

# 000 SCALABLE CIRCUIT LEARNING FOR INTERPRETING 001 002 LARGE LANGUAGE MODELS 003 004

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## 007 008 ABSTRACT 009

010  
011 A prominent research direction within mechanistic interpretability involves learning  
012 sparse circuits to model causal relationships between LLM components,  
013 thereby providing insights into model behavior. However, due to the polysemantic  
014 nature of LLM components, learned circuits are often difficult to interpret.  
015 While sparse autoencoder (SAE) features enhance interpretability, their high di-  
016 mensionality presents a significant challenge for existing circuit learning methods  
017 to scale. To address these limitations, we propose a scalable circuit learning ap-  
018 proach, *CircuitLasso*, that leverages sparse linear regression. Our method  
019 can efficiently uncover relationships among SAE features, showing how human-  
020 interpretable semantic features propagate through the model and influence its pre-  
021 dictions. We empirically evaluate our method against state-of-the-art baselines  
022 on benchmark circuit learning tasks, demonstrating substantial improvements in  
023 efficiency while accurately capturing circuits involving LLM components. Given  
024 its efficiency, we then apply our method to SAE (high dimensional) features and  
025 obtain human-interpretable circuits for a grammatical classification task that has  
026 not been studied before in mechanistic interpretation. Finally, we validate the  
027 utility of our learned circuits by leveraging their insights to improve downstream  
028 performance in domain generalization.

## 029 1 INTRODUCTION 030

031 The fundamental challenge of mechanistic interpretability is to understand the “why” behind the  
032 behaviors of large language models (LLMs). A key technique involves discovering causal circuits,  
033 which are compact subgraphs connecting key components within the model (such as attention heads  
034 and neurons) that drive a specific behavior or capability. However, existing methods for circuit learn-  
035 ing often face a bottleneck. The raw components of an LLM, such as individual neurons, are known  
036 to be polysemantic, meaning that a single neuron can be activated by and contribute to multiple,  
037 seemingly unrelated concepts. This polysemanticity renders the learned circuits dense, noisy, and  
038 challenging for humans to interpret, undermining the very goal of mechanistic interpretability.

039 The limitations of using raw, polysemantic neurons have motivated a shift toward a more promising  
040 foundation for circuit analysis based on Sparse Autoencoders (SAEs) and related tools. SAEs are  
041 neural networks trained to reconstruct the activations of an LLM’s raw components using a high-  
042 dimensional but sparse set of “features”. Remarkably, these SAE features tend to be monosemantic,  
043 i.e., each feature consistently activates for a single, human-interpretable concept, such as “related  
044 to sports,” “a specific emotion,” or “a particular grammatical structure.” The monosemanticity of  
045 SAE features has the potential not only to enhance interpretability in itself but also to yield sparser,  
046 cleaner causal graphs, and perhaps more faithful representations of the model’s internal processing.

047 Our work is motivated by the above potential of SAE features to achieve greater interpretability  
048 in LLM circuit analysis. However, existing circuit learning methods, many of which are designed  
049 for the lower-dimensional space of raw neurons, struggle to scale to the high-dimensional feature  
050 space of SAEs. The computational complexity and the risk of finding spurious correlations increase  
051 dramatically. To address this, we introduce a novel approach to handle the high dimensionality. Our  
052 method, *CircuitLasso*, utilizes the Lasso (i.e.,  $\ell_1$ -penalized linear regression) to find a sparse  
053 set of connections between features that explains the model’s behavior. Sparse linear regression is  
well-suited for high-dimensional data, as it is computationally efficient and the sparsity translates to

more interpretable circuits. An advantage of our approach is its use of observational data only. This

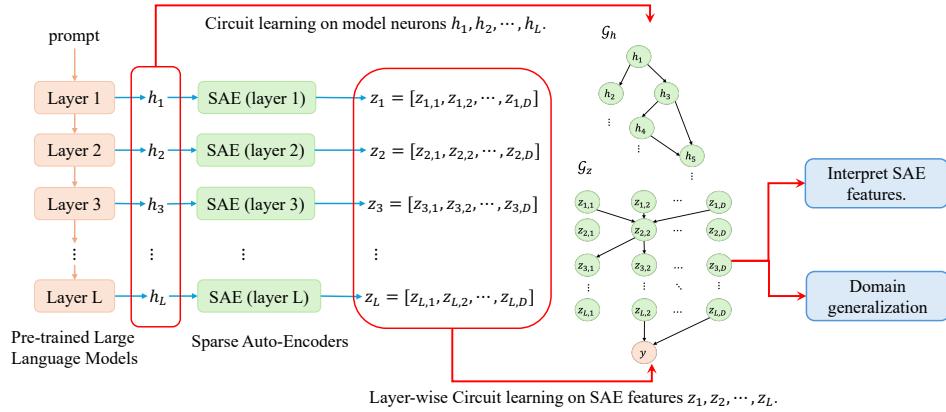


Figure 1: An illustration of our model neuron activation and SAE feature collection procedure, learned circuits, and potential downstream tasks.

broadens its applicability and eliminates the need for interventions used by existing methods, whose cost scales with LLM size. We quantify the efficiency advantage of our regression-based method through a theoretical analysis of its computational cost compared to state-of-the-art intervention-based approaches, establishing conditions under which our method guarantees greater efficiency.

We empirically evaluate `CircuitLasso` against state-of-the-art baselines on a circuit learning benchmark, demonstrating substantial improvements in efficiency while accurately capturing circuits involving LLM components. Leveraging its scalability, we then apply our method to SAE features and obtain human-interpretable circuits for the CoLA dataset, which has not been used before in mechanistic interpretability studies. Finally, we validate the utility of our learned circuits by leveraging them to improve performance in a downstream application of domain generalization.

Our primary contributions are as follows: 1) Inspired by causal graph discovery literature, we introduce an efficient sparse circuit discovery method, `CircuitLasso`, and theoretically analyze its computational cost compared to intervention-intensive approaches. 2) `CircuitLasso` facilitates operating on monosemantic but high-dimensional SAE features, potentially offering clearer explanations of how human-interpretable concepts propagate through LLMs. 3) Extensive experiments across LLMs (up to 9B parameters), SAEs, and datasets demonstrate the efficiency and effectiveness of `CircuitLasso` for circuit discovery and improving generalization performance.

## 2 RELATED WORKS

**Mechanistic Interpretability.** Much of the established work in mechanistic interpretability explains behaviors in terms of raw or coarse-grained model components. [Olsson et al. \(2022\)](#) implicated induction heads in in-context learning, while others ([Meng et al., 2022](#); [Geva et al., 2023](#); [Nanda et al., 2023](#)) examined MLP modules for factual recall. However, due to the polysemantic nature of raw neurons and coarse-grained components ([Elhage et al., 2022](#)), the resulting mechanistic insights are often difficult to apply to downstream tasks. Some prior methods ([Geiger et al., 2023](#); [Zou et al., 2023](#)) attempt to address this issue by fitting model internals to pre-defined hypotheses using curated data, but these approaches fail to generalize to scenarios where researchers lack expert knowledge or cannot anticipate how models implement specific behaviors. Recent work ([Bricken et al., 2023](#); [Cunningham et al., 2023](#)) leverages advances in dictionary learning for interpretability and introduces sparse autoencoders (SAEs) to identify sparse, disentangled features in high-dimensional spaces that align with human-interpretable concepts. Building on this, a number of advanced strategies for learning SAE features have been proposed ([Rajamanoharan et al., 2024](#); [Gao et al., 2024](#); [Bussmann et al., 2024](#); [Dunefsky et al., 2024](#)). Despite this progress, existing mechanistic interpretability methods continue to face challenges in scaling to the high-dimensional SAE feature space.

108 **Circuit Learning.** Intervention-based circuit learning approaches, including causal mediation analysis (Vig et al., 2020; Geva et al., 2023; Hanna et al., 2024) and causal tracing (Meng et al., 2022),  
 109 rely on counterfactual intervention techniques such as activation patching (Nanda, 2023; Syed et al.,  
 110 2023) to quantify the influence of one component on another. However, these interventions are  
 111 computationally intensive, making it difficult to scale such methods to large sets of components, let  
 112 alone to the high-dimensional space of sparse autoencoder (SAE) features. To address this, Marks  
 113 et al. (2025) propose efficient approximations of intervention-based methods for SAE features, but  
 114 in high-dimensional settings they must resort to heuristic pre-processing steps such as clustering.  
 115 These limitations highlight the need for more efficient techniques to learn circuits in LLMs. For  
 116 example, Laptev et al. (2025a) propose a data-free approach that constructs circuit graphs using in-  
 117 formation from SAE decoder weights. While many prior works borrow causal concepts (Meng et al.,  
 118 2022), the broader causal discovery literature has been less explored in the context of circuit learn-  
 119 ing. Notably, Conmy et al. (2024) iteratively prune edges from the computation graph, reminiscent  
 120 of constraint-based causal discovery algorithms such as the PC algorithm (Pearl et al., 2000).  
 121

### 3 CIRCUIT LEARNING FRAMEWORK AND METHODOLOGY

#### 3.1 CIRCUIT DISCOVERY FROM A CAUSAL PERSPECTIVE

122 In this work, we formulate circuit discovery as the task of learning a directed acyclic graph (DAG)  
 123 from data, analogous to approaches in causal discovery. State-of-the-art approaches quantify the im-  
 124 portance of hidden representations or computational graph edges by estimating their causal effects,  
 125 particularly indirect effects, using techniques such as causal mediation analysis (Vig et al., 2020),  
 126 causal tracing (Meng et al., 2022), attribution patching (Nanda, 2023; Syed et al., 2023), and related  
 127 variants (Kramár et al., 2024; Hanna et al., 2024). These approaches share some similarities with  
 128 constraint-based causal discovery, which assesses potential edges among variables via indepen-  
 129 dence tests and retains those with strong dependencies. However, constraint-based causal discovery meth-  
 130 ods are known to face scalability challenges, and circuit discovery methods share this limitation  
 131 since they must separately quantify the importance of every hidden representation and edge in the  
 132 computational graph, which can quickly become infeasible with larger models.  
 133

134 Inspired by the continuous causal discovery literature, we propose a (causal) circuit discovery ap-  
 135 proach, *CircuitLasso*. Assume we extract  $N$  components (which may be MLP neurons, at-  
 136 tention heads, or SAE features) from all the desired locations in the LLMs and concatenate their  
 137 activations to form a vector  $\mathbf{x} = [x_1, x_2, \dots, x_N] \in \mathbb{R}^N$ . Our goal is to learn the DAG  $\mathcal{G}$  with the  
 138  $N$  components as its nodes. We leverage structural equation models (SEM) from continuous causal  
 139 discovery literature to model the causal relations between a component  $x_i$  and its parents  $Pa_{\mathcal{G}}(x_i)$ :  
 140  $x_i = f_i(Pa_{\mathcal{G}}(x_i)) + \varepsilon_i$ , where  $f_i(\cdot)$  is the causal function and  $\varepsilon_i$  is the exogeneous noise. In this  
 141 work, we assume the causal relations between components are linear. Given  $M$  observations of the  
 142  $N$  components, i.e., input matrix  $\mathbf{X} \in \mathbb{R}^{N \times M}$ , we can then obtain the linear SEM in its matrix  
 143 form:  
 144

$$\mathbf{X} = A^T \mathbf{X} + \varepsilon, \quad (1)$$

145 with continuous parameters  $A \in \mathbb{R}^{N \times N}$ , a weighted adjacency matrix;  $\varepsilon \in \mathbb{R}^{N \times M}$  is a matrix of  
 146 mutually independent exogeneous noises.  $A[i, j] \neq 0$  indicates the existence of the causal relation  
 147  $x_i \rightarrow x_j$ . We aim to learn  $A$  by minimizing the reconstruction error between  $\mathbf{X}$  and  $A^T \mathbf{X}$  subject  
 148 to sparsity and acyclicity constraints:  
 149

$$\hat{A} = \arg \min_A \|\mathbf{X} - A^T \mathbf{X}\|_F^2 + \lambda \|A\|_1, \text{ subject to } \mathcal{G}(A) \in \mathbb{D} \quad (2)$$

150 where  $\|\cdot\|_F$  denotes Frobenius norm;  $\|A\|_1$  is the sparsity penalty with tuning coefficient  $\lambda$ ;  $\mathcal{G}(A)$  is  
 151 the circuit structure inferred from  $A$ ; and  $\mathbb{D}$  is the space of acyclic graphs with  $N$  nodes. We lever-  
 152 age the established identifiability conditions (Peters et al., 2014) by assuming causal sufficiency  
 153 and specific noise characteristics (non-Gaussian or equal-variance Gaussian) to ensure the learned  
 154 DAG is uniquely identifiable and thus interpretable as the underlying causal structure. Thus far,  
 155 in Eq. (2), we have not made assumptions about the causal ordering of the components in  $\mathbf{x}$ , i.e.,  
 156 the orientations of potential edges between components. Thus, we require the acyclicity constraint  
 157  $\mathcal{G}(A) \in \mathbb{D}$  to prevent self-loops and cycles, which are unsuitable for interpreting the transmission,  
 158 aggregation, and evolution of model components. However, the acyclicity constraint is the main  
 159 computational challenge in solving the circuit learning problem in Eq. (2). In this paper, we make  
 160

162 simplifying assumptions that remove this constraint and reduce the optimization to sparse linear re-  
 163 gression problems (also known as Lasso), enabling a scalable solution. We discuss the formulations  
 164 for circuit discovery on model neurons and SAE features in Sections 4.1 and 3.3.2, respectively.  
 165

166 **3.2 CIRCUIT DISCOVERY ON NEURONS**  
 167

168 To better understand how models encode and process information, mechanistic interpretability re-  
 169 search (Conmy et al., 2023a; Cao et al., 2021; Syed et al.) has focused on identifying graphical  
 170 structures (circuits) connecting pre-trained language model neurons, including outputs from atten-  
 171 tion and MLP modules. To evaluate the effectiveness of our proposed method in Section 3.1, we  
 172 follow the same setting as these prior works and treat model neurons as the components of interest.  
 173 We first collect neuron activations  $[\mathbf{h}_1, \mathbf{h}_2, \dots, \mathbf{h}_L]$  from  $L$  target locations, each with dimension  $d$ ,  
 174 and for  $M$  LLM inputs (observations), resulting in  $\mathbf{H} \in \mathbb{R}^{L \times d \times M}$ . Existing circuit discovery meth-  
 175 ods typically assume that circuit structures respect the model locations’ computation order, meaning  
 176 that neurons from layer  $i$  precede those from layer  $j$  if  $i < j$ , and within each layer, attention activa-  
 177 tions come before MLP activations. We adopt this assumption to simplify the acyclicity constraint  
 178 in Eq. (2). Accordingly, we reorder  $\mathbf{H}$  according to the computational graph and reshape it to obtain  
 179  $\tilde{\mathbf{H}} \in \mathbb{R}^{N \times M}$ , whereby  $N = Ld$ . Substitute  $\mathbf{X}$  in Eq. (2) with  $\tilde{\mathbf{H}}$  to estimate the weighted adjacency  
 180 matrix  $A$  as

$$181 \hat{A} = \arg \min_A \|\tilde{\mathbf{H}} - A^\top \tilde{\mathbf{H}}\|_F^2 + \lambda \|A\|_1, \quad \text{subject to } A \text{ being block lower triangular.} \quad (3)$$

183 Specifically, each block  $A[i, j]$  is now a  $d \times d$  square matrix, and  $A[i, j] = 0^{d \times d}$  whenever  $i \leq j$ .  
 184 This block lower triangular structure ensures that each block of variables depends only on preceding  
 185 blocks, so later layers cannot influence earlier ones, thereby preserving the causal ordering without  
 186 requiring an explicit acyclicity constraint. **This constraint exploits the known, human-engineered**  
 187 **computational order of the LLM.** The underlying architectural insight provides a justifiable acyclic  
 188 constraint that aligns with the inherent feed-forward nature of the network (activations in later layers  
 189 are computed after, and depend on, those in earlier layers). Causal discovery with such a justified  
 190 acyclicity leads to more accurate identification of the underlying causal relationships, as demon-  
 191 strated by empirical results in Table 1. In practice, we enforce this constraint by initializing the  
 192 upper-triangular blocks to zero matrices and keeping them fixed throughout optimization. The re-  
 193 sulting circuit structure  $\mathcal{G}$  is then inferred from  $\hat{A}$ .

194 We now provide complexity analysis of our proposed circuit discovery approach on model neurons  
 195 versus the existing intervention-based approaches. For our optimization problem in Eq. (3), we have:

196 **Proposition 3.1. Complexity of CircuitLasso on Model Neurons.** Suppose in Eq. (3),  $\tilde{\mathbf{H}} \in$   
 197  $\mathbb{R}^{N \times M}$  contains  $M$  samples of  $N$ -dimensional features, whereby  $N = Ld$ . Assume a first-order  
 198 optimization method is used to solve the problem up to convergence error  $\epsilon$ , then the computational  
 199 complexity of solving Eq. (3) is  $\mathcal{O}\left(\frac{ML(L-1)d^2}{2\epsilon}\right)$ .  
 200

201 Please refer to the detailed proof in Appendix A.1. We aim to theoretically compare the compu-  
 202 tational cost of our CircuitLasso with the state-of-the-art intervention-based circuit discovery  
 203 approach. Specifically, we consider the EAP-ig method, which computes IEs for  $L$  locations of  
 204 model components with dimension  $d$ . EAP-ig relies on the *attribution patching* technique, which  
 205 applies a linear approximation to IEs, enabling them to be computed in parallel. While the additional  
 206 cost of estimating IEs from this linear approximation scales linearly with  $L$  and considered to have  
 207 state-of-the-art efficiency, the primary computational burden arises from the two forward passes and  
 208 one backward pass required for each evaluation of the LLM. Hence, we first provide a computation  
 209 cost estimation for the EAP-ig with the same learning problem in Eq. (3) and provide conditions  
 210 when our CircuitLasso has guaranteed efficiency over EAP-ig.

211 **Proposition 3.2.** Suppose a transformer-based large language model with  $S$  blocks has model neu-  
 212 ron dimension of  $d$ .  $n_{\text{token}}$  is the tokens sequence length,  $h$  is the number of attention heads,  $f$  being  
 213 the feedforward expansion factor, then the approximate computational cost of  $M$  observations for  
 214 EAP-ig is roughly  $\mathcal{O}\left(16MSn_{\text{token}}d^2(2+f) + 16MSn_{\text{token}}^2d + MLd\right)$ , CircuitLasso with  
 215 computational complexity of  $\mathcal{O}\left(\frac{ML(L-1)d^2}{2\epsilon}\right)$  has guaranteed better efficiency compared to EAP-ig

216 if one of the following conditions hold: 1)  $\sqrt{\frac{L(L-1)}{32S(2+f)\epsilon}} < n_{token} \ll d$ . 2)  $n_{token} > \sqrt{\frac{L(L-1)d}{32S\epsilon}}$  and  
 217  $n_{token} \gg d$ .  
 218

219 Please refer to the detailed proof in Appendix A.2. Intuitively, **Proposition 3.2** provides a guide-  
 220 line for selecting the number of component locations of interest ( $L$ ) and determining which circuit  
 221 discovery approach is more efficient.  
 222

### 223 3.3 CIRCUIT DISCOVERY ON SPARSE FEATURES 224

225 Although recent research has shown that learned circuits can carry semantically meaningful information  
 226 and shed light on how information flows through the model, the polysemantic nature of neurons  
 227 makes them difficult to interpret (Elhage et al., 2022). To address this, more recent work (Marks  
 228 et al., 2025; Laptev et al., 2025b) explores circuit discovery on sparse SAE features, but the scal-  
 229 ability challenge posed by their high dimensionality remains. To address this issue, we extend our  
 230 proposed formulation to operate on SAE features.  
 231

#### 232 3.3.1 PRELIMINARIES ON SPARSE AUTOENCODER (SAE) 233

234 Given a model with  $d$ -dimensional latent space and neuron activations  $\mathbf{h} \in \mathbb{R}^d$ , an SAE can represent  
 235  $\mathbf{h}$  as a linear combination of sparse features  $\mathbf{z} \in \mathbb{R}^D, D \gg d$ :  
 236

$$237 \mathbf{z} = \sigma(\mathbf{W}_{\text{enc}}\mathbf{h} + \mathbf{b}_{\text{enc}}), \quad \hat{\mathbf{h}} = \mathbf{W}_{\text{dec}}\mathbf{z} + \mathbf{b}_{\text{dec}},$$

238 where  $\mathbf{W}_{\text{enc}}, \mathbf{b}_{\text{enc}}$  are encoder parameters and  $\mathbf{W}_{\text{dec}}, \mathbf{b}_{\text{dec}}$  are decoder parameters ;  $\sigma(\cdot)$  is a nonlinear  
 239 activation function. The SAEs are usually trained by minimizing the reconstruction error between  
 240 model activations  $\mathbf{h}$  and reconstructed activations  $\hat{\mathbf{h}}$  subject to a sparsity regularizer:  
 241

$$242 \mathcal{L}_{\text{SAE}}(\mathbf{h}, \mathbf{z}; \mathbf{W}_{\text{enc}}, \mathbf{b}_{\text{dec}}, \mathbf{W}_{\text{dec}}, \mathbf{b}_{\text{dec}}) := \|\mathbf{h} - \hat{\mathbf{h}}\|_2^2 + \alpha \mathcal{L}_{\text{reg}}(\mathbf{z}).$$

243 Recent work on sparse autoencoder (SAE) features explores various methods—ReLU with  $L_1$  reg-  
 244 ularization, thresholding, top- $K$  selection, and Transcoders, to enforce sparsity and improve in-  
 245 terpretability. However, our focus is to uncover the causal relations among learned sparse SAE  
 246 features, rather than developing new SAE training methods. For this study, we employ the fol-  
 247 lowing pre-trained SAEs on small (GPT2-small, Pythia-70M), medium (Gemma-2-2b), and large  
 248 (Gemma-2-9b) LLMs. Please refer to Appendix C.1 for details of employed models and SAEs.  
 249

#### 250 3.3.2 LAYER-WISE SPARSE FEATURE CIRCUIT DISCOVERY 251

252 In this work we assume that causal relations follow the computation order of the underlying model  
 253 neurons. To be specific, consider two model neurons with dimension of  $d$  and their activations at  
 254 locations  $i$  and  $j$ , denoted by  $\mathbf{h}_i, \mathbf{h}_j \in \mathbb{R}^d$ , where computation at  $i$  precedes computation at  $j$ . We  
 255 obtain the corresponding SAE features  $\mathbf{z}_i, \mathbf{z}_j \in \mathbb{R}^D$  using trained SAEs:  
 256

$$257 \mathbf{z}_i = \sigma(\hat{\mathbf{W}}_{\text{enc},i}\mathbf{h}_i + \mathbf{b}_{\text{enc},i}), \quad \mathbf{z}_j = \sigma(\hat{\mathbf{W}}_{\text{enc},j}\mathbf{h}_j + \mathbf{b}_{\text{enc},j}).$$

258 If a causal relationship exists between variables in  $\mathbf{z}_i$  and  $\mathbf{z}_j$ , we constrain its direction to be from  $i$   
 259 to  $j$ . Given  $M$  observations of  $\mathbf{z}_i$  and  $\mathbf{z}_j$ , we obtain input data  $\mathbf{Z}_i \in \mathbb{R}^{D \times M}$  and  $\mathbf{Z}_j \in \mathbb{R}^{D \times M}$ . We  
 260 estimate these relations by solving:  
 261

$$\hat{A}_{i,j} = \arg \min_{A_{i,j}} \|\mathbf{Z}_j - A_{i,j}^\top \mathbf{Z}_i\|_F^2 + \lambda \|A_{i,j}\|_1, A_{i,j} \in \mathbb{R}^{D \times D}. \quad (4)$$

262 This procedure is repeated for every pair  $(i, j)$  where  $i$  precedes  $j$  in the computation order. In partic-  
 263 ular, learning  $A_{i,j}$  for all transformer block outputs in consecutive layers provides insight into how  
 264 semantic concepts are transferred, propagated, and evolved across the model. The computational  
 265 cost of the learning problem in Eq. (4) is  $\mathcal{O}(\frac{MD^2}{\epsilon})$ .  
 266

267 We also incorporate the downstream prediction target into circuit discovery to enable explanation of  
 268 the model’s predictive behavior. We formulate the following optimization problem to learn a model  
 269 for predicting the downstream target  $y$  using sparse atuoencoder features  $\mathbf{z}_i$ , derived from model  
 270 neuron activations at location  $i$ :

$$271 \hat{A}_{i,y} = \arg \min_{A_{i,y}} \mathcal{L}_{\text{pred}}(\mathbf{y}, A_{i,y}^\top \mathbf{Z}_i) + \lambda \|A_{i,y}\|_1, A_{i,y} \in \mathbb{R}^D, \quad (5)$$

270 where  $\mathcal{L}_{\text{pred}}(\cdot, \cdot)$  denotes the prediction loss, instantiated as mean squared error for regression tasks  
 271 and cross-entropy loss for classification tasks. Application-wise, with the learned  $A_{i,y}$  and interpre-  
 272 tatable sparse features  $z$ , we can not only explain the model’s predictive behavior, but also rectify  
 273 the prediction model to mitigate spurious or biased behavior. The computational cost of the learning  
 274 problem in Eq. (5) is  $\mathcal{O}(\frac{MD}{\epsilon})$ .  
 275

## 276 4 EXPERIMENTS

277 We evaluate **CircuitLasso** on both model neurons (Section 4.1) and sparse autoencoder fea-  
 278 tures (Section 4.2), demonstrating its effectiveness in accurately capturing relations among model  
 279 components with improved efficiency, providing interpretable insights into model behavior in gram-  
 280 maticality classification, and enhancing downstream performance on a domain generalization task.  
 281

### 283 4.1 CIRCUIT DISCOVERY ON MODEL NEURONS

285 **Models and Baselines.** We first evaluate our circuit discovery methods on the INTERPBENCH  
 286 benchmark datasets (Gupta et al., 2024). INTERPBENCH consists of semi-synthetic yet realistic  
 287 transformers with known circuits, designed for assessing circuit discovery approaches. The trans-  
 288 former models are trained to align their internal computation with a target high-level causal model  
 289 while constraining non-circuit nodes from influencing the output. We compare our method against  
 290 four state-of-the-art circuit discovery approaches: Automatic Circuit DisCovery (ACDC) (Conmy  
 291 et al., 2023b), Subnetwork Probing (SP) (Cao et al., 2021) on nodes and edges, Edge Attribution  
 292 Patching (EAP) (Syed et al., 2023), and EAP with integrated gradients (EAP-ig) (Marks et al.,  
 293 2025). While INTERPBENCH includes 86 semi-synthetic transformer models, we follow the proto-  
 294 col of Gupta et al. (2024) and evaluate on the 5 randomly selected cases, which have been empirically  
 295 verified to be sufficiently realistic for benchmarking circuit discovery techniques.  
 296

296 **CircuitLasso on Neurons.** We begin by collecting activations from the model neurons. To  
 297 ensure fairness, we use the same set of input prompts as the baselines. Given data, we aim to learn  
 298 a weighted adjacency matrix  $A$  that encodes the causal relations between neuron locations, and use  
 299 it to infer the causal circuit. Please refer to the detailed learning procedure in Appendix B.

300 **Metrics and Implementation Details.** We evaluate circuit discovery accuracy using the Structural  
 301 Hamming Distance (SHD) between the ground-truth and estimated circuits, and assess efficiency  
 302 by measuring runtime in seconds. All experiments were performed over three trials on an NVIDIA  
 303 A100 machine. We report the mean and standard deviation results in the Table 1.

304 Cases	ACDC		SP		EAP		EAP-ig		CircuitLasso	
	SHD	Runtime	SHD	Runtime	SHD	Runtime	SHD	Runtime	SHD	Runtime
306 3	7.6 $\pm$ 0.06	78.9 $\pm$ 2.81	9.0 $\pm$ 0.18	112.5 $\pm$ 4.89	12.2 $\pm$ 0.25	25.1 $\pm$ 3.18	5.2 $\pm$ 0.13	42.2 $\pm$ 4.03	4.9 $\pm$ 0.14	10.6 $\pm$ 0.03
307 4	13.7 $\pm$ 3.50	118.8 $\pm$ 45	15.3 $\pm$ 3.91	92.4 $\pm$ 6.82	19.8 $\pm$ 4.76	58.1 $\pm$ 7.69	11.1 $\pm$ 2.25	61.9 $\pm$ 9.16	9.4 $\pm$ 2.88	18.34 $\pm$ 5.30
308 8	9.8 $\pm$ 2.16	121.5 $\pm$ 9.81	11.0 $\pm$ 1.88	204.9 $\pm$ 17.92	20.9 $\pm$ 4.92	54.8 $\pm$ 2.83	7.2 $\pm$ 1.29	87.2 $\pm$ 7.19	7.4 $\pm$ 0.96	50.2 $\pm$ 6.43
309 11	5.5 $\pm$ 0.86	89.1 $\pm$ 11.97	8.7 $\pm$ 1.47	117.6 $\pm$ 9.81	11.7 $\pm$ 2.91	68.7 $\pm$ 5.08	4.3 $\pm$ 0.89	72.1 $\pm$ 6.34	3.9 $\pm$ 0.22	21.3 $\pm$ 3.08
101	14.2 $\pm$ 5.11	90.7 $\pm$ 7.21	19.5 $\pm$ 5.14	118.5 $\pm$ 18.16	20.9 $\pm$ 4.92	48.9 $\pm$ 6.01	10.9 $\pm$ 4.58	51.7 $\pm$ 5.48	9.3 $\pm$ 2.91	20.8 $\pm$ 2.50

310 Table 1: The circuit discovery performance in terms of efficiency (runtime in seconds) and accuracy  
 311 (SHD) on 5 cases from INTERPBENCH.  
 312

313 According the empirical result in Table 1, we can establish that CMINT is capable of identify-  
 314 ing causal relations between model components with accuracy on par with intervention-based ap-  
 315 proaches, while simultaneously offering markedly improved computational efficiency.  
 316

### 317 4.2 CIRCUIT DISCOVERY ON SPARSE AUTOENCODER FEATURES

319 We now turn to applying **CircuitLasso** to popular pre-trained LLMs and more realistic tasks,  
 320 having shown its efficiency advantages over intervention-based methods in Section 4.1. We adapt  
 321 **CircuitLasso** to learn causal circuits on sparse autoencoder features (as described in Sec-  
 322 tion 3.3.2), revealing model behaviors in terms of human-interpretable concepts (Section 4.2.1).  
 323 Following Marks et al. (2025), we also leverage insights from learned circuits to improve domain  
 324 generalization (Section 4.2.2).

324 4.2.1 CASE STUDIES OF PROVIDING INTERPRETATION  
325326 **Data and Model.** We demonstrate our approach on the **Corpus of Linguistic Acceptability** (CoLA)  
327 task (Warstadt et al., 2018) from the GLUE benchmark (Wang et al., 2018), aiming to reveal the  
328 inner workings of gpt2-small (Nanda & Bloom, 2022) through interpretable features derived from  
329 OpenAI’s pre-trained sparse autoencoders for gpt2-small. The CoLA dataset is (to our knowledge)  
330 a new dataset for mechanistic interpretation studies. It contains 10,657 sentences from 23 linguistics  
331 publications, annotated for grammaticality by the original authors. We conduct our interpretability  
332 experiments on the 8,551 training sentences in the public release.333 **CircuitLasso on Sparse Autoencoder Features.** We extract gpt2-small’s neuron activations on  
334 the  $M$  training sentences and corresponding sparse autoencoder features. Please refer to the detailed  
335 learning procedure in Appendix B.336 **Sparse Feature Interpretation within Learned Circuits.** The following paragraphs describe our  
337 method for interpreting the learned circuit and its constituent sparse features by tracing backward  
338 from the prediction target  $y$ . Starting with  $A_{L,y}$ , we select features in  $z_L \in \mathbb{R}^D$  that are important  
339 for predicting  $y$ . The measure of importance can be either the absolute coefficients  $|A_{L,y}|$ , or if we  
340 wish to focus on a particular prompt, the Hadamard product  $s = |A_{L,y}| \odot |z_L| \in \mathbb{R}^D$  between  
341 the absolute coefficients and the absolute activations of  $z_L$  for this prompt. Suppose the  $k^{\text{th}}$  sparse  
342 feature  $z_{L,k} \in z_L$  is chosen as an important feature. To uncover the semantic concept encoded by  
343  $z_{L,k}$ , we apply two complementary, cross-validating procedures:344 **Multi-prompt approach.** We identify multiple prompts and the tokens with them that strongly activate  
345  $z_{L,k}$ . By inspecting the collected tokens, we infer the semantic concept encoded by  $z_{L,k}$ . For  
346 example, words ending in “-self” consistently activate the sparse feature  $z_{12,20726}$ , suggesting that  
347 this feature captures the presence of such words. Examples are illustrated in Table 5, 6, and 7 in  
348 Appendix C.4.349 **Single-prompt approach.** To validate the plausibility of the identified semantic concept for  $z_{L,k}$ ,  
350 we select a single prompt, systematically vary one or more of its tokens according to the concept,  
351 and observe the resulting changes in  $z_{L,k}$ . If altering the tokens causes  $z_{L,k}$  to lose activation, the  
352 inferred concept is considered reasonable. For example, in the prompt “He said that himself was  
353 hungry,” the word “himself” (the fifth token) activates  $z_{12,20726}$  to a value of 1.3509. Replacing  
354 “himself” with “him”, “he”, or other alternatives without the suffix “-self” reduces the activation of  
355  $z_{12,20726}$  to 0. An example is illustrated in Table 8 in Appendix C.4.356 With the above *multi-prompt* and *single-prompt* approaches, we identify the semantics of important  
357 sparse features in the final layer. For example, feature  $z_{12,20726}$  captures the concept of “-self”,  
358  $z_{12,3092}$  corresponds to “ending punctuation”,  $z_{12,776}$  to “thirst/hunger”, and  $z_{12,19322}$  to  
359 “tired/weary”. For each important feature  $z_{L,k}$ , we then trace its most influential parent variables  
360 in the previous layer  $L-1$  using the learned adjacency matrix  $A_{L-1,L}$ . As with layer  $L$ , we may choose to focus on the current prompt and define the importance measure as the product  
361  $s = |\frac{\partial z_{L,k}}{\partial z_{L-1}}| \odot |z_{L-1}| \in \mathbb{R}^D$ . We then select the most important features (for example  $z_{11,6368}$ ,  
362  $z_{11,29778}$ ,  $z_{11,29041}$ , and  $z_{11,21518}$ ), and interpret their semantics using the same *multi-prompt* and  
363 *single-prompt* procedures. Repeating this process across all consecutive pairs of layers yields tree-  
364 shaped circuit paths spanning the transformer blocks, offering intuition into how semantic concepts  
365 are encoded, propagated, and ultimately contribute to task-specific predictions.366 Figure 2 presents such a tree-shaped circuit, consisting of sparse features with human-interpretable  
367 meanings across 5 layers. More examples are provided in Appendix C.5. From the circuits in Figure  
368 2, we make the following observations:369 **Persistence.** Certain semantic concepts persist along circuit paths across multiple layers, particularly  
370 in the later layers. For example, the concept of “-self” is present in the 20726<sup>th</sup> feature of layer 12, the 6368<sup>th</sup>  
371 feature of layer 11, the 2985<sup>th</sup> feature of layer 10, the 9592<sup>th</sup> feature of layer 9, and the 15186<sup>th</sup> feature of layer 8. We highlight circuit paths that capture persistence relations between  
372 consecutive layer features in black.373 **Merging and Dropping.** We also observe that sparse features in later layers can merge semantic  
374 concepts from multiple parent features in the preceding layer, or disregard (i.e., drop) certain  
375 concepts contributed by those parent features. For instance, the 10609<sup>th</sup> feature of layer 9 merges

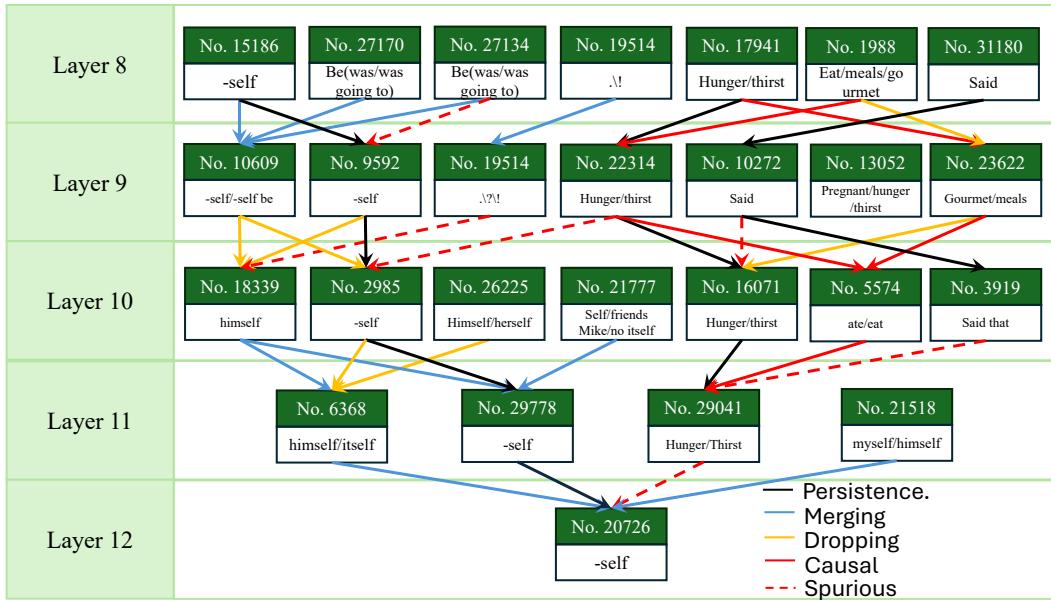


Figure 2: The learned circuits over SAE features on GPT2-small model. Different colors represent different types of edges in the computation graph.

concepts from both the 15186<sup>th</sup> and 27170<sup>th</sup> features of layer 8. In contrast, the 6368<sup>th</sup> feature of layer 11 retains only the concept “himself” and disregards all other forms of “-self” from the 2985<sup>th</sup> feature of layer 10. We highlight circuit paths representing propagation in blue and decomlocation in orange.

**Cause-Effects and Spurious Correlations.** Our circuits can capture causal relations between features that encode cause–effect semantic concepts. For example, the 22314<sup>th</sup> feature of layer 9 represents the concept of “hunger/thirst,” which can be considered a cause of the action “ate/eat,” encoded in the 5574<sup>th</sup> feature of layer 10. However, our assumption that causal orientations align with the computation order results in some circuit paths appearing anti-causal. From a human perspective, one typically feels hungry before taking actions such as “eat food/meals/gourmet,” yet our circuit includes a path from the 1988<sup>th</sup> feature of layer 8 to the 22314<sup>th</sup> feature of layer 9, which implies the reverse. Moreover, our circuits also capture spurious correlations. For example, the 29041<sup>th</sup> feature of layer 12, which represents “-self,” is spuriously correlated with the “hunger/thirst” concept encoded in the 29041<sup>th</sup> feature of layer 11. Such correlations are likely introduced by biases in the training data, such as the frequent co-occurrence of these two semantic concepts within the same sentence. By analyzing these circuit paths, we can infer the nature of dataset biases and potentially mitigate them through targeted model editing. We next show how such insights from a learned circuit can be leveraged to improve downstream domain generalization in Section 4.2.2.

**Faithfulness and Completeness.** To more comprehensively evaluate the quality of our learned circuits on SAE features, we further assess them on the CoLA dataset using the **faithfulness** and **completeness** metrics, following the standard protocol in Marks et al. (2025). In particular, we introduce a new ablation strategy: rather than ablating features outside the circuit by replacing them with their dataset-average values, we ablate edges by removing their direct contributions to the output. Let the learned circuit be  $C$ , and define the model output  $m = p(Y = \text{grammatically correct}) - p(Y = \text{grammatically wrong})$ . We first apply the standard feature ablation method of Marks et al. (2025) and compare our results with the intervention-based circuit-learning method SHIFT. To ensure fairness, we exclude SAE reconstruction errors and attention/MLP SAEs from SHIFT. For our CircuitLasso approach, we focus only on SAE features within the learned circuit and still ablate features in the original LLM. The top two plots in Figure 3 show the node ablation results. Our learned circuit achieves performance comparable to SHIFT, consistent with the findings in Marks et al. (2025) that relatively small feature circuits can explain a substantial portion of a model’s be-

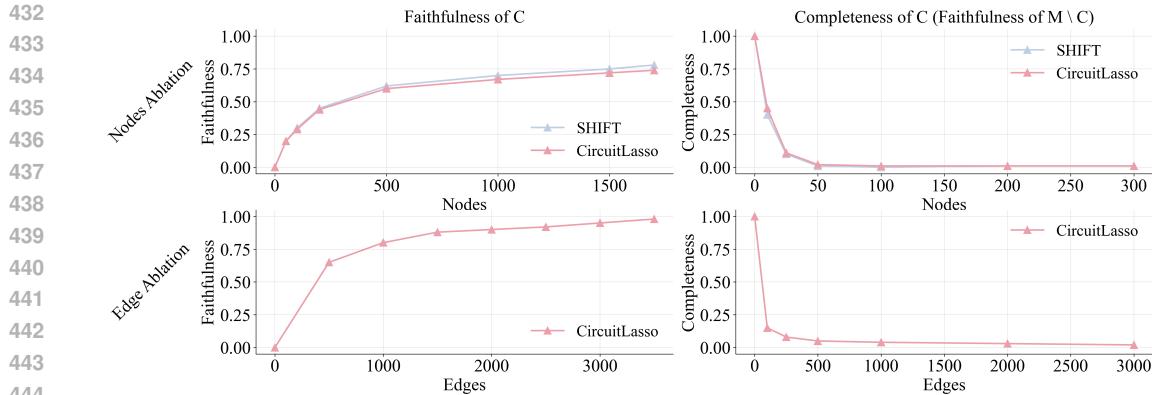


Figure 3: Faithfulness and completeness scores for the learned circuits, evaluated on the CoLA training dataset using both node ablation and novel-edge ablation. Ideal faithfulness is 1, and ideal completeness is 0.

havior. We then perform edge ablation on our circuit. Because our sparse-regression framework explicitly learns edge coefficients, representing the direct influence of each SAE feature on the output, we can ablate a specific edge by setting its coefficient to zero, thereby removing that dependence.<sup>1</sup> The bottom two plots in Figure 3 report these results. The conclusions mirror those from node ablation: a small subset of essential edges, together with their corresponding SAE features, governs the model’s prediction behavior.

#### 4.2.2 DOWNSTREAM TASK: DOMAIN GENERALIZATION

A common approach in domain generalization is to construct predictors that are robust across domains by removing unintended, domain-variant features, which may be predictive in-distribution but fail to generalize. Inspired by the ability of `CircuitLasso` to identify and interpret important features for predicting the downstream target, we investigate whether `CircuitLasso` can remove spurious features.

**Data, Models and Baselines.** We evaluate `CircuitLasso` for domain generalization on the same dataset as Marks et al. (2025), the Bias in Bios dataset (BiB) (De-Arteaga et al., 2019). This dataset consists of professional biographies with the task of classifying an individual’s profession from their biography. The BiB dataset encodes a spurious semantic concept, gender, based on which two subsets are constructed: an ambiguous set, where profession and gender are strongly correlated<sup>2</sup>, and a balanced set, where profession and gender are independent<sup>3</sup>. The goal is to produce a profession classifier that performs accurately on the balanced set but is trained only on the ambiguous set. While Marks et al. (2025) demonstrate their approach on small to moderate LLMs (Pythia-70M (Biderman et al., 2023) and Gemma-2-2B (Team, 2024)), we extend their evaluation to a larger LLM, Gemma-2-9B (Team, 2024). For all three models, we employ the pre-trained SAEs provided by Lan et al. (2024). Following the evaluation protocol in Marks et al. (2025), we compare against several baselines: a predictor trained on the ambiguous set (ORIGINAL); a predictor trained on the balanced set (ORACLE); concept bottleneck probing (CBP, Yan et al., 2023); and spurious human-interpretable feature trimming (SHIFT, Marks et al., 2025). For existing baseline SHIFT, we adopt the variant that operates on SAE features with manual inspection and evaluation, and exclude the versions trained on neurons or without human inspection due to their consistently inferior performance. We report SHIFT results using both the original linear classifier and a retrained classifier.

<sup>1</sup>We do not apply edge ablation to SHIFT, since it does not provide edge-level correlations between SAE features and the output.

<sup>2</sup>For example, all professors are assumed to be male, while nurses are assumed to be female.

<sup>3</sup>The balanced set contains equal numbers of male professors, male nurses, female professors, and female nurses.

486  
**CircuitLasso for Domain Generalization.** We select SAE features from a specific location  
487 of a pre-trained LLM, such as the transformer output at layer 22 in Gemma-2-2B. We ablate spu-  
488 riuous features by setting their values to zero and *directly feed* the resulting SAE feature values into  
489 our trained linear classifier. In addition, similar to SHIFT, we also investigate retraining the linear  
490 classifier on the ablated SAE features. Please refer to Appendix B for more details.  
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492 493 494 495 496 497 498 499 500 501 502 503 504 505 506 507 508 509 510	492 493 494 495 496 497 498 499 500 501 502 503 504 505 506 507 508 509 510			492 493 494 495 496 497 498 499 500 501 502 503 504 505 506 507 508 509 510			492 493 494 495 496 497 498 499 500 501 502 503 504 505 506 507 508 509 510		
Method	Pythia-70M	Gemma-2-2B	Gemma-2-9B	Method	Pythia-70M	Gemma-2-2B	Gemma-2-9B		
ORIGINAL	61.9	87.4	24.4	69.6	79.5	4.1	70.8	78.2	23.4
CBP	83.3	60.1	67.7	90.1	<b>50.2</b>	86.8	94.7	<b>50.0</b>	91.5
ORACLE	93.0	49.4	91.4	<b>95.1</b>	<b>50.2</b>	91.7	95.7	<b>50.0</b>	90.5
SHIFT	88.5	54.0	76.0	72.8	51.6	43.7	77.1	52.8	67.9
SHIFT-retrain	93.1	52.0	<b>89.0</b>	94.2	52.4	92.4	96.0	51.3	90.3
CircuitLasso	90.5	<b>50.1</b>	75.8	77.5	50.7	50.5	81.5	50.3	69.8
CircuitLasso-retrain	<b>94.2</b>	50.6	88.7	<b>95.1</b>	52.8	<b>92.9</b>	<b>96.9</b>	50.5	<b>91.5</b>

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Table 2: Prediction accuracy with different LLMs and domain generalization methods.

504 505 506 507 508 509 510	504 505 506 507 508 509 510		504 505 506 507 508 509 510		504 505 506 507 508 509 510		504 505 506 507 508 509 510		504 505 506 507 508 509 510	
Method	Pythia-70M	Gemma-2-2b	Gemma-2-9b	# of features	Runtime (s) ↓	# of features	Runtime (s) ↓	# of features	Runtime (s) ↓	
SHIFT	49	257.6	65	371.2	71	908.4				
SHIFT-retrain		356.3		476.8		1056.0				
CircuitLasso	41	<b>36.5</b>	55	<b>47.2</b>	59	107.4				
CircuitLasso-retrained		61.9 (17.37%)		72.5 (15.20%)		125.2 (11.98%)				

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Table 3: Runtime and numbers of selected features for SHIFT versus our CircuitLasso method.  
The runtime does not include manual interpretation time.

514  
**Results.** Tables 2 and 3 present the accuracy and efficiency of our approach compared to base-  
515 lines. Overall, CircuitLasso consistently achieves competitive or superior results, with clear  
516 efficiency advantages that become more pronounced as model size increases. The prediction out-  
517 comes in Table 2 demonstrate that CircuitLasso can reliably identify spurious correlations from  
518 the learned circuit. Both CircuitLasso and CircuitLasso-retrain slightly outperform SHIFT,  
519 which we attribute to our design choice of directly feeding SAE features into a linear classifier.  
520 This enables prediction using disentangled semantic concepts, allowing more effective ablation of  
521 spurious features and retraining. Efficiency results in Table 3 further underscore the strengths of  
522 CircuitLasso, as it requires fewer features and substantially less runtime than SHIFT, partic-  
523 ularly for large models. These findings confirm that CircuitLasso not only achieves stronger  
524 generalization but also scales more efficiently without compromising interpretability.

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5 CONCLUSION AND DISCUSSION

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In this work, we presented a new circuit learning method, CircuitLasso, based on Lasso re-  
528 gression. Our work offers a novel and effective solution to the challenges of polysemy and  
529 high dimensionality in LLM circuit learning. By shifting the focus from polysemantic neurons to  
530 the monosemantic features extracted by SAEs and applying a scalable sparse regression approach,  
531 we are able to discover circuits that are both accurate and interpretable. Our method’s ability to  
532 handle high-dimensional data, its reliance on observational data, and the sparsity of its learned cir-  
533 cuits represent significant advantages over existing baselines. We believe this research offers new  
534 insights on how LLMs work and can be impactful for various downstream applications, such as  
535 domain generalization.

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## 653 A THEORETICAL PROOFS

### 654 A.1 PROOF FOR PROPOSITION 3.1

655 *Proof.* Solving Eq. (3) is equivalent to solve  $N$  LASSO problems. The  $n^{\text{th}}$  regression has most  $p_n \leq$   
 656    $\lfloor \frac{n}{d} \rfloor d$  predictors. Per iteration cost for a single regression is roughly  $\mathcal{O}(p_n d M)$ . For  $N$  regressions,  
 657   we have  $\mathcal{O}(Md \sum_{n=1}^N p_n) = \mathcal{O}(\frac{ML(L-1)d^2}{2})$ . For a smooth loss function, first-order methods  
 658   typically require  $\mathcal{O}(\frac{1}{\epsilon})$  iterations to reach an error tolerance  $\epsilon$ . Hence the total computational cost  
 659   over all iterations is  $\mathcal{O}(\frac{ML(L-1)d^2}{2\epsilon})$ .  $\square$   
 660  
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### 662 A.2 PROOF FOR PROPOSITION 3.2

663 *Proof.* Assume  $d$  to be model hidden dimension,  $n_{\text{token}}$  to be the tokens sequence length,  $h$  to be the  
 664   number of attention heads, so head dimension being  $k = \frac{d}{h}$ , and  $f$  being the feedforward expansion  
 665   factor, for one transformer block:

- 666   • Q/K/V projections:  $\approx 6n_{\text{token}}d^2$
- 667   •  $QK^T$  across all heads:  $\approx 2n_{\text{token}}^2 d$ .
- 668   • Attention-weighted  $V$  across heads:  $\approx 2n_{\text{token}}^2 d$
- 669   • Output projection:  $\approx 2n_{\text{token}}d^2$
- 670   • Feed-forward network (two linear layers  $d \rightarrow fd \rightarrow d$ ):  $\approx 4fn_{\text{token}}d^2$

671 For the forward pass, the asymptotic complexity is approximately:  
 672

$$673 \quad \mathcal{O}(n_{\text{token}}d^2(8 + 4f) + 4n_{\text{token}}^2 d)$$

674 For the backward pass, the asymptotic complexity is approximately 2 to 3 times forward passes, we  
 675   take the lower bound here and approximate it as:  
 676

$$677 \quad \mathcal{O}(n_{\text{token}}d^2(16 + 8f) + 8n_{\text{token}}^2 d)$$

678 Hence, for 2 forward passes and one backward pass of  $M$  observations across  $S$  blocks, we have  
 679   computational cost:  
 680

$$681 \quad \mathcal{O}\left(16MSn_{\text{token}}d^2(2 + f) + 16MSn_{\text{token}}^2 d\right)$$

682 The linear approximation regarding  $L$  locations:  $\mathcal{O}(MLd)$ , which is usually ignorable compared to  
 683   the computational cost of forward and backward passes. Hence for EAG-ig, the roughly computa-  
 684   tional cost is  $\mathcal{O}\left(16MSn_{\text{token}}d^2(2 + f) + 16MSn_{\text{token}}^2 d + MLd\right)$ .  
 685

686 If  $n_{\text{token}} \gg d$ , then the dominant term is  $16MSn_{\text{token}}^2 d$ , to have efficiency advantage, we have to  
 687   achieve:  
 688

$$689 \quad \begin{aligned} 16MSn_{\text{token}}^2 d &> \frac{ML(L-1)d^2}{2\epsilon} \\ 690 \quad \implies n_{\text{token}}^2 &> \frac{L(L-1)d}{32S\epsilon} \\ 691 \quad \implies n_{\text{token}} &> \sqrt{\frac{L(L-1)d}{32S\epsilon}} \end{aligned} \quad (6)$$

702 Else if  $d \gg n_{\text{token}}$ , then the domain term is  $16MSn_{\text{token}}d^2(2 + f)$ , to guarantee efficiency, we  
 703 must have:

$$\begin{aligned}
 706 \quad 16MSn_{\text{token}}d^2(2 + f) &> \frac{ML(L-1)d^2}{2\epsilon} \\
 707 \quad \Rightarrow n_{\text{token}}^2 &> \frac{L(L-1)}{32S(2+f)\epsilon} \\
 708 \quad \Rightarrow n_{\text{token}} &> \sqrt{\frac{L(L-1)}{32S(2+f)\epsilon}}
 \end{aligned} \tag{7}$$

□

## 719 B EXPERIMENT DETAILS

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 721  
 722 **CircuitLasso on Neurons.** We begin by collecting activations from the model neurons. To  
 723 ensure fairness, we use the same set of input prompts as the baselines. For example, in each case,  
 724 ACDC employs two sets of data inputs: a clean run with  $M$  input prompts, each with  $n_{\text{token}}$  tokens,  
 725 i.e., an  $M \times n_{\text{token}}$  array of tokens  $\mathbf{T}_{\text{clean}}$ , and a corrupted run of the same dimensionality, an  $M \times$   
 726  $n_{\text{token}}$  array  $\mathbf{T}_{\text{corrupted}}$ . Our approach combines these two runs into a single dataset, an array  $\mathbf{T} =$   
 727  $(\mathbf{T}_{\text{clean}}, \mathbf{T}_{\text{corrupted}})$  of  $2M \times n_{\text{token}}$  tokens, which is then used to generate neuron activations at various  
 728 locations in the LLM. Given  $\mathbf{T}$  and a pre-trained model, we obtain neuron activations at a location  $i$   
 729 with shape  $d \times 2M \times n_{\text{token}}$  and average over tokens to produce activations  $\mathbf{H}_i \in \mathbb{R}^{d \times 2M}$ . Repeating  
 730 this process across all  $L$  locations and sorting them according to the computation order yields  $\tilde{\mathbf{H}} \in$   
 731  $\mathbb{R}^{Ld \times 2M}$ . Substituting  $\tilde{\mathbf{H}}$ , the collected data matrix with  $N = Ld$  dimensions and  $2M$  observations  
 732 into Eq. (3), we aim to learn a weighted adjacency matrix  $A \in \mathbb{R}^{N \times N}$  that encodes the causal  
 733 relations between neuron locations. Finally, we infer the causal circuit.

734 **CircuitLasso on Sparse Autoencoder Features.** We extract gpt2-small’s neuron activations  
 735 on the  $M$  training sentences. We select the final outputs from each transformer block (layer) as  
 736 our locations of interest. Given a prompt with  $n_{\text{token}}$  tokens, we obtain transformer outputs at the  
 737  $i^{\text{th}}$  layer with shape  $d \times n_{\text{token}}$  and the corresponding sparse autoencoder features with shape  $D \times$   
 738  $n_{\text{token}}$ . We then collect sparse autoencoder features for all  $M$  prompts and average across tokens to  
 739 produce sparse feature activations  $\mathbf{Z}_i \in \mathbb{R}^{D \times M}$ . Repeating this across all  $L$  layers yields our dataset  
 740  $\{\mathbf{Z}_1, \mathbf{Z}_2, \dots, \mathbf{Z}_L\}$ . In our setting,  $L = 12$ ,  $d = 768$ ,  $D = 32,768$ , and  $M = 8,551$ . For the CoLA  
 741 task, the prediction target  $y$  indicates whether a sentence is linguistically acceptable. Substituting  
 742  $\{\mathbf{Z}_i\}_{i=1}^L$  and  $y$  into Eq. (4) and Eq. (5), we learn weighted adjacency matrices between consecutive  
 743 layers,  $\{A_{i,i+1}\}_{i=1}^{L-1}$ , and the weighted adjacency matrix between the final layer sparse autoencoder  
 744 features  $\mathbf{z}_L$  and the prediction target  $y$ , i.e.,  $A_{L,y}$ .

745 **CircuitLasso for Domain Generalization.** We select SAE features from a specific location of  
 746 a pre-trained LLM, such as the transformer output at layer 22 in Gemma-2-2B. For each prompt, we  
 747 average the  $D$ -dimensional SAE features at this location over tokens and collect them across all  $M$   
 748 prompts in the training data, producing  $\mathbf{Z}_s \in \mathbb{R}^{D \times M}$ . Substituting  $\mathbf{Z}_s$  and the target observations  
 749  $y = (y_1, y_2, \dots, y_M) \in \mathbb{R}^M$  into Eq. (5), we estimate the weighted adjacency matrix  $A_{s,y} \in \mathbb{R}^D$   
 750 and identify important features with large absolute coefficients. This process is equivalent to training  
 751 a sparse linear classifier on the SAE features, which we later exploit for profession prediction. From  
 752  $A_{s,y}$ , we further interpret the semantics of the important features using our proposed *multi-prompt*  
 753 and *single-prompt* approaches (Section 4.2.1) and manually identify spurious features associated  
 754 with gender. Unlike the SHIFT method of Marks et al. (2025), which *decodes* SAE features into  
 755 neuron activations after ablation, we ablate spurious features by setting their values to zero and  
 directly *feed* the resulting SAE feature values into our trained linear classifier. In addition, similar  
 to SHIFT, we also investigate retraining the linear classifier on the ablated SAE features.

756 C INTERPRETABILITY ON SPARSE FEATURES CIRCUITS  
757758 C.1 PRELIMINARY OF SPARSE AUTOENCODERS  
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760 Cunningham et al. (2023) uses a ReLU activation with  $L_1$  sparsity regularization. Subsequent work  
761 explores alternative activation functions  $\sigma(\cdot)$  to extract desired SAE features. Rajamanoharan et al.  
762 (2024) introduces a threshold to determine the minimum pre-activation for feature activation, while  
763 Gao et al. (2024) and Bussmann et al. (2024) enforce sparsity by selecting the top  $K$  features.  
764 Dunefsky et al. (2024) proposes Transcoders, which are similar to SAEs, but focusing on training  
765 interpretable approximations of MLPs. In this work, we employ the following pre-trained LLMs  
766 and SAEs:

- 767 • The open-source GPT2-small SAEs for all sublayers of the open-weights GPT2-small  
768 model. These SAEs use a ReLU-linear encoder with  $D = 32768$  and  $L_1$  sparsity regu-  
769 larization.
- 770 • The open-source Pythia-70M SAEs for all sublayers of the open-weight Pythia-70M. These  
771 SAEs use a ReLU-linear encoder with  $D = 64 \times d$  and  $L_1$  sparsity regularization.
- 772 • The open-source Gemma Scope SAEs for all sublayers of the open-weights Gemma-2-2B,  
773 Gemma-2-9B models. These SAEs use the JumpReLUlinear encoder and set  $D = 8 \times d$ .

775 C.2 ABLATION STUDY OF SPARSITY CONSTRAINT  
776

777 Table 4 presents an ablation study on the sparsity coefficient  $\lambda$  for circuit discovery between the last  
778 layer sparse features and prediction target. When  $\lambda = 0$ , the model achieves the highest training  
779 accuracy (99.36%) but suffers severe overfitting, as reflected in a large performance drop on the test  
780 set (71.10%). Introducing a small sparsity constraint ( $\lambda = 10^{-5}$ ) improves test accuracy to 72.77%,  
781 the best among all settings, indicating enhanced generalization. Larger values of  $\lambda$  further enforce  
782 sparsity but lead to higher training loss and a notable decline in both training and test accuracy,  
783 suggesting that excessive sparsity harms the model’s capacity to capture meaningful circuit structure.  
784 We therefore select  $\lambda = 10^{-5}$  as the optimal setting, as it achieves the best test accuracy and  
785 generalization ability while preserving a sparse, interpretable circuit structure.

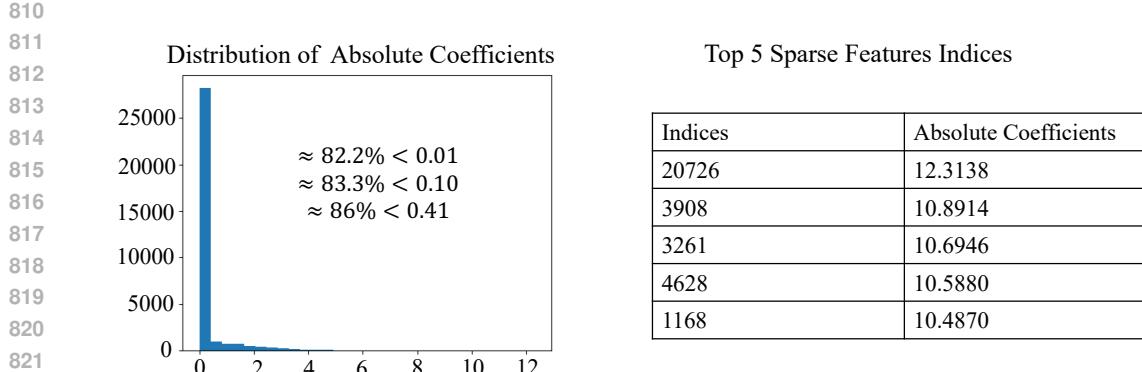
$\lambda$	Prediction Loss	Training Set		Prediction Loss	Test Set Prediction Accuracy (%)
		L1 Loss	Prediction Accuracy (%)		
0	0.0612	-	<b>99.36</b>	0.9977	71.10
$10^{-5}$	0.1741	9257.6	95.70	0.6684	<b>72.77</b>
$5 \times 10^{-5}$	0.3498	1898.7	85.44	0.5566	72.48
$5 \times 10^{-4}$	0.5535	45.3	72.14	0.5566	70.28
$10^{-4}$	0.6143	0.5	70.44	0.6283	69.14

793 Table 4: Ablation study of sparsity constraint coefficient  $\lambda$  for circuit discovery between last layer  
794  $z_L$  and prediction target  $y$ .

796 C.3 STATISTICS OF LEARNED CIRCUIT WEIGHTED ADJACENCY MATRICES  
797

798 Figure 5 examines the coefficient distribution  $|A_{L,y}|$  under the best setting ( $\lambda = 10^{-5}$ ). We observe  
799 that most coefficient values are extremely small, with 82.2% below 0.01, 83.3% below 0.10, 86%  
800 below 0.41, suggesting that only a small subset of features contribute substantially to the prediction.  
801 The top 5 essential features clearly dominate the distribution, highlighting the effectiveness of the  
802 sparsity constraint in filtering out irrelevant features and isolating semantically interpretable ones.

804 C.4 SEMANTIC CONCEPTS ENCODED IN SPARSE FEATURES  
805806 C.5 SPARSE FEATURES CIRCUITS  
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Figure 4: The distribution of  $|A_{L,y}|$  and the selected top 5 essential features.

Prompts	Values of $z_{12,20726}$	Values of $z_{12,20726}$ for each token
Kiss <b>himself</b> .	0.3051	(0, 0, 0, <b>1.5254</b> , 0)
This movie just watches <b>itself</b> .	0.1861	(0, 0, 0, 0, 0, <b>1.3027</b> , 0)
This window just opens <b>itself</b> .	0.1759	(0, 0, 0, 0, 0, <b>1.2311</b> , 0)
This list includes my name on <b>itself</b> .	0.1697	(0, 0, 0, 0, 0, 0, <b>1.5277</b> , 0)
This silver polishes <b>itself</b> .	0.1692	(0, 0, 0, 0, 0, <b>1.1844</b> , 0)
He said that <b>himself</b> was hungry	0.1689	(0, 0, 0, 0, <b>1.3509</b> , 0, 0, 0)
Every picture of <b>itself</b> arrived.	0.1665	(0, 0, 0, 0, <b>1.1652</b> , 0, 0)
Bill understands Mary and <b>himself</b> .	0.1638	(0, 0, 0, 0, 0, <b>1.1467</b> , 0)
<b>Myself</b> saw me	0.1602	(0, 0, <b>0.8009</b> , 0, 0)

Table 5: *Multi-prompt* approach for identifying semantic concepts for sparse features  $z_{12,20726}$ .

Prompts	Values of $z_{12,776}$ for each token
<b>Hun</b> <b>ger</b> fainted Sharon.	(0, <b>0.9980</b> , <b>3.3986</b> , 0, 0, 0, 0, 0)
Many people were dying of <b>thirst</b> .	(0, 0, 0, 0, 0, <b>2.0910</b> , 0)
One people was dying of <b>thirst</b> .	(0, 0, 0, 0, 0, <b>1.8140</b> , 0)
John whined that he was <b>hungry</b> .	(0, 0, 0, 0, 0, 0, 0, <b>1.9004</b> , 0)
Many soldiers have claimed bottled water satisfies <b>thirst</b> best.	(0, 0, 0, 0, 0, 0, 0, <b>1.9243</b> , 0, 0)

Table 6: *Multi-prompt* approach for identifying semantic concepts for sparse features  $z_{12,776}$ .

Prompts	Values of $z_{12,19322}$ for each token
The teacher became <b>tired</b> <b>of</b> the students.	(0, 0, 0, 0, <b>2.7252</b> , <b>1.0383</b> , 0, 0, 0)
The president looked <b>weary</b> .	(0, 0, 0, 0, <b>2.1888</b> , 0)
Genie intoned that she was <b>tired</b> .	(0, 0, 0, 0, 0, 0, 0, <b>2.6658</b> )
John placed him <b>busy</b> .	(0, 0, 0, 0, <b>1.5510</b> , 0)
Visiting relatives can be <b>boring</b> .	(0, 0, 0, 0, 0, 0, <b>1.8287</b> , 0)

Table 7: *Multi-prompt* approach for identifying semantic concepts for sparse features  $z_{12,19322}$ .

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Prompts	Values of $z_{12,3092}$ for each token
He said that himself was hungry .	(0, 0, 0, 0, 0, 0, 6.0688 )
He said that himself was hungry yet	(0, 0, 0, 0, 0, 0, 0 )
He said that himself was hungry ,	(0, 0, 0, 0, 0, 0, 0 )
He said that himself was hungry ?	(0, 0, 0, 0, 0, 0, 3.4722 )
He said that himself was hungry !	(0, 0, 0, 0, 0, 0, 3.7391 )

878 Table 8: *Single-prompt* approach for identifying semantic concepts for sparse features  $z_{12,3092}$ .  
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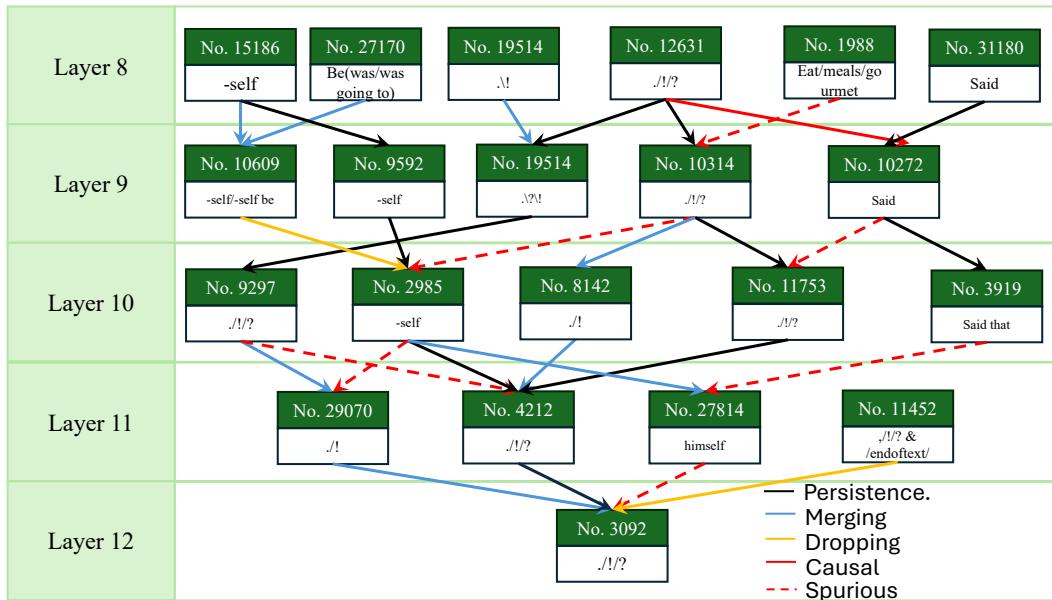


Figure 5: The learned circuit over SAE features on GPT2-small model. Starting with feature No.3072 in layer 12.