representations from the outputs of relevant attention heads and then matches later heads.

This latent subspace can be viewed as a sophisticated example of feature superposition [25] for compositional tasks.

We experiment on a variety of LLMs and highlight key findings in Figure 5(b)–(f), where we use GPT-2 as a recurring example and summarize results of other models. Top-scoring PTHs and IHs are distributed across different layers of LLMs, though more PTHs appear in early layers. We sample sequences of the format  $(s^\#, s^\#, s^\#)$  and calculate the average token-wise probability/accuracy for predicting the third segment  $s^\#$ . See experiment details in Section C.

**Experiments with two interventions.** For both experiments, we apply screening to top PTHs and IHs based on diagonal scores, resulting in an average of 9 effective PTHs and 7 effective IHs. The first intervention experiment involves shuffling heads. We randomly permute matrices  $\mathbf{W}_{QK}$  within the list of IHs, yielding an edited model (“shuffle within”). As comparison, we replace each  $\mathbf{W}_{QK}$  within the list wby a random  $\mathbf{W}_{QK}$  outside the list, yielding another edited model (“shuffle outside”). In a parallel experiment, we shuffle  $\mathbf{W}_{OV}$  circuits within PTHs similarly. We evaluate the original model and edited models by calculating the average probability of predicting correct tokens.

The second intervention experiment involves projection of weight matrices. First, we stack the QK matrices from IHs into a matrix  $[\mathbf{W}_{QK}^1, \dots, \mathbf{W}_{QK}^K]$  and extract the top right singular vectors  $\mathbf{V} \in \mathbb{R}^{d \times r}$  for a pre-specified  $r$ . We call the column linear span of  $\mathbf{V}$  as the *bridge subspace*. Then, we edit 25% of all attention heads by weight projection  $\mathbf{W}_{QK} \leftarrow \mathbf{W}_{QK} \mathbf{V} \mathbf{V}^\top$ . After the edit ('keep'), the attention calculation can only use the component of embeddings within the bridge subspace. In a parallel experiment, we make a projection edit ('remove') with an orthogonal complement  $\mathbf{W}_{QK} \leftarrow \mathbf{W}_{QK} (\mathbf{I}_d - \mathbf{V} \mathbf{V}^\top)$  to force attention



**Figure 5: Common bridge representation hypothesis as the mechanism of composition in LLMs.** (a) Linear maps from circuits in relevant attention heads are connected by an intermediate *bridge subspace*. (b) We visualize  $\mathbf{W}_{\text{QK}} \mathbf{W}_{\text{OV}}$  using highest-ranking PTH and IH. (c) Distributions of diagonal scores, comparing pairs from top-10 PTHs/IHs and pairs from random QK/OV circuits. (d) Distributions of subspace matching scores. (e) Shuffling  $\mathbf{W}_{\text{QK}}$  (or  $\mathbf{W}_{\text{OV}}$ ) among top-scoring attention heads mildly changes probabilities of correct prediction, whereas replacing these QK or OV matrices with random heads significantly reduces the probabilities. (f) Removing a low-rank ( $r = 50$  for GPT-2,  $r = \frac{1}{20}d$  for others) bridge subspace from attention calculation ('remove') heavily reduces prediction accuracy, whereas only using this subspace for attention calculation ('keep') yields mild loss of accuracy.

calculation not to use component in the bridge subspace. We evaluate the edited models by calculating the average accuracy of predicting correct tokens.

**Results: Subspace matching is a pervasive mechanism of compositions.** Fig. 5(b)(c) show that  $\mathbf{W}_{\text{QK}} \mathbf{W}_{\text{OV}}$  contains large diagonal entries when the circuits are selected from PTHs and IHs. Further, Fig. 5(d) shows that leading (left) singular spaces of  $\mathbf{W}_{\text{OV}}$  and (right) singular spaces of  $\mathbf{W}_{\text{QK}}$  are highly aligned. Among many PTHs and IHs across different layers, subspace matching is a pervasive mechanism, which extends the findings from the synthetic example to realistic models.

**Results: relevant attention heads share a common latent subspace.** We further show that the pairwise matching between circuits is not a coincidence; instead, a global latent subspace provides a “bridge” connecting relevant OV/QK circuits. The result of the shuffling experiment in Fig. 5(e) indicates that  $\mathbf{W}_{\text{QK}}$  (or  $\mathbf{W}_{\text{OV}}$ ) from IHs (or PTHs) are approximately exchangeable, since permuting  $\mathbf{W}_{\text{QK}}$  (or  $\mathbf{W}_{\text{OV}}$ ) does

not reduce prediction probabilities significantly. Moreover, Fig. 5(f) further supports that  $\mathcal{V}$  contains nearly complete information about copying, because removing/keeping this low-rank subspace from attention calculation drastically changes prediction accuracy in opposite directions.

The common bridge subspace is connected to the statistical literature on spiked matrices [39]. Roughly speaking, the principal subspaces of  $\mathbf{W}_{\text{OV}}^j, \mathbf{W}_{\text{QK}}^j$  correspond to a shared spike, which contains relevant information for the compositional task.

## 4 Related work

There are many recent papers on analyzing and interpreting Transformers [95, 12, 75, 35]; see [9] for a comprehensive survey. We highlight a few key threads of research.

**Mechanistic interpretability and induction heads.** Mechanistic interpretability (MI) aims to provide microscopic interpretability of inner workings of Transformers [57]. In particular, [26, 58] proposed IHs as crucial components of Transformers. In particular, they suggested that matching OV circuits and QK circuits is crucial for ICL. A line of research extends IHs in various aspects [84, 66, 52, 74, 27, 5, 29, 4]. Compared with the existing literature, we conducted extensive experiments on both small Transformers and a variety of LLMs, demonstrating that IHs are crucial components for many reasoning tasks. Further, we propose that subspace matching—and more broadly common bridge representation hypothesis—as the compositional mechanism.

**OOD generalization and compositions.** Historically, studies of generalization on novel domains focus on extrapolation, distribution shift, domain adaptation, etc. Since GPT-3 [16], recent studies of OOD generalization focus on arithmetic and algebraic tasks [43, 96], formal language and deductive reasoning [71, 67, 77, 83], learning boolean functions [1], etc. Our copying task is an example of length generalization [7, 99]. Compositional tasks are strongly related to reasoning abilities of LLMs, such as arithmetic tasks [24, 42], formal language [32], logical rules [14, 91], and so on. Despite recent insights [10, 24], a systematic analysis remains challenging. Our work is a first step toward understanding sophisticated compositional capabilities of LLMs.

**Linear Representation Hypothesis.** Linear Representation Hypothesis (LRH) states that monosemantic (meaning basic or atomic) concepts are represented by linear subspaces (or half-spaces) in embeddings [11, 25, 63]. This hypothesis is empirically verified in not only in LLMs but also in simpler statistical models [53, 64]. LRH treats subspaces as fundamental units for representing linguistic concepts, but it does not explain how models solve reasoning tasks or achieve OOD generalization. Our CBR hypothesis furthers this view by linking intermediate outputs in compositions to interpretable subspaces.

## 5 Limitations and future work

First, our hypothesis is a general conjecture on the mechanism of compositions in Transformers, based on our analysis of IHs. While IHs are pervasive in LLMs, other components or mechanisms for compositions may exist. Additionally, our interpretations are based on a simplified form of self-attention. It would be interesting to explore alternative mechanisms for compositions, and examine variants or practical techniques in LLMs that may impact our hypothesis.

Second, we did not develop insights to explain the emergence of the bridge subspace during training. The sharp transition in prediction accuracy is related to the *emergent abilities* of LLMs observed in broader

contexts [86]. In simpler settings, feedforward networks learning algebraic rules also exhibit phase transitions from memorization to generalization, a phenomenon known as *Grokking* [65, 56, 98, 48, 46, 51]. Analyzing the training dynamics of Transformers for copying and other compositional tasks would be an interesting avenue for further research

## Code and data availability

The code for replicating the experiments and analyses can be found in GitHub page:

<https://github.com/JiajunSong629/ood-generalization-via-composition>

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# Appendix

## Table of Contents

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<b>A Notations</b>	<b>21</b>
<b>B Experiment details for the synthetic example</b>	<b>22</b>
B.1 Two-layer Transformer model . . . . .	22
B.2 ID error and OOD error . . . . .	22
B.3 One-layer Transformer . . . . .	22
B.4 Larger Transformers . . . . .	22
B.5 Details about models . . . . .	23
B.6 Details about measurements . . . . .	24
<b>C Experiment details for experiments with LLMs</b>	<b>25</b>
C.1 Models . . . . .	25
C.2 Prompt examples . . . . .	25
C.3 Shuffle intervention experiment . . . . .	26
C.4 Projection intervention experiment . . . . .	27
C.5 Connection to spiked matrices . . . . .	27
<b>D Additional results for the synthetic example</b>	<b>28</b>
D.1 Larger models show similar sharp transitions . . . . .	28
D.2 Progress measures under varying pool sizes . . . . .	28
D.3 Attention matrices . . . . .	29
D.4 Measurements for subspace matching . . . . .	29
D.5 Rotary positional embedding . . . . .	31
<b>E Additional results for the LLMs experiments</b>	<b>32</b>
E.1 Additional results for symbolized language reasoning . . . . .	32
E.2 Details about PTHs and IHs in LLMs . . . . .	34
E.3 Histograms for PTH/IH matching . . . . .	35
E.4 Histograms for shuffling experiments . . . . .	38
E.5 Histograms for projection experiments . . . . .	38
<b>F Additional Related Work</b>	<b>41</b>

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## A Notations

- $\mathcal{A}$  is the vocabulary which is a discrete set. A token  $s$  is an element in  $\mathcal{A}$ .  $\mathcal{A}^L$  denotes the product of  $L$  copies of  $\mathcal{A}$ .
- $s = (s_1, s_2, \dots, s_T)$  denotes a sequence of tokens where  $s_t \in \mathcal{A}$  for  $t \leq T$ , and  $s_{<t} = (s_1, \dots, s_{t-1})$ .
- $p_t(s|s_{<t})$  is a conditional probability mass function given by a pretrained language model, where  $t$  is up to a maximum sequence length.
- $\mathcal{S} \subset \mathcal{A}^L$  is the set of all possible repeating pattern  $s^\# = (s_1, s_2, \dots, s_L)$ . We use  $S$  to denote the cardinality of  $\mathcal{S}$ , which we call the pool size.
- $\mathbf{A} \in \mathbb{R}^{T \times T}$  is the attention matrix. The attention weight satisfies  $A_{t,t'} \in [0, 1]$  and  $\sum_{t'} A_{t,t'} = 1$  for each  $t$ . LLMs are GPT-styled Transformers, which apply a mask to attention matrices that effectively sets  $A_{t,t'} = 0$  for  $t' > t$  (“no look into the future”).
- $\mathbf{I}_d \in \mathbb{R}^{d \times d}$  is the identity matrix.
- $\text{span}(\mathbf{V})$  is a  $r$ -dimensional subspace in  $\mathbb{R}^d$  representing the column linear span of a matrix  $\mathbf{V} \in \mathbb{R}^{d \times r}$ .
- $\sigma_{\max}(\mathbf{M})$  is the largest singular value of a matrix  $\mathbf{M}$ , and  $\sigma_j(\mathbf{M})$  is the  $j$ -th largest singular value.
- $\text{Ave}_{i \in \mathcal{I}}(a_i)$  denotes the average of a collection of numbers  $a_i$  indexed by  $i \in \mathcal{I}$ , namely  $\frac{1}{|\mathcal{I}|} \sum_{i \in \mathcal{I}} a_i$ . Similarly,  $\text{Std}_{i \in \mathcal{I}}(a_i)$  denotes the standard deviation of a collection of numbers  $a_i$ .

## B Experiment details for the synthetic example

### B.1 Two-layer Transformer model

We detail the model hyperparameters in our synthetic example. The embedding dimension (or model dimension) is 64, maximum sequence length is 64. We sample both 5000 sequences for calculating ID errors and OOD errors. The  $\theta$  parameter in RoPE is 10000. We apply layer normalization before the self-attention in each layer. We use Rotary positional embedding in each of the two layers.

Optimization related hyperparameters are listed below.

- Learning rate: 0.001
- Weight decay: 0.0005
- Batch size: 50
- Dropout: 0.1

### B.2 ID error and OOD error

We provide explanations for the ID error and the OOD error for Figure 1. At any give training step, the Transformer model gives the conditional probability  $p_t(s|s_{<t})$  and makes prediction based on the token that maximizes the probability, namely  $\hat{s}_t = \arg \max_{s \in \mathcal{A}} p_t(s|s_{<t})$  for input sequence  $s_{<t}$ .

Given the  $i$ -th ID/OOD test sequence of the format  $s_i = (*, s_i^\#, *, s_i^\#, *)$ , we are interested in how well the model predicts the second segment  $s_i^\#$ . Let the length of  $s_i^\#$  be  $L_i$  and the starting index of the second  $s_i^\#$  be  $m_i$ . Note that  $L_i \in \{10, 11, \dots, 19\}$  for ID and  $L_i = 25$  for OOD. We calculate ID/OOD errors:

$$\text{Err} = \text{Ave}_{i \leq n, m_i+5 \leq t \leq m_i+L_i} (\mathbf{1}((\hat{s}_i)_t \neq (s_i)_t)).$$

We choose  $m_i + 5$  instead of  $m_i + 1$  as the starting position for calculating errors, because the model needs a burn-in period before starting repeating patterns due to the presence of ‘noise’ tokens.

### B.3 One-layer Transformer

Figure 1 shows that one-layer Transformers do not learn the rule of copying under 20K training steps. We used the same model architecture and hyperparameters for training as detailed in Section C.1.

Here we measure the prediction probabilities of the one-layer Transformer after 20K training steps, namely  $p_t(s_t|s_{<t})$ . Recall that we used a power law distribution  $\mathcal{P}$  to generate training sequences and ID test sequences, and a uniform distribution  $\mathcal{P}_{\text{OOD}}$  to generate OOD test sequences. Figure 6 shows the probabilities  $p_t(s_t|s_{<t})$  gathered over different positions  $t$  and sequences the ID test dataset, OOD test dataset respectively. We also plot the power law distribution  $\mathcal{P}$ .

The three curves are almost identical, which suggests that one-layer Transformer only learns the marginal distribution of input sequences—which is the token distribution  $\mathcal{P}$ —for predicting the next token, and that it fails to learn the rule of copying.

### B.4 Larger Transformers

We believe that the 2-layer 1-head Transformer with no MLP is a minimal yet representative model for analyzing the sharp transition. To demonstrate this, we consider training other Transformers using the same dataset:

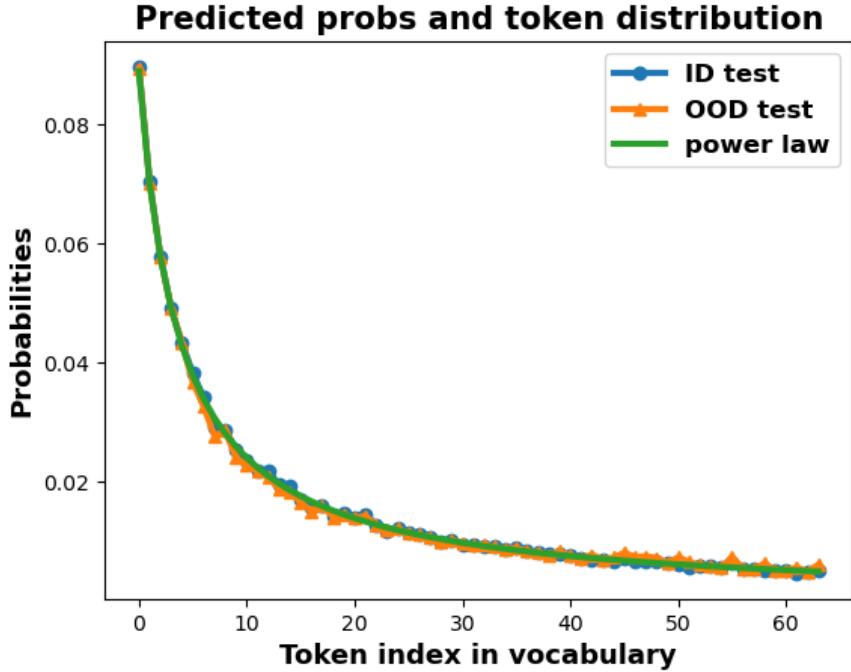


Figure 6: Prediction probabilities of one-layer Transformers on the copying task after 20K training steps.

1. 2-layer 1-head Transformer with MLP,
2. 4-layer 4-head Transformer without MLP,
3. 8-layer 8-head Transformer without MLP.

The results of the three models are similar to the minimal model (2-layer 1-head Transformer with no MLP) we analyzed in the paper. See plots in Section D.1.

## B.5 Details about models

We make connections to the original Transformer [81]. Let  $\mathbf{x}_1, \dots, \mathbf{x}_T \in \mathbb{R}^d$  be a sequence of input embedding vectors or hidden states in the intermediate layers, and denote  $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_T]^\top \in \mathbb{R}^{T \times d}$ . Let  $d_{\text{head}} \leq d$  be the head dimension. Given the query/key/value weights  $\mathbf{W}^q, \mathbf{W}^k, \mathbf{W}^v \in \mathbb{R}^{d \times d_{\text{head}}}$  respectively, a self-attention head calculates

$$\text{AttnHead}(\mathbf{X}; \mathbf{W}^q, \mathbf{W}^k, \mathbf{W}^v) = \text{softmax}\left(\frac{\mathbf{X}\mathbf{W}^q(\mathbf{W}^k)^\top \mathbf{X}^\top}{\sqrt{d_{\text{head}}}}\right) \mathbf{X}\mathbf{W}^v \quad (5)$$

where  $\text{softmax}(\mathbf{Z})_{ij} = \exp(Z_{ij}) / \exp(\sum_t Z_{it})$ . Now let the number of attention heads be  $H$  where  $Hd_{\text{head}} = d$ , and suppose that there are  $H$  sets of matrices  $(\mathbf{W}^{q,j}, \mathbf{W}^{k,j}, \mathbf{W}^{v,j})$  where  $j \leq H$ . Given an output matrix  $\mathbf{W}^o \in \mathbb{R}^{d \times d}$ , we partition it into  $H$  blocks of equal sizes  $\mathbf{W}^o = [\mathbf{W}^{o,1}, \dots, \mathbf{W}^{o,H}]$ . Let  $\mathbf{W}$  be the collection  $\mathbf{W} = (\mathbf{W}^{q,j}, \mathbf{W}^{k,j}, \mathbf{W}^{v,j}, \mathbf{W}^{o,j})_{j \leq H}$ . Then, the MultiHead attention calculates

$$\text{MultiHead}(\mathbf{X}; \mathbf{W}) = \sum_{j=1}^H \text{softmax}\left(\frac{\mathbf{X}\mathbf{W}^{q,j}(\mathbf{W}^{k,j})^\top \mathbf{X}^\top}{\sqrt{d_{\text{head}}}}\right) \mathbf{X}\mathbf{W}^{v,j}(\mathbf{W}^{o,j})^\top \quad (6)$$

Comparing with Eq. 1, we identify  $\mathbf{W}^{q,j}(\mathbf{W}^{k,j})^\top / \sqrt{d_{\text{head}}}$  with  $\mathbf{W}_{\text{QK},j}$  and  $\mathbf{W}^{v,j}(\mathbf{W}^{o,j})^\top$  with  $\mathbf{W}_{\text{OV},j}^\top$ .

Now we explain the major differences between our simplified Transformer in Eq. 1 and Transformers in practice. We note the following differences.

- Practical Transformers usually contain layer normalization and sometimes bias terms.
- Practical Transformers contain an MLP sublayer following every multihead self-attention.
- Early Transformers use the absolute positional embedding whereas more recent Transformers use rotary positional embedding.

The justification for the simplified Transformer is discussed in [26]. We provide some comments about positional embeddings.

**Positional embedding.** There are two major variants of positional embedding: absolute positional embedding (APE) and rotary embedding (RoPE). APE is proposed in the original Transformer paper [81] and used widely in early LLMs such as GPT-2. The input vector to a Transformer is obtained by adding a token-specific embedding vector and a position-specific embedding vector, thus encoding both token information and positional information. RoPE [76] is often used in recent LLMs such as Llama-2. The positional information is not encoded at the input layer; instead, RoPE directly modifies the attention by replacing  $\mathbf{W}^q(\mathbf{W}^k)^\top$  in Eq. 5 with  $\mathbf{W}^q \mathbf{R}_{\Delta t}(\mathbf{W}^k)^\top$  where  $\mathbf{R}_{\Delta t} \in \mathbb{R}^{d_{\text{head}} \times d_{\text{head}}}$  is a matrix that depends on relative distance of two tokens. In particular, if  $\Delta t = 0$  then  $\mathbf{R}_{\Delta t} = \mathbf{I}_d$ . Our analysis in Section 2 and 3 essentially treats  $\Delta t = 0$ .

Section D.5 explores the impact of  $\mathbf{R}_{\Delta t}$  on our results. We did not find significant differences when we repeat our measurements with a nonzero  $\Delta t$ .

## B.6 Details about measurements

**Subspace matching score.** Note that the above definition is invariant to the choice of bases  $\mathbf{U}, \mathbf{V}$ . Indeed, for different orthonormal matrices  $\mathbf{U}' = \mathbf{U}\mathbf{O}_1, \mathbf{V}' = \mathbf{V}\mathbf{O}_2$  where  $\mathbf{O}_1, \mathbf{O}_2$  are two orthogonal matrices, we have  $\sigma_{\max}(\mathbf{U}^\top \mathbf{V}) = \sigma_{\max}((\mathbf{U}')^\top (\mathbf{V}'))$ .

This score is a generalization of vector cosine similarity since

$$\sigma_{\max}(\mathbf{U}^\top \mathbf{V}) = \max_{\|\mathbf{y}_1\|_2 = \|\mathbf{y}_2\|_2 = 1} \langle \mathbf{U}\mathbf{y}_1, \mathbf{V}\mathbf{y}_2 \rangle.$$

which is equivalent to the inner product between two optimally chosen unit vectors in the two subspaces. In the special case  $r = 1$ ,  $\mathbf{U}, \mathbf{V}$  are two vectors, and this definition reduces to the regular cosine similarity between two vectors (after taking the absolute values).

## C Experiment details for experiments with LLMs

### C.1 Models

We list the models in the experiments.

- **GPT2:** 12 layers, 12 attention heads, and a hidden size of 768.
- **GPT2-XL:** 48 layers, 25 attention heads, and a hidden size of 1600.
- **Llama2-7B:** 32 layers, 32 attention heads, and a hidden size of 4096.
- **Gemma-7B:** 36 layers, 32 attention heads, and a hidden size of 3072.
- **Gemma2-9B:** 28 layers, 16 attention heads, and a hidden size of 3072.
- **Falcon-7B:** 32 layers, 32 attention heads, and a hidden size of 4544.
- **Falcon2-11B:** 60 layers, 32 attention heads, and a hidden size of 4096.
- **Mistral-7B:** 32 layers, 32 attention heads, and a hidden size of 4096.
- **Olmo-7B:** 32 layers, 32 attention heads, and a hidden size of 4096.
- **Llama3-8B:** 32 layers, 32 attention heads, and a hidden size of 4096.
- **Pythia-7B:** 32 layers, 32 attention heads, and a hidden size of 4096.
- **Llama2-70B:** 64 layers, 80 attention heads, and a hidden size of 8192 (for chain-of-thought experiments in Section E.1).

All models are downloadable from Huggingface.

### C.2 Prompt examples

Here we list a few examples for the three tasks in Section 3.1.

#### Fuzzy copying.

Prompt : bear snake fox poppy plate butterfly caterpillar boy  
aquarium\_fish motorcycle BEAR SNAKE FOX POPPY PLATE BUTTERFLY CATERPILLAR BOY

Solution : AQUARIUM\_FISH MOTORCYCLE

Prompt : willow\_tree bee orchid man plain bicycle pear crab otter possum  
WILLOW\_TREE BEE ORCHID MAN PLAIN BICYCLE PEAR CRAB

Solution : OTTER POSSUM

### **Indirect Object Identification.**

English Version

Prompt : Then, Anna and Matthew went to the station. Anna gave a basketball to  
Solution : Matthew

Symbolized Version

Prompt : Then, &^ and #\\$ went to the station. &^ gave a basketball to  
Solution : #\\$

### **In-context Learning.**

English Version

Prompt : baseball is sport, celery is plant, sheep is animal,  
volleyball is sport, rugby is sport, cycling is sport,  
camel is animal, llama is animal, hockey is sport, panda is animal,  
football is sport, onions is plant, cucumber is plant, zucchini is plant,  
zebra is animal, billiards is sport, golf is sport, horse is animal,  
kale is plant, volleyball is sport, lettuce is

Solution : plant

Symbolized Version

Prompt : baseball is \\$#, celery is !%, sheep is &\*, volleyball is \\$#,  
rugby is \\$#, cycling is \\$#, camel is &\*, llama is &\*, hockey is \\$#,  
panda is &\*, football is \\$#, onions is !%, cucumber is !%, zucchini is !%,  
zebra is &\*, billiards is \\$#, golf is \\$#, horse is &\*, kale is !%,  
volleyball is \\$#, lettuce is

Solution : !%

### **C.3 Shuffle intervention experiment**

We reported in Figure 5(e) the probability of predicting correct tokens for the copying task under two edits. We detail the calculations used in the figure.

**Evaluation.** First, we uniformly sample tokens from the vocabulary  $\mathcal{A}$  (i.e.,  $|\mathcal{A}| = 50257$ )  $L$  times, forming the segment  $s^\#$ . Then we repeat this segment using two replicas, yielding the input sequence  $(s^\#, s^\#, s^\#)$ . We repeat this  $N_0 = 50$  times and obtain a batch of input sequences.

Then, using the edited models as well as the original model, we calculate the probability of predicting the correct token

$$p_{2L+t}(s_t^\# | (s^\#, s^\#, s_{<t})). \quad (7)$$

For GPT2, we gather the above probability for  $t \in \{6, 7, 8, \dots, L\}$  and every input sequence. Finally, in the left plot in Figure 5(e), we compare the histogram of the prediction probabilities of the original model, the edited model with shuffling, and the edited random baseline.

We also summarize the result of each LLM by averaging the probability in Eq. 7 over  $i \in \{6, 7, 8, \dots, L\}$  and input sequences. We obtained three averaged probabilities: the original LLM, the edited model with shuffling, and the edited random baseline with random replacement. Then we measure how much probability is reduced from the original probability to the two edited models. Finally we report the result in the right plot of Figure 5(e).

#### C.4 Projection intervention experiment

**Calculating bridge subspace.** As mentioned in Section 3.2, we calculated the bridge subspace of rank  $r$  based on the top- $K$   $\mathbf{W}_{QK}$  from the list of IHs. We chose to edit 25% of all heads using the projection matrices  $\mathbf{V}\mathbf{V}^\top$  or  $\mathbf{I}_d - \mathbf{V}\mathbf{V}^\top$  because we believe that 25% of all heads are likely to be relevant to the copying task. These heads are selected as the 25% top-ranking heads according to the IH attention score.

**Evaluation.** Similar to the shuffling experiment, we use  $N_0 = 50$  input sequences  $(s^\#, s^\#, s^\#)$  where the segment  $s^\#$  consists of uniformly sampled tokens. Here we consider the prediction accuracy. Namely, we use 0-1 loss to measure whether a predicted token matches the target token

$$\mathbf{1}\left(\arg \max_s p_{2L+t}(s | (s^\#, s^\#, s_{<t})) = s_t^\#\right)$$

For GPT2, we measure the change of the average prediction accuracy under projection edits  $\mathbf{V}\mathbf{V}^\top$  and  $\mathbf{I}_d - \mathbf{V}\mathbf{V}^\top$  for varying rank parameter  $r$ , which we report in the left plot of Figure 5(f).

We also measure each LLM and summarize the result by selecting a fixed rank parameter. The rank is selected to be 5% of the model dimension  $d$ . Table 1 lists the value of  $r$  for each LLM.

GPT2	GPT2-XL	Gemma-7b	Gemma2-9b	Llama2-7b	Llama3-8b	Mistral-7b	Olmo-7b	Pythia-7b	Falcon-7b
50	80	150	170	200	200	200	200	200	220

Table 1: The rank  $r$  of  $\mathbf{V}$  used in the projection calculation.

#### C.5 Connection to spiked matrices

We notice that common bridge subspace is connected to the statistical literature on spiked matrices [39]. Consider an ideal scenario, where the weight matrices are spiked with a shared spiked

$$\mathbf{W}_{OV}^j = \mathbf{V}\mathbf{U}^\top + \text{noise}, \quad \mathbf{W}_{QK}^j = \mathbf{U}\mathbf{V}^\top + \text{noise},$$

where  $\mathbf{U}, \mathbf{V} \in \mathbb{R}^{d \times r}$  are orthonormal matrices and the noise matrices have much smaller magnitude. The observed properties are realized by this ideal case. Indeed, the QK and OV circuits are all matched through a common subspace  $\text{span}(\mathbf{V})$ , QK circuits (or OV circuits) play exchangeable roles, and compositional information goes through  $\text{span}(\mathbf{V})$ . Moreover,  $\mathbf{W}_{QK,j}\mathbf{W}_{OV,j} \approx \mathbf{U}\mathbf{U}^\top$ , so diagonal entries are generally larger for  $\mathbf{U}$  in a generic position.

## D Additional results for the synthetic example

### D.1 Larger models show similar sharp transitions

We believe that the 2-layer 1-head Transformer with no MLP is a minimal yet representative model for analyzing the sharp transition. We show similar results on three larger Transformer models in Figure 7 to 10.

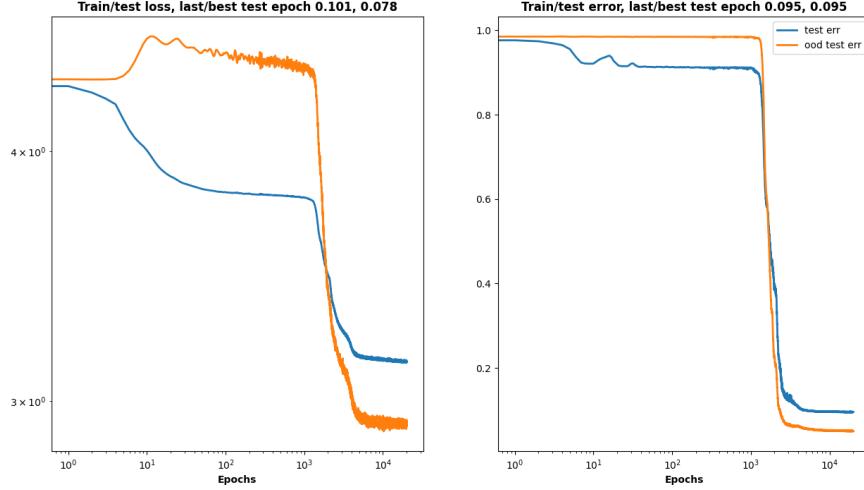


Figure 7: 2-layer 1-head Transformer **with MLP**. ID/OOD test errors vs. training steps.

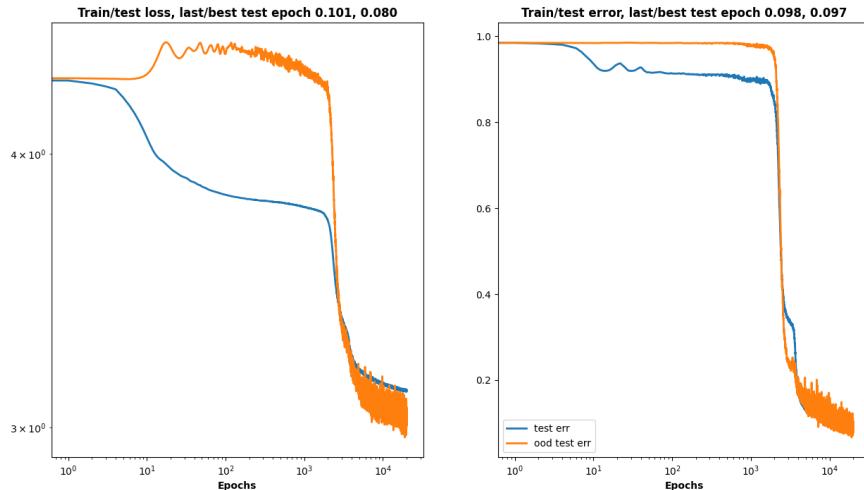


Figure 8: 4-layer 4-head Transformer **without MLP**. ID/OOD test errors vs. training steps.

### D.2 Progress measures under varying pool sizes

We consider the same model/training settings as in Section 2 but we choose two different pool sizes  $S = 1000$  and  $S = 100$ . In Figure 11 and 12, the progress measures under  $S = 1000$  are similar to Figure 2 but very different under  $S = 100$ .

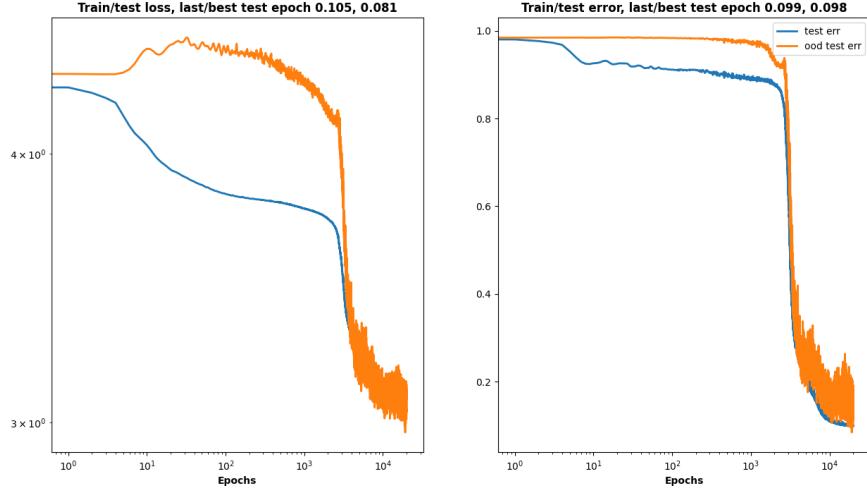


Figure 9: 8-layer 8-head Transformer without MLP. ID/OOD test errors vs. training steps.

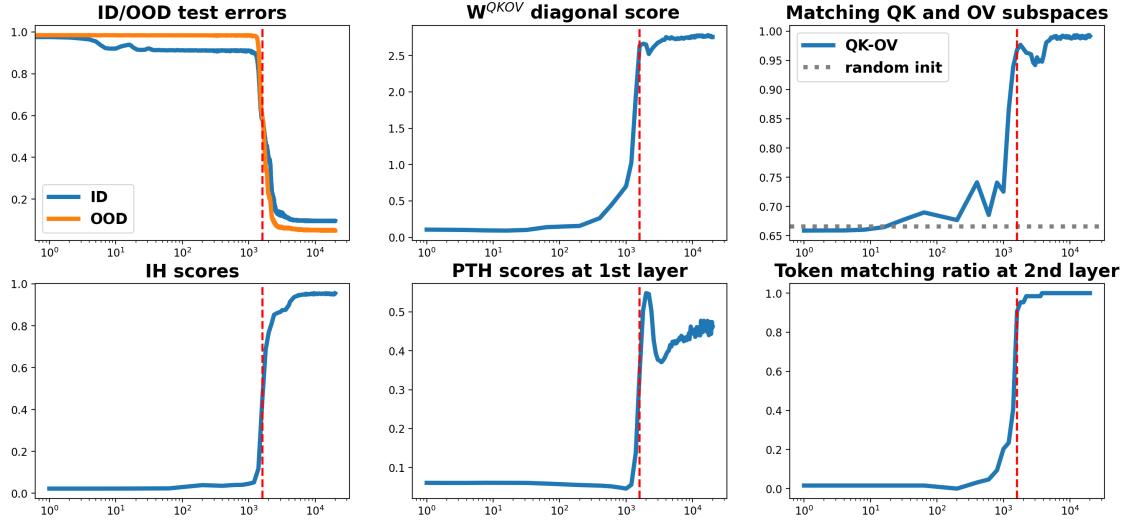


Figure 10: Progress measures for 2-layer 1-head Transformer **with MLP**.

### D.3 Attention matrices

The heatmaps in Figure 3 indicate that the memorizing model ( $S = 100$ ) are qualitatively different from that generalizing model ( $S = 1000$ ). In Figure 13 and 14, we further plot attention matrices  $\mathbf{A}$  based on one OOD sequence at training step 16K to support our claim that the memorizing model does not learn compositional structure for OOD generalization.

### D.4 Measurements for subspace matching

We explore two factors that may impact the subspace matching score. Recall that we defined the score as

$$\sigma_{\max}(\mathbf{U}^\top \mathbf{V})$$

where  $\mathbf{U}, \mathbf{V} \in \mathbb{R}^{d \times r}$  are the principal subspaces of  $\mathbf{W}_{\text{QK}}$  and  $\mathbf{W}_{\text{OV}}$ . We consider alternative measurements.

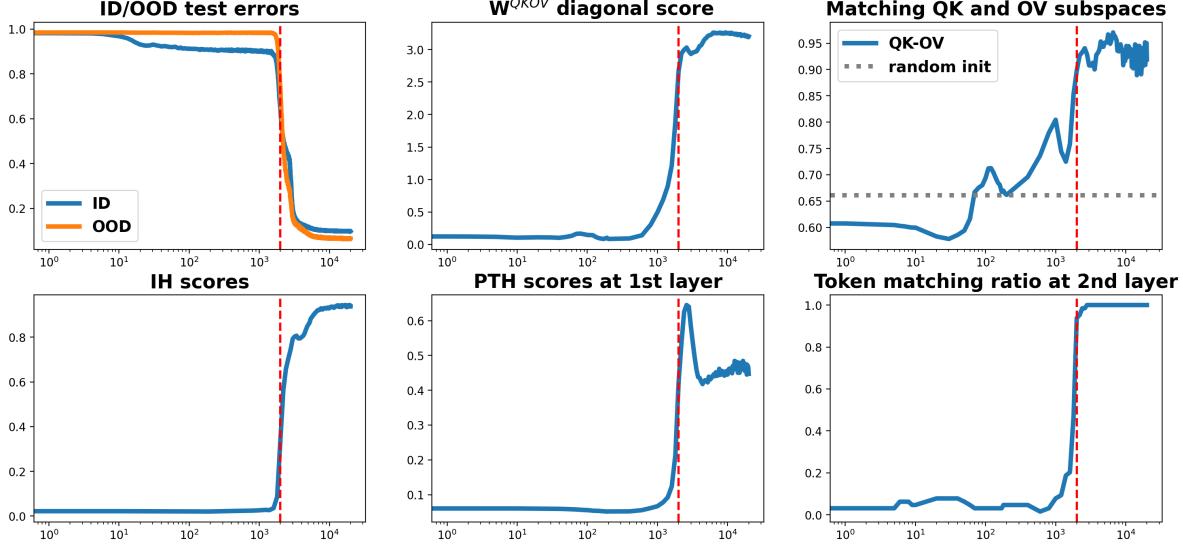


Figure 11: Progress measures for synthetic data with a large pool size  $S = 1000$ . Plots are similar to Figure 2.

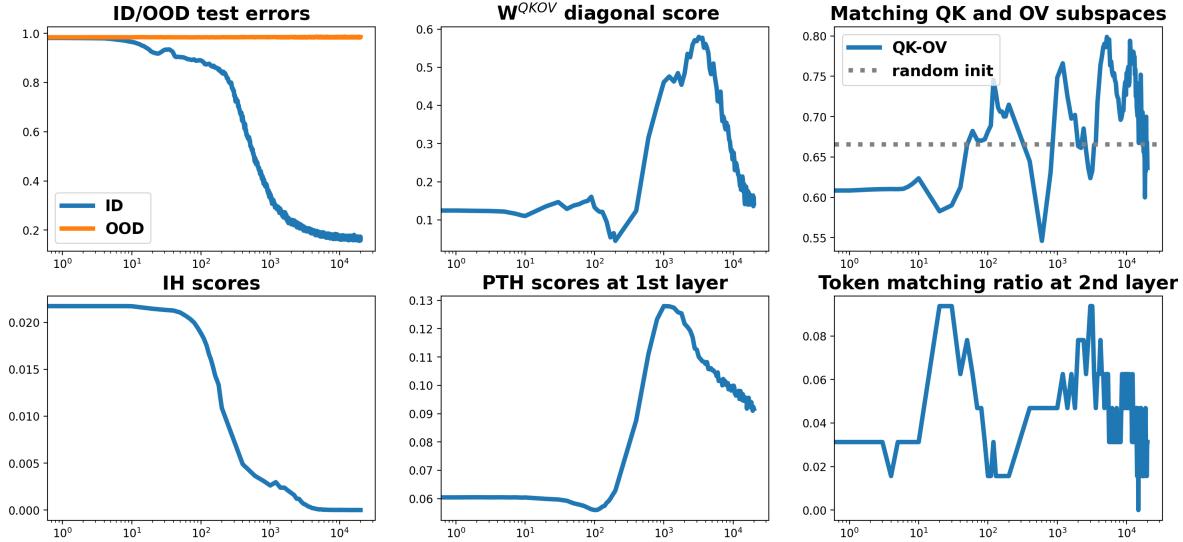


Figure 12: Progress measures for synthetic data with a small pool size  $S = 100$ . Plots are dissimilar to Figure 2.

- Replace the largest singular value by an average quantity  $(r^{-1} \sum_{j \leq r} \sigma_j^2 ((\mathbf{U}^\top \mathbf{V}))^{1/2}$  where  $\sigma_j$  denotes the  $j$ -th largest singular value.
- Vary the rank parameter  $r$ .

First, the average score reflects the alignment of two subspaces by picking two vectors randomly from the subspaces. Second, we investigate whether the rank parameter  $r$  has impact on the subspace matching measurement on the synthetic example. We consider the same setting as in Section 2 but use different  $r \in \{5, 10, 15, 20\}$  when measuring the subspace matching scores.

We find that the two alternative measurement yield qualitatively similar results; see Figure 15 and 16.

**PTH/IH attention: pool size None, step 16000**

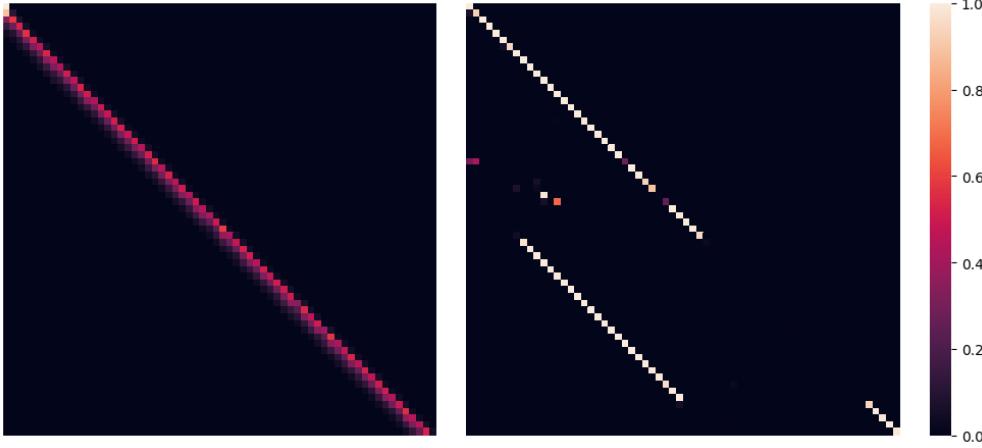


Figure 13: Attention matrices of the generalizing model (pool size is 1000). As claimed, the PTH (left) largely attends to the previous position (diagonal line shifted down by 1), and IH (right) attends to to-be-copied positions of the repeated segment.

**PTH/IH attention: pool size 100, step 16000**

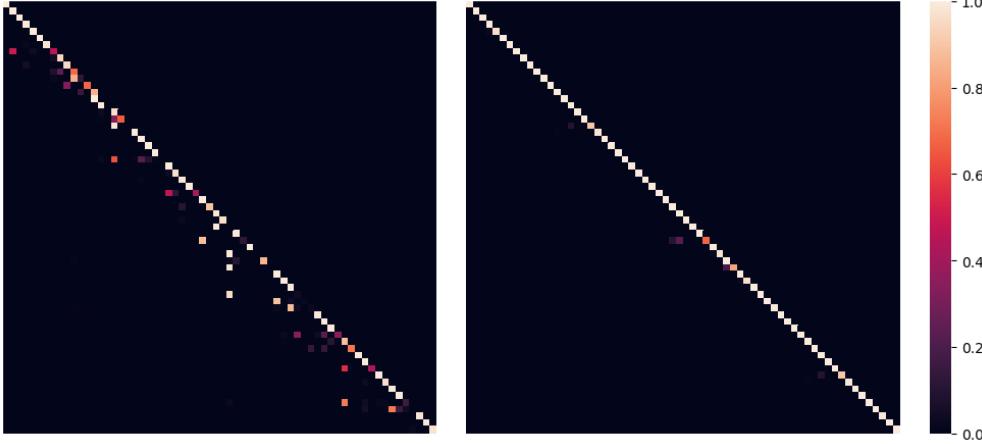


Figure 14: Attention matrices of memorizing model (pool size is 100). Both PTH (left) and IH (right) exhibit diagonal lines, which do not reflect the repetition pattern in the OOD instance.

## D.5 Rotary positional embedding

As we explained in Section B.5, there is a nuance with rotary positional embedding (RoPE) in the attention calculation. To calculate the attention in a head, we need a set of QK matrices  $(\mathbf{W}_{QK,\Delta t})_{\Delta t \geq 0}$  where

$$\mathbf{W}_{QK,\Delta t} = \mathbf{W}^q \mathbf{R}_{\Delta t} (\mathbf{W}^k)^\top$$

The matrix  $\mathbf{Z} \in \mathbb{R}^{T \times T}$  before softmax operation is given by  $Z_{t,t'} = \mathbf{x}_t^\top \mathbf{W}_{QK,|t-t'|} \mathbf{x}_{t'}$ . In particular, if  $\Delta t = 0$ , then  $\mathbf{R}_0 = \mathbf{I}_d$  and thus  $\mathbf{W}_{QK,0} = \mathbf{W}^q (\mathbf{W}^k)^\top$ . We used exactly  $\mathbf{W}_{QK,0}$  for Figure 2.

We show that  $\mathbf{W}_{QK,\Delta t}$  with nonzero  $\Delta t$  yields similar results. This is demonstrated in Figure 17–20 where  $\Delta t \in \{5, 10, 15, 20\}$ . Note that  $\Delta t$  only affects the 2nd, 3rd, and 6th subplots in each figure.

## Matching QK and OV subspaces

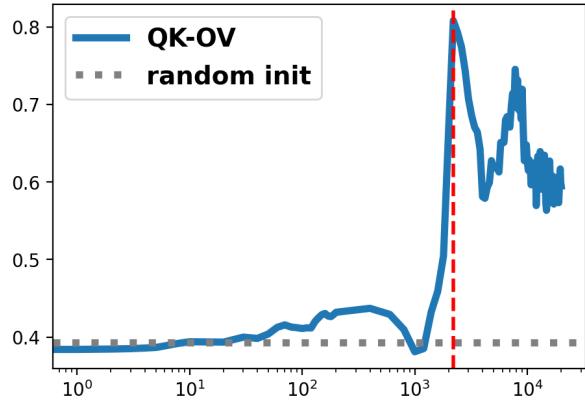


Figure 15: Subspace matching on the synthetic example with an average score.

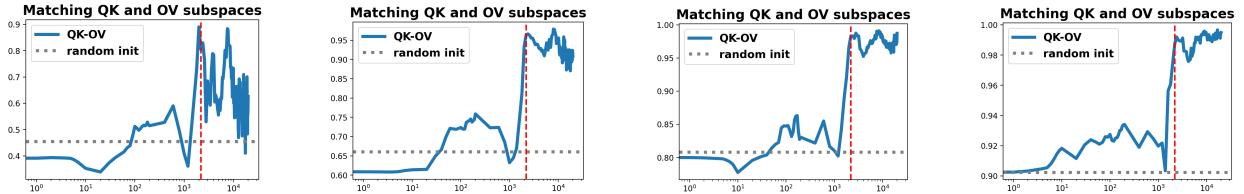


Figure 16: Subspace matching on the synthetic example with different rank  $r \in \{5, 10, 15, 20\}$ .

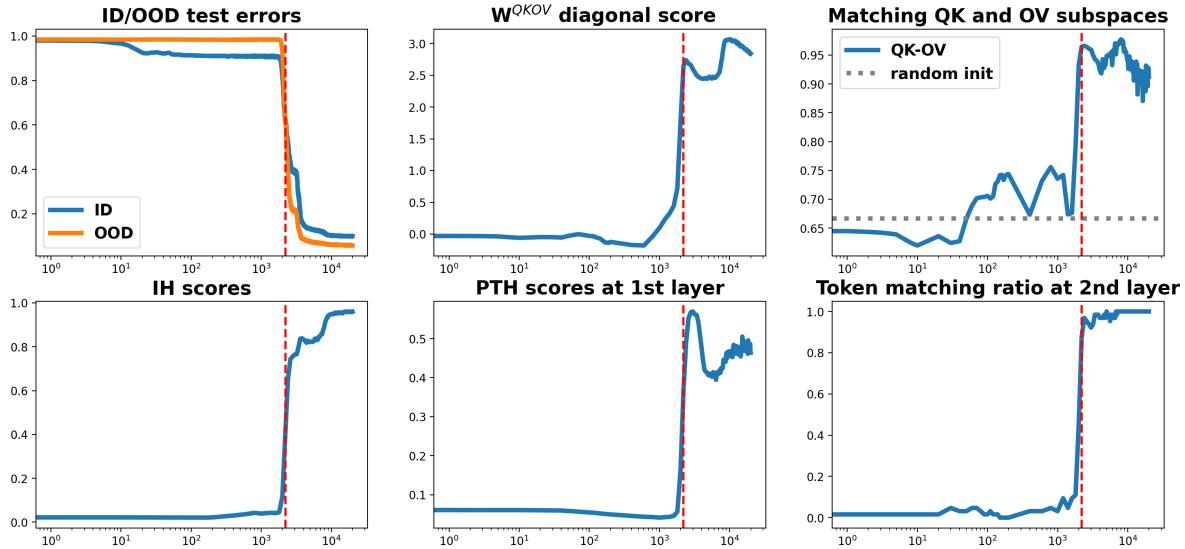


Figure 17: Progress measures using  $W_{QK,\Delta t}$  where  $\Delta t = 5$ .

## E Additional results for the LLMs experiments

### E.1 Additional results for symbolized language reasoning

Apart from the three tasks in Section 3.1, we offer an additional task. Chain-of-thought (CoT) reasoning empirically works well on mathematical tasks. It usually involves a step-by-step manner. We demonstrate

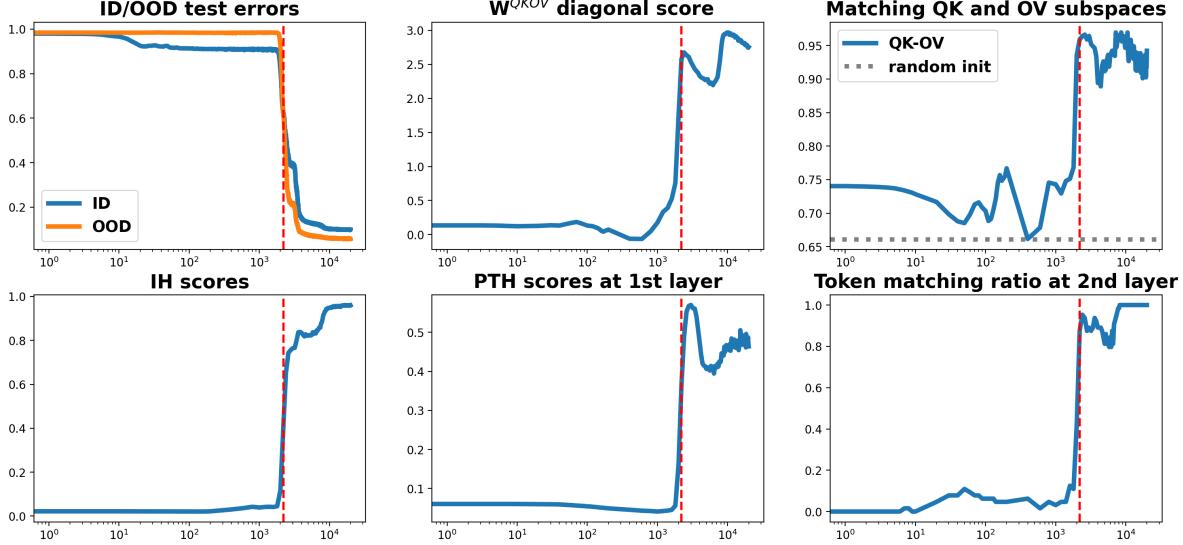


Figure 18: Progress measures using  $W_{QK,\Delta t}$  where  $\Delta t = 10$ .

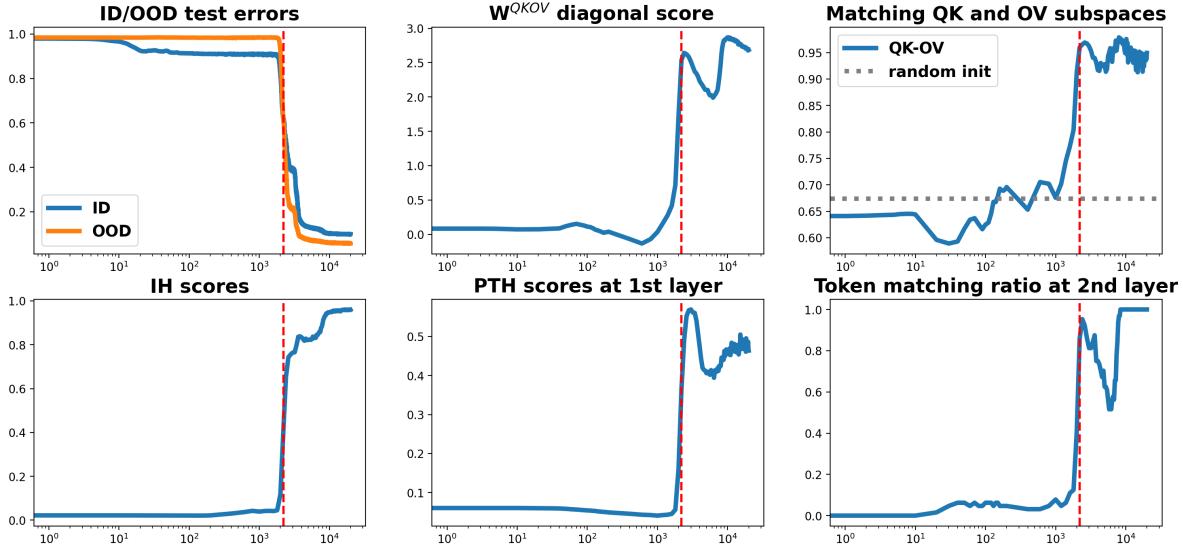


Figure 19: Progress measures using  $W_{QK,\Delta t}$  where  $\Delta t = 15$ .

that IHs also have a large impact on CoT reasoning.

4. Chain-of-thought (CoT): we sample instances from the GSM8K Dataset [19] which contain grade school math problems.

For instance, “Ivan had \$10 and spent 1/5 of it on cupcakes. He then spent some money on a milkshake and had only \$3 left. How much is the milkshake?” We concatenate pairs of a problem description and a step-by-step solution as in-context examples in the prompt. We use Llama2-70B as the pretrained LLM to generate answers. We measure the accuracy of the original/edited model by generating 256 tokens, extracting the first numeric number from generated tokens, and comparing it with the correct number.

Each problem consists of several base arithmetic subproblems. While the subproblems are likely ID, due to the freedom of combining the subproblems, the problem may be OOD. Figure 21 shows that removal

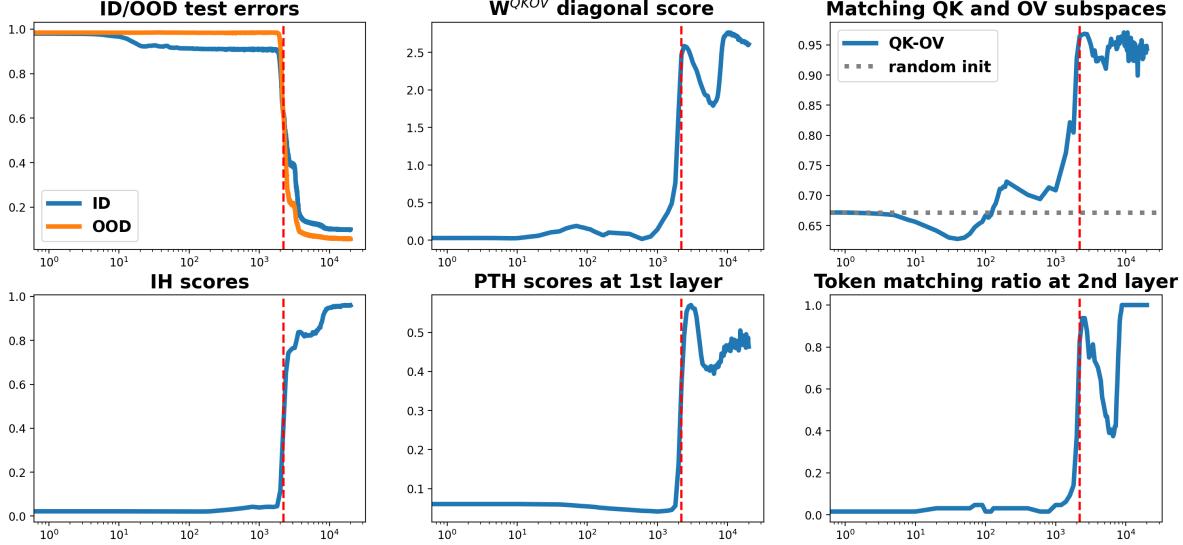


Figure 20: Progress measures using  $W_{QK, \Delta t}$  where  $\Delta t = 20$ .

of IHs causes significant accuracy drop.

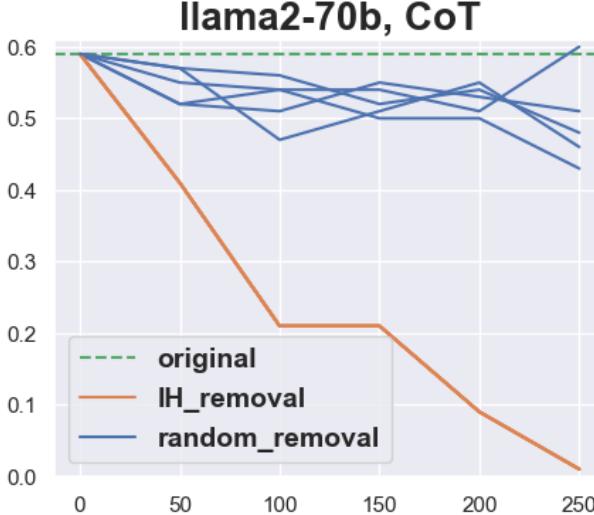


Figure 21: Chain-of-thought depends on IHs. Accuracy drops as we increase the number of removed IHs from the model.

## E.2 Details about PTHs and IHs in LLMs

We find that PTHs and IHs are distributed across many layers. In particular, Figure 5(c)(d) shows that the top-10 PTHs and IHs are strongly aligned compared with random pairs.

For the shuffling experiments and projection experiments in Section 3, we selected PTHs and IHs from top-scoring attention heads. Here we detail the procedure and [layer, head] pairs for each model.

**Selecting relevant IHs and PTHs.** Here we show the list of PTHs and IHs for each models in Table 2.

The screening process for IHs and PTHs in the shuffling and projection experiments in Section 3.2 is as follows. For each LLM, we first sort the IH/PTH pairs by their diagonal score and then filter out pairs with scores below the cutoff of  $\delta = 2.3$ ,

$$\text{diagonal}(\text{IH}_1, \text{PTH}_1) \geq \text{diagonal}(\text{IH}_2, \text{PTH}_2) \geq \dots \geq \text{diagonal}(\text{IH}_{K'}, \text{PTH}_{K'}) \geq \delta$$

We obtain an ordered list  $\text{IH}_\delta$  as the deduplicated IH heads appearing in the top- $K'$  pairs above. Similarly, the ordered list  $\text{PTH}_\delta$  contains the deduplicated PTH heads appearing in the top- $K'$  pairs above. To avoid too many heads, we select at most 10 heads from  $\text{PTH}_\delta$  and  $\text{IH}_\delta$ .

Model	IH	PTH
<b>GPT2</b>	$[[5, 1], [6, 9], [5, 5], [7, 2], [7, 10], [5, 8], [5, 0], [8, 1], [7, 11], [9, 6]]$	$[[4, 11], [5, 6], [8, 7], [6, 8], [6, 0], [9, 3], [3, 3], [7, 0], [5, 2], [1, 0]]$
<b>GPT2-XL</b>	$[[17, 6], [16, 21], [16, 3], [13, 0], [18, 0], [17, 14], [20, 0], [19, 18], [22, 20], [21, 3]]$	$[[15, 19], [12, 21], [13, 20], [14, 12], [16, 5], [11, 2], [9, 7], [14, 20], [10, 15], [13, 12]]$
<b>Llama2-7B</b>	$[[6, 9], [6, 30], [7, 4], [8, 26], [7, 12], [7, 13], [6, 11], [8, 31], [6, 16], [11, 15]]$	$[[5, 15], [6, 5], [10, 3], [15, 11]]$
<b>Gemma-7B</b>	$[[5, 0], [14, 15], [20, 1], [20, 13], [18, 13], [21, 1], [16, 1]]$	$[[3, 9], [13, 3], [19, 13], [3, 15], [2, 4], [17, 0], [1, 0], [13, 2], [15, 3]]$
<b>Gemma2-9B</b>	$[[28, 6], [17, 5], [7, 1], [25, 13], [28, 2], [11, 2], [15, 2], [5, 1], [15, 3], [34, 14]]$	$[[27, 2], [16, 0], [6, 9], [24, 2], [10, 4], [14, 2], [10, 1], [3, 14], [3, 15], [14, 11]]$
<b>Falcon-7B</b>	$[[5, 65], [5, 18], [5, 13], [5, 10], [5, 2], [5, 1], [5, 69], [5, 43], [5, 41], [5, 14]]$	$[[3, 38]]$
<b>Mistral-7B</b>	$[[12, 6], [12, 4], [12, 7], [18, 2], [18, 1], [18, 3]]$	$[[11, 17], [17, 22]]$
<b>Olmo-7B</b>	$[[27, 14], [15, 15], [24, 7], [2, 28], [2, 10], [26, 17]]$	$[[26, 25], [14, 30]], [14, 18], [23, 24], [1, 7], [24, 3], [25, 6], [1, 15], [26, 30]]$
<b>Llama3-8B</b>	$[[15, 28], [15, 30], [8, 1], [15, 1], [5, 11], [5, 8], [5, 10], [5, 9], [16, 20], [16, 23]]$	$[[14, 26], [7, 2], [4, 13], [7, 1], [4, 12], [1, 20], [9, 11], [25, 20]]$
<b>Pythia-7B</b>	$[[7, 26], [7, 2], [7, 1], [6, 30], [8, 11], [8, 17], [4, 18], [8, 4], [6, 13], [7, 20]]$	$[[6, 9], [5, 10], [3, 7], [3, 23], [14, 3], [6, 23], [11, 19]]$

Table 2: Table of selected IHs/PTHs in the shuffling experiments and projection experiments

### E.3 Histograms for PTH/IH matching

In Figure 5(c)(d), we only presented the histogram plots based on GPT2. We show that results from other LLMs are consistent with our findings. In Figure 22 and 23, we present the histograms of diagonal scores and the histograms of subspace matching scores.

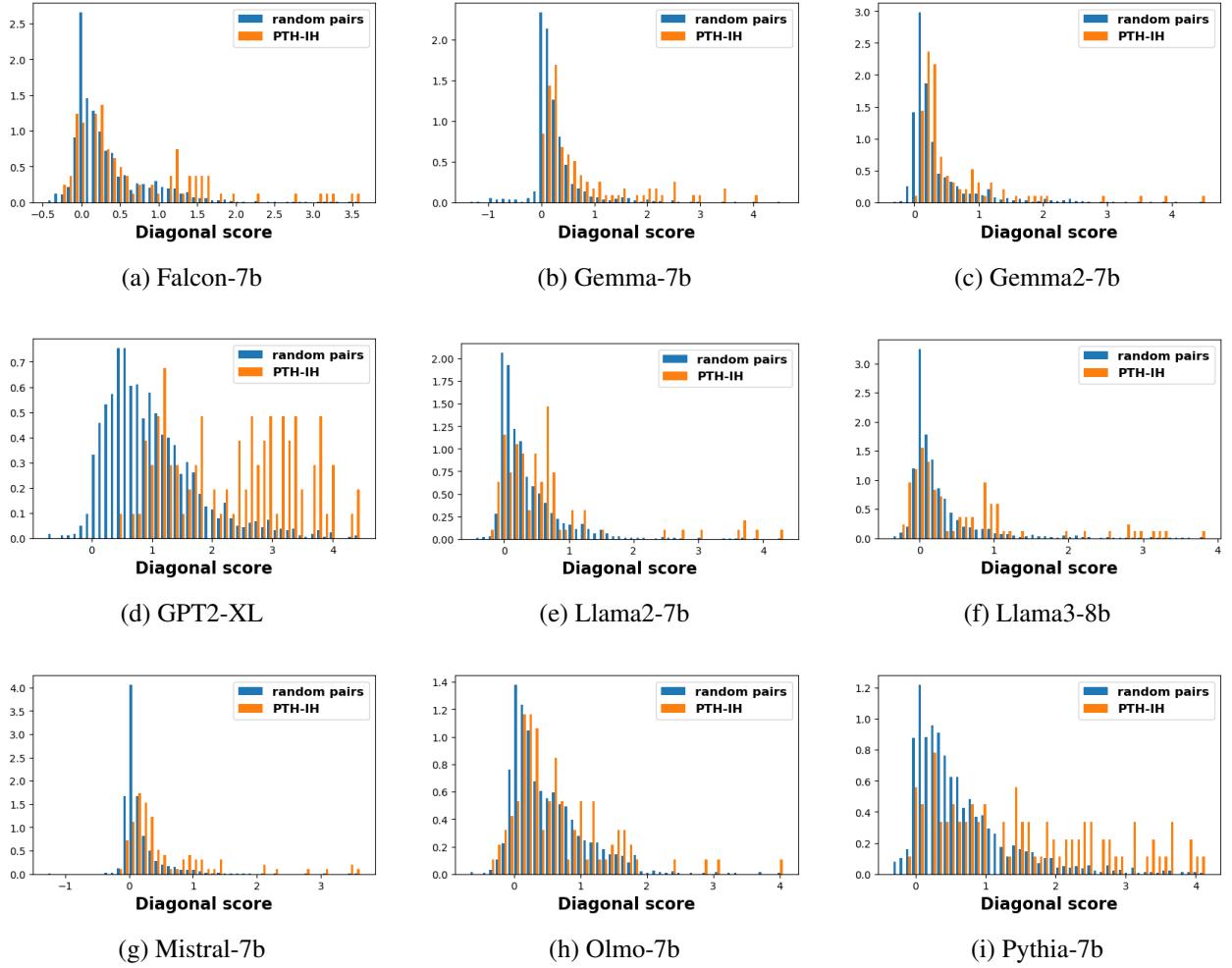


Figure 22: Diagonal scores: histograms showing matching of pairs from PTH/IH.

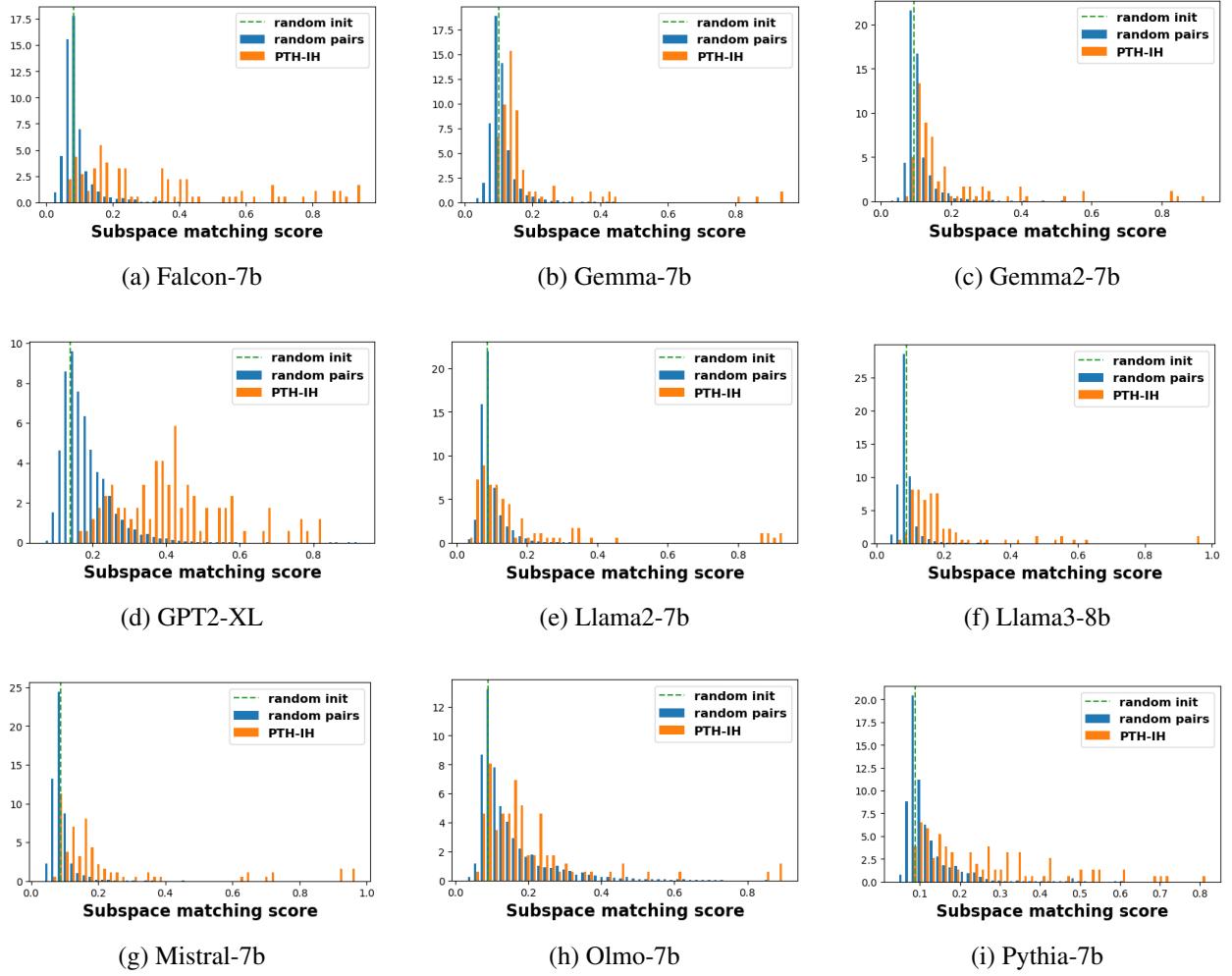


Figure 23: Subspace matching scores: histograms showing matching of pairs from PTH/IH.

#### **E.4 Histograms for shuffling experiments**

In Figure 5(e), we only presented the histogram plot based on GPT2. We show in Figure 24 that results from other LLMs are consistent with our findings.

#### **E.5 Histograms for projection experiments**

In Figure 5(f), we only presented the histogram plots based on GPT2. We show in Figure 25 that results from other LLMs are similar to the plot from GPT2.

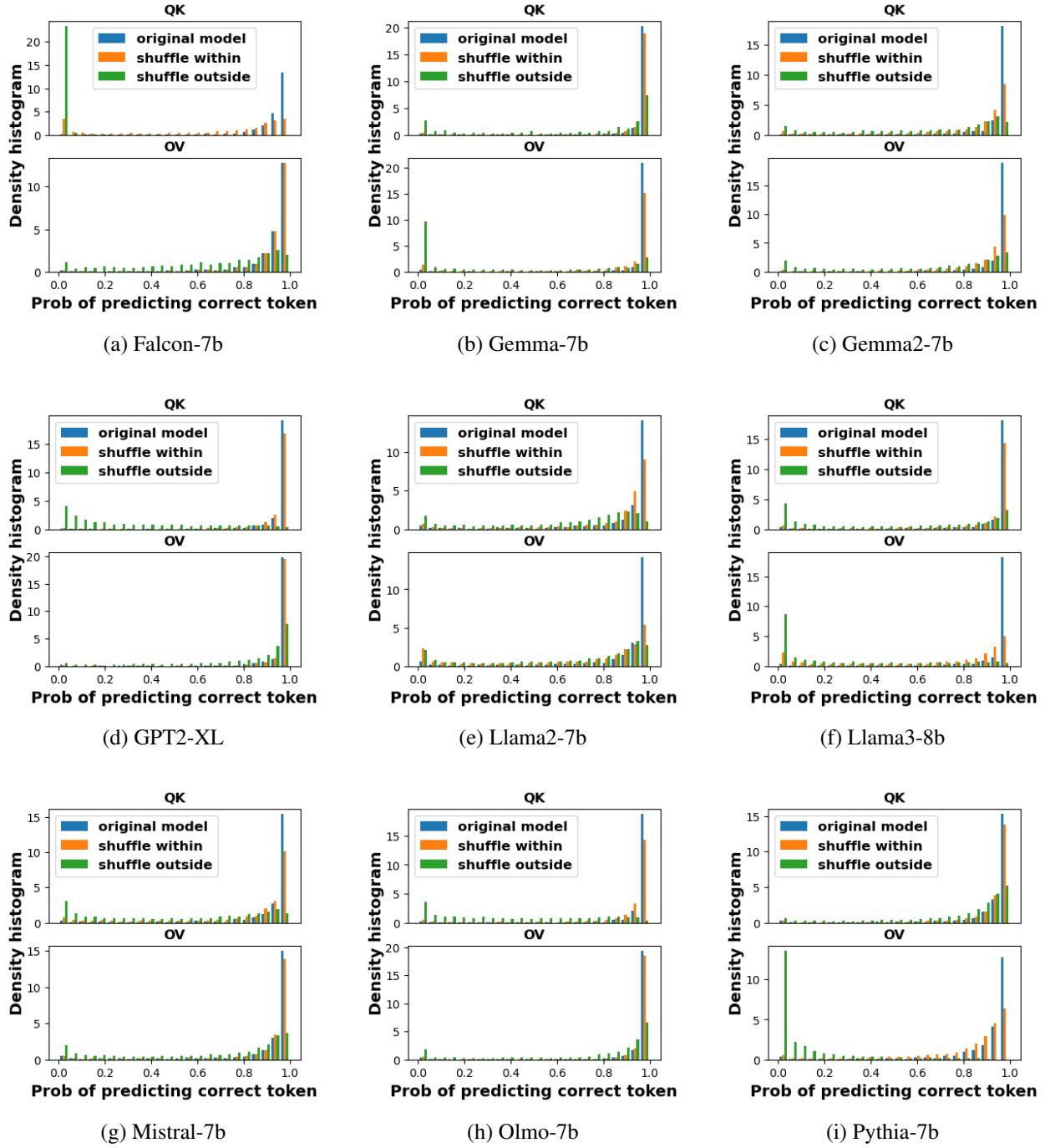


Figure 24: Shuffling experiments: histograms showing the effects of editing in various models.

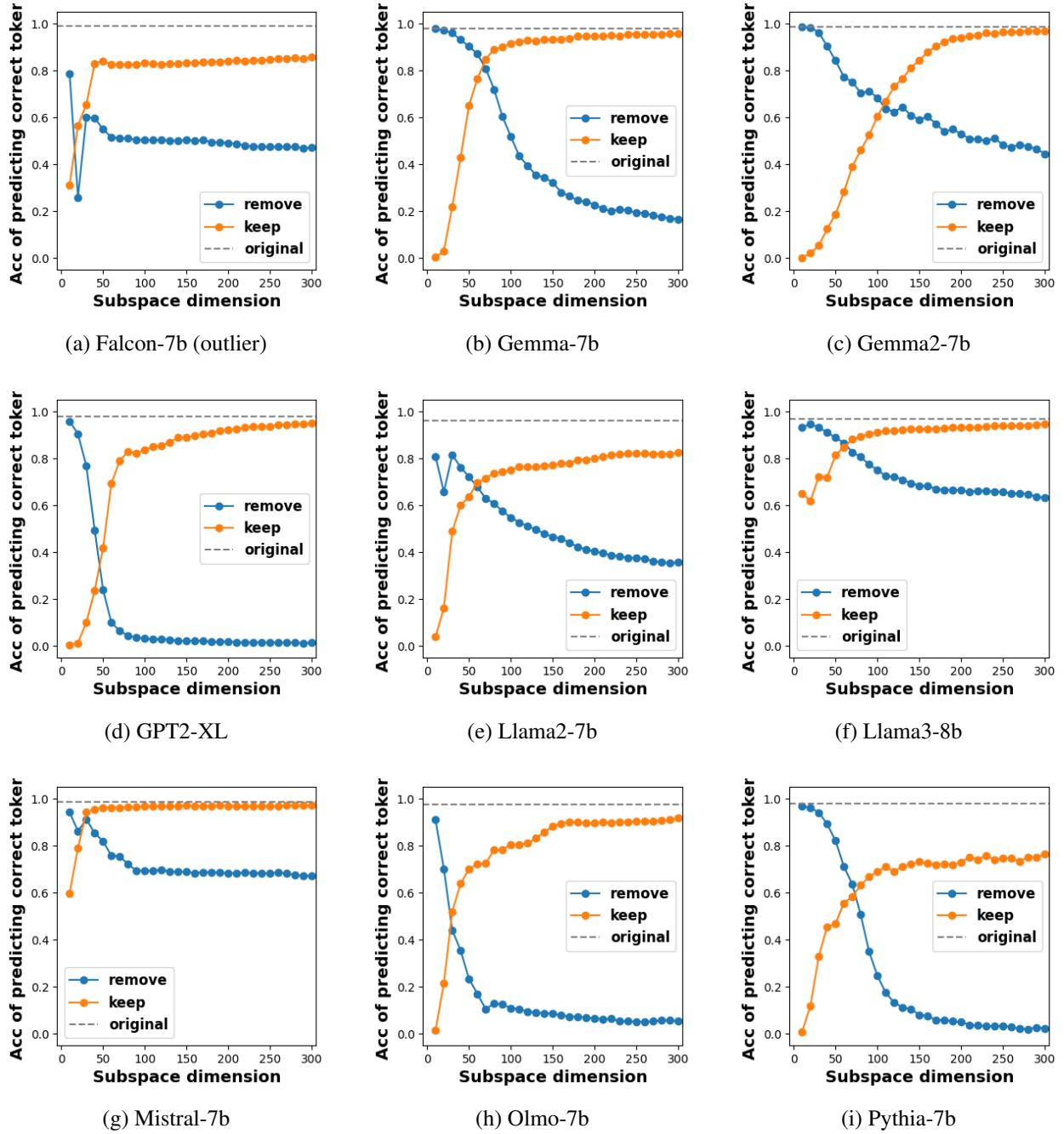


Figure 25: Projection experiments: histograms showing the effects of editing in various models.

## F Additional Related Work

**Large Language Models.** Large Language Models (LLMs) are typically based on the Transformer architecture and are characterized by their enormous number of parameters and extensive pretraining on vast datasets. Notable examples include LLaMA[80], ChatGPT [59], GPT4 [60] and Claude [8]. These models utilize various pretraining methods such as masked language modeling [20, 45], and autoregressive pre-training [16]. Researchers have investigated the effects of pretraining on language model performance. Adapting LLMs to various downstream tasks has garnered significant attention in the field. This adaptation can take many forms, including the use of adapters [36, 37], multitask fine-tuning [85, 92, 93], in-context learning [55, 21, 72], reinforcement learning from human feedback (RLHF) [61], and methods for accelerating inference [31, 90]. Each of these approaches aims to enhance LLM performance or efficiency for specific applications or domains, allowing these powerful models to be tailored to a wide range of tasks and requirements.

**In-context Learning.** LLM exhibits a remarkable ability for in-context learning (ICL) [16], particularly for generative models. This ability allows models to construct new predictors for test examples based on a prompt containing a sequence of labeled examples, without requiring parameter updates. The behavior of ICL has been the subject of several empirical studies. [97, 34, 47] have formulated the problems and reported on its sensitivity. To enhance performance, [18, 54] have employed meta-training with an explicit in-context learning objective. On the theoretical front, [89, 28] have provided frameworks to explain the underlying mechanisms of in-context learning. Studies by [82, 3, 49, 94], using linear models, have demonstrated how transformers can represent gradient descent and perform linear regression. On contrastive to these works, we present an mechanistic analysis that illustrates how LLMs can demonstrate OOD capability in ICL.