# CIRCUIT COMPOSITIONS: EXPLORING MODULAR STRUCTURES IN TRANSFORMER-BASED LANGUAGE MODELS

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### Abstract

A fundamental question in interpretability research is to what extent neural networks, particularly language models, implement reusable functions via subnetworks that can be composed to perform more complex tasks. Recent developments in mechanistic interpretability have made progress in identifying subnetworks, often referred to as circuits, which represent the minimal computational subgraph responsible for a model's behavior on specific tasks. However, most studies focus on identifying circuits for individual tasks without investigating how functionally similar circuits relate to each other. To address this gap, we examine the modularity of neural networks by analyzing circuits for highly compositional subtasks within a transformer-based language model. Specifically, given a probabilistic context-free grammar, we identify and compare circuits responsible for ten modular string-edit operations. Our results indicate that functionally similar circuits exhibit both notable node overlap and cross-task faithfulness. Moreover, we demonstrate that the circuits identified can be reused and combined through subnetwork set operations to represent more complex functional capabilities of the model.

### 1 INTRODUCTION

Neural networks can be effectively modeled as causal graphs that illustrate how inputs are mapped to the output space (Mueller et al., 2024). For instance, the feed-forward and attention modules within the Transformer architecture (Vaswani et al., 2017) can be interpreted as a series of causal nodes that guide the transformation from input to output via the residual stream (Ferrando et al., 2024). This abstraction is commonly used in mechanistic interpretability to identify computational subgraphs, or *circuits*, responsible for the network's behavior on specific tasks (Wang et al., 2023). Circuits are typically identified through causal mediation analysis, which quantifies the causal influence of model components on the network's predictions (Mueller et al., 2024). Techniques such as activation patching (Meng et al., 2022), attribution patching (Nanda, 2023; Syed et al., 2023), and their variants (Hanna et al., 2024b) have been successfully applied to identify circuits in language models for tasks such as indirect object recognition (Wang et al., 2023; Merullo et al., 2024), entity tracking (Prakash et al., 2024), and factual recall (Meng et al., 2022).

However, a notable limitation of existing studies is their focus on identifying circuits for isolated, individual tasks. Few studies compare circuits responsible for different functional behaviors of the model, and those that do primarily focus on tasks with limited cross-functional similarity (Hanna et al., 2024b). This limitation may be due to the rigid task structures imposed by common circuit identification methods, which typically analyze the causal effect of individual model components on predictions related to a *specific token* of interest (Meng et al., 2022; Nanda, 2023; Syed et al., 2023). For instance, Meng et al. (2022) identify circuits responsible for recalling factual associations, such as "The Eiffel Tower is located in", by analyzing the causal effect of model components on predicting a single token representing the association, e.g., "Paris". As a result, more complex functional capacities, which are difficult to capture through the causal effect on a single token prediction, are often overlooked.

In this study, we explore the modularity of neural networks by comparing circuits responsible for highly compositional subtasks within a transformer-based sequence-to-sequence model. Specifically, we identify circuits associated with ten modular string-edit operations on a probabilistic context-free grammar, introduced by PCFG SET (Hupkes et al., 2020). We analyze the circuits discovered in terms of both node overlap and cross-task faithfulness, assessing their performance for functionally related tasks. To facilitate the study of circuits related to sequence-prediction tasks that extend beyond single-token predictions, we propose an automatic circuit identification method that builds upon continuous sparsification (Savarese et al., 2020), jointly optimizing for *faithfulness* and *minimality*—two key objectives in circuit discovery (for further details, see Section 2.2). Moreover, we demonstrate that the circuits identified can be reused and combined through subnetwork set operations to explain more complex functional capabilities of the model. In summary, our contributions are as follows: 1) we demonstrate the application of continuous sparsification to automatically discover both faithful and minimal circuits for sequence-to-sequence tasks from PCFG SET; 2) we analyze the relationships between functionally related circuits by examining node overlap and cross-task faithfulness, providing insights into the model's modular structure; and 3) we show that computational subgraphs from functionally related circuits can be combined using subnetwork set operations, resulting in novel subnetworks that explain model behavior on tasks beyond the scope of the initial circuits.

### 2 BACKGROUND

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In this section, we provide a brief overview of key concepts related to circuit discovery and continuous sparsification. For a more comprehensive perspective of interpretability research rooted in causal mediation analysis, including the circuits framework, we direct interested readers to the work of Mueller et al. (2024).

### 2.1 ACTIVATION PATCHING

A widely used approach for identifying circuits within neural networks, particularly language models, is activation patching (Vig et al., 2020; Meng et al., 2022; Wang et al., 2023; Zhang & Nanda, 2024). Grounded in causal mediation analysis, activation patching assesses the causal influence of nodes within the model's computation graph by quantifying their *indirect effect* (IE) (Pearl, 2001) on downstream nodes, typically the model's final output (Mueller et al., 2024). Given a counterfactual intervention  $\tilde{z}$  applied to a mediator z—commonly another node within the model's computation graph—, the indirect effect of a node x on some downstream node y through z can be calculated as the difference in a metric  $\mathbb{P}$  that captures the state of y before and after the intervention:

$$\operatorname{IE}\left(\mathbb{P}, \boldsymbol{x}, \boldsymbol{z}, \boldsymbol{z}_{x}, \tilde{\boldsymbol{z}}\right) = \mathbb{P}\left(\boldsymbol{y}(\boldsymbol{x}) | \, \boldsymbol{z} = \boldsymbol{z}_{x}\right) - \mathbb{P}\left(\boldsymbol{y}(\boldsymbol{x}) | \operatorname{do}\left(\boldsymbol{z} = \tilde{\boldsymbol{z}}\right)\right) \tag{1}$$

078 In this context, x typically represents the model's input for the task at hand, while y denotes the model's output. The 079 variable  $z_x$  corresponds to the mediator's natural value for x without intervention, and  $\tilde{z}$  represents its counterfac-080 tual value. Various types of counterfactual interventions are explored in the literature. For example, zero and mean ablations modify the mediator's value by setting it to either zero or its mean value across a reference distribution, 081 respectively (Wang et al., 2023). Another approach, symmetric token replacement, involves substituting the mediator's value with the value obtained when the model is exposed to a slightly altered input, where key tokens related to the task 083 are replaced with similar tokens of the same sequence length (Zhang & Nanda, 2024). For instance, when exploring 084 model components responsible for predicting factual information, Meng et al. (2022) use the mediator's value with respect to a *clean* input like "The Eiffel Tower is in" as the counterfactual intervention  $\tilde{z}$ , while assessing its indirect 086 effect on the model output y over a similar but slightly *corrupted* input x, such as "The Colosseum is in," for which the mediator takes the value  $z_x$ .

In its original form, activation patching iteratively assesses the indirect effect across a set of mediators, assigning 089 causal significance to a mediator's influence on the model's task behavior when the observed indirect effect exceeds 090 a defined threshold (Vig et al., 2020; Meng et al., 2022; Wang et al., 2023). The choice of mediator z varies between 091 studies, ranging from the entire output activation vector  $a \in \mathbb{R}^d$  of a module (e.g., the multi-head attention module) 092 or a submodule (e.g., the linear layer within a module), to individual neurons  $a_i \in a$  (Mueller et al., 2024). Similarly, 093 the intervention's downstream targets can be configured. For example, node patching directs the intervention to the residual stream, while edge patching affects the input to a specific model component (Miller et al., 2024). Overall, 095 a high level of granularity with respect to the intervention can lead to a combinatorial explosion of the search space 096 when exhaustively exploring all mediators (Mueller et al., 2024). To address this, several variations of activation patching have been developed—most notably, attribution patching and its derivatives (Nanda, 2023; Syed et al., 2023; Hanna et al., 2024b)-which balance accuracy and causal guarantees with improved search efficiency. In this study, we overcome the combinatorial problem by optimizing over a continuous approximation of the discrete search space 099 (see Section 3 for further details). 100

### 2.2 CIRCUIT PROPERTIES

Once a circuit has been successfully identified for a given model  $\mathcal{M}$  and task T, it can be represented as a binary mask that signifies whether a specific model component is causally relevant to the model's behavior for the task at hand. Let  $z_i \in \mathcal{Z}$  represent a single node<sup>1</sup> in the model's causal graph, denoted as  $\mathcal{G} = (\mathcal{Z}, \mathcal{E})$ , where  $\mathcal{E} \subseteq \mathcal{Z} \times \mathcal{Z}$  and  $|\mathcal{Z}| = N$ .

<sup>&</sup>lt;sup>1</sup>Depending on the granularity of the identification method, this can range from entire modules to individual neurons within the model.

- The circuit can be defined as the binary mask  $m \in \{0, 1\}^N$  over the model's node space, where each entry specifies whether a node  $z_i$  is causally relevant to the model's task behavior  $(m_i = 1)$  or not  $(m_i = 0)$ .
- Circuits are generally evaluated based on three key criteria (Wang et al., 2023):
  - 1. *Faithfulness*: A circuit is considered faithful to the task T if it accurately captures the full model's task behavior while ablating all nodes not identified as causally relevant ( $m_i = 0$ ) by replacing them with some ablation value  $\tilde{z}$  (Hanna et al., 2024b; Miller et al., 2024). Given a metric P that compares the outputs of two models for task T, task faithfulness  $F_T$  is typically quantified as:

$$F_T = P\left(\mathcal{M}\left(\cdot\right), \mathcal{M}\left(\cdot \mid \operatorname{do}\left(\boldsymbol{z} = \boldsymbol{m} \odot \boldsymbol{z}_x + (\boldsymbol{1} - \boldsymbol{m}) \odot \tilde{\boldsymbol{z}}\right)\right)\right)$$
(2)

where essentially, the causally relevant nodes identified by the circuit  $(m_i = 1)$  are preserved, while the remaining nodes  $(m_i = 0)$  are ablated via element-wise multiplication of (1 - m) with  $\tilde{z}$ .

- 2. *Minimality*: A circuit is deemed minimal if it avoids falsely identifying causally irrelevant nodes as causally relevant (Mueller et al., 2024). Formally, given a candidate set of circuits C, minimality is encouraged by selecting the circuit with the smallest norm:  $\min_{m \in C} ||m||_1$ .
- 3. Completeness: A circuit is said to be complete if it captures all nodes necessary to explain the model's behavior on task T.

While faithfulness and minimality are typically straightforward to measure, assessing completeness is more challenging. For further discussion, please refer to Section 6.

### 2.3 CONTINUOUS SPARSIFICATION

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Continuous sparsification originates from model pruning and has been introduced to sparsify networks, specifically their weight space, without causing performance degradation (Savarese et al., 2020). Unlike other pruning approaches (Srinivas et al., 2017; Louizos et al., 2018), continuous sparsification approximates  $l_0$  regularization by learning a deterministic mask  $m \in \{0, 1\}^N$  over the network's parameters  $w \in \mathbb{R}^N$  that indicates which weights to prune. The search for such a sparse subnetwork can be represented by the following minimization problem:

$$\min_{\boldsymbol{w}\in\mathbb{R}^{N},\,\boldsymbol{m}\in\{0,1\}^{N}}\mathcal{L}\left(\mathcal{M}\left(\,\cdot\,;\boldsymbol{m}\odot\boldsymbol{w}\right)\right)+\lambda\,\|\boldsymbol{m}\|_{1}$$
(3)

which uses the fact that  $\|\boldsymbol{m}\|_0 = \|\boldsymbol{m}\|_1$  for binary masks, and where  $\mathcal{L}$  denotes the loss of the network  $\mathcal{M}$ , while  $\lambda$  controls the trade-off between loss and number of parameters  $\|\boldsymbol{w}\|_0$ . To circumvent the combinatorial constraint imposed by the discrete space of  $\boldsymbol{m} \in \{0, 1\}^N$ , the mask is deterministically re-parameterized as a sigmoid function  $\sigma(\cdot)$  of the new variable  $\boldsymbol{s} \in \mathbb{R}^N$ . Specifically, this yields:

$$\min_{\boldsymbol{w}\in\mathbb{R}^{N},\,\boldsymbol{s}\in\mathbb{R}^{N}}\mathcal{L}\left(\mathcal{M}\left(\,\cdot\,;\sigma\left(\boldsymbol{\beta}\cdot\boldsymbol{s}\right)\odot\boldsymbol{w}\right)\right)+\lambda\,\|\sigma\left(\boldsymbol{\beta}\cdot\boldsymbol{s}\right)\|_{1}\tag{4}$$

where  $\beta \in [1, \infty]$  represents a temperature parameter for which the sigmoid function converges to the Heaviside function with  $\lim_{\beta \to \infty} \sigma (\beta \cdot s) = H(s)$ . By minimizing the above loss via gradient descent while jointly annealing  $\beta$ , and recovering the binary mask from the re-parameterization via m = H(s), a sparse representation of the network's parameters can be learned.

### 3 ACTIVATION PRUNING THROUGH CONTINUOUS SPARSIFICATION

To automatically identify circuits for sequence-to-sequence prediction tasks, we adopt an approach similar to the subnetwork probing method proposed by Conmy et al. (2023) and formulate the identification process as a minimization problem. For this, we leverage techniques from both causal mediation analysis (Pearl, 2001) and model pruning, specifically *continuous sparsification* (Savarese et al., 2020). Unlike traditional pruning, which aims to reduce model complexity by creating a sparse and efficient representation of the model's weight space (see Section Section 2.3), we focus on intervening on the model's activations, thereby linking our method to the causal mediation analysis that underlies activation patching.

As outlined in Section 2.2, we represent a circuit as a binary mask  $m \in \{0, 1\}^N$  over the model's mediator space—here the activation space of the model components considered—, indicating which activations z of a frozen model  $\mathcal{M}$  are

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responsible for its behavior on a given task T. To find a circuit, or binary mask m, that is both *faithful* and *minimal* (we exclude *completeness* for now; see Section 6 for a detailed discussion on *completeness*), we aim to minimize the following loss term:

$$\min_{\boldsymbol{m} \in \{0,1\}^{N}} \mathcal{L}_{T} \left( \mathcal{M}(\cdot), \mathcal{M}\left( \cdot \,|\, \operatorname{do}\left(\boldsymbol{z} = \boldsymbol{m} \odot \boldsymbol{z}_{x} + (1 - \boldsymbol{m}) \odot \tilde{\boldsymbol{z}} \right) \right) \right) + \lambda \cdot \mathcal{L}_{reg} \left( \boldsymbol{m} \right)$$
(5)

where  $\mathcal{L}_T$  captures the circuit's task faithfulness, with lower values indicating greater faithfulness, while  $\mathcal{L}_{reg}$  assesses 170 the size of the circuit. The hyperparameter  $\lambda$  controls the influence of  $\mathcal{L}_{reg}$  on the total loss term. Note that the circuit's task faithfulness is computed by comparing the output of the full model with the output when activations outside the 172 circuit  $(m_i = 0)$  are ablated by  $\tilde{z}$ , while activations inside the circuit  $(m_i = 1)$  are kept unperturbed  $(z = z_r)$ , as 173 illustrated in Equation (2). Given the combinatorial complexity of optimizing binary masks over a potentially large 174 activation space, direct optimization of m can be computationally prohibitive. However, as discussed in Section 2.3, 175 the mask can be deterministically re-parameterized using a sigmoid function  $\sigma(\cdot)$  over a new variable  $s \in \mathbb{R}^N$ , 176 following the approach of continuous sparsification (Savarese et al., 2020). Consequently, the optimization reduces to 177 the following term:

$$\min_{\boldsymbol{s}\in\mathbb{R}^{N}}\mathcal{L}_{T}\left(\mathcal{M}(\cdot),\mathcal{M}\left(\cdot\,|\,\operatorname{do}\left(\boldsymbol{z}=\sigma\left(\boldsymbol{\beta}\cdot\boldsymbol{s}\right)\odot\boldsymbol{z}_{x}+\left(1-\sigma\left(\boldsymbol{\beta}\cdot\boldsymbol{s}\right)\right)\odot\tilde{\boldsymbol{z}}\right)\right)\right)+\lambda\cdot\mathcal{L}_{reg}\left(\sigma\left(\boldsymbol{\beta}\cdot\boldsymbol{s}\right)\right)\tag{6}$$

where the sigmoid function  $\sigma$  is applied element-wise, and  $\beta$  serves as a temperature parameter that increases progressively after each training epoch, following an exponential schedule until it reaches a maximum value,  $\beta_{max}$ , as proposed by Lepori et al. (2023). As  $\beta$  approaches infinity ( $\beta \to \infty$ ), the sigmoid function converges to the Heaviside step function, i.e.,  $\sigma(\beta \cdot s) \to H(s)$ . To assess the circuit's task faithfulness, we use the Kullback-Leibler divergence  $D_{KL}(y^m \parallel y^M)$ , which captures the difference between the circuit's predicted output distribution and that of the full model. Since the full model's predicted output distribution  $y^{\mathcal{M}}$  is independent of the variable s, minimizing the KL divergence is equivalent to minimizing the cross-entropy between  $y^m$  and  $y^M$ . Accordingly, we define the crossentropy loss  $\mathcal{L}_{CE}$  as our task faithfulness loss. For regularization, we apply  $l_1$  regularization in line with continuous sparsification (see Equation (4)). Thus, the final minimization problem is formulated as follows:

$$\min_{\boldsymbol{s} \in \mathbb{R}^{N}} \mathcal{L}_{CE}\left(\mathcal{M}(\cdot), \mathcal{M}\left(\cdot \,|\, \operatorname{do}\left(\boldsymbol{z} = \sigma\left(\boldsymbol{\beta} \cdot \boldsymbol{s}\right) \odot \boldsymbol{z}_{x} + \left(1 - \sigma\left(\boldsymbol{\beta} \cdot \boldsymbol{s}\right)\right) \odot \tilde{\boldsymbol{z}}\right)\right)\right) + \lambda \cdot \|\sigma\left(\boldsymbol{\beta} \cdot \boldsymbol{s}\right)\|_{1}$$
(7)

By minimizing the expression in Equation (7), we obtain an approximation of m that strikes a balance between *faithfulness* and *minimality*, with  $\lambda$  governing the emphasis on the latter. It is important to note that during training, we optimize solely with respect to the mask approximation, specifically s, while the original model's weights and activations remain unchanged. Once training converges, the binary mask is derived through re-parameterization via m = H(s), representing the final circuit identified.

In comparison to the subnetwork probing method proposed by Conmy et al. (2023), our approach identifies circuits through deterministic re-parameterization of the binary mask  $m \in \{0,1\}^N$  as a sigmoid function of the new variable  $s \in \mathbb{R}^N$ . In model pruning, this deterministic approach has demonstrated superior performance over stochastic methods (Savarese et al., 2020; Lepori et al., 2023; Gale et al., 2019). Additionally, unlike activation patching, our approach automates the search for causally relevant nodes, enabling simultaneous assessment of the causal effects of all nodes considered, guided by the optimization process. Finally, our method supports different levels of node granularity; in this study, we focus on neuron-level interventions.

### 4 **EXPERIMENTS**

211 This work studies the modularity of a transformer-based sequence-to-sequence model by analyzing circuits responsi-212 ble for its behavior on highly compositional subtasks. Specifically, we employ activation pruning through continuous sparsification (as outlined in Section 3) to identify circuits associated with the ten string-edit operations introduced by 213 PCFG SET (Hupkes et al., 2020), a dataset designed to study compositionality within neural networks. The experi-214 mental setup, including an overview of the dataset and details on the training and evaluation processes, is outlined in 215 Section 4.1. The corresponding results are presented in Section 4.2.

Unary operation	Input	Output		
сору	$x_1 \dots x_n$	$x_1 \dots x_n$		
echo	$x_1 \dots x_n$	$x_1 \dots x_n x_n$		
repeat	$x_1 \dots x_n$	$x_1 \dots x_n x_1 \dots x_n$		
reverse	$x_1 \dots x_n$	$x_n \dots x_1$		
swap	$x_1 \dots x_n$	$x_n x_2 \dots x_{n-1} x_1$		
shift	$x_1 \dots x_n$	$x_2 \ldots x_n x_1$		

Table 1: The string-edit operations in PCFG SET from Hupkes et al. (2020).

# Binary operationInputOutputappendx, yx yprependx, yy xremove\_firstx, yyremove\_secondx, yx

### 220 227 4.1 SETUP

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### 4.1.1 DATASET

We use the PCFG SET dataset (Hupkes et al., 2020) to analyze and compare circuits for functionally related tasks. 230 As illustrated in Table 1, the dataset (Hupkes et al., 2020) comprises ten different string-edit operations (SET) applied 231 to sequences generated by a probabilistic context-free grammar (PCFG). All tasks resemble translation problems, 232 where an input sequence is transformed into a corresponding output sequence through the recursive application of the 233 string-edit operations specified within the input sequence. The dataset includes two types of functions: unary and 234 binary string-edit operations. Unary functions operate on a single string sequence, whereas binary functions require 235 two input arguments. For instance, the binary function prepend places the second argument before the first (e.g., 236 prepend  $A1, B1 \rightarrow B1 A1$ ). The input alphabet in PCFG SET consists of three categories: i) words representing 237 string-edit operations (e.g., copy or echo), ii) symbols forming the input sequence (e.g., A1, B1, etc.), and iii) a 238 separator "," that distinguishes the two arguments for binary operations. For additional information and examples, 239 please refer to Appendix A.1.

Hupkes et al. (2020) construct PCFG SET in such a way that compositionality is a salient feature of the dataset.
Notably, all operators in PCFG SET are functionally related. For example, the repeat operator can be replicated by applying the copy operation two times in succession (see Table 1). Our objective is to identify circuits for each of the ten string-edit operations in PCFG SET. To this end, we generate ten distinct data subsets, each containing examples from a specific string-edit operation. For each task, we generate 20,000 samples, with 16,000 allocated to the training set and 4,000 to the test set. Details regarding the data generation process and the individual sub-datasets can be found in Appendix A.2.

### 248 4.1.2 TRAINING

Base Model Training. As a first step, we train a base model *M* to perform all ten string-edit operations in PCFG
SET. Specifically, we use an encoder-decoder model based on the Transformer architecture (Vaswani et al., 2017), comprising six encoder and decoder layers with a hidden state dimension of 512, resulting in approximately 58 million parameters. The model is trained on the official data splits of PCFG SET Hupkes et al. (2020), which include around 83,000 training samples covering all string-edit operations and their compositions. Additional details on the training procedure and corresponding hyperparameters can be found in Appendix B.3.

256 **Mask Training.** Next, we aim to identify circuits corresponding to each subtask. This is accomplished by training 257 a binary mask  $m \in \{0,1\}^N$  over the base model's causal node space  $\mathcal{Z}$ , as described in Section 3. For each sub-258 task, we minimize the loss as described in Equation (7) by training the mask on the respective subtask dataset (see 259 Section 4.1.1). We consider individual output activations from the feed-forward and multi-head attention modules as 260 mediators  $z = a_i \in a$ . For the ablation value  $\tilde{z}$ , we conduct experiments with both zero and mean ablations. We use the same ablation value across all token positions and adopt an approach similar to node patching, where interven-261 tions target the model's residual stream. When employing mean ablations, we follow the approach proposed by Wang 262 et al. (2023) and use the mediator's mean value across a reference distribution, specifically the subtask dataset. This 263 removes variation-specific information while preserving constant information from the reference distribution. Further 264 details on the mask training procedure and associated hyperparameters can be found in Appendix B.4. 265

It is worth noting that while we choose to apply neuron-level ablations for the feed-forward and multi-head attention modules, activation pruning as introduced in Section 3 can be extended to other levels of granularity. For instance, one could adopt an approach similar to edge attribution patching (Syed et al., 2023) by applying a mask to individual edges representing inputs to other layers of interest. Alternatively, entire modules could be ablated rather than individual neurons, thereby reducing the dimension of the mask.

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Figure 1: Task faithfulness performance  $F_T$  and accuracy for the **unary** tasks. The y-axis corresponds to the circuit, while the x-axis represents the evaluation task. When we only evaluate selected positions, we omit the diagonal, as there are no applicable tokens for comparison.

### 4.1.3 EVALUATION

We evaluate circuits according to two primary criteria: performance and node overlap. Regarding performance, we assess each circuit on each string-edit operation in PCFG SET (see Section 4.1.1 for details). Specifically, we measure both the circuit's faithfulness to the original model's behavior, as defined by Equation (2), and its accuracy on the assigned task. As outlined in Section 3, the circuit's faithfulness is quantified via the KL-divergence  $D_{KL}(y^m || y^M)$ , which captures the difference between the circuit's predicted output distribution and that of the full model. However, since the KL-divergence is unbounded and therefore unsuitable for cross-task comparisons, we also use a normalized version of the Jensen–Shannon divergence JSD<sub>norm</sub> to evaluate the similarity between the circuit's predictions and those of the model (see Equation (8) in Appendix B.5). Note that  $0 \leq JSD_{norm} \leq 1$ . For visualization purposes, and to convert the loss into a performance metric, we define the circuit's *faithfulness performance* on task T as  $F_T = 1 - JSD_{norm}$ , where values approaching 1 indicate higher task faithfulness. Moreover, the circuit's accuracy is assessed by comparing the exact match between the circuit's predicted and the ground truth output sequence. When evaluating a circuit identified for task T on a different task  $\hat{T}$ , we retain the mean values from task T as ablation values for nodes with  $m_i = 0$  when using mean ablations. For a discussion on this approach, please refer to Section 6.

In addition to performance, circuits are compared based on their node overlap. For this, we use two metrics: Intersection over Union (IoU) and Intersection over Minimum (IoM), as defined in Equation (9) in Appendix B.5. Note that the IoU captures the overall overlap of the circuits relative to their combined size, whereas the IoM measures how much of the smaller circuit is contained within the larger one.

### 4.2 RESULTS

We begin by presenting the performance results of the base model on PCFG SET. After training, the encoder-decoder model exhibits strong performance across all ten string-edit operations, achieving accuracy rates exceeding 95% on unary functions and ranging between 83% and 99% on binary tasks. A detailed breakdown of the base model's taskspecific accuracy is provided in Appendix B.3. As shown in Table 3 in the appendix, the most challenging operations for the model are prepend and append.

In the following sections, we report results for the circuits identified in this study. Due to space constraints, we focus primarily on the circuits discovered via mean ablation. For additional results concerning circuits identified through zero ablation, please refer to Appendix C.2.

3173184.2.1 CIRCUIT PERFORMANCE

We first analyze the circuits' performance across different string-edit operations. Figure 1 illustrates both the task faithfulness performance,  $F_T$ , as defined in Section 4.1.3, as well as the accuracy of each circuit with respect to the six unary operations. Due to the functional similarities between the string-edit operations, multiple operators may produce the same output tokens at various token positions. Therefore, we assess faithfulness performance under two configurations: one where  $F_T$  is averaged across all output tokens (Figure 1a) and another where faithfulness is calculated only at positions where the ground truth output sequences of the circuit-task and evaluation-task diverge



Figure 2: Task faithfulness performance  $F_T$  and accuracy for the **binary** tasks. The y-axis corresponds to the circuit, while the x-axis represents the evaluation task. When we only evaluate selected positions, we omit the diagonal, as there are no applicable tokens for comparison.

(Figure 1b). For example, when evaluating the copy circuit on the echo task, the evaluation focuses on measuring task faithfulness at the final token of the target output sequence —specifically, the additional  $x_n$  in echo which differs from the end-of-sequence token in copy (see Table 1).

Unary Circuits. Analyzing the diagonal in Figure 1a, it is evident that all unary circuits demonstrate a high level of 346 faithfulness performance, with rates exceeding 0.94 on their respective tasks. Additionally, several circuits, such as 347 echo, repeat, and swap, exhibit strong cross-task faithfulness and accuracy on the copy task. This observation 348 aligns with human intuition, as the copy operation is either a significant component of these string-edit operations or 349 can be effectively performed by these functions. In contrast, operators like reverse and shift, which substantially 350 alter the input sequence, demonstrate lower functional similarity to the copy operation. This is reflected in both the reduced cross-task faithfulness (see Figure 1a; 1b) and the lower accuracy (Figure 1c) of the reverse and shift 351 circuits on the copy task. Interestingly, while the repeat and swap circuits perform well on the copy task, the 352 copy circuit does not perform as effectively on these tasks, despite the theoretical possibility of completing the repeat 353 operation through two consecutive applications of the copy operator. 354

355 For many circuits, we observe high cross-task faithfulness performance when considering all tokens, as illustrated 356 in Figure 1a. However, their faithfulness scores on tokens that differ between the circuit and the evaluation task, as well as their cross-task accuracy, tend to be low. For example, the copy circuit demonstrates a notable cross-task 357 faithfulness score of 0.64 on the swap task when evaluated across the entire output sequence, as shown in Figure 1a. 358 When focusing solely on the tokens that differ between the ground truth output sequences of copy and swap, the 359 faithfulness score drops significantly to 0.01 (see Figure 1b). This suggests that the copy circuit predominantly 360 adheres to its designated copy function, even when the input sequence demands a swap operation. The instances 361 where the copy circuit generates the correct output for the swap task —reflected in its cross-task accuracy of 0.16362 -may be attributed to the fact that applying the swap operation twice yields the same result as copy. 363

364 **Binary Circuits.** Figure 2 illustrates the performance of circuits associated with the binary string-edit operations. 365 Similar to the unary circuits, these binary circuits exhibit a high level of faithfulness for their respective tasks, with 366 performance values ranging from 0.90 to 0.99, as illustrated in Figure 2a. Notably, the remove\_first circuit 367 demonstrates strong cross-task faithfulness and accuracy when applied to the remove\_second task, although the 368 reverse is not true. Additionally, the prepend circuit shows consistently strong performance across all binary tasks. When analyzing the size of each circuit —i.e., the fraction of nodes with causal relevance to the model's task behavior, 369 expressed as a fraction of remaining activations, as displayed in Figure 3a —we observe that the prepend circuit is 370 the largest among all circuits, retaining 39% of its activations. Similarly, the remove\_first circuit is notably larger 371 than the remove\_second circuit. A potential hypothesis for this pattern is that more complex operations, such as 372 prepend, append, or remove\_first engage a larger portion of the model's activation space compared to simpler 373 functions.<sup>2</sup> For example, the remove\_second operation may be accomplished through a straightforward copy op-374 eration while producing an end-of-sequence token at the position of the separator ",". In contrast, the remove\_first 375 operation might not be executed as easily. 376

<sup>&</sup>lt;sup>2</sup>Although there is currently insufficient evidence to confirm this hypothesis, we consider it a valuable perspective worthy of inclusion. For a more detailed discussion, we refer to Section 6.



Figure 3: Node overlap for circuits identified via activation pruning with mean ablation.

Local sparsity. In Figure 3b, we visualize the local sparsity of the copy circuit, which is the smallest among all circuits. Specifically, we depict the percentage of remaining activations of the feed-forward (FFW), multi-head self-attention (MHSA), and multi-head cross-attention (MHCA) modules for each layer. Interestingly, in the decoder, we observe that the MHCA modules are predominantly active, whereas the activations in the FFW and MHSA modules are nearly entirely pruned. This might be expected, as the copy task primarily involves directing the input data processed by the encoder to the output. Additional visualizations for other circuits can be found in Appendix C.1.2.

**Zero vs. mean ablations.** The results so far relate to circuits identified via mean ablation. It is also possible to zero-ablate nodes, respectively. However, similar to prior work by Miller et al. (2024), we find circuits identified via zero ablations to be less faithful. For a detailed overview of respective results, please refer to Appendix C.2.

### 4.2.2 CIRCUIT OVERLAP

409 We compare the circuits identified for all ten string-edit operations by illustrating their respective node overlap in 410 Figure 4. Specifically, we assess the IoU and IoM between all circuit pairs, as described in Section 4.1.3. Upon 411 analyzing the overall IoU among circuits, we observe that most circuit pairs exhibit values of around 0.20 to 0.30. 412 However, certain clusters of circuits show a higher degree of node overlap. For example, the circuits for reverse, 413 swap, and shift demonstrate IoU values ranging from 0.36 to 0.42. This is further reflected in their IoM, which is 414 with values around 0.60 notably higher than for most other circuit pairs. This suggests that the base model  $\mathcal{M}$  may 415 reuse a subset of the shared activations for all three tasks. Given the functional similarities of these operations, this 416 finding aligns with intuitive expectations. However, it is worth noting that the cross-task performance of reverse, swap, and shift on their respective tasks, as depicted in Figure 1, is lower than that of other circuits. A similarly 417 high node overlap is observed for the append and prepend circuits, both associated with tasks that the base model 418 finds particularly challenging. 419

In Section 4.2.1, we demonstrated that the echo, repeat and swap circuits exhibit high cross-task performance on the copy task. This raises the question to what extent the copy circuit is embedded within these circuits. Upon examining the node overlap between the copy circuit and the aforementioned circuits, we find their IoM values to range from 0.42 to 0.56, indicating that approximately half of the nodes in the copy circuit are contained within these other circuits. For a more detailed discussion of the implications of these findings, please refer to Section 6.

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### 4.2.3 CIRCUIT COMPOSITIONS: SUBNETWORK SET OPERATIONS

Given that we can define a circuit as binary mask  $m \in \{0, 1\}^N$  over the model's mediator space, we extend our study on *cross-circuit relationships* by creating compositions through basic set operations on these masks. Specifically, for a circuit-pair  $(m^{T_1}, m^{T_2})$ , we define their composite as the union  $m^{T_1,T_2} = m^{T_1} \cup m^{T_2}$ . Importantly, this union is not symmetric: we use the ablation values  $\tilde{z}^{T_1}$  of the first circuit for nodes deemed causally irrelevant after the union  $(m_i^{T_1,T_2} = 0)$ . For additional details on how this union is applied, we refer to Appendix B.6.



Figure 4: Node overlap for circuits identified via activation pruning with mean ablation.

452 Figure 5 illustrates the cross-task accuracy of various circuits and their composites, derived from the union operation 453 previously described. The results demonstrate the existence of composite circuits which acquire functional capacities 454 for subtasks that the original base circuits could not handle individually. For example, while neither the repeat nor 455 the reverse circuit can solve the echo task alone, their union achieves a notable accuracy of 78%. Similarly, the 456 composite of swap and reverse shows a performance improvement on the shift task, reaching an accuracy of 33%. For tasks that can be solved by at least one of the original circuits, the performance of their composite generally 457 reflects a combination of their individual accuracies. For instance, the repeat circuit achieves 90% accuracy on the 458 copy task, while the reverse circuit yields 0.0% accuracy. Their union achieves an intermediate accuracy of 80%459 on the task. Similarly, the swap circuit achieves 27% accuracy on the reverse task, whereas the reverse circuit 460 reaches up to 96%. Their composite circuit achieves a balanced performance of 45%. This implies that improvements 461 in accuracy for novel tasks may be accompanied by a decline in performance on previously mastered skills. Further 462 experiments and results on subnetwork set operations can be found in Appendix C.1.4. 463

464 A possible explanation for these observations is that the union operation  $m^{T_1,T_2} = m^{T_1} \cup m^{T_2}$  shifts the activation 465 space of  $m^{T_1}$  towards  $m^{T_2}$ , effectively transforming the input into a feature space that aligns with one of the subtasks 466 the model  $\mathcal{M}$  can solve. For instance, the union  $m^{\text{swap}} \cup m^{\text{reverse}}$  might shift the activation space of  $m^{\text{swap}}$  towards 467  $m^{\text{reverse}}$ , essentially allowing the new circuit  $m^{\text{swap}, \text{reverse}}$  to to perform the shift operation, while sacrificing 468 some performance on the swap task.

### 5 RELATED WORK

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Techniques that discover circuits through causal mediation analysis have been successfully applied across various domains and tasks, including the study of gender bias in language models (Jeoung & Diesner, 2022; Chintam et al., 2023), different forms of factual recall (Meng et al., 2022; Geva et al., 2023), subject-verb agreement (Chintam et al., 2023), and arithmetic operations (Nanda et al., 2023; Hanna et al., 2024a). Finding subnetworks has also been of interest outside of the mechanistic interpretability literature. Previous work has studied task-specific subnetworks through clustering approaches (Casper et al., 2022; Watanabe, 2019), pruning Csordás et al. (2020); Cao et al. (2021); Lepori et al. (2023), sparse fine-tuning (Ansell et al., 2022), and adapters (Pfeiffer et al., 2021; Rücklé et al., 2021).

### 6 DISCUSSION

In this section, we discuss the implications of our findings, particularly focusing on the nature of the identified circuits and their significance for the model's modularity.

**What constitutes a circuit?** We introduce *activation pruning through continuous sparsification*, a method that formulates the circuit discovery process as an optimization problem balancing *task faithfulness* and *minimality*. Our

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Figure 5: The results of combining circuits through a union operation on their respective binary masks.

498 results demonstrate that this method successfully identifies circuits that are both faithful and sparse for each subtask 499 within PCFG SET. However, as discussed in Section 2.2, circuits are further expected to be *complete*, meaning they should include all nodes involved in the model's computations for a given task. We emphasize that our current ap-500 proach does not guarantee completeness. While some methods attempt to evaluate completeness by analyzing circuit 501 behavior under ablations (Wang et al., 2023), these approaches are computationally expensive, especially when dealing with large circuit sizes. Future work is needed to develop more efficient ways to quantify completeness and incorpo-503 rate this objective into the optimization framework described in Equation (7). In addition, we observe that the circuits 504 identified are influenced by the ablation value  $\tilde{z}$  used during the identification process. For example, when comparing 505 circuits based on mean versus zero ablation, we find notable differences in the nodes identified as causally relevant, 506 even for zero-ablated circuits that demonstrate high task faithfulness (see results in Appendix C.2, specifically Fig-507 ure 14). This raises a broader question about what truly defines a circuit. In our setup, a circuit's behavior in response to an input is influenced not only by the nodes deemed causally significant  $(m_i = 1)$  but also by the values  $\tilde{z}$  of the nodes where  $m_i = 0$ . Essentially, the behavior of a circuit is determined not merely by what it includes but also by what it excludes, as similarly noted by Miller et al. (2024). We believe this is a general characteristic of methods that 510 rely on constant perturbations, such as zero and mean ablations (Olsson et al., 2022; Wang et al., 2023). 511

513 Modularity in Neural Networks. Our results presented in Section 4.2 demonstrate that circuits responsible for tasks such as echo, repeat and swap are capable of successfully completing the copy task, whereas the copy 514 circuit does not perform effectively on these other tasks. This raises the question: do the echo, repeat, and swap 515 circuits leverage the copy operation for their respective functions? Our analysis on node overlap suggests that the 516 copy circuit —which is notably the smallest among those identified, as shown in Figure 3a—is largely embedded 517 within these other circuits. Moreover, circuits that share functional similarities exhibit greater node overlap compared 518 to those that are functionally distinct. While it is premature to draw definitive conclusions based on this experimental 519 evidence, we underscore the general observation that more complex operations tend to engage a larger portion of 520 the model's activations and are capable of solving multiple tasks. Furthermore, we find that circuits combined via 521 the union operator can represent novel functional capabilities. This might suggest some level of modularity within 522 the network. One might argue that our identification process has not produced truly minimal circuits. While it is 523 inherently challenging to determine whether a circuit is truly minimal, we have mitigated this concern by conducting 524 an extensive hyperparameter search, ensuring a fair balance between faithfulness and minimality. Lastly, it is important to note that our study focuses on a small encoder-decoder model trained on a single dataset like PCFG SET. Naturally, the question arises as to whether these findings will generalize to larger models commonly used in practice. This 526 touches on a broader concern within the field of mechanistic interpretability, where many studies are conducted on 527 smaller models and datasets (Elhage et al., 2022). While scaling our findings to larger models is an area for future 528 research, we believe the methodology used in this study offers valuable insights for future investigations into the 529 compositionality of larger, more complex models. 530

### 7 CONCLUSION

This study explores modularity in neural networks by analyzing circuits in a transformer-based language model for highly compositional subtasks. Specifically, we train an encoder-decoder model using the PCFG SET dataset and identify circuits responsible for ten modular string-edit operations. To achieve this, we introduce *activation pruning through continuous sparsification*, a method that allows us to formulate circuit identification as minimization problem. Our results demonstrate that this approach successfully identifies both faithful and sparse circuits for each subtask within PCFG SET. Additionally, we assess all circuits by examining their cross-task performance and node overlap. Finally, we show that new functional circuits can be composed through set operations, such as the union of two circuits.

### 8 **REPRODUCIBILITY STATEMENT**

542 To ensure the reproducibility of our experiments, we make all code publicly available as supplementary material 543 and provide comprehensive instructions along with user-friendly bash scripts for replicating our results. Details of 544 the training process, including the computational setup, model implementation, and hyperparameter selection, are thoroughly documented in Section 4.1.2 and Appendix B. Similarly, a detailed account of the evaluation procedure can be found in Section 4.1.3 and Appendix B.5. Furthermore, all data used in this work is either publicly available 546 or accompanied by a detailed description of the data generation process in Appendix A, supported by scripts that 547 facilitate its reproduction. 548

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Unary operation	Input	Output	Example
copy echo repeat reverse swap shift	$\begin{array}{c} x_1 \dots x_n \\ x_1 \dots x_n \end{array}$	$\begin{array}{c} x_1 \dots x_n \\ x_1 \dots x_n x_n \\ x_1 \dots x_n x_1 \dots x_n \\ x_n \dots x_1 \\ x_n x_2 \dots x_{n-1} x_1 \\ x_2 \dots x_n x_1 \end{array}$	copy K1 Y1 W1 K1 $\rightarrow$ K1 Y1 W1 K1 echo E1 K1 A1 X1 J $\rightarrow$ E1 K1 A1 X1 J1 J1 repeat J1 F1 S1 $\rightarrow$ J1 F1 S1 J1 F1 S1 reverse G1 T1 X1 J1 $\rightarrow$ J1 X1 T1 G1 swap B1 Z1 V1 I1 W1 $\rightarrow$ W1 Z1 V1 I1 B1 shift Y1 I1 D1 H1 K1 $\rightarrow$ I1 D1 H1 K1 Y1
Binary operation	Input	Output	Example
append prepend remove_first remove_second	$egin{array}{c} x,y\ x,y\ x,y\ x,y\ x,y\ x,y\ x,y\ x,y\$	x y y x y x	append F1 B1, U1 A1 G1 $\rightarrow$ F1 B1 U1 A1 G1 prepend F1 B1, U1 A1 G1 $\rightarrow$ U1 A1 G1 F1 B1 remove_first Z1 P1 N1, A1 D1 $\rightarrow$ A1 D1 remove_second F1 B1, U1 A1 G1 $\rightarrow$ F1 B1

Table 2: The string-edit operations in PCFG SET from Hupkes et al. (2020).

# A DATASET

### A.1 PCFG SET

Hupkes et al. (2020) construct PCFG SET in such a way that compositionality is a salient feature of the dataset, while aligning its statistical properties with those of natural language corpora, specifically English. We present examples for each string-edit operation in Table 2 to help the reader get more familiar with the functions employed in PCFG SET Hupkes et al. (2020).

### A.2 GENERATING ISOLATED FUNCTION DATA

We use the probabilistic context-free grammar proposed by Hupkes et al. (2020) to generate datasets for each of the string-edit operations originally used to construct PCFG SET. Using the same vocabulary, consisting of letters [A - Z] combined with numbers in  $(0, \infty] \in \mathbb{Z}^+$ , we restrict the grammar to produce samples that use only specific string-edit operation for each subtask dataset, e.g. copy W1 O1 Z5 G1. For each SET operation, we generate 160000 samples for training and 4000 for validation. Each subtask dataset includes samples of both single-use and composed applications of that function, such as remove\_first remove\_first A1, B1, B1A1  $\rightarrow$  B1A1.

### **B** EXPERIMENTAL DETAILS

We provide all code for our experiments through the supplementary material. In this section, we outline key details regarding our experiments, such as our computational setup and the hyperparameters selected.

### B.1 SOFTWARE AND COMPUTING

All experiments are implemented using PyTorch (Paszke et al., 2019) as the primary framework. Detailed information about supporting software and specific versions can be found in our code repository. All experiments have been conducted using AMD Instinct MI250X accelerators.

### B.2 BASE MODEL ARCHITECTURE

The base model  $\mathcal{M}$  is a transformer-based encoder-decoder, as proposed by Vaswani et al. (2017), but with the Gated Linear Unit (GLU) variant from Shazeer (2020). We use sinusoidal positional encoding, delimit tokens on whitespace, and disjoint embedding matrices for the input and output sequences. The base model  $\mathcal{M}$  consists of six encoder and six decoder layers, with a hidden size of dimension 512, and eight attention heads per layer.

### 752 B.3 BASE MODEL TRAINING

We train the base model  $\mathcal{M}$  using a learning rate of  $5 \cdot 10^{-7}$ , a batch size of 64 without gradient accumulation, a gradient clipping value of 15, and a dropout rate of 0.2. Furthermore, the model is trained using the original datasets from Hupkes et al. (2020). In Table 3, we report the accuracy of the base model on each of the isolated subtask

Unary operation	Accuracy	Binary operation	Accuracy
yqoo	1.0	append	0.848
echo	0.999	prepend	0.832
repeat	0.943	remove_first	0.975
reverse	0.989	remove_second	0.999
swap	0.996		
shift	0.992		

Table 3: The generation accuracy of the base model on the different subtasks(Hupkes et al., 2020).

datasets. The base model  $\mathcal{M}$  achieves final accuracy of 87.8% on the official PCFG test set, which is slightly lower than the performance of 92.0% reported by Hupkes et al. (2020).

### B.4 MASK TRAINING

In this study, we conduct experiments for both mean and zero ablation. Following the approach of Wang et al. (2023), the mean ablation value  $\tilde{z}$  is derived from a reference distribution. Specifically, when training a mask for task  $T_l$  on dataset  $D_l$ , we assign the ablated value  $\tilde{z}_i$  for each potential mediator  $z_i$  in  $\mathcal{M}$  as the average activation of  $z_i$  across samples in  $D_l$ , which only includes samples corresponding to task  $T_l$ . For instance, when training a mask for the copy task, the ablated value  $\tilde{z}_i$  for each mediator  $z_i$  is set to the average activation of  $z_i$  over samples exclusively containing the copy function, i.e.,  $D_{copy}^{train}$ , averaged across all token positions.

The final optimization problem, described in Equation (7), requires the predicted output probabilities  $y^{\mathcal{M}}$  of the base model  $\mathcal{M}$  for each dataset sample across all of the subtask datasets. In practice, this is achieved through caching: a forward pass is performed on all datasets using  $\mathcal{M}$ , and  $y^{\mathcal{M}}$  is stored for later use during mask training.

### B.4.1 HYPERPARAMETERS

In Table 4 we report the final hyperparameters for the mask training for each subtask, using the same notation as in Section 3. These are selected based on a random search over the following hyperparameters: learning rate:  $\{1 \cdot 10^{-3}, 1 \cdot 10^{-4}, 1 \cdot 10^{-5}\}$ ,  $\lambda$ :  $\{1 \cdot 10^{-3}, 1 \cdot 10^{-4}, 1 \cdot 10^{-5}\}$ ,  $s_{initial}$ :  $\{0.2, 0.05, 0\}$ ,  $\beta_{max}$ :  $\{100, 200, 300\}$ .

Circuit	lr	$\lambda$	$m{s}_{ ext{initial}}$	$\beta_{max}$	Epochs
echo	$1\cdot 10^{-4}$	$1\cdot 10^{-4}$	0.05	200	500
сору	$1\cdot 10^{-4}$	$1\cdot 10^{-4}$	0.05	200	500
repeat	$1\cdot 10^{-4}$	$1\cdot 10^{-4}$	0.05	200	500
reverse	$1 \cdot 10^{-4}$	$1 \cdot 10^{-4}$	0.05	200	500
swap	$1 \cdot 10^{-4}$	$1\cdot 10^{-4}$	0.05	200	500
shift	$1\cdot 10^{-4}$	$1\cdot 10^{-4}$	0.05	200	500
append	$1 \cdot 10^{-3}$	$1 \cdot 10^{-5}$	0	200	500
prepend	$1\cdot 10^{-3}$	$1\cdot 10^{-5}$	0	100	500
remove_first	$1 \cdot 10^{-4}$	$1 \cdot 10^{-5}$	0.05	300	500
remove_second	$1 \cdot 10^{-3}$	$1 \cdot 10^{-5}$	0.05	100	300

Table 4: Final hyperparameters used for mask training.

### **B.5** EVALUATION

We evaluate circuits according to two primary criteria, performance and node overlap, as described in Section 4.1.3. Specifically, we quantify the performance of a circuit by its *faithfulness* score, which is calculated via the KL divergence,  $D_{KL}$ , between the output distribution of the circuit  $y^m$  and the base model  $y^M$ . However, to get a bounded metric, we instead use the normalized version of the Jensen-Shannon divergence between the two output distributions:

$$JSD_{norm}\left(\boldsymbol{y^{m}} \parallel \boldsymbol{y^{\mathcal{M}}}\right) = \frac{1}{2\log(2)}\left(D_{KL}\left(\boldsymbol{y^{m}} \parallel \boldsymbol{y^{m\mathcal{M}}}\right) + D_{KL}\left(\boldsymbol{y^{\mathcal{M}}} \parallel \boldsymbol{y^{m\mathcal{M}}}\right)\right), \text{ where } \boldsymbol{y^{m\mathcal{M}}} = \frac{\boldsymbol{y^{m}} + \boldsymbol{y^{\mathcal{M}}}}{2}$$
(8)

where  $y^{m\mathcal{M}}$  is a mixture distribution of  $y^m$  and  $y^{\mathcal{M}}$ . Note that the Jensen-Shannon divergence is symmetric. Furthermore, it is bounded, i.e.,  $0 \leq \text{JSD}_{\text{norm}} \leq 1$ .

To measure the circuits' node overlap we compute their Intersection over Union (IoU) and Intersection over Minimum (IoM). Given two circuits  $m^{T_1} \in \{0,1\}^N$  and  $m^{T_2} \in \{0,1\}^N$  defined over the same node space, the IoU and IoM are computed as follows:

$$IoU = \frac{\|\boldsymbol{m}^{T_1} \cap \boldsymbol{m}^{T_2}\|_1}{\|\boldsymbol{m}^{T_1} \cup \boldsymbol{m}^{T_2}\|_1} \qquad IoM = \frac{\|\boldsymbol{m}^{T_1} \cap \boldsymbol{m}^{T_2}\|_1}{\min\left(\|\boldsymbol{m}^{T_1}\|_1, \|\boldsymbol{m}^{T_2}\|_1\right)}$$
(9)

where  $m^{T_1} \cap m^{T_2}$  represents the intersection of the two binary masks, while  $m^{T_1} \cup m^{T_2}$  denotes their union. Specifically, the intersection between two circuits  $m^{T_1,T_2} = m^{T_1} \cup m^{T_2}$  is defined as:

$$m_i^{T_1,T_2} = m_i^{T_1} \cap m_i^{T_2} = m_i^{T_1} \wedge m_i^{T_2} = \begin{cases} 1 & \text{if } m_i^{T_1} = 1 \text{ and } m_i^{T_2} = 1, \\ 0 & \text{otherwise.} \end{cases}$$
(10)

Similarly, the union between two circuits  $m^{T_1,T_2} = m^{T_1} \cup m^{T_2}$  can be computed as:

$$m_i^{T_1,T_2} = m_i^{T_1} \cup m_i^{T_2} = m_i^{T_1} \vee m_i^{T_2} = \begin{cases} 0 & \text{if } m_i^{T_1} = 0 \text{ and } m_i^{T_2} = 0, \\ 1 & \text{otherwise.} \end{cases}$$
(11)

### **B.6** SUBNETWORK COMPOSITIONS

When creating circuit compositions, we apply the union operator between the binary masks of two circuits, as illustrated in Equation (11). For zero-ablated circuits, this operation remains symmetric. However, in the case of mean-ablated circuits, symmetry is not preserved. This is primarily due to the fact that the mediator value,  $z_i$ , for which  $m_i = 0$  after the union, is ablated by the mean value across the reference distribution associated with the first circuit's task,  $\tilde{z}_i^{T_1}$ . Specifically, for the union  $m^{T_1,T_2} = m^{T_1} \cup m^{T_2}$ , the mediator value  $z_i$  is determined as follows:

$$\boldsymbol{z}_{i} = \begin{cases} \tilde{\boldsymbol{z}}_{i}^{T_{1}} & \text{if } m_{i}^{T_{1}} = 0 \text{ and } m_{i}^{T_{2}} = 0, \\ \boldsymbol{z}_{T_{i}} & \text{otherwise,} \end{cases}$$
(12)

This means that  $m^{T_1} \cup m^{T_2} \neq m^{T_2} \cup m^{T_1}$  for mean ablations if  $\tilde{z}_i^{T_1} \neq \tilde{z}_i^{T_2}$ . For zero ablation, the ablation value remains the same for both cases  $\tilde{z}_i^{T_1} = \tilde{z}_i^{T_2} = 0$ , thus yielding symmetry of the operator. Please refer to Section 6 for further discussion.

### C SUPPLEMENTAL RESULTS

In this section, we report supplemental results that complement the paper's key findings.

C.1 MEAN ABLATION

We first report additional results related to circuits identified via mean ablation.

### C.1.1 CIRCUIT PERFORMANCE

In Figure 6 and Figure 7 we report the KL divergence between the predicted output distributions of the mean-ablated circuits, m, and the base model,  $\mathcal{M}$ , for both unary and binary string-edit operations. The results exhibit a trend consistent with the observations discussed in Section 4.2.1.



Figure 6: Task faithfulness measured via  $D_{KL}(y^m || y^M)$  for the **mean-ablated unary** circuits. The y-axis corresponds to the circuit, while the x-axis represents the evaluation task. When we only evaluate selected positions, we omit the diagonal, as there are no applicable tokens for comparison.



Figure 7: Task faithfulness measured via  $D_{KL}(y^m || y^M)$  for the **mean-ablated binary** circuits. The y-axis corresponds to the circuit, while the x-axis represents the evaluation task. When we only evaluate selected positions, we omit the diagonal, as there are no applicable tokens for comparison.

### C.1.2 LOCAL SPARSITY

Figure 16 illustrates the local sparsity of each unary circuit identified via mean-ablations, while 17 presents the local sparsity of each binary circuit, respectively. It is evident that unary circuits are highly sparse, with no module retaining more than 45% of activations. Notably, the feed-forward (FFW) and multi-head self-attention (MHSA) modules within the decoder demonstrate pronounced sparsity across all layers, typically retaining only 0.0% to 10% of activations. In contrast, the multi-head cross-attention (MHCA) modules retain a higher proportion of activations. As shown in Figure Figure 17, binary circuits generally retain a greater number of activations. Specifically, the append and prepend circuits show substantial remaining activations in both the encoder and decoder.

### C.1.3 DETERMINISTIC MASK APPROXIMATION.

915 As discussed in Section 3, a key advantage of learning a binary mask through continuous sparsification is the deter-916 ministic nature of the approach. To assess whether our method consistently converges to the same circuits despite the 917 stochastic elements of the training process (e.g., dataset shuffling), we examine the node overlap of circuits trained 918 using different random seeds. Our findings demonstrate that the method reliably converges to the same mask for identical subtasks, regardless of the random seed. This holds true for both mean and zero ablation. For example, we report an IoU and IoM of 1.0 when comparing five prepend circuits trained with varying random seeds.

## C.1.4 SET OPERATIONS

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Figure 8: The results of combining circuits through a union operation on their respective binary masks.

In Figure 8 we present the cross-task accuracy of additional composite circuits as supplementary results to Section 4.2.3. Consistent with previous observations, the union of two circuits acquires functional capacities for subtasks that the original base circuits cannot perform independently. For example, the union  $m^{\text{swap}} \cup m^{\text{repeat}}$  achieves a 56% accuracy on the reverse task and 31% on shift, representing significant improvements over the performance of these circuits in isolation. Similarly, the union  $m^{\text{reverse}} \cup m^{\text{echo}}$  reaches 31% accuracy on swap. In the case of  $m^{\text{shift}} \cup m^{\text{echo}}$ , we observe that while the composite retains approximately half of the performance on the individual tasks, it also enhances performance on the copy task.

### 949 C.2 ZERO ABLATION

While the main paper focuses on circuits obtained through mean ablation, this section presents the results from the same set of experiments conducted using zero ablation.

### C.2.1 CIRCUIT PERFORMANCE

In Figure 9 and Figure 10, we present the task faithfulness performance  $F_T$  and generation accuracy for the zeroablated circuits. Similarly, Figure 11 and Figure 12 illustrate task faithfulness in terms of the KL divergence between the predicted output distributions of the zero-ablated circuits, m, and the base model,  $\mathcal{M}$ , for both unary and binary string-edit operations. The key finding from these experiments is that zero ablation yields results closely aligned with those of mean ablation for binary operations, but not for unary operations. Similarly, patterns observed in mean-ablated unary circuits are not evident here. As noted in the literature, zero ablation can significantly shift the distribution, leading to degraded performance, which is one of the reasons for adopting mean ablation (Miller et al., 2024).

962 963 C.2.2 NODE OVERLAP

Figure 13 illustrates the IoU and IoM between all circuit-pairs under zero ablation. The observed patterns are consistent
 with those identified under mean ablation (Figure 4), where unary circuits tend to exhibit higher node overlap compared
 to binary circuits.

### 968 C.3 COMPARISON BETWEEN MEAN AND ZERO ABLATION 969

Figure 14 illustrates the overlap between the mean and zero ablated circuits for identical subtasks. As discussed in
Section 6, we find significant differences in the circuits identified, specifically for unary circuits that tend to engage a smaller portion of the base model's activation space (refer to Figure 15 for comparison).



Figure 9: Task faithfulness performance  $F_T$  and accuracy for the **unary** tasks for the **zero** ablated circuits. The y-axis corresponds to the circuit, while the x-axis represents the evaluation task. For task faithfulness with respect to positions where the ground truth tokens differ between the circuit and the evaluation task, the diagonal is omitted, as there are no applicable token positions for comparison.



Figure 10: Task faithfulness performance  $F_T$  and accuracy for the **binary** tasks for the **zero** ablated circuits. The y-axis corresponds to the circuit, while the x-axis represents the evaluation task. For task faithfulness with respect to positions where the ground truth tokens differ between the circuit and the evaluation task, the diagonal is omitted, as there are no applicable token positions for comparison.

### C.4 GLOBAL SPARSITY

In Figure 15 we present the global sparsity of the circuits for both mean and zero ablation. As touched upon in Section 6, we observe that while the two ablation strategies identify circuits of comparable sizes, they do not necessarily yield identical circuits. Additionally, the ordering of circuits in terms of remaining activations is nearly the same for both methods, with the only notable difference being the internal ordering of swap and reverse.



Figure 11: Task faithfulness measured via  $D_{KL}(y^m || y^M)$  for the **zero-ablated unary** circuits. The y-axis corresponds to the circuit, while the x-axis represents the evaluation task. When we only evaluate selected positions, we omit the diagonal, as there are no applicable tokens for comparison.



Figure 12: Task faithfulness measured via  $D_{KL}(y^m || y^M)$  for the **zero-ablated binary** circuits. The y-axis corresponds to the circuit, while the x-axis represents the evaluation task. When we only evaluate selected positions, we omit the diagonal, as there are no applicable tokens for comparison.



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Figure 17: The local sparsity of the **binary** circuits achieved via mean ablation. Considered are feed-forward (FFW), multi-head self-attention (MHSA), and multi-head cross-attention (MHCA) modules for each layer.