

000 HOW DO LANGUAGE MODELS COMPOSE FUNCTIONS?

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ABSTRACT

010 While large language models (LLMs) appear to be increasingly capable of solving
011 compositional tasks, it is an open question whether they do so using compositional
012 mechanisms. In this work, we investigate how feedforward LLMs solve two-hop
013 factual recall tasks, which can be expressed compositionally as $g(f(x))$. We first
014 confirm that modern LLMs continue to suffer from the “compositionality gap”: i.e.
015 their ability to compute both $z = f(x)$ and $y = g(z)$ does not entail their ability
016 to compute the composition $y = g(f(x))$. Then, using logit lens on their residual
017 stream activations, we identify two processing mechanisms, one which solves tasks
018 *compositionally*, computing $f(x)$ along the way to computing $g(f(x))$, and one
019 which solves them *directly*, without any detectable signature of the intermediate
020 variable $f(x)$. Finally, we find that which mechanism is employed appears to be
021 related to the embedding space geometry, with the idiomatic mechanism being
022 dominant in cases where there exists a linear mapping from x to $g(f(x))$ in the
023 embedding spaces.

1 INTRODUCTION

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025 *Compositional behavior* (McCurdy et al., 2024) is widely considered essential for flexible and
026 general intelligence (Szabó, 2024). A long-running debate has asked whether compositional *behavior*
027 necessarily entails compositional *representations* and *processes*. One the one hand, formal languages
028 based on compositional syntax and semantics are guaranteed to support certain types of invariance
029 and generalization, making them compelling models for how humans might achieve abstract cognitive
030 abilities like language and logic (Fodor, 1975; Quilty-Dunn et al., 2023). On the other hand, critics
031 are quick to point out that humans frequently deviate from ideal compositional and logical behavior,
032 suggesting that some other mechanism must underlie our advanced cognition (Kahneman & Tversky,
033 1972; Evans, 2002).

034 Large language models (LLMs) provide an opportunity to revisit this debate in a new light. LLMs
035 exhibit behavior that is at least ostensibly compositional, and which is not easily explained away
036 by trivially non-compositional mechanisms (McCoy et al., 2023; Griffiths et al., 2025). However,
037 LLMs also lack the kinds of explicit symbolic architectural components that have long been assumed
038 necessary for such compositionality. This provides an opportunity to ask: do LLMs produce
039 compositional behavior by invoking compositional processes, or do they rely on something more
040 idiomatic instead?

041 We offer an initial investigation into this question, focusing on a set of two-hop factual retrieval tasks,
042 such as: given a book’s title, output that book’s author’s birth year. All of the tasks we consider
043 can be formally expressed as $y = g(f(x))$ and are thus defensibly “compositional” in the sense
044 invoked in traditional symbolic models. We are interested in whether LLMs solve such tasks by
045 approximating the mapping from x to y *compositionally*, by computing the intermediate variable
046 $z = f(x)$, or *directly*, without a readily-detectable representation of any such z . We find that:

047

- 048 1. Models’ ability to compute both $x \rightarrow f(x)$ and $f(x) \rightarrow g(f(x))$ does not entail their ability
049 to compute $x \rightarrow g(f(x))$. This extends earlier findings on the “compositionality gap” (Press
050 et al., 2022), showing that the gap holds for modern models and on a larger set of tasks.
051 This gap is not trivially reduced in larger models or even necessarily by reasoning models
052 (Sec. 3).

054

055 2. Models exhibit both *compositional* processing mechanisms and *direct* processing mecha-

056 nisms, as defined above. The type of mechanism is only weakly associated with accuracy,

057 suggesting that LLMs are able to use both effectively to compute correct answers (Sec. 4).

058

059 3. The choice of mechanism is mediated by the geometry of the input embedding space.

060 Specifically, when there exists a linear mapping from x in the input embedding space to

061 $g(f(x))$ in the output unembedding space, the LLM tends to favor direct computation over

062 compositional processing (Sec. 5).

063

2 TASK SETUP

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065 Our tasks involve solving a composition $g(f(x))$ from an input x , using in-context learning (ICL)

066 and where f and g are some pre-defined functions. See Table 1 for the full list of tasks we use. We

067 choose common functions f and g that models might learn through their pre-training and for which

068 the inputs and outputs are lexical units. This enables us to use well-established tools for analyzing

069 the mechanisms and latent computations in Transformer models, focusing on a few token positions

070 (i.e. residual streams) and a single autoregressive forward pass.

071 We design the set of tasks in our investigation to cover a qualitative variety of functions, such

072 as arithmetic, factual recall, lexical functions, translation, rotation, and string manipulation. By

073 construction, all of our tasks can be computed by applying f and then g , yielding the causal hops

074 $x \rightarrow f(x) \rightarrow g(f(x))$. Some tasks (e.g. commutative tasks) can also be computed through the hops

075 $x \rightarrow g(x) \rightarrow g(f(x))$ — in which case, the intermediate z may also equal $g(x)$. We differentiate

076 these further, and also describe our dataset construction methodologies (including our sources and

077 pre-processing), in Appendix A.

078 In our experiments, we randomly sample 10 in-context examples for a given task and query. Each

079 in-context example is formatted with a “Q: {input} \n A: {output} \n\n” prompting structure

080 and the test query is formatted with “Q: {input} \n A:”.

081

082 **Limitations** Our experimental design primarily focuses on autoregressive language models per-

083 mitted one token for generation (rather than e.g. reasoning models) and on mechanisms that are

084 discoverable using current widely-accepted interpretability methods. There are certainly many inter-

085 esting compositional and non-compositional mechanisms that are employed by LLMs which are not

086 in the scope of the present study. The mechanisms we describe here are part of the larger story and

087 thus warrant study, but we do not intend to imply that such mechanisms are the whole story of how

088 LLMs process complex tasks.

089 Table 1: List of our tasks. The compositional function $(g \circ f)$ is constructed by f and g here. We list

090 the number of examples (#) in each task’s dataset, along with the variables x , $f(x)$, and $g(f(x))$ for

091 one random example. We list $g(x)$ and $f(g(x))$ for tasks that define them in Appendix A.

f	g	#	$x \rightarrow f(x) \rightarrow g(f(x))$
Word → Antonym	English → Spanish	2398	bogus → authentic → auténtico
Word → Antonym	English → German	2398	philosophical → practical → praktisch
Word → Antonym	English → French	2398	excessive → insufficient → insuffisant
Book → Author	Author → Birth Year	2228	The Boy in the Striped Pyjamas → John Boyne → 1971
Song → Artist	Artist → Birth Year	958	Heartbreak Hotel → Elvis Presley → 1935
Landmark → Country	Country → Capital	1385	Taq-i Kisra → Iraq → Baghdad
Park → Country	Country → Capital	743	Mount Rainier National Park → United States → Washington, D.C.
Movie → Director	Director → Birth Year	2180	Cape Fear → Martin Scorsese → 1942
Person → University	University → Year	4992	Andi Gutmans → Technion – Israel Institute of Technology → 1924
Person → University	University → Founder	4996	Ezra Abbot → Bowdoin College → James Bowdoin
Product → Company	Company → CEO	1904	NES-101 → Nintendo → Shuntaro Furukawa
Product → Company	Company → HQ	2276	Toyota Alphard → Toyota → Toyota
x + 10	2x	1000	699 → 709 → 1418
x + 100	2x	1000	922 → 1022 → 2044
x mod 20	2x	1000	891 → 11 → 22
Word → Numeric	2x	1000	one hundred and forty-eight → 148 → 296
Word[:-1]	Word[::-1]	2946	responsible → responsibl → lbisnopser
Rotate(RGB, 120°)	RGB → Name	1000	8a735a → 598a73 → dimgray

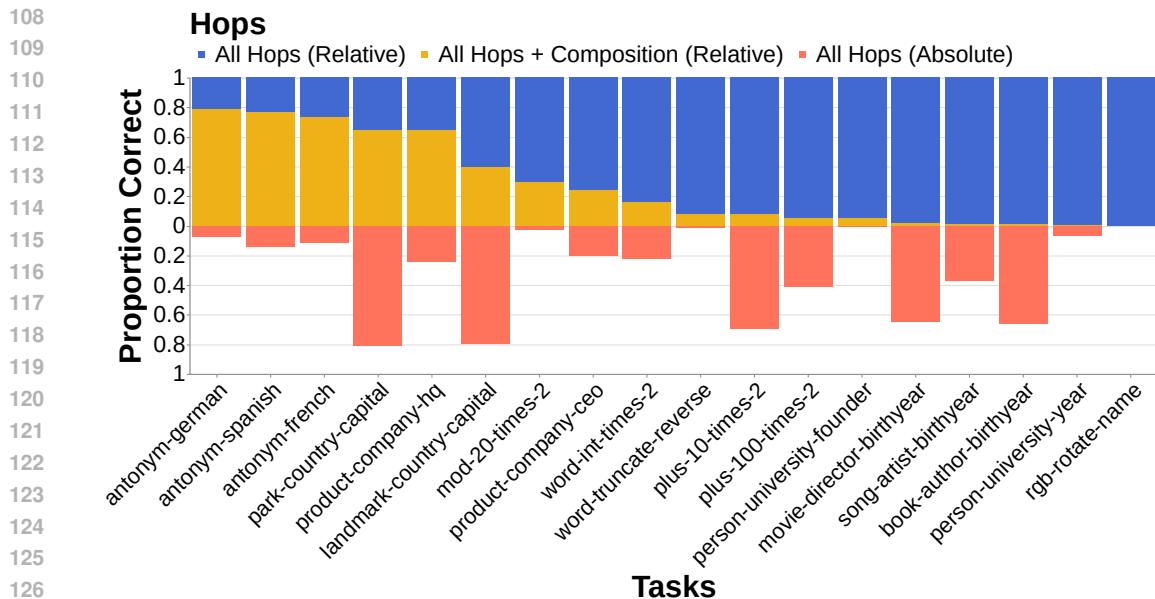


Figure 1: Compositionality gap for Llama 3 (3B) on our tasks. Red bar represents examples for which the model is able to solve all causal hops, out of all examples (absolute). Blue and yellow bars are relative to the red bar: they show proportions of examples out of those in the red bar. Blue represents the same examples as red and yellow represents those for which the model is able to additionally solve the composition. Correlation between red and yellow bars is $r^2 = 0.00$.

3 COMPOSITIONALITY GAP

Press et al. (2022) documented a “compositionality gap” in LLMs, showing that they consistently fail to solve compositions, despite solving the hops independently. Press et al. (2022) tested the GPT-3 family of models with natural language questions about celebrities and encyclopedic knowledge that required two-hops of factual recall. We confirm and extend this finding by testing modern LLMs on a larger set of compositional tasks.

3.1 EXPERIMENTAL DESIGN

We prompt models with $\text{input} \rightarrow \text{output}$ mappings between lexical units.¹ We measure models’ predictive accuracies using the ICL prompts from Sec. 2, greedy sampling, and the exact match evaluation metric. The *compositionality gap* is defined as the proportion of examples for which a model answers both $x \rightarrow f(x)$ and $f(x) \rightarrow g(f(x))$ correctly,² but $x \rightarrow g(f(x))$ incorrectly.

We test the Llama 3 (3B) model on all of our tasks, using all available examples. We also test a wider set of models (including those from Llama 3, OLMo 2, DeepSeek, and GPT model families) on 4 tasks: antonym-spanish, plus-100-times-2, park-country-capital, and book-author-birthyear (which capture a representative set of processing signatures from Sec. 4). We aggregate metrics over these tasks and use 100 examples per task for testing.

3.2 RESULTS

We show performance of the Llama 3 (3B) model on our tasks in Fig. 1. We clearly find a compositionality gap: the model is unable to solve the composition in 20–100% (varying by task) of examples for which it can solve all hops. We show the performances of our other models in Fig. 2.

¹Note that this represents a methodological difference from Press et al. (2022), who prompted with long-form questions. Our format is chosen to fit with the interpretability methods we use in later sections.

²We extend this definition to further require success at $x \rightarrow g(x)$ and $g(x) \rightarrow g(f(x))$ in tasks where these are valid hops.

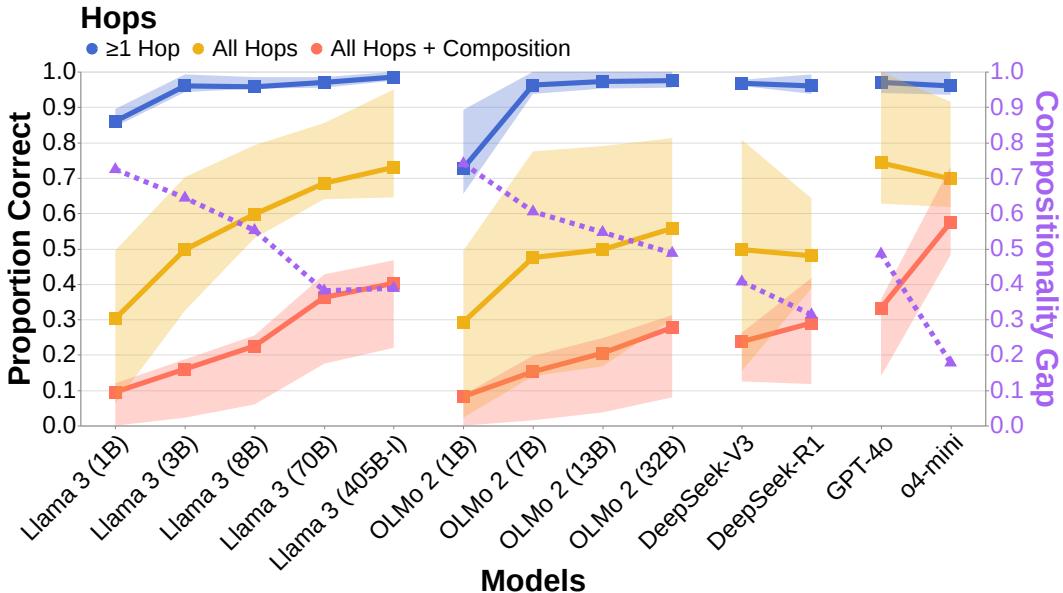


Figure 2: Compositionality gap (dashed purple line; lower is better) of various models aggregated over 4 tasks (100 examples each). Blue, yellow, and red lines show proportions of examples for which models correctly solve combinations of hops and the composition. Purple line shows the relative gap between yellow and red: the proportion of examples for which the model cannot solve the composition, out of those for which it can solve all hops. “-I” indicates the instruction-tuned variant of Llama 3 (405B). Error bands show interquartile range.

We find the compositionality gap does reduce with size from $72\% \rightarrow 39\%$ (Llama 3, 1B \rightarrow 405B) and $74\% \rightarrow 49\%$ (OLMo 2, 1B \rightarrow 32B). However, the gap clearly remains and we find monotonically diminishing improvements for both model families with respect to size. We plot the gap against model parameters and layers in Appendix C. In fact, the gap shows no improvement at all between the 70B and (instruction-tuned) 405B parameter Llama 3 models.

We also compare reasoning models (o4-mini and DeepSeek-R1; allotted a budget of 2000 reasoning tokens) against same-generation, non-reasoning models (GPT-4o and DeepSeek-V3) in Fig. 2. We find some reduction ($41\% \rightarrow 31\%$) in the compositionality gap in the case of DeepSeek’s reasoning model and significant reduction ($49\% \rightarrow 18\%$) in the case of o4-mini. As o4-mini is proprietary (and both this and GPT-4o have additional “external tool-use” capabilities), it is difficult to speculate about the exact causes for these improvements. However, it is notable that even with advanced reasoning models, the gap does not necessarily disappear entirely.

4 ANALYZING PROCESSING MECHANISMS

We next try to understand *how* the model correctly computes compositions in cases where it is successful. Our intuition is based on prior work from Merullo et al. (2024) which identifies a processing signature in models that solve one-hop relational tasks. That work shows that models predicting $y = f(x)$ iteratively surface vocabulary representations — first for x and then for y — in the residual stream. This “crossover” point was interpreted as evidence of the function f being applied to the argument x in order to yield the final answer $f(x)$ and was localized to specific computations in the MLPs.

In this section, we ask whether an analogous signature will emerge in the case of compositional functions, $g(f(x))$. That is, can we find distinct intermediate representations for x , followed by $f(x)$, and then $g(f(x))$ during the model’s processing?

Here, we employ analyses most similar to Biran et al. (2024) and Yang et al. (2025) in the context of our evaluation (see Sec. 7 for further discussion on these works). We also join other works in

216 identifying stages of processing within language models (Tenney et al., 2019; Merullo et al., 2024;
 217 Lepori et al., 2024).

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220 4.1 EXPERIMENTAL DESIGN

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We rely on existing methods which allow us to analyze processing signatures that are interpretable
 222 using the vocabulary space of the model (nostalgebraist, 2020; Geva et al., 2022). We specifically
 223 use *logit lens* (nostalgebraist, 2020), a method which projects intermediate representations into the
 224 vocabulary space using the language modeling head. We also include results in Appendix F using the
 225 token identity patchscope (Ghandeharioun et al., 2024) as an alternative decoding method to logit
 226 lens. We find that both methods yield similar findings.

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We follow the approach from Merullo et al. (2024) to identify the processing signature of models that
 228 solve our compositional tasks and, in particular, representations of the intermediate variables, $f(x)$
 229 and $g(x)$, prior to those for $g(f(x))$. We specifically use logit lens to analyze the residual streams
 230 corresponding to the computation $x \rightarrow g(f(x))$ and measure the reciprocal rank of our variables
 231 at each layer (see Appendix B for more details). We also use the maximum reciprocal rank of our
 232 intermediate variables across the layers as a heuristic for their overall presence in the computation.

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We conduct this analysis with the Llama 3 (3B) model. We exclusively analyze examples where the model can solve all requisite hops. To ensure sufficient sample sizes, we exclude any task with fewer than 10 such examples where the model can also successfully solve the composition. In particular, these excluded tasks include song-artist-birthyear, person-university-year, person-university-founder, mod-20-times-2, word-truncate-reverse, and rgb-rotate-name. We show results for these tasks in Appendices D and E.

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4.2 RESULTS

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243 Fig. 3a shows the relative presence of each of the variables, across layers and aggregated over all
 244 instances in which the model ultimately produced the correct answer. In such cases, we see a very
 245 clear peak signal for the intermediate variable $f(x)$, as expected, between those for x and $g(f(x))$.
 246 Interestingly, this signal is much less clear for cases in which the model ultimately produces the
 247 incorrect answer (Fig. 3b). However, upon further inspection, there is little evidence of a causal
 248 relationship here, which we discuss further in Appendix E.

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253 There are also plenty of individual examples in which the model produces a correct answer without
 254 showing any signature of the intermediate variables, and there is only a weak correlation by task
 255 ($r^2 = 0.22$) between predictive accuracy (measured as in Sec. 3.1) and the presence of intermediate
 256 variables as measured by our heuristic (Sec. 4.1).

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262 Figs. 3c to 3f show model processing signatures for a few tasks, aggregated over cases in which
 263 the model produces correct answers. We see, for example, that there is a clear signature in the
 264 antonym-spanish task (Fig. 3c) for the intermediate computation of $f(x)$, the word’s antonym,
 265 before it is translated into Spanish. In contrast, for the movie-director-birthyear task (Fig. 3d),
 266 there is no decodable signal for $f(x)$, the movie’s director, before the model produces their birth year.
 267 This variation can be seen in qualitatively similar tasks as well: tasks with the same basic arithmetic
 268 structure (Figs. 3e and 3f) only sometimes carries detectable signatures of $f(x)$ or $g(x)$, depending
 269 on the task’s operand (e.g. 10 or 100). We show processing signatures for the remaining tasks in
 Appendix D and for all tasks, aggregated over unsuccessful cases, in Appendix E.

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5 COMPOSITIONAL PROCESSING AND EMBEDDING SPACE LINEARITY

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Given that there is significant variation in whether or not the LLM solves a task compositionally
 (i.e. how strongly they appear to compute the intermediate variables), we next ask why this variation
 occurs. It is well-known that embedding spaces can capture relational information in their geometry
 (Mikolov et al., 2013; Hewitt & Manning, 2019). Moreover, Hernandez et al. (2024) shows that some
 subject → object relations can be represented by a single linear transformation from a language
 model’s residual stream activations to its unembedding space. Following this, we propose and test a

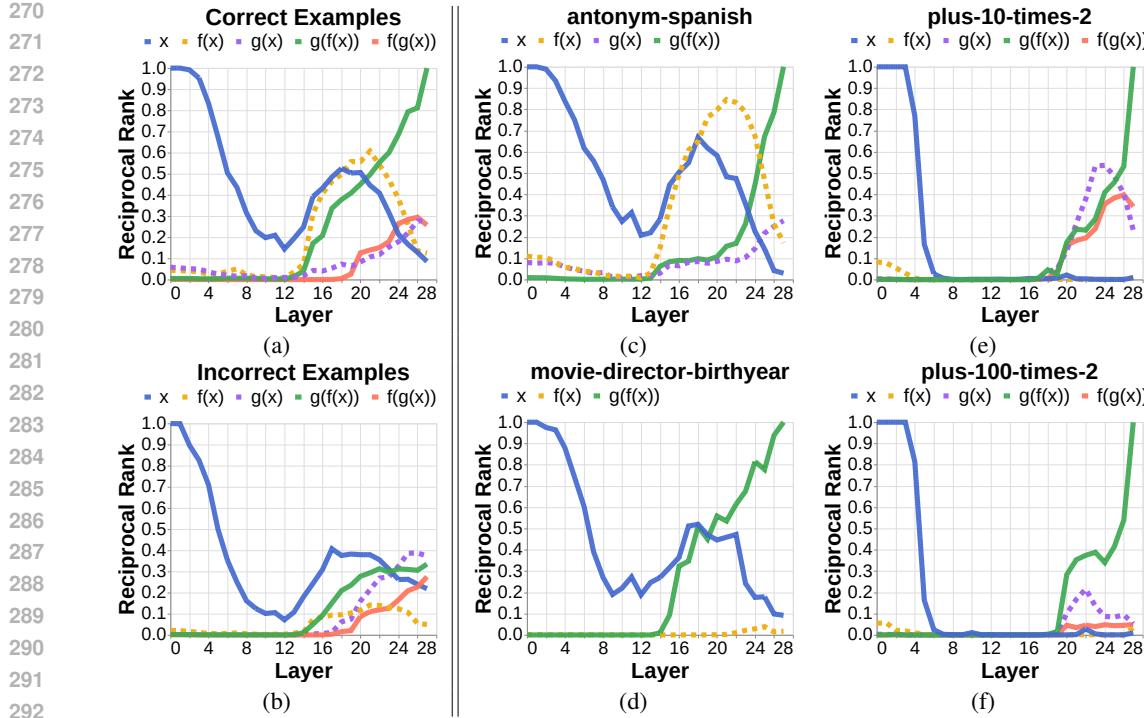


Figure 3: (a–b) Processing signatures aggregated over examples (across all tasks) in which Llama 3 (3B) solves all hops correctly, but the composition (a) correctly or (b) incorrectly. (c–f) Processing signatures for particular tasks — aggregated over examples where the model correctly solves all hops and the composition. (a–f) Lines show reciprocal ranks of relevant variables (decoded using logit lens) from residual streams corresponding to $x \rightarrow g(f(x))$. Intermediate variables are shown with dashed lines. The incorrect composition, $f(g(x))$, is shown by the red line when not distinct from $g(f(x))$.

hypothesis that language models could process compositional functions in one hop if they are directly represented as a linear transformation between the embedding and unembedding spaces.

5.1 EXPERIMENTAL DESIGN

To investigate our hypothesis, we fit a linear transformation for each task using least squares regression from x (average embedding across tokens) to $g(f(x))$ (first token unembedding) on 100 examples.³ We quantify the “linearity” of this transformation using its reconstruction accuracy (measured via cosine similarity) on the remaining examples. We quantify how “compositional” the processing is using our heuristic metric which captures the strength of the signal for the intermediate variables, $f(x)$ and $g(x)$ (see Sec. 4). We again restrict our analysis to examples where the model is successful on all hops and the composition, as well as tasks with at least 10 such examples.

5.2 RESULTS

Fig. 4a shows the that there is a strong inverse correlation ($r^2 = 0.53$) between the linearity of the representation and the compositionality of the processing. That is, the more linear the representation of a relation is in the embedding spaces, the more likely the model is to display *idiomatic* (as opposed to *compositional*) processing.

This correlation is computed by averaging linearity and compositionality across instances for each task. Fig. 4b shows the de-aggregated distribution of our “compositionality” metric across the

³See Appendix H for additional analyses which consider correlations with the linearities of the individual hops (rather than the compositional task).

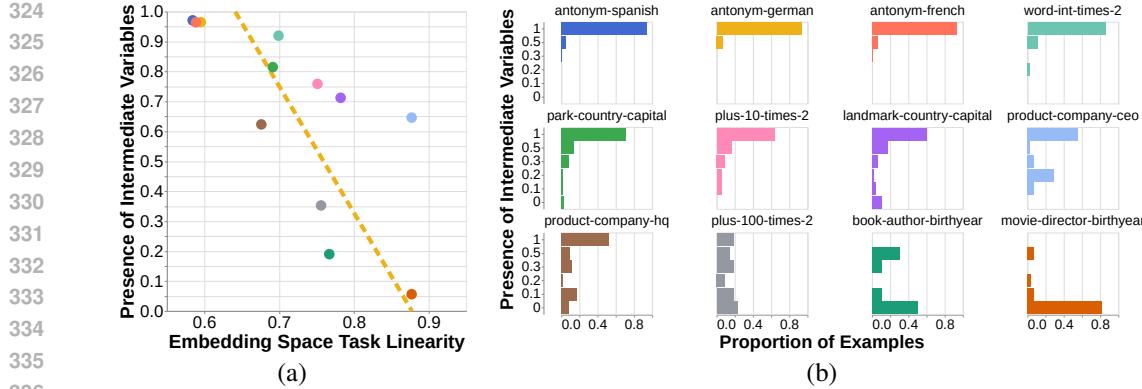


Figure 4: (a) Strong correlation across tasks between presence of intermediate variables (heuristic from Sec. 4.1 based on reciprocal rank; on average across examples) and embedding space linearity ($r^2 = 0.53$). Conversely, accuracy is weakly correlated with these intermediate variable ($r^2 = 0.22$) and linearity ($r^2 = 0.13$) metrics. (b) Distribution of examples for each task, shown as a histogram of intermediate variable reciprocal ranks. (a–b) Colors refer to corresponding tasks between points in (a) and histograms in (b).

examples. For some tasks, it appears that nearly all individual examples behave the same way. For example, nearly every instance of the antonym-spanish task displays a compositional processing signature, while almost every instance of the movie-director-birthyear task displays an idiomatic one. On the other hand, this distribution is more uniform for other tasks, such as plus-100-times-2. This distribution appears to be bimodal across all examples: 82% have very low (< 0.1) or high (≥ 0.5) values for compositionality.

6 DISCUSSION

Summary of Findings Our results suggest that tasks which appear to have the same computational structure may nonetheless be processed differently by LLMs. In particular, we consider functions which appear compositional in a formal sense — i.e. they can be represented as $y = g(f(x))$ for some reasonably defined f and g . We find evidence that LLMs only sometimes process such functions compositionally, showing evidence of representing or computing the value of $z = f(x)$ on the way to computing y . In other cases, LLMs appear to map x to y directly. Which of these processes is invoked appears to be related to how well the relationship between x and y is represented in the embedding space, e.g. as a result of pretraining (Merullo et al., 2025).

Implications for Theories of Compositionality There is a long-running debate about the degree to which compositional behavior (McCurdy et al., 2024) requires compositionality at the level of mechanisms. The two sides of this debate have often talked past each other, often using different types of computational architectures in order to model different aspects of behavior, for example, using explicitly compositional symbolic systems to model formal domains (Lake et al., 2017; Ellis et al., 2023) and using distributional or neural systems to model humans’ more idiomatic performance (Erk, 2012; Lampinen et al., 2024).

Attempts to find compromises or “hybrid” systems often consist of neuro-symbolic systems which are designed top-down (Andreas et al., 2016; Ellis et al., 2018). Large language models offer an alternative approach for advancing this debate. LLMs have proven capable of a range of behaviors that have traditionally required compositionality — e.g. generating language and writing formal computer code. However, LLMs lack the explicit symbolic mechanisms traditionally associated with such behaviors. Using methods from interpretability to understand how LLMs represent such functions internally enables us to approach the question in a “bottom up” manner, potentially offering novel hypotheses about the mechanisms that can generate behavior that is sometimes systematic and other times heuristic, as is the case in humans (Russin et al., 2025).

378 Our results suggest that LLMs employ a mix of compositional and idiomatic processing, and that the
 379 choice of mechanism is related to the representations of the functions that result from pretraining.
 380 This offers an interesting perspective on one question that is frequently at the heart of discussions of
 381 compositionality — i.e. what are the primitives and where do they come from Carey (2011)? The
 382 relationship between linearity in embedding space and compositionality of processing presented here
 383 suggests an attractive hypothesis that the primitives are those things which are well represented as a
 384 result of (pre-)training, and that compositional mechanisms are invoked to handle those things which
 385 are not sufficiently well represented. Future work in this direction would likely yield interesting new
 386 results and topics for debate.

387 **Relationship to work on compositional generalization** The work presented here concerns the
 388 (apparent) compositionality of the processing mechanism, but does not directly relate this mechanism
 389 to an LLM’s capacity for compositional generalization. The majority of work on compositionality
 390 in neural networks (and LLMs) concerns compositional generalization, and the compositionality
 391 researchers surveyed by McCurdy et al. (2024) overwhelmingly agree that existing language models
 392 are insufficient in this regard. This belief is supported by evidence from many prior works (Sec. 7)
 393 and our investigation in Sec. 3.

394 Our work suggests that models employ both compositional and direct mechanisms to solve tasks.
 395 Intuitively, we would expect there to be a relationship between the use of the mechanism and the
 396 ability to generalize — i.e. the compositional mechanism should support generalization better than
 397 the idiomatic mechanism (“memorization”). However, we do not test this intuition directly in this
 398 paper. Future work could do so by employing causal interventions on the intermediate variables, for
 399 example (see Appendix G for some initial investigations). This would likely present new complexities
 400 and challenges that would enrich our understanding of compositionality, and of the relationships
 401 between mechanisms and behaviors in LLMs in general.

403 7 RELATED WORK

404 **Latent multi-hop reasoning** Our work is most closely related to recent or concurrent works
 405 which also study latent two-hop reasoning in large language models. Yang et al. (2024a) use causal
 406 interventions to identify the existence of the hops in the latent computation and whether they co-occur.
 407 Biran et al. (2024) employ the entity description patchscope (Ghandeharioun et al., 2024) to inspect
 408 intermediate representations and localize the hops, finding they are resolved in different layers and
 409 token positions. They propose a representational intervention (“backpatching”) to correct failures
 410 based on this finding. Finally, Yang et al. (2025) use logit lens to analyze intermediate representations
 411 and consistently find a “compositional” processing signature across their tasks. Our work employs all
 412 of these interpretability methods (Sec. 4 and Appendices F and G) to analyze the hops, but specifically
 413 highlights and investigates the duality of the compositional vs. direct processing mechanisms. All
 414 works (including our own) test different sets of tasks, make experimental design decisions according
 415 to their independent goals,⁴ and make findings in context of their own experiments.

416 Among other works in this domain, Wang et al. (2024) trains a language model on synthetic compositional
 417 data and identifies a multi-hop reasoning circuit in this model. Shalev et al. (2024) conduct a
 418 distributional analysis (considering semantic category spaces, rather than individual tokens) using
 419 logit lens. Li et al. (2024); Yu et al. (2025) also propose interventions on intermediate representations
 420 and mechanisms to solve failure cases. Yang et al. (2024b) conduct an evaluation that is intentionally
 421 designed to omit opportunities for models to exploit shortcuts.

422 **Compositionality** Compositionality is long-studied (Fodor & Pylyshyn, 1988; Partee, 2004) but
 423 exact definitions evade general consensus. Russin et al. (2024) and McCurdy et al. (2024) offer
 424 recent overviews on the topic in the context of large language models. Russin et al. (2024) provide a
 425 historic account of compositionality and review studies of compositionality generalization in neural
 426 networks. McCurdy et al. (2024) survey compositionality researchers on how to define and evaluate
 427 compositional behavior in neural networks. These researchers agree that our current representational

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 430 ⁴One notable example is that, while Yang et al. (2024a) and Biran et al. (2024) prompt their models with f
 431 and g (e.g. “The mother of the singer of $\{x\}$ is $\{y\}$ ”), we omit this information from our prompts (i.e.
 432 more simply “Q: $\{x\}$ \n A: $\{y\}$ ”) to avoid inducing bias towards the compositional mechanism.

432 analyses are insufficient for evaluating models, but are divided about whether our behavioral analyses
 433 are sufficient.

434 In a partial effort towards defining compositionality, Hupkes et al. (2020) identify five particular aspects
 435 of compositionality and propose tests for each using a synthetic, fully compositional translation
 436 task. Systematicity is one such aspect and is prominently studied: see Vegner et al. (2025) for a
 437 survey of benchmarks for systematic generalization. Our work — in which we test whether $f(x)$ is
 438 evaluated before $g(f(x))$ — is closest to Hupkes et al. (2020)’s aspect of localism, in which “smaller
 439 constituents are evaluated before larger constituents”.

440 Among many other works, Johnson et al. (2017), (Keyser et al., 2019), Lake & Baroni (2018),
 441 Hupkes et al. (2020), and Kim & Linzen (2020) offer prominent benchmarks that behaviorally test for
 442 compositional generalization in neural networks trained from scratch on compositional data. These
 443 works generally show that such models perform poorly on generalization, or at least poorly implement
 444 the compositional processes that underlie the data. Press et al. (2022) and Ma et al. (2023) continue
 445 to show significant failures in compositional generalization in pre-trained models. On the other
 446 hand, Furrer et al. (2020) points out that pre-training a masked language model rivals or outperforms
 447 architectures specifically designed for the SCAN (Lake & Baroni, 2018) and CFQ (Keyser et al.,
 448 2019) generalization benchmarks. Lepori et al. (2023) finds that neural networks learn to implement
 449 compositionality structurally in their weights, supporting this claim against the need for specialized
 450 symbolic mechanisms.

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 452 **Compositionality of functions** Several works consider how language models solve compositions
 453 of functions (rather than specifically multi-hop reasoning tasks). Dziri et al. (2023) studies how
 454 language models autoregressively solve such tasks, like multi-digit multiplication, by inspecting their
 455 scratchpads. Wattenberg & Viégas (2024) propose mechanisms which neural networks could use to
 456 implement relational compositions. Yu et al. (2023); Todd et al. (2024) propose zero-shot methods
 457 to invoke compositions of functions in language models that have learned the primitive functions.
 458 Zhou et al. (2024) find that language models can compose functions with meta-learning in a way that
 459 imitates human behavior.

460
 461 **LIMITATIONS**

462 In this work, we primarily analyze the computation that occurs in a single forward pass of the Llama
 463 3 (3B) model. It is also necessary to understand how other models (e.g. larger models, reasoning
 464 models, or those with different inductive biases) implement compositional functions. Our findings
 465 reflect the tasks we happen to test (often, factual recall) under our specific experimental design.
 466 Further work should test other kinds of compositional functions, and try to more deeply understand
 467 the relationship between compositional mechanisms, behavior, and generalization.

468 We investigate a limited subset of mechanisms in language models and use current methods to conduct
 469 our analyses. These permit us to decode some, but not all, relevant representational structure. Some
 470 signals that we do decode may be a result of feature multiplicity or are not guaranteed to be causal.
 471 Finally, some of our tasks (e.g. arithmetic) may be solved by algorithms that we do not consider.

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 473 **REPRODUCIBILITY STATEMENT**

474 We make our code fully available so that all of our experiments can be replicated as closely as
 475 possible and all computational artifacts (datasets, plots, results) can be reconstructed. We do our best
 476 to include all experimental details in the main text and appendices of our paper.

477
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A DATA CREATION

672 Table 2: List of our tasks, showing x , $g(x)$, and $f(g(x))$ for the random example in Table 1. Tasks
 673 with neither $g(x)$ nor $f(g(x))$ are omitted. $f(g(x))$ only shown if distinct from $g(f(x))$.
 674

f	g	x	$g(x)$	$f(g(x))$
Word \rightarrow Antonym	English \rightarrow Spanish	bogus	false	—
Word \rightarrow Antonym	English \rightarrow German	philosophical	philosophisch	—
Word \rightarrow Antonym	English \rightarrow French	excessive	excessive	—
$x + 10$	$2x$	699	1398	1408
$x + 100$	$2x$	922	1844	1944
$x \bmod 20$	$2x$	891	1782	2
Word \rightarrow Numeric	$2x$	one hundred and forty-eight	two hundred and ninety-six	—
Word $[-1]$	Word $[-1]$	responsible	elbisnopser	elbisnopse
Rotate(RGB, 120°)	RGB \rightarrow Name	8a735a	dimgray	—

684
 685 All tasks in Table 2 permit the additional computational pathway $x \rightarrow g(x) \rightarrow g(f(x))$. Those
 686 which don’t list $f(g(x))$ are commutative and so $f(g(x)) = g(f(x))$ and applying f to $g(x)$ results
 687 in $g(f(x))$. The remaining tasks are not commutative, but their formal construction permits the hop
 688 $g(x) \rightarrow g(f(x))$ anyway. In particular, $g(f(x))$ equals $g(x) + 20$ in plus-10-times-2, $g(x) + 200$ in
 689 plus-100-times-2, $g(x) \bmod 40$ in mod-20-times-2, and $g(x)[1:]$ in word-truncate-reverse.
 690

A.1 TASK CONSTRUCTION

693 **Antonyms & Translations** We obtain a list of antonyms from Todd et al. (2024) — further derived
 694 from Nguyen et al. (2017) — and obtain translations from Opus-MT (Tiedemann & Thottingal,
 695 2020).

697 **Factual Relations** We obtain various factual relations from WikiData and IMDb Non-Commercial
 698 Datasets (Vrandečić & Krötzsch, 2014; IMDb.com, Inc., 2024; Bast & Buchhold, 2017). We apply
 699 a number of heuristics to obtain well-known and unambiguous mappings. For example, we filter
 700 entities by their “sitelinks” on WikiData or “votes” on IMDB (heuristics for popularity) to obtain
 701 well-known subjects. To avoid ambiguity, we identify subjects (songs, books, movies, people, etc.)
 with a single corresponding object (authors, attended universities, etc.). We omit parks and landmarks

702 that exist in their country’s capital. Our exact queries for generating each task can be found in our
 703 source code.
 704

705 **Arithmetic** We use the range of numbers from 0 to 999 as x in our tasks. These numbers typically
 706 result in one token. We use the `num2words` library to obtain a mapping between words and numeric
 707 values. We use the list of antonyms as our list of words for the `word-truncate-reverse` task.
 708

709 **Colors** In the `rgb-rotate-name` task, we randomly sample RGB colors, rotate them 120° by their
 710 hue, and map the resulting color value to that color’s name (using the `webcolors` library and the
 711 common CSS 3 specification).
 712

713 B IMPLEMENTATION DETAILS

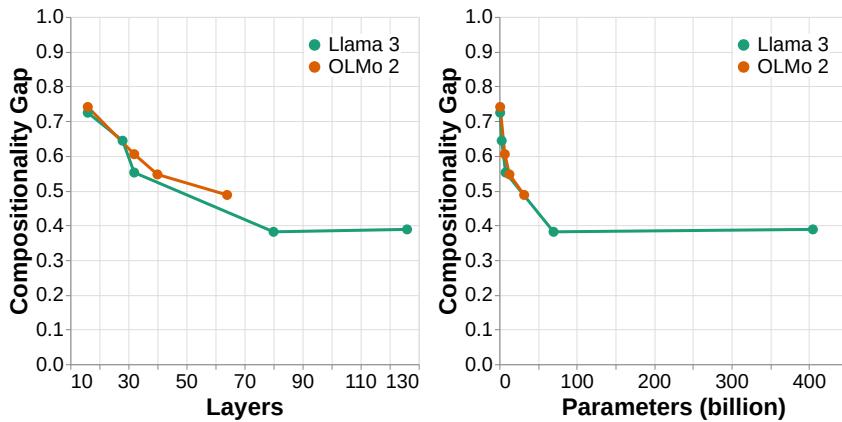
714
 715 **Examples & Prompts** We prevent sampling of in-context examples that intersect in the vari-
 716 ables $\{x, f(x), g(x), g(f(x)), f(g(x))\}$ with the query. And, as mentioned in Sec. 4.1, we exclude
 717 examples in Secs. 4 and 5 which overlap in the first token among their variables. So, although
 718 $x = \text{“excessive”}$ for the `antonym-french` task is listed in Table 2, this trivially shares the same first
 719 token as $g(x) = \text{“excessive”}$ and would be omitted from our analyses.
 720

721 Our prompts are tokenized differently when predicting numbers or words, e.g. “... \n A: 99”
 722 results in [] [99] whereas “... \n A: modern” results in [modern]. We accordingly include the
 723 trailing space in our prompts when predicting numbers and omit it otherwise. We would then test for
 724 the single-token prediction of [99] and [modern] in this example.
 725

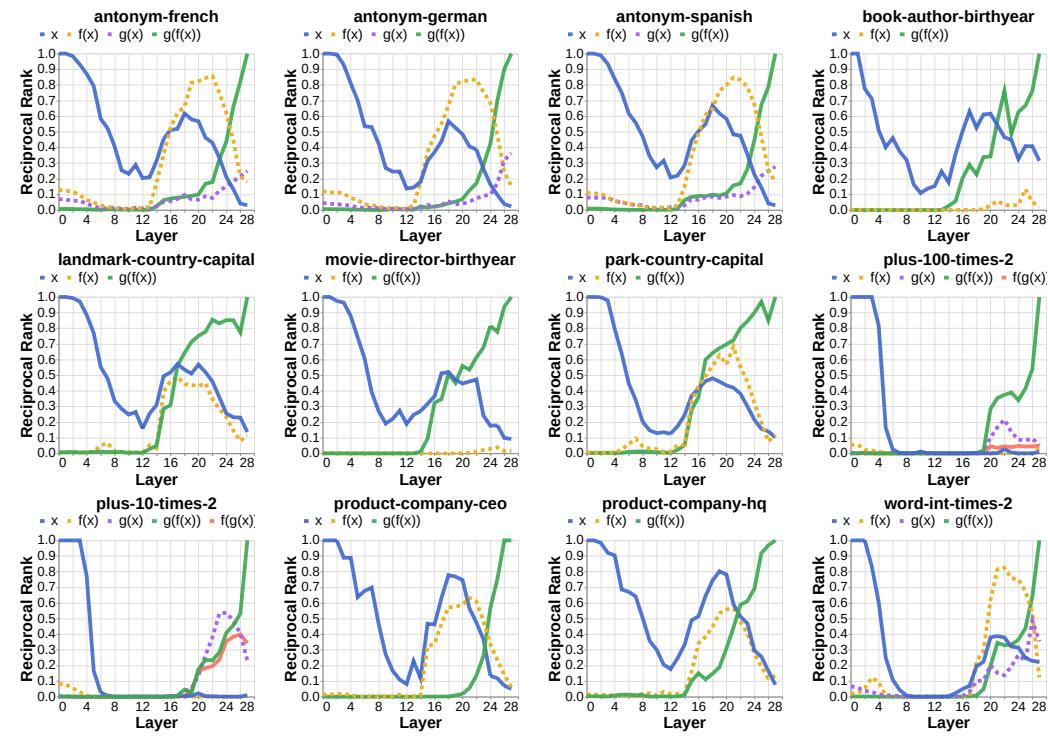
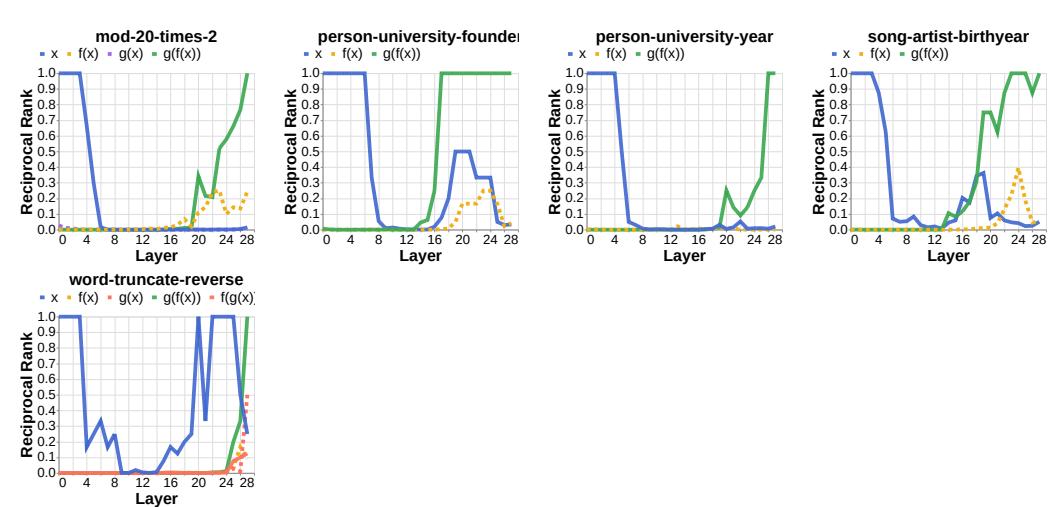
726 **Representational analysis** In Sec. 4, we analyze the model’s computation from $x \rightarrow g(f(x))$.
 727 Consider the query for “Heartbreak Hotel” \rightarrow “1935”: i.e. “... Q: Heartbreak Hotel \n A: ”.
 728 Here, multiple tokens ([Heart] [break] [Hotel] [\] [n] [A:] []) are central to the computation.
 729 We therefore analyze all residual streams for these tokens. At each layer, we measure the signal for
 730 each variable by its maximum reciprocal rank across the streams. This procedure yields processing
 731 signatures, which quantify the presence of our variables at every layer.
 732

733 We additionally represent each variable by its first token (since our decoding methods can only produce
 734 single-token probabilities) and exclude examples where different variables share the same first token
 735 and would be hard to differentiate. For example, $f(x) = \text{“modern”}$ and $g(f(x)) = \text{“moderno”}$ both
 736 share the first token [modern].
 737

C COMPOSITIONALITY GAP BY SIZE

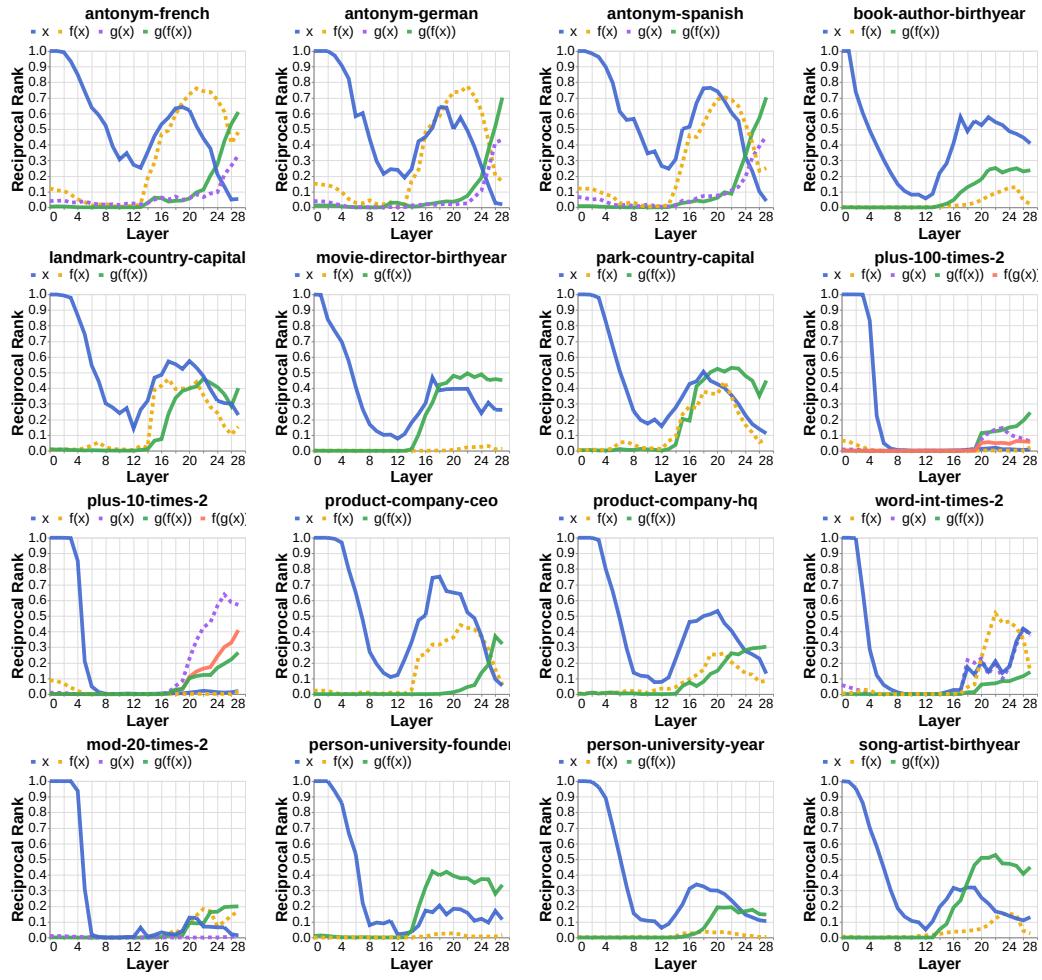


753 Figure 5: We illustrate the monotonically diminishing improvements to the compositionality gap
 754 resulting from increased model size (layers and parameters). We re-visualize results for the OLMo 2
 755 and Llama 3 model families from Fig. 2.
 756

756 **D PROCESSING SIGNATURES (CORRECT)**
757783 Figure 6: Aggregate processing signatures for each of our tasks, in which Llama 3 (3B) correctly
784 solves all hops and the composition for at least 10 examples.803 Figure 7: Aggregate processing signatures for each of our tasks, in which Llama 3 (3B) correctly
804 solves all hops and the composition for less than 10 examples.805 **E PROCESSING SIGNATURES (INCORRECT)**
806807 Although we see a difference in aggregate processing signatures (Figs. 3a and 3b), where the signal
808 for the intermediate variables is clearer in the correct cases than the incorrect cases, this does not

810 appear to be generally true (and is more likely due to data imbalances). We can see significant
 811 presence of the intermediate variables when considering incorrect examples, de-aggregated by task
 812 (Fig. 8).

813



845

846 Figure 8: Aggregate processing signatures for each of our tasks, in which Llama 3 (3B) correctly
 847 solves all hops but not the composition for at least 10 examples.

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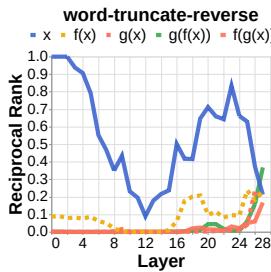
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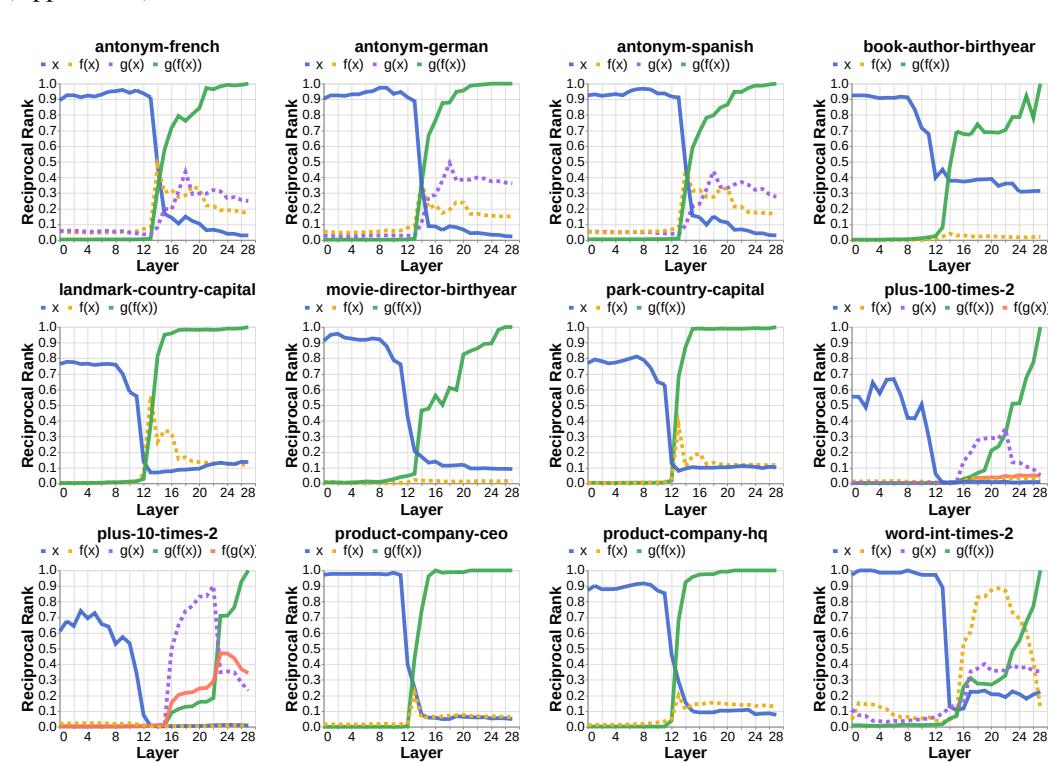
864 Figure 9: Aggregate processing signatures for each of our tasks, in which Llama 3 (3B) correctly
 865 solves all hops but not the composition for less than 10 examples.

864 F TOKEN IDENTITY PATCHSCOPE
865

866 Here, we repeat the analyses in Secs. 4 and 5, but use the token identity patchscope (Ghandeharioun
867 et al., 2024) instead of logit lens. This method is proposed as one that is more closely aligned with a
868 language model’s computation than other methods (such as logit lens).

869 We would specifically like to use this method to decode a representation into vocabulary-space logits.
870 To do so, we prompt a model with the “token identity prompt”, in which random tokens are repeated
871 twice each, such as “[A] [A] ; [B] [B] ; . . . ; [?]”. We patch our representation of interest
872 into the residual stream of this forward pass (at the corresponding layer and final token position).
873 The language modeling logits resulting from our intervention then serve as the decoding for our
874 representation.

875 We generally find similarities with our logit lens analyses: in tasks with “compositional” processing
876 signatures, we continue to see growth of the signals for the intermediate variables with or before
877 that for $g(f(x))$. Please zoom in to observe simultaneous growth, which may be difficult to see due
878 to overlapping lines. And, although these plots may show growth of $f(x)$ and $g(f(x))$ in the same
879 layers, recall that these computations can occur in different (e.g. earlier or later) residual streams
880 (Appendix B).



906 Figure 10: Aggregate processing signatures (using the token identity patchscope) for each of our
907 tasks, in which Llama 3 (3B) correctly solves all hops and the composition for at least 10 examples.
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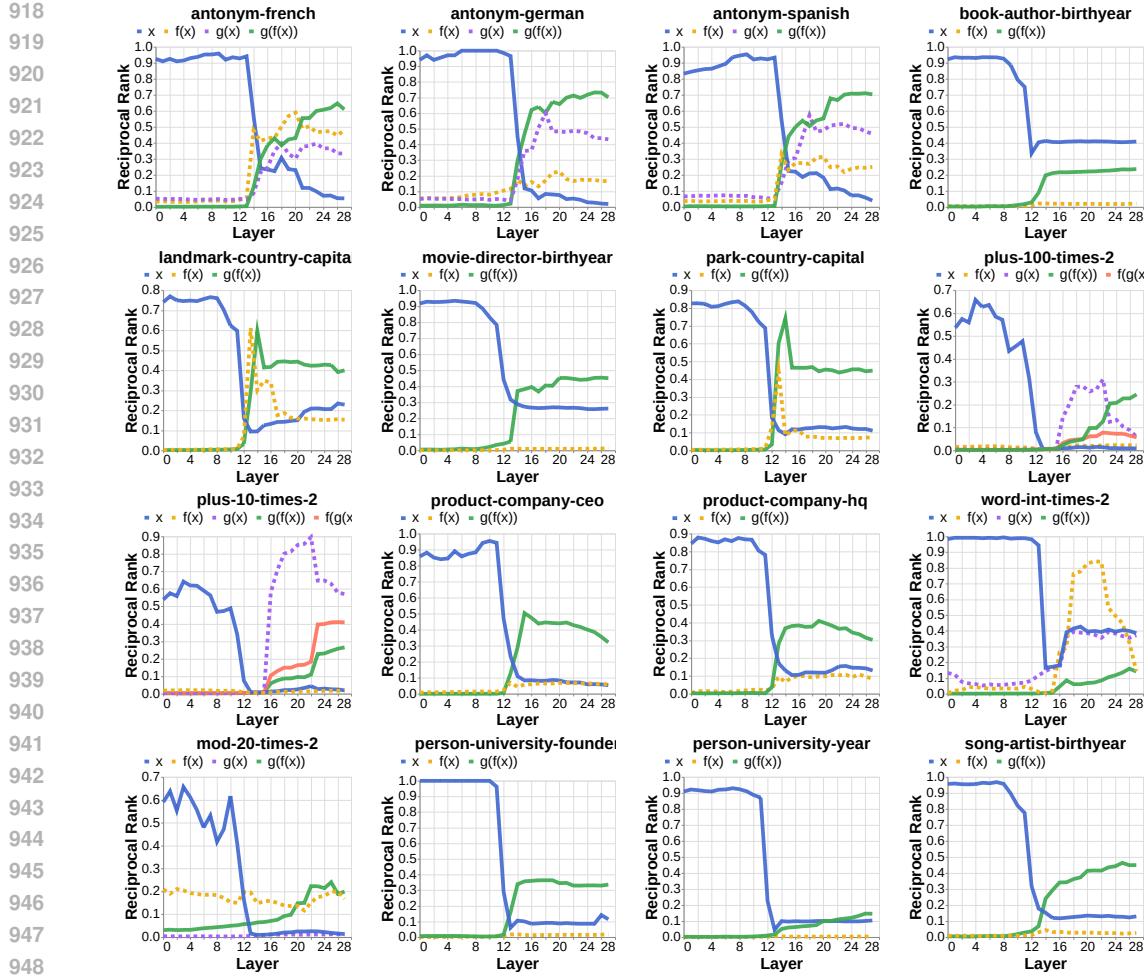


Figure 11: Aggregate processing signatures (using the token identity patchscope) for each of our tasks, in which Llama 3 (3B) correctly solves all hops but not the composition for at least 10 examples.

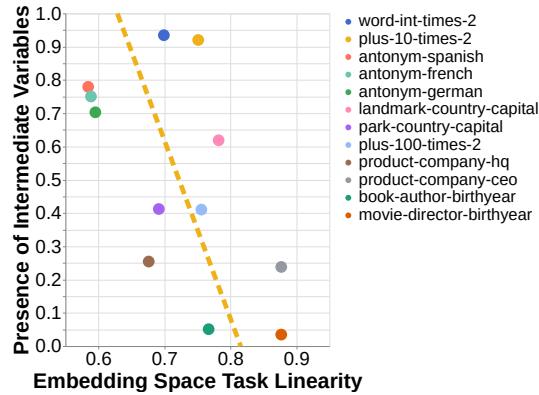


Figure 12: Correlation across tasks ($r^2 = 0.35$) for embedding space task linearity and presence of intermediate variables. Analogous to Fig. 4a, using the intermediate variable metric from the token identity patchscope.

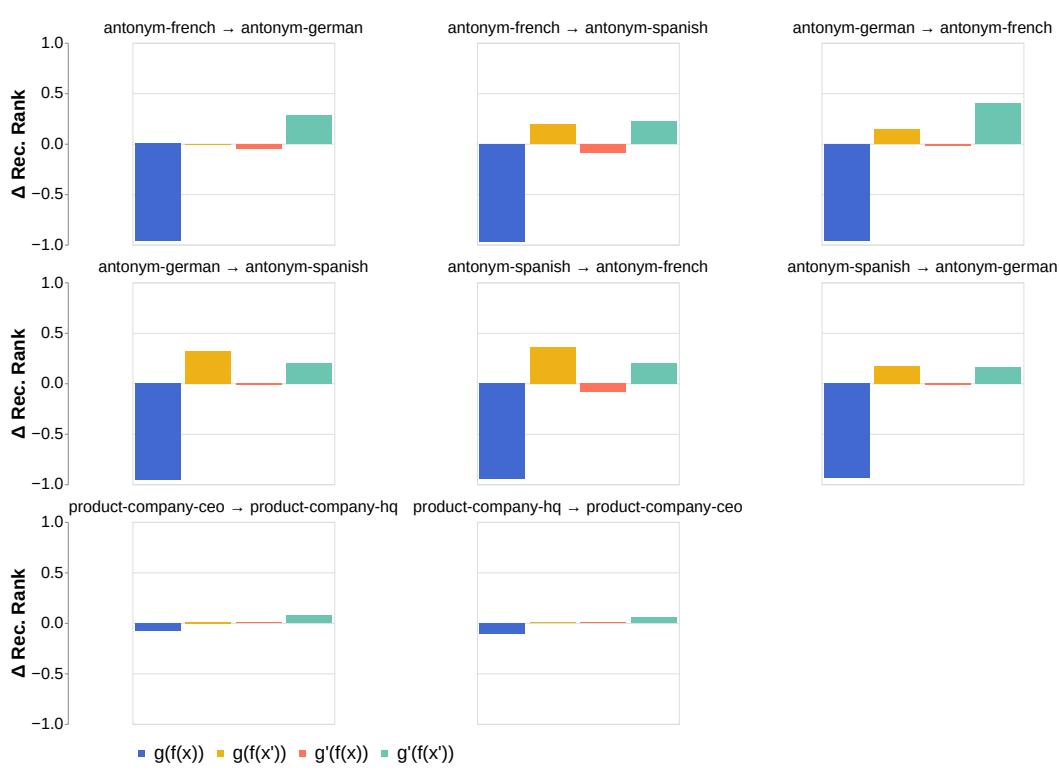
972 G CAUSALITY OF INTERMEDIATE VARIABLES

974 We would like to determine whether the variables, $f(x)$ and $g(x)$, we identify in models' intermediate
 975 representations have a causal effect on the outcome. We describe a preliminary investigation below.
 976

977 We use activation patching (Vig et al., 2020), a common method for conducting causal interventions
 978 in interpretability, and patch representations across tasks.
 979

980 We first identify tasks with the same f but different g , such as `antonym-spanish` ($g \circ f$) and
 981 `antonym-german` ($g' \circ f$). For some x and x' , we extract a single intermediate representation from
 982 the forward pass of $g'(f(x'))$ and patch it into the forward pass of $g(f(x))$. On average (over many x
 983 and x'), we measure the causal effects on the predictions $g(f(x))$, $g(f(x'))$, $g'(f(x))$, and $g'(f(x'))$.
 984

985 We extract the representation from $g'(f(x'))$ at the position and layer where $f(x)$ or $g(x)$ have
 986 the highest reciprocal rank (and only use instances where this value is at least 0.5). We patch this
 987 representation into the forward pass for $g(f(x))$ at the median location where intermediate values are
 988 highest (layer 18 and 71st percentile query token position; identified among variables that reach RR
 989 ≥ 0.5). We apply this intervention to two groups: instances with intermediate values that reach a peak
 990 RR ≤ 0.2 and ≥ 0.5 . In other words, instances with direct or compositional processing signatures.
 991



1014 Figure 13: Causal effects on predicted values after patching from $g'(f(x'))$ to $g(f(x))$ for instances
 1015 with compositional processing signatures.
 1016

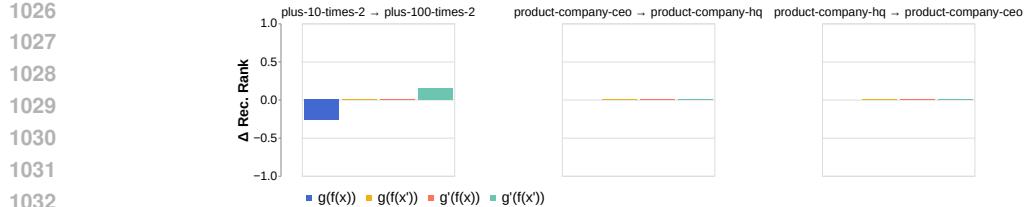


Figure 14: Causal effects on predicted values after patching from $g'(f(x'))$ to $g(f(x))$ for instances with direct processing signatures.

The Antonym–Translation tasks (which tend to have compositional signatures) show the most significant causal effect: on average, $g(f(x))$ and $g'(f(x))$ decrease by -0.95 and -0.4, and $g(f(x'))$ and $g'(f(x'))$ increase by 0.20 and 0.24. The effect on $g(f(x'))$ clearly implicates the existence and causality of $f(x')$ in the patched activation; that on $g'(f(x'))$ indicates the additional existence of either itself or the function vector (Todd et al., 2024) for g' in that representation. The causal effects on compositional instances of product-company-hq and product-company-ceo are smaller.

But we can also see a clear difference between the causal effects on the compositional and direct instances. Indeed, the effects on product-company-hq and product-company-ceo are larger in their compositional instances. Patching activations from plus-10-times-2 into plus-100-times-2 primarily decreases $g(f(x))$ and increases $g'(f(x'))$, perhaps only implying the existence of the representation for $g'(f(x'))$ in the patched activation.

H LINEARITY CORRELATIONS

Similarly to the experiment in Sec. 5 and Fig. 4a, we investigate the relationship between our compositionality heuristic and embedding space linearity for variations of the hops (rather than of the compositional task).

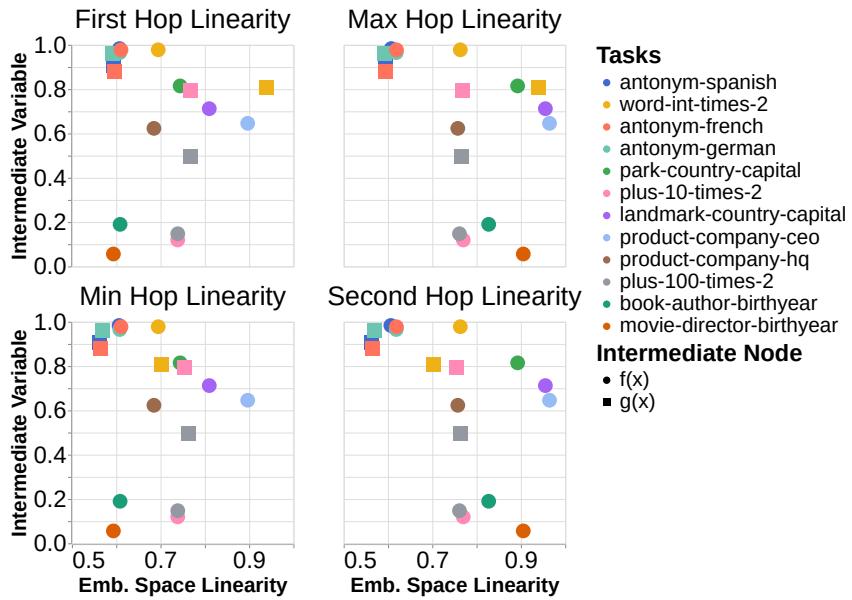


Figure 15: Relationships between presence of intermediate variables and embedding space linearity for the hops. We find weaker correlations in all cases. $r^2 = 0.01$ against the linearity of the first hop; $r^2 = 0.28$ against the second hop; $r^2 = 0.05$ using the minimum linearity between the hops; and $r^2 = 0.20$ using the maximum.