Toward a Theory of Generalizability in LLM Mechanistic Interpretability Research

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Abstract

Research on Large Language Models (LLMs) increasingly focuses on identifying mechanistic explanations for their behaviors, yet the field lacks clear principles for determining when (and how) findings from one model instance generalize to another. This paper addresses a fundamental epistemological challenge: given a mechanistic claim about a particular model, what justifies extrapolating this finding to other LLMs—and along which dimensions might such generalizations hold? I propose five potential *axes of correspondence* along which mechanistic claims might generalize, including: functional (whether they satisfy the same functional criteria), developmental (whether they develop at similar points during pretraining), positional (whether they occupy similar absolute or relative positions), relational (whether they interact with other model components in similar ways), and configurational (whether they correspond to particular regions or structures in weight-space). To empirically validate this framework, I analyze "1-back attention heads" (components attending to previous tokens) across pretraining in random seeds of the Pythia models (14M, 70M, 160M, 410M). The results reveal striking consistency in the *developmental trajectories* of 1-back attention across models, while positional consistency is more limited. Moreover, seeds of larger models systematically show earlier onsets, steeper slopes, and higher peaks of 1-back attention. I also address possible objections to the arguments and proposals outlined here. Finally, I conclude by arguing that progress on the generalizability of mechanistic interpretability research will consist in mapping constitutive design properties of LLMs to their emergent behaviors and mechanisms.

1 Introduction

The field of *mechanistic interpretability* aims to uncover the internal structures (e.g., circuits or representations) that give rise to observable behavior in Large Language Models (LLMs) and other neural network-based systems [Olah et al., 2020, Merullo et al., 2023, 2024]. This research has the potential to deliver novel insights about the behavior of LLMs and even help build safer, more aligned models. Yet the scientific study of LLMs has yet to establish firm *epistemological foundations*: although connectionist models have of course been studied for decades [Elman, 1990, McClelland and Rumelhart, 1981], mechanistic interpretability of LLMs is still arguably in a "pre-paradigmatic" stage [Olah et al., 2020, Gurnee et al., 2023, Olah, 2023] and requires further refinement of what constitutes an explanation [Ayonrinde and Jaburi, 2025a,b]. The field thus faces a number of challenges relating to how knowledge is produced and evaluated. Some of these challenges have been discussed in recent literature, e.g., accurately benchmarking model "capabilities" [Raji et al., 2021, Ivanova, 2023, Saxon et al., 2024], but others have received only cursory treatments.

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In this paper, I focus on the question of **generalizability**, specifically of *mechanistic claims* about LLMs. For instance, given a particular claim about the circuits present in a particular model instance, **which aspects of this claim might generalize across model instances and which do not—and what principles can we use to guide those scientific generalizations**? I first argue that the field currently lacks a coherent theory of generalizability, and point to several potential features that might help predict whether two model instances share the same mechanisms (Section 2). This raises the question of what it means for two circuits to be the "same" in the first place (Section 3). Building on recent research, I propose several potential *axes of correspondence* along which mechanistic claims could plausibly generalize (Section 3.1), and also enumerate *functional criteria* that help identify which kinds of mechanisms we might expect to be robust across models (Section 3.2). I then validate the utility of the proposed theoretical framework in an empirical study focusing on the *positional* and *developmental* properties of "1-back attention heads" across random seeds of models in the Pythia suite (14M, 70M, 160M, 410M) [Biderman et al., 2023, van der Wal et al., 2025] (Section 4). I find striking *inter-seed* developmental consistencies within each model; developmental milestones are also highly correlated *across* models, albeit with some subtle differences in timing. Finally, I consider and respond to possible objections (Section 5).

2 Samples, populations, and the generalizability problem

Many scientific disciplines aim to draw general conclusions about the target of inquiry. This approach, sometimes called "nomothetic", contrasts with a more descriptive approach aimed at characterizing individual cases ("idiographic") [Beck, 1953]. In certain fields (e.g., Cognitive Science), this target of inquiry (e.g., human cognition) is too large or abstract to be observed in its entirety: consequently, researchers rely on *samples* to make inferences about the underlying *population of interest*. When drawing generalizations is the goal of scientific inquiry, this *unbiased* sample should be representative of the population of interest.[1]

Research on mechanistic interpretability is arguably nomothetic in nature [Li et al., 2015, Olah et al., 2020, Olah, 2023], i.e., the aim is to produce generalizable or "universalizable" claims about model behaviors or mechanisms. Of course, in practice, interpretability research is not (and cannot be) conducted on the entire "population" of possible LLMs; rather, it is conducted on specific **model instances**. Here, we define a "model instance" $m_{A,\theta,D}$ as a system with some particular architecture A, initialized with some particular parameter set θ, and trained on some particular dataset D.[2] While some recent work has begun to explore the issue of typologizing model instances [Klabunde et al., 2025, Yax et al., 2024], clear principles remain elusive: what would constitute a "representative sample" of LLMs? This makes it difficult for researchers to specify the "population of interest" in any particular study, or to explain the rationale behind which model instances were sampled.

Thus, given a *mechanistic claim* obtained by studying a particular model instance (or instances), what (if anything) have we learned about model instances not in the sample? For instance, if researchers identify a putative "circuit" in GPT-2, what other language models are likely to possess that same circuit—and on what basis could we justify this extrapolation? In principle, the answer to these questions should be informed by the factors known to influence the behaviors and mechanisms of individual model instances, such as: **architectural properties** like model size [Kaplan et al., 2020, Biderman et al., 2023, Rivière et al., 2024, Schrimpf et al., 2021] or depth [Mueller and Linzen, 2023, Petty et al., 2023]; the amount and variety of **training data** [Kaplan et al., 2020, Grieve et al., 2025, Aryabumi et al., 2024, Chang et al., 2024, Conneau et al., 2020, Zhang et al., 2025]; and the **initial parameters** of a model [Bencomo et al., 2025, McCoy and Griffiths, 2023, Marinescu et al., 2024, Hu et al., 2025, Frankle and Carbin, 2018, Belrose and Scherlis, 2024].

Indeed, some recent work has taken exactly this approach [Tigges et al., 2024], mapping the developmental trajectories of multiple circuits (e.g., subject-verb agreement) among models in the Pythia suite [Biderman et al., 2023]; one crucial finding of this work was that these trajectories were relatively *aligned* across model sizes (see also 3.1). Another potentially relevant piece of evidence

[1] This is not always the case: for instance, in Cognitive Science research, English speakers from Western, industrialized countries have long been overrepresented, threatening the external validity of claims made on the basis of those samples [Henrich et al., 2010, Blasi et al., 2022].

[2] Note that additional axes of variation could augment this definition (e.g., particular prompts), which would further complicate the question of identifying a suitable reference class.

comes from work on the Platonic Representation Hypothesis [Huh et al., 2024], which predicts that we should observe more representational convergence between larger models trained on larger volumes of data—if this hypothesis is correct, we might also expect larger, better language models to converge on more similar mechanistic solutions.

The question of which model instances will develop a particular kind of circuit is no doubt challenging. Yet this framing points to a further, even more philosophically complicated challenge: what does it even mean to assert that two different models have the "same" circuit?

3 In what ways are two circuits the "same"?

Interpretability research typically involves the application of specific techniques to particular model instances, allowing researchers to determine which model components (e.g., which attention heads) perform a particular function or embed a specific concept [Clark et al., 2019, Wang et al., 2022, Olsson et al., 2022, Merullo et al., 2023, Manning et al., 2020, Merullo et al., 2024, Park et al., 2025, Zhang et al., 2024]. The result of applying such techniques might (for example) consist in a set of *head indices* believed to correspond to that function, e.g., $(L3, H1), (L4, H2)$. If a researcher's goal is idiographic (i.e., characterizing a given model instance), identifying this set might be sufficient: the circuit has been mapped in a particular model. But if a researcher's goal is nomothetic (i.e., drawing generalizations about other models), they face the question of what, in particular, could plausibly be generalized across model instances.

Yet, with some exceptions [Binhuraib et al., 2024], the position of a head *within* a layer in the standard transformer architecture is arbitrary: even among models with the same architecture trained on the same data, there is no intrinsic reason to expect that $(L3, H_{i=1})$ should consistently perform the same function, as opposed to some other head in the same layer $(L3, H_{i\neq1})$. Thus, what exactly do we mean when we assert that two circuits in different model instances are "the same"?

3.1 Axes of Potential Correspondence

Here, I take inspiration from research in neurophysiology: although mechanistic heterogeneity in biological networks is well-attested [Prinz et al., 2004], researchers nonetheless strive to make generalizations about cell types and cell functions using various axes of correspondence. These include gene expression [Mukamel and Ngai, 2019], putative function [Moser et al., 2008, Knierim et al., 1995, Alexander and Nitz, 2015], temporal patterns [Rivière et al., 2022, Rivière and Rangel, 2017], and anatomical connectivity [Bates et al., 2019, Haber and Schneidman, 2022]. Mechanistic interpretability researchers might therefore identify analogous *axes of potential correspondence* between model instances:

- **Function**: Intuitively, the minimal standard for asserting circuit identity across model instances is whether components in each instance meet certain functional definitions, regardless of where in each model those components are located [Tigges et al., 2024]. Here, a claim might look like: *Attention heads*[3] *performing function X were identified across model instances $m_1, ..., m_n$.*
- **Position**: One might also expect certain functions to be performed by components in similar positions across models. Here, researchers might differentiate between *absolute* position (e.g., always layer 3) and *relative* position (e.g., middle layers) [Rivière et al., 2024, Cheng and Antonello, 2024]. Here, a claim might look like: *Attention heads performing function X were identified at a layer depth of 0.5 across model instances $m_1, ..., m_n$.*
- **Developmental**: Just as human development is associated with particular milestones [Murray et al., 2007], some functions might plausibly emerge at similar points in the course of training, e.g., after having encountered a given number of tokens. Indeed, empirical research suggests that multiple specialized circuits begin forming at around 2B-10B tokens [Tigges et al., 2024, Olsson et al., 2022, Rivière and Trott, 2025, van der Wal et al., 2025, Jumelet et al., 2024]; we might also expect such findings to be marked by relative discontinuities or "phase transitions" during development [Chen et al., 2023, Hu et al., Kangaslahti et al., 2025]. Here,

[3]Note that this framework could in principle be applied to any model component at varying levels of granularity; attention heads are simply used as an illustrative example.

a claim might look like: *Attention heads performing function X emerged after $2B$ tokens were observed across model instances $m_1, ..., m_n$.*

- **Relational**: Model components could also be defined in terms of how they interact with other components. For example, induction circuits consist of an "induction head" and a "previous token head" [Olsson et al., 2022, Singh et al., 2024]. Similarly, [Zhang et al., 2024] report analogous circuit structures across model instances trained on different languages (or different combinations of languages). Here, a claim might look like: *Attention heads performing function X were identified in the layer immediately following attention heads performing function Y across model instances $m_1, ..., m_n$.*
- **Configurational**: Finally, particular functions or concepts might correspond to particular geometric configurations (e.g., in weight-space or activation-space). Here, a claim might look like: *Attention heads performing function X consistently occupied Y region of weight-space across model instances $m_1, ..., m_n$.*

This list is not exhaustive, but rather, provides a set of initial organizing principles that help ground claims about which mechanisms might generalize across model instances (and how). For example, this framework suggests that **induction heads** might be particularly promising candidates as generalizable model components. Induction heads participate in *induction circuits*, which are responsible for detecting whether a given token t has appeared earlier in a sequence (e.g., position s), then predicting that the subsequent token will be the one that previously occurred at position $s + 1$ [Elhage et al., 2021, Olsson et al., 2022]. Notably, induction heads satisfy multiple of the criteria discussed above: first, heads meeting the *functional* definition emerge in model instances of various sizes [Olsson et al., 2022, Singh et al., 2024]; second those heads follow similar *developmental* trajectories during training [Singh et al., 2024]; third, they (by definition) share a common *relational* structure with other heads, i.e., they participate in induction circuits [Olsson et al., 2022, Singh et al., 2024]; and fourth, they tend to occupy similar *relative positions* across model instances [Olsson et al., 2022].

3.2 On finding plausible mechanistic candidates

Mechanistic interpretability research aimed at identifying robust, generalizable model components might also benefit from focusing on identifying plausible candidates for mechanistic functions. The relative "success" of induction heads in this regard points to two additional criteria that may prove useful. First, their function is closely tied to the units over which models operate (i.e., token sequences) and was not defined *a priori* in terms of abstract human constructs—in this sense, they may even satisfy the definition of "concept enrichment" explored by Ayonrinde [2025]. Crucially, tracking previous sequences of tokens in the context is an intuitive solution to the problem faced by language models (predicting upcoming tokens); there is thus a clear link between induction head function and the language model training objective.

Second, while this operation is very concrete, it may be amenable to compositional abstraction [Olsson et al., 2022]: in some cases, induction heads may attend not only to exact repetitions of a token but more abstract correspondences (i.e., "types"). This could make them relevant for *in-context learning*, or ICL [Olsson et al., 2022, Singh et al., 2024], which in turn suggests that they could play a useful explanatory role in higher-level accounts of LLM behavior. Although there is debate about the extent to which induction heads are directly involved in ICL [Yin and Steinhardt, 2025, Feucht et al., 2025], efforts to connect *microscopic phenomena* to *macroscopic behavior* [Olah, 2023] can serve as a useful "North Star" for future research.

4 1-back Attention: An Empirical Case Study

If generalizability is to be a realistic ambition, then we should hope to observe some degree of robustness across *minimally different* model instances, such as different random seeds of the same (or similar) architecture trained on the same data.

The current section presents an empirical study exploring this question, focusing on **1-back attention heads**—defined as heads that direct attention from some target token to the immediately preceding token [Clark et al., 2019]. From a definitional perspective, these **1-back heads** satisfy the proposed criterion of closely tracking the actual units over which models operate (i.e., token sequences; see Section 3.2); as with induction heads (see Section 3.2), tracking the immediately preceding token

seems intuitively helpful for making predictions about upcoming tokens, therefore tying the putative function of these heads to the overall training objective of the model.

Because 1-back heads are likely very useful—and also quite simple in terms of their behavior—one might expect them to emerge across many model instances, including small models, making them a suitable test case for the proposed axes of correspondence (Section 3.1). For the *reference class*, I limit the analysis to (arguably) the simplest possible "population": different random seeds of four model architectures (Pythia-14M, Pythia-70M, Pythia-160M, Pythia-410M) trained on the same data [Biderman et al., 2023]. Note also that the approach adopted below focuses on characterizing the *behavior* of these heads (in terms of their attention patterns), which is a necessary but not sufficient prerequisite for firmly establishing their function as 1-back heads.

This approach allows us to address three related research questions:

- RQ1 To what extent do we observe *inter-seed* and *inter-model* regularities in terms of the developmental trajectories and relative position of 1-back heads? Here, we find striking *developmental regularities*, consistent with prior work on other model components [Jumelet et al., 2024, Olsson et al., 2022, Tigges et al., 2024]; evidence for positional regularity is more mixed.
- RQ2 What divergences do we observe across model instances, and which (if any) properties allow us to predict these divergences? Here, I find that larger models show an *earlier onset* of 1-back heads than smaller models, a steeper *slope* of 1-back attention over pretraining, and a higher *peak* of 1-back attention.
- RQ3 What predicts *convergences* in developmental trajectories across model instances? Here, different seeds of the same architecture show the strongest correlation; when comparing model instances of different sizes, higher correlations were predicted by the size of each model being compared.

A link to a GitHub repository with code and data required to reproduce these analysis can be found at `https://github.com/seantrott/mechinterp_generalizability`.

4.1 Methods

I selected the Pythia suite of auto-regressive English models [Biderman et al., 2023], focusing on the nine random seeds released for Pythia-14M, 70M, 160M, and 410M [van der Wal et al., 2025]. Each model was assessed at 16 training checkpoints (i.e., all available checkpoints up to and including step 1000, followed by step 1000, 50000, 100000, and 143000). As described in Biderman et al. [2023], each model was trained on approximately 300B tokens. All models were accessed through the HuggingFace *transformers* library Wolf et al. [2020] and run on a 2022 Mac laptop. The Pythia models are licensed under an Apache License, Version 2.0.

Each model at each checkpoint was presented with sentences from the Natural Stories Corpus [Futrell et al., 2021]. The Natural Stories Corpus consists of 10 English-language stories, each containing approximately 1000 words. This served as a repository of naturalistic sentences with which to probe attention head behavior (note that the behavior of attention heads was remarkably consistent across different stories; see Appendix B). The corpus is licensed under a Creative Commons Attribution-NonCommercial-ShareAlike 4.0 International License.

The goal was to assess the developmental and positional properties of putative **1-back attention heads**. Here, "1-back attention" was defined as directing attention from a target token to the immediately preceding token. For each head in each model (at each checkpoint), I calculated the average 1-back attention for each sentence.[4] More precisely, if $A_h(i, j)$ represents the attention assigned by head h from token i to token j, and n represents the number of tokens in a given sentence I calculated:

[4]Note that qualitatively identical results for the developmental analyses (though not the positional analyses) were obtained with alternative operationalizations, such as the ratio between the average 1-back attention and the average self-attention. The two metrics were generally highly correlated within each model at the final step ($r \geq 0.68$ for all models). Average 1-back attention was favored in the final analysis because it did not depend upon arbitrary assumptions about the appropriate baseline; moreover, because the attention scores are normalized, the average 1-back attention can be interpreted as the proportion of attention directed by a given head to previous tokens.

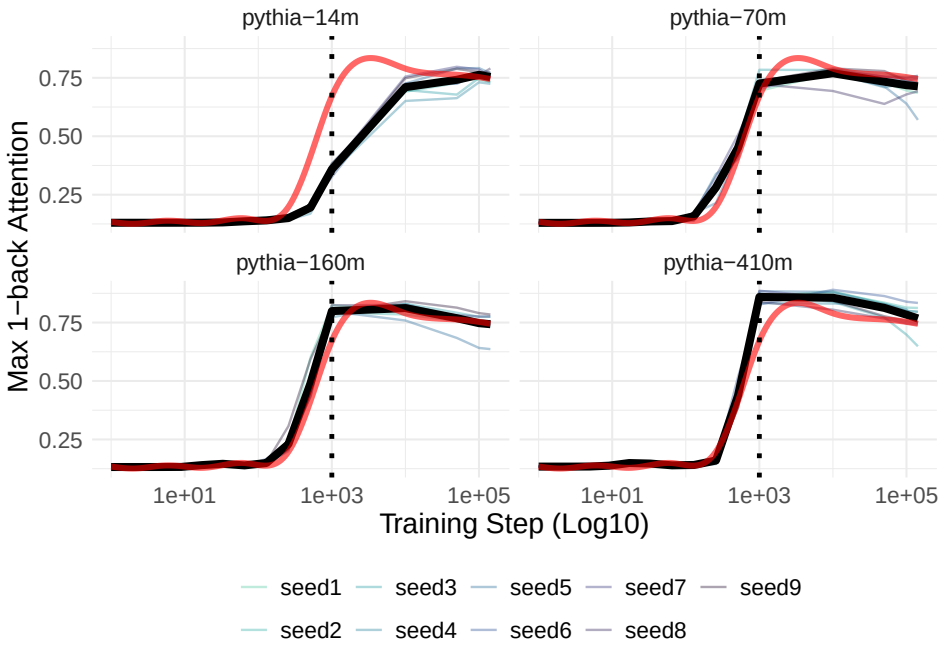


Figure 1: Maximum 1-back attention for each seed of Pythia 14M, 70M, 160M, and 410M. Dark black line indicates average across each seed for that model. Red reference line indicates predictions from a generalized additive model (GAM) fit to all data points (i.e., across models).

$$R_h = \frac{1}{n-1} \sum_{i=2}^{n} A_h(i, i-1) \tag{1}$$

Note that i starts at 2 to exclude the first token in the sequence. All analyses and visualizations were conducted in R [R Core Team, 2025].

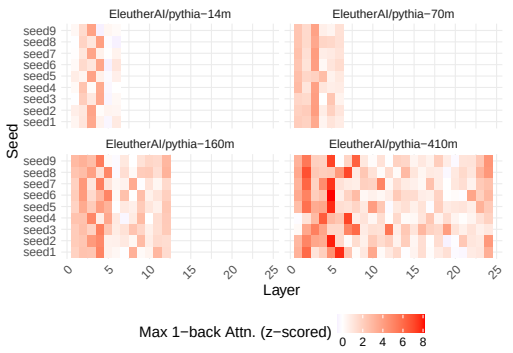
4.2 Results

4.2.1 RQ1: Inter-seed consistency

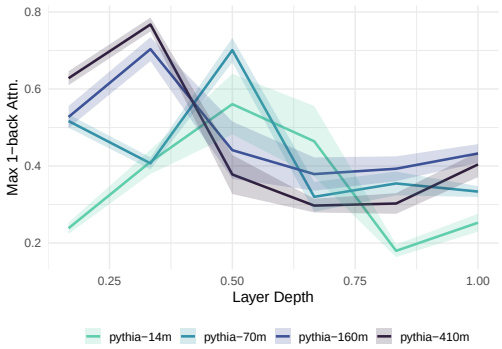
First, I asked about the developmental and positional consistency of putative 1-back attention across different seeds of the same architecture. As depicted in Figure 1, different seeds of the same model showed striking regularity in their developmental trajectories. Even different models exhibited remarkably similar patterns: selective 1-back attention tended to emerge around 10^3 training steps, corresponding to roughly $2B$ tokens of exposure. A generalized additive model (GAM) fit to all data points from all models (i.e., the maximum attention at each step for each seed of each model) using Log Training Step as a predictor achieved an $R^2 = 0.95$; as depicted in Figure 1, the GAM's predictions (in red) are consistent with an expected onset in 1-back attention occurring between 512 and 2000 steps.

The *position* of these putative 1-back heads exhibited considerably more variance across seeds and especially across models. Figure 2a depicts the maximum 1-back attention at each *layer* of each random seed for each model at the final pre-training step. For $14M$, 1-back heads tended to emerge either in layer 3 or in layer 4[5]; see also Appendix A. Overall, positional consistency across model architectures was relatively low, though there was some evidence for middle layers showing a peak in 1-back attention. A linear mixed effects model predicting average 1-back attention at the final step

[5]This echoes other work revealing *bimodal* distributions in the mechanisms and behaviors that emerge across random seeds [Zhao et al., 2025], and suggests that there might be multiple "attractors" in weight-space with the respect to 1-back attention head emergence.



(a) Z-scored 1-back attention for each head at the final step of each Pythia-14M random seed. Dotted red line represents 3 standard deviations from the mean for that seed.



(b) Maximum attention to previous tokens at each *binned layer depth* across models (shading indicates one standard error calculated across seeds).

Figure 2: Different random seeds of the same architecture showed considerable variance in where putative 1-back attention heads formed.

from each individual head of each model instance revealed a significantly negative effect of Layer Depth [$\beta = -0.11, SE = 0.005, p < 0.001$], i.e., *later* layers were associated with significantly less attention to previous tokens on average.

Together, these results point to a high degree of *developmental correspondence* in putative 1-back attention heads across model instances in the Pythia suite, but also suggest a limited degree of *positional correspondence*: 1-back heads are systematic in *when* but not *where* they appear.

4.2.2 RQ2: Model divergences in timing

Although 1-back attention heads were extremely consistent in *when* they developed across model instances, subtle differences in timing are revealed by comparing the trajectory of each individual model to the fit GAM predictions (Figure 1). Relative to the predictions, smaller models (like $14M$) had a delayed *onset* of 1-back heads, a shallower *slope* of 1-back attention over time, and a reduced *peak*; conversely, larger models (like $410M$) showed a sharper *slope* and a higher *peak*.

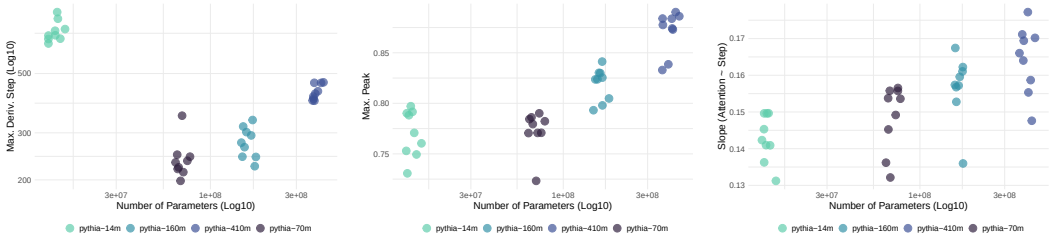
To quantify these apparent divergences, I first operationalized each construct (onset, slope, and peak) as follows. The *onset* of 1-back attention for a given seed was defined as the earliest step where the change in maximum 1-back attention relative to the change in log training step (d_{ratio}) exceeded some threshold; in order to avoid dependence on a particular threshold, this was assessed for a range of thresholds $(0.01, 0.3)$ for each seed and averaged across the resulting values for that range. Intuitively, this measure reflects the average *earliest step* at which 1-back attention sharply increased for a given instance.[6] The *slope* was identified by regressing the maximum 1-back attention at each step against Log Training Step and extracting the resulting slope estimate. Finally, the *peak* was defined as the maximum 1-back attention (i.e., across all steps for that seed).

Each measure was then regressed (in a separate linear mixed effects model) against Log Parameters, with seed as a random intercept. Log Parameters was significantly related with each dependent variable in the expected direction. That is, larger models displayed a reduced *onset* of 1-back attention [$\beta = -0.18, SE = 0.05, p < .001$], increased *slope* [$\beta = 0.01, SE = 0.003, p < .001$], and a higher *peak* [$\beta = 0.07, SE = 0.01, p < 0.001$]. These relationships are also depicted in Figure 2.

4.2.3 RQ3: What predicts convergence?

A central question concerning generalizability is what, if anything, predicts that two model instances will belong to the same "reference class" with some respect to some *axis of correspondence* (Section 3.1). As described in Section 4.2.1, I observed striking convergence in the developmental trajectories

[6] Note that the results are robust to different thresholds, as well as different operationalizations of 1-back attention onset.



(a) Earliest *onset* of 1-back attention heads in each seed of each model.

(b) Max *peak* of 1-back attention heads in each seed of each model.

(c) *Slope* of 1-back attention (against pretraining step) in each seed of each model.

Figure 3: Larger Pythia models tended to show a slightly earlier *onset* of 1-back attention, a higher *peak*, and a steeper *slope*.

of 1-back attention across random seeds of the same model, and even relatively strong temporal alignment between models of different sizes. Here, still focusing on the *temporal axis*, I asked a related question: which properties predict higher temporal convergence between two model instances?

First, I calculated the Pearson's correlation between every pair of 1-back attention trajectories (i.e., for each pair of model instances). Unsurprisingly, random seeds of the same *architecture* exhibited substantially higher correlation ($M = 0.99, SD = 0.04$) on average than instances from different architectures ($M = 0.95, SD = 0.003$). I then constructed a linear regression with correlation between each pair of model instances ($r_{i,j}$) as a dependent variable; predictors included a factor indicating whether the two instances were the Same Model, as well as the Number of Parameters (Log10) of model m_i and model m_j. Consistent with the descriptive results, Same Model positively predicted higher $r_{i,j}$ [$\beta = 0.05, SE = 0.002, p < .001$]; holding Same Model constant, both Number of Parameter predictors were also positively related with higher $r_{i,j}$ [$\beta = 0.03, SE = 0.002, p < .001$]. That is, stronger temporal convergence was observed among instances belonging to the *same* architecture and among instances of *larger* (different) architectures; similar results are reported in the Appendix (Section C).

4.3 Discussion

The primary goal of this empirical case study was as a *demonstration of viability* for the proposed *axes of correspondence* (Section 3.1)—specifically focusing on the positional and temporal axes of model similarity. 1-back attention heads were selected because they were a well-established phenomenon [Clark et al., 2019] that would likely emerge in even small models, and which also satisfied the proposed criteria for plausible mechanistic candidates (Section 3.2).

Concretely, the case study addressed three research questions. First, I observed considerable *inter-seed* and *inter-model* convergence along the temporal axis (see Figure 1), though there was less positional consistency: 1-back heads were highly systematic in *when* but not *where* they emerged. Second, I observed subtle timing differences as a function of model size: larger models showed an earlier onset, steeper slope, and higher peak of 1-back attention (see Figure 2). Finally, inter-seed temporal convergence was (unsurprisingly) highest among instances of the same architecture; among instances of different architectures, temporal convergence was higher when both instances were larger (Section 4.2.3), possibly consistent with the Platonic Representation Hypothesis [Huh et al., 2024]. Together, these results suggest that at least when it comes to putative 1-back attention heads, model mechanisms are more constrained by *developmental* features than *positional ones*, which is itself informative about the nature of various constraints operating over head specialization.

A key limitation of this work is that candidate 1-back heads were defined in terms of their attentional behavior—their *functional* role in model predictions was not investigated. Future work could conduct further analyses to investigate the functional axis specifically, perhaps connecting these heads to broader circuits in which they may or may not participate; the latter goal would also connect to other potential proposed axes of correspondence, such as the *relational* structure of heads to other model components.

5 Objections and Limitations

Thus far, I have argued: first, that *generalizability* is a central epistemological challenge in the science of LLM interpretability; and second, that progress could be made by considering particular *axes of correspondence* among model instances. I have also presented a case study illustrating the value of using these proposed axes to guide empirical investigation. Here, I consider possible objections to the key arguments in the paper, as well as potential replies to each objection.

Objection: Interpretability *is* idiographic, not nomothetic.

Reply: If interpretability is idiographic, then generalizability is indeed not a concern. That said, interpretability research does (arguably) appear to be nomothetic in nature, with identifying "universal" circuits as a high-level goal [Olah et al., 2020, Olah, 2023]. Further, as argued in Olah et al. [2020], (near-)universality would also make interpretability a much more *tractable* field:

> In the same way, the universality hypothesis determines what form of circuits research makes sense. If it was true in the strongest sense, one could imagine a kind of "periodic table of visual features" which we observe and catalogue across models. On the other hand, if it was mostly false, we would need to focus on a handful of models of particular societal importance and hope they stop changing every year. There might also be in between worlds, where some lessons transfer between models but others need to be learned from scratch. [Olah et al., 2020]

Objection: Automated interpretability techniques reduce the need for generalization, as putative circuits can quickly be discovered in new model instances.

Reply: In a world of fully automated interpretability [Conmy et al., 2023], a suite of methods would simply be applied to each model instance as necessary, perhaps reducing the need to speculate about "unobserved" instances. However, my position is that a coherent theory of generalizability would still be of value in such a world for two reasons. First, a theory of generalizability is, at root, an articulation of what makes two model instances similar or different along some dimension; it is not only *useful* for conducting research but could also be seen as a *progress marker* of research. Second, in such a world there would presumably be vast empirical data characterizing large numbers of individual model instances—a theoretical framework such as the one proposed here (Section 3.1) would give researchers a *lexicon* [Kuhn, 1982, Contreras Kallens and Dale, 2018] to describe observed convergences and divergences between model instances and make sense of this landscape.

Objection: The case study is limited—1-back heads are simple, and a narrow reference class was chosen.

Reply: The goal of the case study was to investigate the viability of identifying correspondences across model instances, which is why a simple phenomenon (1-back heads) was selected, as well as a relatively narrow reference class (different seeds or sizes of the same underlying architecture trained on the same data). The underlying logic was that if generalizability is to be a goal of interpretability research, we should be able to establish it in at least this case, which perhaps reflects a "lower bound" of tractability. The relative success of the case study suggests these axes of correspondence may serve as fruitful guides for future work, which could expand to more complex circuits or mechanisms.

Objection: The functional axis is sufficient to establish circuit identity.

Reply: The functional axis of correspondence (Section 3.1) is arguably the *minimal standard* for establishing whether components of different model instances "do the same thing". My argument is not that other axes are *necessary*, but rather that they are additional organizing principles for assessing similarities and differences between circuits. It is informative to be able to assert that two circuits satisfy the same functional criteria but emerge at different timepoints in different models—particularly if those divergences can be related to other points of departure between those models (see Section 4.2.2). Moreover, finding correspondences along these other dimensions might also strengthen our confidence in the robustness of a particular result or in the identity of circuits across model instances: intuitively, two circuits seem more conceptually and mechanistically similar if they not only satisfy the same functional definition [Wang et al., 2022] but also exhibit similar *developmental trajectories* (or converge along other axes of correspondence). That said, functional alignment is probably the only strictly necessary axis to assert that two circuits are implementing the

same function; as in evolutionary biology, different systems often achieve the same goals or perform the same computations in different ways.

Objection: Random seeds (and pretraining checkpoints) are not available for most models, making generalizability too difficult to investigate.

Reply: Indeed, the problem is even worse—the space of *actual* model instances is also not itself a representative sample of the distribution of *possible* models. With some exceptions [Biderman et al., 2023], available models are driven by specific research or commercial interests and not necessarily with the goal of exhaustively characterizing the space of possible models. However, the fact that generalizability will be hard to investigate is not a refutation of its epistemological importance for the field of interpretability. Fully addressing the gap is beyond the scope of this paper (and will likely require large-scale coordination between institutions in multiple sectors), but individual researchers do still have options available to them, such as the Pythia suite [Biderman et al., 2023, van der Wal et al., 2025] and OLMo 2 [OLMo et al., 2025]. Moreover, not every interpretability study needs to address every axis of correspondence: a study investigating developmental convergences across seeds might focus on the Pythia suite [Biderman et al., 2023], but a study focused on positional or relational consistency would not necessarily need pretraining checkpoints. Nonetheless, the field would clearly benefit from a larger number of open-source models subjected to controlled training regimes.

6 The Path Forward

The shift from a pre-paradigmatic stage of research [Olah et al., 2020, Olah, 2023] to more established research practices and inferential principles will require a combination of theoretical and methodological refinement. In this paper, I have argued that *generalizability* is a major epistemological gap in the scientific study of LLM mechanisms. Yet enumerating challenges is often straightforward; identifying markers of progress on those challenges can be much more difficult. In that spirit, I have drawn on the growing body of existing research [Tigges et al., 2024, Zhang et al., 2024, Olsson et al., 2022] to propose *axes of correspondence* that might serve as organizing principles with which to guide questions about generalizability. I have also presented the results of a case study validating the utility of this framework in identifying areas of convergence and divergence between model instances. Moving forward, one marker to look for is the construction of a theoretically legible typology (or "phylogeny") that makes clearly articulable predictions about which pairs of model instances will share similar mechanisms along which axes of correspondence.

7 Reproducibility Statement

A link to a GitHub repository with code and data required to reproduce these analyses can be found at `https://github.com/seantrott/mechinterp_generalizability`.

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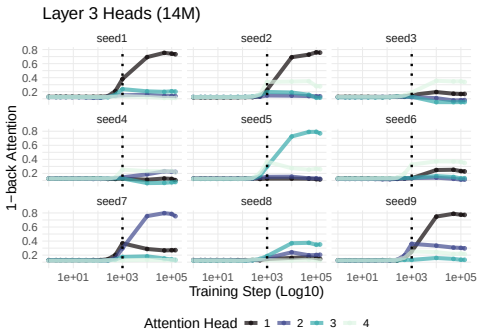
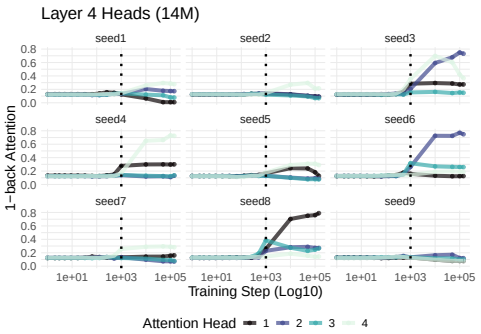


(a) 1-back attention for layer 3 heads across Pythia-14M seeds and pre-training checkpoints.



(b) 1-back attention for layer 4 heads across Pythia-14M seeds and pre-training checkpoints.

Figure 4: In each random seed of Pythia-14M, 1-back attention heads emerged at roughly similar training checkpoints.

A Individual head trajectories in 14m

The developmental trajectories depicted in the primary manuscript collapsed across heads and layers for the purpose of illustrating temporal patterns across all models tested. Here, I depict the trajectories of 1-back attention for each individual head in each random seed of Pythia-14M for layer 3 (Figure 4a) and layer 4 (Figure 4b).

B Consistency across stories

One question that arises is about the generalizability of the results reported in the primary manuscript across *input sentences*. That is, how dependent is the developmental trajectory observed upon the corpus used to assess attention head function? To address this, I plotted the maximum 1-back attention for each random seed of Pythia-14M for each *story* from the Natural Stories Corpus. The developmental trajectories are extremely similar, with changes in attention beginning around 10^3 training steps for all random seeds, for all stories.

C Multi-dimensional scaling of seeds

In the primary manuscript, I reported the average correlation between seeds belonging to the same architecture and between seeds belonging to different architectures; a key finding was among seeds of *different architectures*, stronger temporal convergences were observed when both instances being compared were larger.

Another perspective on this result comes from embedding the correlation matrix of all model instances in a $2D$ space using multi-dimensional scaling (MDS) [Carroll and Arabie, 1998]. As depicted in Figure 6, the first MDS component appeared to track model size. Moreover, seeds of smaller models ($14M$) exhibited tight clustering and relatively larger separation from larger models.

I quantified this trend by first calculating the centroid among each set of seeds (i.e., for 14M, 70M, etc.). I then calculated the Separation Ratio, defined as the mean distance of each centroid to other centroids, divided by the mean distance of each point within a model class to the centroid of that class. It decreases systematically with model size, reflecting the combination of wider internal spread and closer inter-cluster proximity in larger models. The Separation Ratio systematically declined with model size: 14M was the largest (11.4), followed by 70M (3.37), and 160M (2.42). The results are nuanced, however, as 410M exhibited a larger Separation Ratio than 70M and 160M (4.0), though still considerably smaller than 14M; see also Figure 1.

Together, this suggests that at least along the temporal axis, smaller model instances of the same architecture are relatively different from other models—conversely, larger models of different architectures are relatively more similar to each other.

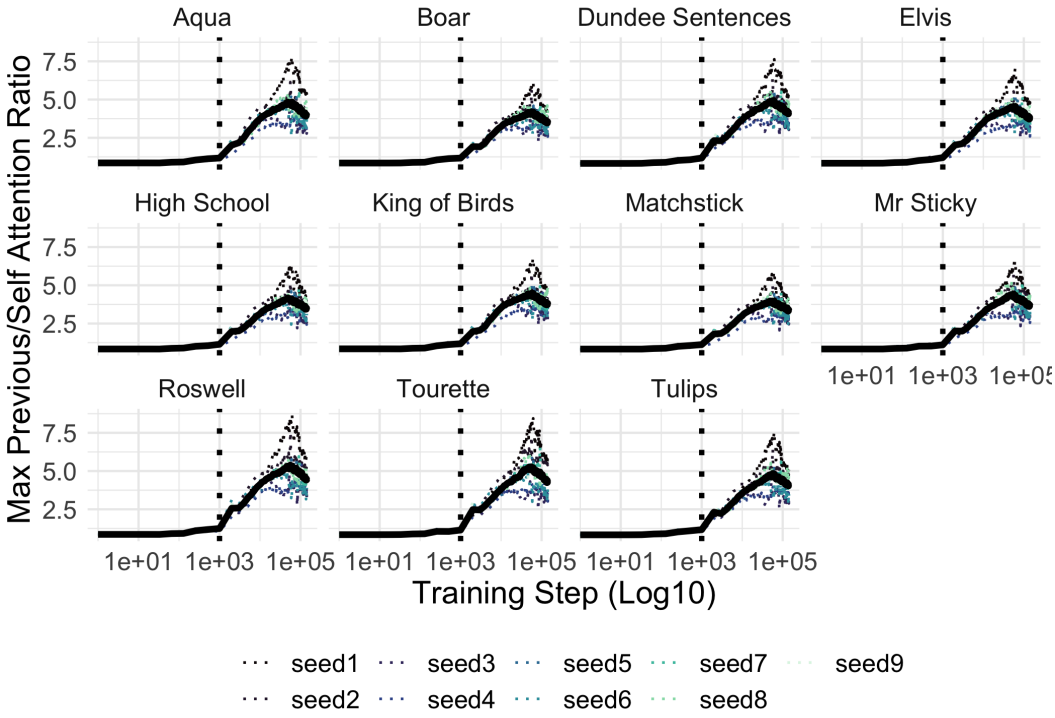


Figure 5: Developmental trajectory of putative 1-back attention heads across random seeds of Pythia-14M and across the story corpora used to assess this behavior. Across all heads at a given checkpoint for a given model, the maximum 1-back attention was calculated.

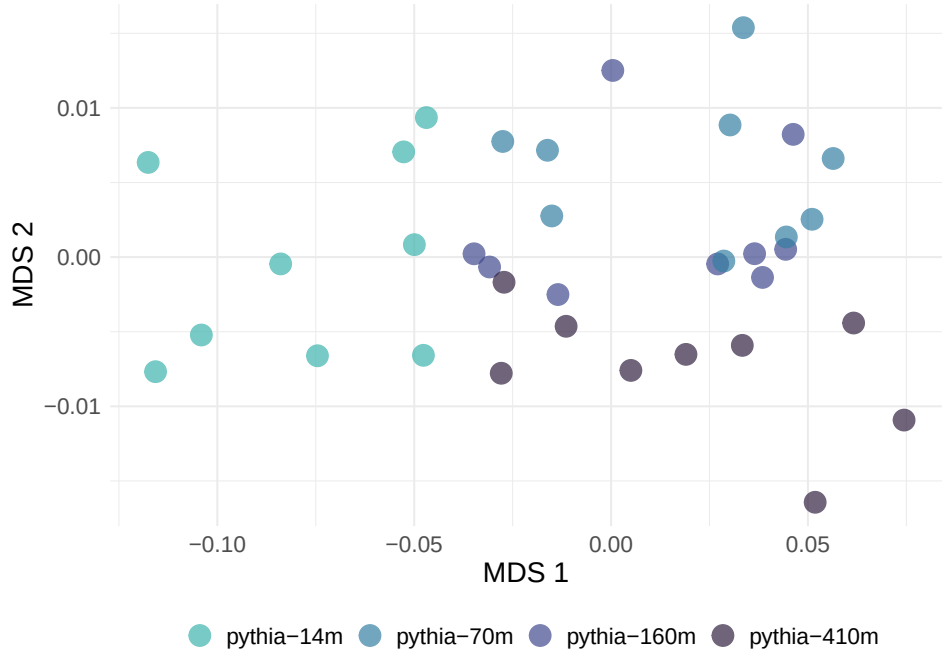


Figure 6: Results of applying multi-dimensional scaling (MDS) to the correlation matrix of all model instance pairs. Each MDS point represents a given seed of a particular model.

NeurIPS Paper Checklist

1. **Claims**

   Question: Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope?

   Answer: [Yes]

   Justification: The goal of the paper is to argue that generalizability is a major epistemological challenge in the study of LLMs, propose a theoretical framework for investigating it, and present the results of a novel case study; the abstract and introduction summarizes this.

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   - The answer NA means that the abstract and introduction do not include the claims made in the paper.
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   - It is fine to include aspirational goals as motivation as long as it is clear that these goals are not attained by the paper.

2. **Limitations**

   Question: Does the paper discuss the limitations of the work performed by the authors?

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