Emergent Symbol-like Number Variables in Artificial Neural Networks

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Abstract

What types of numeric representations emerge in neural systems? What would a satisfying answer to this question look like? In this work, we interpret Neural Network (NN) solutions to sequence based counting tasks through a variety of lenses. We seek to understand how well we can understand NNs through the lens of interpretable Symbolic Algorithms (SAs), where SAs are defined by precise, abstract, mutable variables to perform computations. We use GRUs, LSTMs, and Transformers trained using Next Token Prediction (NTP) on numeric tasks in which the solutions to the tasks depend on latent information in the task structure. We show through multiple causal and theoretical methods that we can interpret NN's raw activity through the lens of simplified SAs when we frame the neural activity in terms of interpretable subspaces rather than individual neurons. Depending on the analysis, however, these interpretations can be graded, existing on a continuum, highlighting the philosophical question of what it means to "interpret" neural activity, motivating us to introduce Alignment Functions to add flexibility to the existing Distributed Alignment Search (DAS) method. Through our specific analyses we show the importance of causal interventions for NN interpretability; we show that recurrent models develop graded, symbollike number variables within their neural activity; we introduce a generalization of DAS to frame NN activity in terms of linear functions of interpretable variables; and we show that Transformers must use anti-Markovian solutions—solutions that avoid using cumulative, Markovian hidden states—in the absence of sufficient attention layers. We use our results to encourage interpreting NNs through the lens of SAs using a variety of theoretic and causal analyses.

1 Introduction

We can see examples of the power of Neural Networks (NNs) in biological NNs (BNNs) from the impressive capabilities of human cognition, and in artificial NNs (ANNs) where recent advances have had such great success that ANNs have been crowned the "gold standard" in many machine learning communities (Alzubaidi et al., 2021). The inner workings of NNs, however, are still often opaque. This is, in part, due to their representations being highly distributed. Individual neurons can play multiple roles within a network in what's called population encoding. In these cases, human-interpretable information is encoded across populations of neurons rather than within any individual unit (Rumelhart et al., 1986; McClelland et al., 1986; Smolensky, 1988; Olah et al., 2017; 2020; Elhage et al., 2022; Scherlis et al., 2023; Olah, 2023).

Symbolic Algorithms (SAs), in contrast, defined as processes that manipulate distinct, typed entities according to explicit rules and relations, can have the benefit of consistency, transparency, and generalization when compared to their neural counterparts. A concrete example of an SA is a computer program, where the variables are abstract, mutable entities, able to represent many different values, processed by well defined functions. There are many existing theories that posit the necessity of algorithmic, symbolic, processing for higher level cognition (Do & Hasselmo, 2021; Fodor & Pylyshyn, 1988; Fodor, 1975; 1987; Newell, 1980; 1982; Pylyshyn, 1980; Marcus, 2018; Lake et al., 2017). Human designed symbolic cognitive systems, however, can lack the expressivity and performance of NNs. This is apparent in the field of natural language processing where neural architectures trained on vast amounts of data (Vaswani et al., 2017; Brown et al., 2020; Kaplan

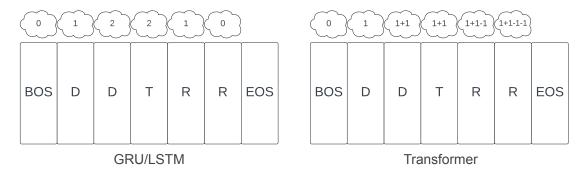


Figure 1: Different architecture's solutions achieving the same accuracy on a numeric equivalence task. The rectangles represent tokens for a task in which the model must produce the same number of R tokens ending with the EOS token as it observed D tokens. The T token indicates the end of the D tokens (see Methods 3.1). The thought bubbles represent the values of causally discovered neural variables encoded within the models' representations. The recurrent models encode a single count variable that increments up before the T token and down after the T token, with 0 indicating the end of the task. Transformers learn a solution in which they recompute the task relevant information from the input tokens at each step in the sequence. All NoPE transformers align with the displayed Transformer solution. RoPE transformers can partially rely on positional information unless they are trained on a variant of the task that breaks number-position correlations.

et al., 2020) have swept the field, surpassing the pre-existing symbolic approaches. Despite the differences between NNs and SAs, it might be argued that NNs actually implement simplified SAs; or, they may approximate them well enough that seeking neural analogies to these simplified SAs would be a powerful step toward an interpretable, unified understanding of complex neural behavior. In one sense, this pursuit is trivial for ANNs, in that ANNs are by definition aligned to the computer program that defines them. The complexity of these programs, however, is so great that simplified SAs become useful for explaining and predicting their behavior. This approach of seeking to characterize NNs in terms of *simplified* SAs is, in some sense, the goal of most cognitive science, neuroscience, and mechanistic interpretability.

In this work, we narrow our focus to numeric cognition and ask, how we can understand neural implementations of numeric concepts at the level of SAs? Numeric reasoning has the advantage of being well studied in humans of different ages and experience levels, which provides a powerful domain for comparisons between BNNs and ANNs (Di Nuovo & Jay, 2019). And numeric domains provide the benefit of tasks built upon well defined variables. We focus on a numeric equivalence task that was used to test the numeric abilities of humans whose language lacks explicit number words (Gordon, 2004). The task is formulated as a sequence of tokens, requiring the subject to produce the same number of response tokens as a quantity of demonstration tokens initially observed at the beginning of the task. This task is interesting for computational settings because the training labels vary in both identity and sequence length, and numbers are never explicitly labeled. Similar versions of this task have also been used in previous theoretical and computational work (El-Naggar et al., 2023; Weiss et al., 2018; Behrens et al., 2024), providing a platform to expand our understanding seemingly disparate systems in unified ways.

What sorts of representations do ANNs use to solve such a task and how do they arrive at these representations? Do the networks represent numbers in a shared system, or do they use different systems for different situations? Is it propitious to think about their representations as though they are discrete variables in an SA, or would it be better to think of their neural activity on a graded continuum? Do the answers to these questions change over the course of training, and do the answers vary based on task and architectural details? How can we unify the way we understand NN solutions in satisfying ways for cognitive scientists, neuroscientists, and computer scientists alike? We set out to understand NN neural activity through the lens of simplified, interpretable SAs using causal interventions to support our interpretations.

In this work, we pursue these questions by training Gated Recurrent Units (GRUs)(Cho et al., 2014), Long Short-Term Memory cells (LSTMs) (Hochreiter & Schmidhuber, 1997), and Transformers on numeric

equivalence tasks using Next Token Prediction (NTP). We then provide causal, correlative, and theoretical analyses such as activation patching, Principal Component Analysis (PCA), attention visualizations, and Distributed Alignment Search (DAS) (Geiger et al., 2021; 2023) to understand the networks' representations and solutions, and we introduce the notion of a Alignment Function to the DAS framework to allow us to frame neural activity in terms of linear functions of interpretable variables. We summarize our contributions as follows:

- 1. We show through causal interventions the emergence of graded neural variables in RNNs. These emergent neural variables are representational subspaces that causally align with variables in an SA, but still exhibit signatures of a continuum rather than being fully discrete.
- 2. We show that seemingly insignificant task variations can drastically affect the NN's alignment to the SAs, motivating us to introduce the notion of a Alignment Function to the DAS framework. This allows us to understand neural activity as a function of the variables from interpretable SAs.
- 3. We show empirically that Transformers use an anti-Markovian solution to the numeric tasks, and we show theoretically that Transformers must use anti-Markovian solutions in all tasks in the absence of sufficient attention layers.
- 4. Through our specific analyses, we demonstrate the importance of interpreting NNs at the level of neural subspaces and using causal interventions to make claims.

We use our results to encourage use of multiple causal interpretability tools for any representational analysis, to highlight functional differences that might emerge from architectural constraints, and to highlight the subjectivity involved in answering the question, "what does it mean to understand a neural system?"—adding nuance to philosophical discussions on mechanistic interpretability.

2 Related Work

We wish to highlight the importance of using causal manipulations for interpreting neural functions in this work. Causal inference broadly refers to methods that isolate the particular effects of individual components within a larger system (Pearl, 2010). An abundance of causal interpretability variants have been used to determine what functions are being performed by the models' activations (or circuits) (Olah et al., 2018; 2020; Wang et al., 2022; Geva et al., 2023; Merrill et al., 2023; Bhaskar et al., 2024; Wu et al., 2024). Vig et al. (2020) provides an integrative review of the rationale for and utility of causal mediation in neural model analyses. We rely heavily on DAS for our analyses. This method can be thought of as a specific type of activation patching (also referred to as causal tracing) (Meng et al., 2023; Vig et al., 2020).

Many publications explore ANNs' abilities to perform counting tasks (Di Nuovo & McClelland, 2019; Fang et al., 2018; Sabathiel et al., 2020; Kondapaneni & Perona, 2020; Nasr et al., 2019; Zhang et al., 2018; Trott et al., 2018) and closely related tasks (Csordás et al., 2024). Our tasks and modeling paradigms differ from many of these publications in that numbers are only latent in the structure of our tasks without explicit teaching of distinct symbols for distinct numeric values. El-Naggar et al. (2023) provided a theoretical treatment of Recurrent Neural Network (RNN) solutions to a parentheses closing task, and Weiss et al. (2018) explored Long Short-Term Memory RNNs (LSTMs) (Hochreiter & Schmidhuber, 1997) and Gated Recurrent Units (GRUs) (Cho et al., 2014) in a similar numeric equivalence task looking at the activations. These works showed correlates of a magnitude scaling solution in both theoretical and practically trained ANNs. Our work builds on their findings by using causal methods for our analyses, expanding the models considered, and introducing new type of analyses. Behrens et al. (2024) explored transformer counting solutions in a task similar to ours. Our work extends beyond theirs by exploring positional encodings, avoiding explicit labels of the numeric concepts, using causal analyses, and different theoretical explorations.

3 Methods

3.1 Numeric Equivalence Tasks

Each task we consider is defined by varying length sequences of tokens as shown in Figure 1. The goal of the task is to reproduce the same number of tokens as those observed before the Trigger (T) token. Each sequence starts with a Beginning of Sequence (BOS) token and ends with an End of Sequence (EOS) token. Each sequence is defined by first uniformly sampling an object quantity from the inclusive range of 1 to 20. The sequence is then constructed as the combination of two phases. The first phase, called the demonstration phase (demo phase), starts with the BOS token and continues with a series of demo tokens equal in quantity to the sampled object quantity. The end of the demo phase is indicated by the trigger token after the demo tokens. This also marks the beginning of the response phase (resp phase). The resp phase consists of a series of resp tokens equal in number to the demo tokens. After the resp tokens, the end of the sequence is denoted by the EOS token.

During the autoregressive model training, we include all tokens in the next token prediction loss. During model evaluation and DAS trainings, we only consider tokens in the resp phase—which are fully determined by the demo phase. During model trainings, we hold out the object quantities 4, 9, 14, and 17. A trial is considered correct when all resp tokens and the EOS token are correctly predicted by the model after the trigger. We include three variants of this task differing only in their demo and resp token types.

Multi-Object Task: there are 3 demo token types $\{D_1, D_2, D_3\}$ with a single response token type, R. The demo tokens are uniformly sampled from the 3 possible token types. An example input sequence with an object quantity of 2 could be: "BOS D_3 D_1 T", with a ground truth response of "R R EOS". All possible tokens are contained in the set $\{BOS, D_1, D_2, D_3, T, R, EOS\}$.

Single-Object Task: there is a single demo token type, D, and a single response token type, R. An example of the input sequence with an object quantity of 2 is: "BOS D D T", with a ground truth response of "R R EOS". All possible tokens are contained in the set {BOS, D, T, R, EOS}.

Same-Object Task: there is a single token type, C, used by both the demo and resp phases. An example of the input sequence with an object quantity of 2 is: "BOS C C T", with a ground truth response of "C C EOS". All possible tokens are contained in the set {BOS, C, T, EOS}.

For some transformer trainings, we include **Variable-Length (VL)** variants of each task to break count-position correlations. In these variants, each token in the demo phase has a 0.2 probability of being sampled as a unique "void" token type, V, that should be ignored when determining the object quantity of the sequence. The number of demo tokens will still be equal to the object quantity when the trigger token is presented. As an example, consider the possible sequence with an object quantity of 2: "BOS V D V V D T R R EOS".

3.2 Model Architectures

The recurrent models in this paper consist of Gated Recurrent Units (GRUs) (Cho et al., 2014), and Long Short-Term Memory networks (LSTMs) (Hochreiter & Schmidhuber, 1997). These architectures both have a Markovian, hidden state vector that bottlenecks all predictive computations following the structure:

$$h_{t+1} = f(h_t, x_t) \tag{1}$$

$$\hat{x}_{t+1} = g(h_{t+1}) \tag{2}$$

Where h_t is the hidden state vector at step t, x_t is the input token at step t, f is the recurrent function (either a GRU or LSTM cell), and g is a multi-layer perceptron (MLP) used to make a prediction, denoted \hat{x}_{t+1} , of the token at step t+1.

We contrast the recurrent architectures against transformer architectures (Vaswani et al., 2017; Touvron et al., 2023; Su et al., 2023) in that the transformers use a history of input tokens, $X_t = [x_1, x_2, ..., x_t]$, at each time step, t, to make a prediction:

$$\hat{x}_{t+1} = f(X_t) \tag{3}$$

Where f now represents the transformer architecture. We show results from 2 layer, single attention head transformers that use No Positional Encodings (NoPE) (Haviv et al., 2022) and Rotary Positional Encodings (RoPE) (Su et al., 2023). Refer to Supplemental Figure 5 for more model and architectural details. We also consider one-layer transformers with No Positional Encodings (NoPE) in Results section 4.2.2. For all of our analyses except the training curves in Figure 4, we first train the models to >99% accuracy on their respective tasks before performing analyses. One seed from the transformer models in both the Variable-Length Multi-Object and Variable-Length Same-Object tasks were dropped for low accuracy. The models are evaluated on 15 sampled sequences of each of the 16 trained and 4 held out object quantities. We train 5 model seeds for each training condition.

3.3 Symbolic Algorithms (SAs)

In this work, we examine the alignment of 3 different SAs to the models' distributed representations.

Up-Down Program: uses a single numeric variable, called the **Count**, to track the difference between the number of demo tokens and resp tokens at each step in the sequence. It also contains a **Phase** variable to determine whether it is in the demo or resp phase. The program ends when the Count is equal to 0 during the resp phase.

Up-Up Program: uses two numeric variables—the **Demo Count** and **Resp Count**—to track quantities at each step in the sequence. It uses a Phase variable to track which phase it is in. This program increments the Demo Count during the demo phase and increments the Resp Count during the resp phase. It ends when the Demo Count is equal to the Resp Count during the resp phase.

Context Distributed (Ctx-Distr) Program: queries a history of inputs at each step in the sequence, assigns a numeric value to each, and sums their values to determine when to stop (contrasted against encoding a cumulative, Markovian quantity variable). More specifically, this program uses an Input Value variable for each input token, and assigns the Input Value a value of 1 for demo tokens and -1 for resp tokens and computes the sum of the Input Values at each step in the sequence to determine the count. This program outputs the EOS token when the sum is 0 and the sequence contains the T token.

We include Algorithms 1, 2, and 3 in the supplement which show the pseudocode used to implement the Up-Down, Up-Up, and Ctx-Distr programs in simulations. Refer to Figure 1 for an illustration of the Up-Down strategy and the Ctx-Distr strategy that is observed in some transformers.

It is important to note that there are an infinite number of causally equivalent implementations of these SAs. For example, the Up-Down program could immediately add and subtract 1 from the Count at every step of the task in addition to carrying out the rest of the program as previously described. We do not discriminate between programs that are causally indistinct from one another in this work.

3.4 Distributed Alignment Search (DAS)

DAS measures the degree of alignment between a representational subspace from an NN and a symbolic variable from a symbolic algorithm (SA) by testing the assumption that the model hidden state $h \in R^{d_m}$ can be written as an orthogonal rotation h = Qz, where $Q \in R^{d_m \times d_m}$ is orthonormal, $z \in R^{d_m}$ consists of contiguous subspaces encoding high-level variables from SAs, and d_m is the size of the hidden state. The benefit of this alignment is that it allows us understand the NN's activity through interpretable variables and it allows us to manipulate the value of these variables without affecting other information.

Concretely, DAS performed on the Up-Down program tests the hypothesis that z is composed of subspaces c_{count} encoding the Count, c_{phase} encoding the Phase, and c_{extra} encoding extraneous, irrelevant activity.

$$z = \begin{bmatrix} c_{\text{count}} \\ c_{\text{phase}} \\ c_{\text{extra}} \end{bmatrix} \tag{4}$$

Each $c_{\text{var}} \in R^{d_{\text{var}}}$ is a column vector of potentially different lengths satisfying the relation $d_{\text{count}} + d_{\text{phase}} + d_{\text{extra}} = d_m$. Under this assumption, the value of a high-level variable encoded in h can be freely exchanged

through causal interventions using:

$$h^{v} = Q((1 - D_{\text{var}})Q^{-1}h^{trg} + D_{\text{var}}Q^{-1}h^{src})$$
(5)

Where $D_{\text{var}} \in R^{d_m \times d_m}$ is a manually chosen, diagonal, binary matrix with d_{var} non-zero elements used to isolate the dimensions corresponding to the subspace for variable var, h^{src} is the source vector from which the subspace activity is harvested, h^{trg} is the target vector into which activity is substituted, and h^v is the resulting intervention vector that can then replace h^{trg} in the model's processing, allowing the model to make predictions following the intervention.

DAS relies on the notion of counterfactual behavior to create intervention data to train and evaluate Q. For a given SA, we know what the SA's behavior will be after performing a causal intervention on one of its variables. The resulting behavior from the SA after intervening on a specific variable and keeping everything else in the algorithm and task constant is the counterfactual behavior. This counterfactual behavior can be used as a training signal for Q using next-token prediction. Q can equivalently learn any row permutation of the subspaces in z, thus we can restrict our searches to values of D_{var} that have contiguous non-zero entries. We can then brute-force search over independent trainings with different values of d_{var} , selecting the Q- D_{var} pair with the best results. Unless otherwise stated, we try values of d_{var} equal to 16 or half of d_m and take the better performing of the two. See Supplemental Figure 8 for a closer examination of how d_{var} affects results.

We perform our causal interventions on individual time steps in the sequence. We run the model up an independently sampled a timestep t on the target sequence, taking its latent representation a that point as the target vector, h_t^{trg} . We do the same for the source vector, h_u^{src} , at timestep u from a separate source sequence. We then construct h_t^v using Equation 5, and continue the model's predictions starting from time t, using h_t^v in place of h_t^{trg} .

For the LSTM architecture, we perform DAS on a concatenation of the h and c recurrent state vectors (Hochreiter & Schmidhuber, 1997). In the GRUs, we operate on the recurrent hidden state. In the transformers, we operate on the residual stream following the first transformer layer (referred to as the Layer 1 Hidden States in Supplementary Figure 5) or the input embedding layer. We use 10000 intervention samples for training and 1000 samples for validation and testing. For all data, we uniformly sample trial object quantities, and unless otherwise stated, we uniformly sample intervention time points, t and u, from sequence positions containing demo tokens or response tokens (excluding BOS, trigger, and EOS tokens). We orthogonalize the rotation matrix using PyTorch's orthogonal parameterization with default settings. We train Q with a batch size of 512 until convergence, selecting the checkpoint with the best validation performance for analysis. We use a learning rate of 0.001 and an Adam optimizer. See more detail in Supplement A.3.

DAS Evaluation: Once our rotation matrix has converged, we can evaluate the quality of the alignment using the accuracy of the model's predictions on the counterfactual outputs on held out intervention data. We consider a trial correct when all deterministic tokens are predicted correctly using the argmax over logits. We report the proportion of trials correct as the Interchange Intervention Accuracy (IIA) (as used in previous work (Geiger et al., 2023)).

DAS Alignment Functions: In an effort to understand the solutions employed by the Same-Object RNNs, we can relax the orthogonal constraint on the transformation function used in DAS. We do this by generalizing the matrix Q to an invertible function f(h) before performing the interchange intervention. We name these functions alignment functions due to their potential to encode the relationship between the neural activity and the specified interpretable variables. Formally, we can write the model's latent representation, h, in terms of an invertible function, f, where z = f(h). In this work, we only examine linear cases of f of the form f(h) = X(h + b) where $X \in \mathbb{R}^{d_m \times d_m}$ is an invertible symmetric definite matrix and $b \in \mathbb{R}^{d_m}$ is a bias vector. Using $\phi \in \{trg, src\}$ to denote that the same alignment function is applied to both the target and source vectors before the intervention, we reformulate Equation 5 in terms of f:

$$z^{\phi} = f(h^{\phi}) = X(h^{\phi} + b) \tag{6}$$

$$h_t^v = X^{-1}((1-D)z_t^{trg} + Dz_u^{src}) - b$$
 (7)

With this formulation, we are able to train X and b using the same counterfactual sequences used to train Q in Equation 5. We refer to the original DAS analyses as using an **Orthogonal Alignment** and the

linear formulation from Equations 6 and 7 as the **Linear Alignment**. In our experiments, we construct $X = SMM^{\top}$ where $M \in R^{d_m \times d_m}$ is a matrix of learned parameters initially sampled from a gaussian distribution with a standard deviation of $\frac{1}{d_m}$ and $S \in R^{d_m \times d_m}$ is a diagonal scaling matrix with diagonal values $s_{i,i} = \text{Tanh}(a_i) + 0.1(\text{sign}(\text{Tanh}(a_i)))$ where each a_i is a learned parameter.

3.4.1 Activation Substitutions

RNN Individual Activation Substitutions: We explore direct substitutions of individual ANN neuron activations in the Multi-Object trained RNN models to demonstrate the relative ineffectiveness of individual neuron patching compared to the rotated subspace interventions used in DAS. In these individual activation experiments, we directly replace the activation value of a specific neuron within its recurrent hidden state vector at time step t with the value of the same neuron at time step t from a different sequence. This is equivalent to Equation 5 using an identity rotation with a single non-zero value in D corresponding to the index of the desired neuron. We perform these interventions for every model neuron, and we evaluate the model's IIA using the expected behavior from the Count interventions.

Transformer Hidden State Substitutions: A sufficient experiment to determine whether a Transformer is using Markovian states is to examine its behavior after replacing all activations in its most recent hidden state vector from time t from a target sequence with representation from time u from a source sequence. If the post-intervention behavior matches that of the source sequence after time u, then the state has encoded all behaviorally relevant information in its activation vector and we can conclude that the intervened transformer state is Markovian. If the post-intervention behavior ignores the substitution and matches the target sequence after time t, then we can conclude that the states are anti-Markovian. In two layer transformers, we only need to perform this intervention on the residual stream hidden states after Layer 1 as the residual stream after Layer 2 can no longer transmit information between token positions (see Supplement A.4 for more detail). See Supplement A.3.6 for specific intervention data examples.

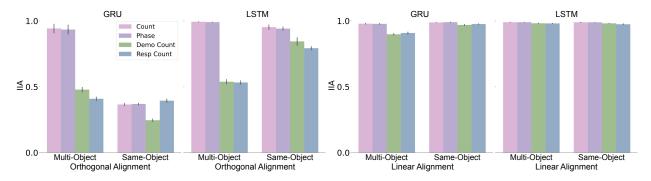


Figure 2: The Interchange intervention accuracy (IIA) for variables from different SAs for different tasks and architectures. The displayed IIA for the Count and Phase variables comes from the Up-Down program. The IIAs for the Demo Count and Resp Count variables come from the Up-Up program. IIA measurements show the proportion of trials where the model correctly predicts all counterfactual R and EOS tokens following a causal intervention. The DAS alignment function is displayed below each panel.

4 Results

4.1 Recurrent Neural Networks

4.1.1 Individual Activation Substitutions

We performed direct substitutions of individual activation values in recurrent models' hidden state vectors to demonstrate the importance of operating on a subspace of the neural population rather than on individual neurons. We turn our attention to the raw activation traces in the topmost panel (b) of Figure 3, and note that neurons 12 and 18 (shown in blue and black) have a high correlation with the Count of the sequence.

These traces came from an LSTM with $d_m=20$. In this model, we attempted interchange interventions that transferred the raw activity from both neurons 12 and 18 in an attempt to transfer the value of the Count. These interventions achieved an IIA of 0.399 on the behavior generated from the Up-Down program. Furthermore, we observed no consistent pattern of behavior (i.e. off by one errors) following the interventions. We include this result as a cautionary demonstration that interpreting and intervening raw NN activations can be misleading and difficult.

4.1.2 DAS

The left side of Figure 2 shows the DAS alignments using the orthogonal alignment function for RNNs trained on the Multi-Object and Same-Object tasks. In the Multi-Object recurrent models, we see that the most aligned SA is the Up-Down program from the higher IIA in the Count and Phase variables compared to the Demo Count and Resp Count variables from the Up-Up program. We use this as evidence in favor of the interpretation that the Multi-Object GRUs and LSTMs develop a count up, count down solution to track quantities within the task using a neural variable to encode quantity. The existence of numeric neural variables stands as a proof of principle that neural systems do not require explicit exposure to discrete numeric symbols, nor do they need built in counting principles, for symbol-like representations of number to emerge.

4.1.3 Graded Symbols

By increasing the granularity of our analyses, we uncovered a continuous effect of the content of the values involved in the interchange interventions. We can see this in Figure 4 (c) and (d). We see a gradience in the IIA, where the interventions have a relatively smooth decrease in IIA when the quantities involved in the intervention are large and when the intervention quantities have a greater absolute difference. This indicates that the neural variables possess some level of graded continuity. We refer to such neural variables

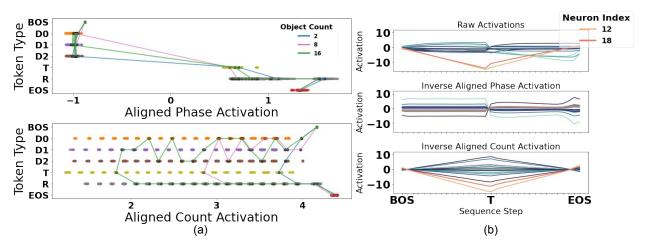


Figure 3: (a) The top panel shows h projected onto the aligned dimension of a Linear Alignment function $DX^{-1}(h-b)$ trained using a single dimension on the Phase variable. The bottom panel shows the same for an alignment with the Count variable. The h vectors are collected from 15 trials for each object count ranging from 1-20 from a single Multi-Object LSTM of size 20. The IIA for the was 84.7% and the Count was 82.6%. The connecting lines trace the states from individual trials with object counts of 2, 8, and 16. The dot colors redundantly encode token type. (b) Each trace within the three panels shows the mean activation value for an individual neuron at each step in the trial averaged over 15 trials each with object counts of 15. The topmost panel shows the raw activation values. We label two specific neurons (index 12 and 18 within the $h \in R^{20}$ vector) that have a high correlation with the Count of the sequence. We show in Section 4.1.1 that these two neurons are insufficient to causally transfer a consistent representation of the Count to different steps in the sequence. The middle panel shows the inverse of the aligned projected activity from the Phase alignment in (a), equal to $X^{-1}(DX(h+b)) - b$. Similarly, the bottom-most panel shows the inverse aligned activity from the Count alignment.

as symbol-like, or graded neural variables. We point out that the task training data provides more experience with smaller numbers, as the models necessarily interact with smaller quantities every time they interact with larger quantities. This is perhaps a causal factor for the more graded representations at larger numbers, but we do not explore this further. The DAS training data suffers from a similar issue due to the fact that we use a uniform sampling procedure for the object quantities that define the training sequences and we uniformly sample the intervention indices from appropriate tokens in these sequences. This results in a disproportionately large number of training interventions containing smaller values.

The graded neural variables raise the question of how best to interpret neural networks. We remind ourselves that the ANN is built on a symbolic computer program, and thus, this program will always align perfectly with the ANN by definition. The non-trivial goal of our work is to find SAs that simplify the computations of the ANN in interpretable ways. The symbolic gradience that we observe in our models serves as partial motivation for the alignment functions examined in Section 4.1.5.

4.1.4 Model Width, Developmental Trajectories, and Task Variations

Model Width: We see in Figure 4(a) that although many model widths can solve the Multi-Object task, increasing the number of dimensions in the hidden states of the GRUs seems to improve the IIA of the Up-Down alignment. We can also see from Figure 4 (b) that the larger models tend to have better IIA. Although our results are for RNNs on linear tasks, an interesting related phenomenon in the LLM literature is the effect of model scale on performance (Brown et al., 2020; Kaplan et al., 2020). We do not concretely explore why increasing dimensionality improves IIA, but we speculate that with greater dimensionality comes a greater likelihood of any two variable subspaces to be orthogonal to one another.

Developmental Trajectories: Turning our attention to the learning trajectories in Figure 4, we can see that the models' task accuracy and IIA begin to transition away from 0% at similar epochs and plateau at similar epochs. This finding can be contrasted with an alternative result in which the alignment curves significantly lag behind the task performance of the models. Alternatively, there could have been a stronger upward slope of the IIA following the initial performance jump and plateau. In these hypothetical cases, a possible interpretation could have been that the network first develops more complex solutions, or it could have developed unique solutions for many different input-output pairs and subsequently unified them with further training. The pattern we observe instead is consistent with the idea that the networks are biased towards simple, unified strategies early in training. Perhaps our result is expected from works like Saxe et al. (2019) and Saxe et al. (2022) which show an inherent tendency for NNs trained via gradient descent to find solutions that share network pathways. This would provide a driving force towards the demo and resp phases sharing the same representation of a Count variable.

Task Variations: An interesting result is the impact of demonstration token type on the resulting alignments of the RNNs with the Up-Down program. Figure 2 shows that RNNs trained on the Same-Object task—in which the demo tokens are the same type as the resp tokens—have poor alignment with our proposed SAs. This result serves as a contrast to the high IIA in the Multi-Object and Single-Object models. It also helps motivate the use of linear alignment functions.

4.1.5 Linear Alignment Functions

The right side of Figure 2 shows the IIA using the linear alignment function. We can see that the resulting IIAs for all models and all variables is higher than the orthogonal alignment function. We ask, why does the linear relaxation improve IIA? To answer this, we reformulate the model's neural activity, h, in terms of activity component vectors $u_i \in R^{d_m}$: $h = X^{-1}z - b = Uz - b = \sum_{i=1}^{d_m} z_i u_i - b$, where X and b are the linear alignment function, $U = X^{-1}$ for notational ease, z is a vector composed of interpretable subspaces from Equation 4, and z_i refers to the value of the ith dimension of z. The interchange intervention in Equation 7

is equivalent to exchanging weighted activity components $z_i u_i$:

$$h^{v} = U(Dz^{src} + (1-D)z^{trg}) - b = \sum_{i=1}^{d_{\text{var}}} z_{i}^{src} u_{i} + \sum_{i=d_{\text{var}}}^{d_{m}} 0z_{i}^{src} u_{i} + \sum_{i=1}^{d_{\text{var}}} 0z_{i}^{trg} u_{i} + \sum_{i=d_{\text{var}}}^{d_{m}} z_{i}^{trg} u_{i} - b$$
 (8)

$$h^{v} = \sum_{i=1}^{d_{\text{var}}} z_{i}^{src} u_{i} + \sum_{i=d_{\text{var}}}^{d_{m}} z_{i}^{trg} u_{i} - b = \sum_{i=1}^{d_{\text{var}}} z_{i}^{src} u_{\text{var},i} + \sum_{i=d_{\text{var}}}^{d_{m}} z_{i}^{trg} u_{\text{yar},i} - b$$
(9)

Where $u_{\text{var},i}$ indicates that the activity corresponds to the intervened variable subspace and $u_{\text{yar},i}$ is all other activity. We know that the inner product $\langle (1-D)z^{trg}, Dz^{src} \rangle = 0$. If U is orthogonal, then $\langle U(1-D)z^{trg}, UDz^{src} \rangle = 0$ due to the fact that orthogonal matrices preserve angles and inner products. Thus, when using an orthogonal alignment function, the intervened subspace needs to be orthogonal to the other variable's subspaces in the original neural space for interventions to avoid operating on overlapping subspaces. This is not the case, however, for the general linear alignment because $\langle X(1-D)z^{trg}, XDz^{src} \rangle$ need not be equal to 0. This means that the linear alignment function can potentially allow the intervened subspaces to be non-orthogonal in the original neural space. This is a possible reason for why IIA improves when using the linear alignment function. We note that it is possible to compose the Count as a linear combination of the Demo Count and Resp Count variables, which is a possible reason for why they have comparable alignments to the Count in cases using the linear alignment function. We leave to future work explorations on how alignment functions can be used to understand NN solutions that use informational superposition (Elhage et al., 2022; Olah, 2023).

An interesting case of alignment functions occurs when we set d_{var} , the aligned subspace size, to 1. This allows us to decompose h into a linear combination of vectors corresponding to each variable. Concretely, using the Count and Phase variables, we can decompose h into $h = z_{\text{count}} u_{\text{count}} + z_{\text{phase}} u_{\text{phase}} + c$ where $c = \sum_{i=2}^{d_m} z_{\text{extra},i} u_{\text{extra},i} - b$. This can be thought of as an explanatory relationship between the high-level, interpretable variables and the raw neural activity.

To visually examine linear alignment cases where $d_{\text{var}} = 1$, we provide Figure 3 (a) and (b). (a) shows many different h vectors from many different time steps and trials, each projected into 1-dimensional aligned Phase and Count subspaces. In Figure 3 (b), we show the inverse of aligned activity, $z_{\text{phase}}u_{\text{phase}} - b$ and $z_{\text{count}}u_{\text{count}} - b$, over the same trials as the raw activity in the top panel. This exemplifies a way to view the neural activity, in the original neural space, through the lens of the interpretable variables. We can see that many of the neurons play a role in both the Phase and Count neural coding.

4.2 Transformers

In this section, we demonstrate through empirical and theoretical means that transformers solve the task by recomputing the solution to the task at each step in the sequence. We refer to this class of solutions as anti-Markovian, named for their inductive bias against cumulative, Markovian states. We begin by demonstrating that using the previous layer's hidden states as the inputs to the attention mechanism restricts transformers from using Markovian solutions that use more steps than attention layers. We then demonstrate a theoretical solution for simplified versions of the Single-Object and Multi-Object numeric equivalence tasks in one layer NoPE transformer architectures, and we causally verify that such a solution emerges empirically. We then show through causal interventions that similar solutions can emerge in two layer RoPE transformers, and lastly we examine the degree to which the computations can be localized to a single attention head.

4.2.1 Anti-Markovian States

In this section, we demonstrate why Transformer solutions that use Markovian states in the residual stream require a new attention layer for every new step in the sequence. To show this, we focus on a simplified transformer architecture that only includes an embedding layer and the self-attention mechanism within each layer. To justify this simplification, we note that the attention mechanism is the only mechanism in the transformer that provides an opportunity to transmit information between token positions in the sequence.

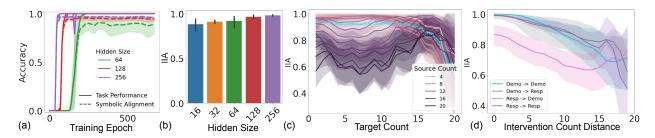


Figure 4: In all panels, the IIA comes from DAS using an Orthogonal Alignment trained on the Count variable in the Up-Down program. The models are all Multi-Object GRUs. (a) Shows task accuracy and IIA over the course of training for architectures with different sizes of the recurrent state h. We note the correlation between IIA and accuracy, with relatively little change as training continues. (b) Shows the final IIA for the GRUs as a function of increasing hidden state sizes. (c) Shows the IIA from the 128d GRU as a function of the Count value from the source h_u^{src} (denoted by color) and the Count before the intervention in the target h_t^{trg} (shown on the x-axis). The cyan, dashed line represents the mean IIA over all interventions for a given target count—highlighting the unequal distribution over target source pairs. (d) DAS IIA from the 128d GRU as a function of the absolute difference between the target and source counts. The colors indicate the Phase of h^{src} on the left and h^{trg} on the right. Panels (c) and (d) show that the value of the variable during the interventions somewhat smoothly affect the resulting IIA. See Supplemental Section A.3.7 for detail on the data used in panels (c) and (d).

With this simplification, we can write the output of a single transformer layer as:

$$\begin{bmatrix} h_0^{\ell} & h_1^{\ell} & \dots & h_t^{\ell} \end{bmatrix} = \begin{bmatrix} h_0^{\ell-1} & h_1^{\ell-1} & \dots & h_t^{\ell-1} \end{bmatrix} + \operatorname{attn}_{\ell} (\begin{bmatrix} h_0^{\ell-1} & h_1^{\ell-1} & \dots & h_t^{\ell-1} \end{bmatrix})$$
(10)

where $h_t^{\ell} \in \mathbb{R}^d$ are column vectors from the transformer residual stream, ℓ denotes the attention layer where $\ell=0$ is the output of the embedding layer, t refers to the positional index in the sequence, and attn $_{\ell}(x)$ refers to the attention mechanism. If we denote residual stream vectors that have encoded an updated cumulative state as h, assume that the attn function can only transmit state information to time t that has already been encoded at time t-1, and assume that the cumulative state is already trained into the embedding for time t=0, then the cumulative state gets updated with each transformer layer as follows:

$$\begin{bmatrix} \hat{h}_0^0 & h_1^0 & h_2^0 & \dots & h_t^0 \end{bmatrix} = \text{Embedding}(x_0, x_1, x_2, \dots, x_t)$$
(11)

$$\begin{bmatrix} \hat{h}_0^1 & \hat{h}_1^1 & h_2^1 & \dots & h_t^1 \end{bmatrix} = \begin{bmatrix} \hat{h}_0^0 & h_1^0 & h_2^0 & \dots & h_t^0 \end{bmatrix} + \operatorname{attn}_1(\begin{bmatrix} \hat{h}_0^0 & h_1^0 & h_2^0 & \dots & h_t^0 \end{bmatrix})$$
(12)

$$[\hat{h}_0^2 \quad \hat{h}_1^2 \quad \hat{h}_2^2 \quad \dots \quad h_t^2] = [\hat{h}_0^1 \quad \hat{h}_1^1 \quad h_2^1 \quad \dots \quad h_t^1] + \operatorname{attn}_2([\hat{h}_0^1 \quad \hat{h}_1^1 \quad h_2^1 \quad \dots \quad h_t^1])$$
 (13)

$$... = ...$$
 (14)

$$\begin{aligned}
& \dots &= \dots \\
& [\hat{h}_0^t \quad \hat{h}_1^t \quad \hat{h}_2^t \quad \dots \quad \hat{h}_t^t] &= [\hat{h}_0^{t-1} \quad \hat{h}_1^{t-1} \quad \hat{h}_2^{t-1} \quad \dots \quad h_t^{t-1}] + \operatorname{attn}_t([\hat{h}_0^{t-1} \quad \hat{h}_1^{t-1} \quad \hat{h}_2^{t-1} \quad \dots \quad h_t^{t-1}]) \quad (15)
\end{aligned}$$

Where x_t denotes the input token id at time t. We can see from Equations 11 that in the best case scenario, the cumulative state can only be transmitted and updated one layer at a time. Thus the two layer transformers in our work are architecturally restricted from using a solution that involves a cumulative state.

We experimentally verify that the two layer RoPE transformers used in this work use anti-Markovian states by performing the Transformer Hidden State Substitutions outlined in Methods Section 3.4.1. Indeed, these substitutions leave the NNs' behavior largely unaffected with an IIA of 0.964 on the original behavior in the Multi-Object RoPE transformers and 0.949 for the Variable-Length Multi-Object RoPE transformers.

We note that generative techniques like scratch pad (Nye et al., 2021) and Chain-of-Thought (CoT) (Wei et al., 2023) allow for transformers to track a cumulative state in the form of self-generated input embeddings. We might expect recurrent models to benefit less from CoT in this respect.

Simplified NoPE Transformers 4.2.2

To better understand how an anti-Markovian solution to the Multi-Object and Single-Object tasks could be implemented in a transformer, we include a theoretical treatment of a single-layer NoPE Transformer that is trained on the Simplified Single-Object task. This task is simplified in that it excludes the BOS and T tokens from the sequences. The self-attention calculation for a single query $q_r \in \mathbb{R}^d$ from a response token, denoted by the subscript r, is as follows:

Attention
$$(q_r, K, V) = V(\text{softmax}(\frac{K^{\top}q_r}{\sqrt{d}})) = \sum_{i=1}^n \frac{e^{\frac{q_r^{\top}k_i}{\sqrt{d}}}}{\sum_{j=1}^n e^{\frac{q_r^{\top}k_j}{\sqrt{d}}}} v_i = \sum_{i=1}^n \frac{s_i^r}{\sum_{j=1}^n s_j^r} v_i = \frac{1}{\sum_{j=1}^n s_j^r} \sum_{i=1}^n s_i^r v_i$$
 (16)

Where d is the dimensionality of the model, n is the sequence length, $K \in \mathbb{R}^{d \times n}$ is a matrix of column vector keys, $V \in \mathbb{R}^{d \times n}$ is a matrix of column vectors v_i , and $s_i^r = e^{\frac{q_r^T k_i}{\sqrt{d}}}$, using i to denote the positional index of the key and the superscript r to denote that the q came from a response token. We refer to $s_i^r v_i$ as the strength-value of the ith token for the query q_r .

In the first layer following the embeddings in a NoPE transformer, each of the queries for the response tokens will produce equal strength-values for a given key-value pair regardless of the position from which the response token and demo tokens originated. This is because NoPE does not add positional information to the embeddings. Thus, assuming that the attention mechanism is performing a sum of the count contributions from each token in the sequence, we should be able to use the $s_i^r v_i$ to increment and decrement the model's decision to produce the EOS token from any given response token in the following way:

IncrementedAttention
$$(q_r, K, V) = \frac{1}{s_r^r + \sum_{j=1}^n s_j^r} \left(s_r^r v_r + \sum_{i=1}^n s_i v_i \right)$$
 (17)

Where the subscript r in the strength s_r and value v_r denotes that the originating token for the key-value pair is a response token. We can decrement the count using a key-value pair from a demonstration token. To verify our theoretical treatment, we performed a simulation using a single-layer NoPE transformer trained on the simplified Single-Object task. Using the strength-value additions outlined in Equation 17, we were able to change the position at which the transformer produced the EOS token with 100% accuracy. We include results for other transformer architecture variants in Supplemental Figure 6 (c).

4.2.3 RoPE Transformers

To determine how the RoPE transformers perform the tasks, we first looked at the attention weights for both of its two layers (see Supplemental Figure 10). The resp and EOS queries give surprisingly little attention to the resp tokens. In Supplemental Figure 6, we show DAS results on the Input Value variable from the Ctx-Distr SA where a numeric value is assigned to each token and the values of all previous tokens are summed at each step in the sequence. The Multi-Object transformers achieved an IIA of 0.800. We also examined a set of transformers trained on the Variable-Length variant of the Multi-Object task that disrupts count-position correlations. The Variable-Length transformers achieved a higher IIA of 0.935 for the same DAS analysis. The lower IIA of the Multi-Object transformers is consistent with the notion that they rely, in part, on a positional readout, rather than a summing operation, to solve the task.

5 Conclusion

In this work we used causal interpretability methods to interpret emergent representations of numbers in various types of NNs. We discovered the existence of graded, symbol-like number variables within RNN representations; we introduced an extension of DAS allowing us to formulate neural activity in terms of interpretable symbolic variables; we explored theoretical and empirical transformer solutions to the the tasks; and we showed the general finding that transformers must use anti-Markovian solutions in the absence of sufficient layers. We conclude by noting that it is, by definition, always possible to find an SA with high alignment to the ANN due to the fact that ANNs are implemented using computer (symbolic) programs. Our goal of NN to SA alignment is to find simplified, unified ways of understanding complex ANNs. If an ANN has poor alignment for a specific region of the symbolic variables, we argue that the SA simply needs to be refined. Any choice of SA refinement is dependent on the goals of the work. We leave further refinements to the SAs presented in this work to future directions.

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A Appendix / supplemental material

A.1 Additional Figures

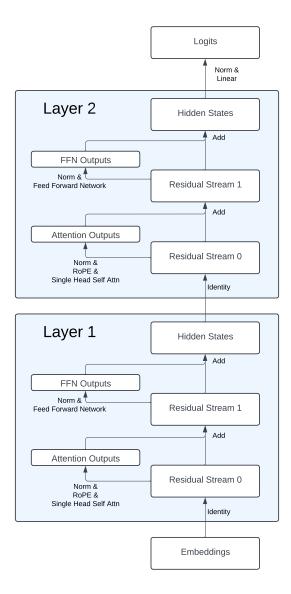


Figure 5: Diagram of the main transformer architecture used in this work. The white rectangles represent activation vectors. The arrows represent model operations. All normalizations are Layer Norms (Ba et al., 2016). The majority of the DAS interchange interventions are performed on Hidden State activation vectors from Layer 1 at individual time-steps. We offer further granularity in the Input Value interventions by performing DAS on the embeddings that are projected into the key and value vectors for the Layer 1 self-attention.

Table 1: The DAS results for each model and task variant. Each alignment function was trained on a single causal variable with a d_{var} (subspace size) of the better performing out of 16 or 64 dimensions. Performance values are reported as IIA under the task name.

\mathbf{Model}	Alignment	Algorithm	Variable	Multi-Object	Same-Object	Single-Object
GRU	Orthogonal	Up, Down	Count	0.9464	0.3698	0.908
GRU	Orthogonal	Up, Down	Phase	0.9368	0.373	0.889
GRU	Orthogonal	Up, Up	Demo Count	0.4807	0.2503	0.606
GRU	Orthogonal	Up, Up	Resp Count	0.4173	0.4024	0.477
GRU	Linear	Up, Down	Count	0.9906	0.991	0.995
GRU	Linear	Up, Down	Phase	0.9884	0.9922	0.991
GRU	Linear	Up, Up	Demo Count	0.9174	0.9744	0.984
GRU	Linear	Up, Up	Resp Count	0.9223	0.9808	0.989
LSTM	Orthogonal	Up, Down	Count	0.993	0.958	0.989
LSTM	Orthogonal	Up, Down	Phase	0.991	0.95	0.991
LSTM	Orthogonal	Up, Up	Demo Count	0.5416	0.86	0.409
LSTM	Orthogonal	Up, Up	Resp Count	0.5374	0.8007	0.439
LSTM	Linear	Up, Down	Count	0.9928	0.9922	0.992
LSTM	Linear	Up, Down	Phase	0.9914	0.9912	0.99
LSTM	Linear	Up, Up	Demo Count	0.9846	0.9846	0.990
LSTM	Linear	Up, Up	Resp Count	0.9862	0.9697	0.991

Table 2: The DAS results for each model and task variant using a linear alignment function with a $d_{\rm var}=1$ (subspace size). Each alignment function was trained on a single causal variable. Performance values are reported as IIA under the task name.

\mathbf{Model}	Alignment	${f Algorithm}$	Variable	$d_{\mathbf{var}}$	Multi-Object	Same-Object
GRU	Linear	Count Up, Count Down	Count	1	0.9436	0.68
GRU	Linear	Count Up, Count Down	Phase	1	0.8568	0.870
GRU	Linear	Count Up, Count Up	Demo Count	1	0.758	0.507
GRU	Linear	Count Up, Count Up	Resp Count	1	0.8339	0.890
LSTM	Linear	Count Up, Count Down	Count	1	0.9236	0.864
LSTM	Linear	Count Up, Count Down	Phase	1	0.955	0.86
LSTM	Linear	Count Up, Count Up	Demo Count	1	0.912	0.775
LSTM	Linear	Count Up, Count Up	Resp Count	1	0.9494	0.900

Table 3: The DAS results for the transformers. Each DAS training was performed on a single causal variable with a d_{var} (subspace size) of the better performing out of 24 or 64 dimensions. Performance values are reported as IIA under the task name.

\mathbf{Model}	Alignment	${f Algorithm}$	Variable	Multi-Object	Same-Object
NoPE Transformer	Orthogonal	Context Distributed	Input Value	0.882	0.982
NoPE Transformer	Orthogonal	Count Up, Count Down	Count	0.1112	0.110
RoPE Transformer	Orthogonal	Context Distributed	Input Value	0.8004	0.935
RoPE Transformer	Orthogonal	Count Up, Count Down	Count	0.1274	0.124

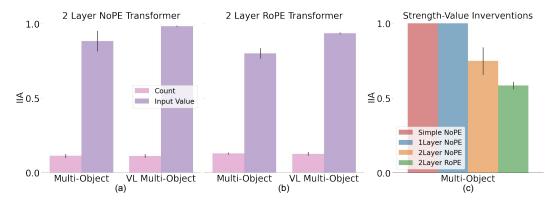


Figure 6: (a) and (b) show the interchange intervention accuracy (IIA) on the Count from the Up-Down program and the Input Value from the Ctx-Distr program aligned to the Transformer architectures using DAS with an Orthogonal alignment function. VL denotes models trained on the Variable-Length version of the task. The Input Value encodes an assigned value (+1, -1, or 0) to each incoming token that is used to recalculate the count at each step in the sequence. The DAS analysis is applied to the model embeddings for the Input Value, and the residual stream after the first transformer layer for the Count. We can see that the Variable-Length transformers have stronger alignment to the Input Value variable—consistent with an interpretation in which the Multi-Object transformers can rely, to some degree, on positional information. (c) IIA for strength-value interventions described in Section 4.2.2. These interventions add and subtract from the count using the strength-value within an attention computation. Strength-values are computed from the last response query, key, and value in the sequence from the layer in which interventions are performed. The displayed IIA is taken from the better performing of the possible attention layers.

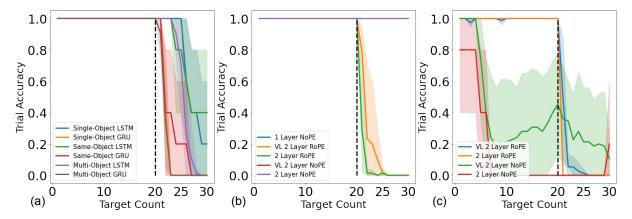


Figure 7: (a) RNN task performance measured as the proportion of trials correct. Object quantity refers to the number of demo tokens in a sequence preceding the trigger token. The evaluation data consists of 15 sampled sequences (even when only one configuration exists for that object quantity). (b) Transformer performance on the Multi-Object task. VL indicates the Variable-Length version of the task. One model seed was dropped from each the NoPE and RoPE models trained on the Variable-Length Multi-Object task due to lower than 99% accuracy. (c) Transformer performance on the Same-Object task. VL indicates the Variable-Length version of the task. All NoPE model seeds performed below 99% accuracy on the Same-Object task.

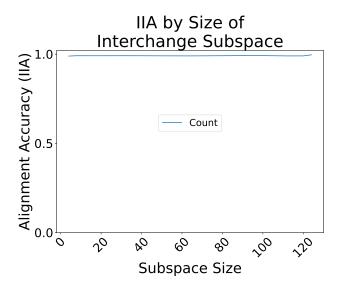


Figure 8: An exploration of the performance of the orthogonal DAS alignment as a function of the size of the interchange subspace for a randomly selected Multi-Object LSTM model seed on the Count variable. The x axis shows d_{count} while the y axis shows IIA. This is the number of dimensions substituted in the intervention.

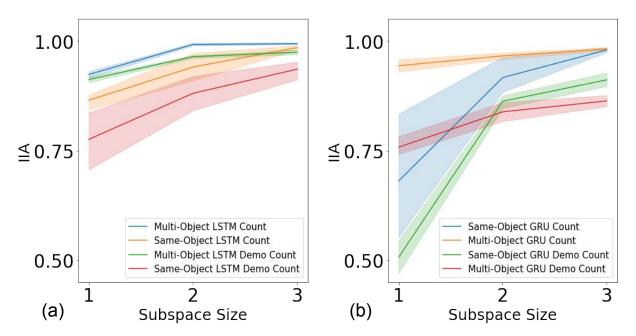


Figure 9: (a) An exploration of the DAS IIA on the y-axis using the Linear Alignment function with varying sizes of d_{var} (the size of the intervention subspace) on the x-axis for the LSTM models. (b) An exploration of the DAS IIA on the y-axis using the Linear Alignment function with varying sizes of d_{var} (the size of the intervention subspace) on the x-axis for the GRU models.

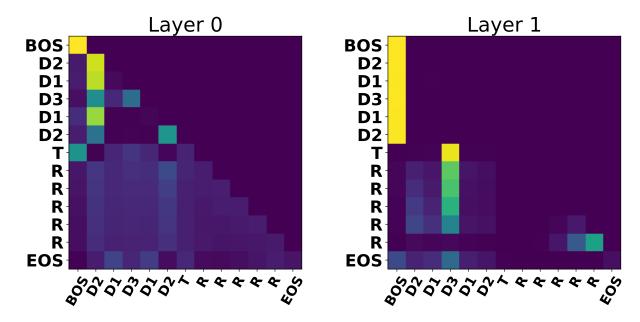


Figure 10: Attention weights for a single transformer with two layers using rotary positional encodings trained on the Multi-Object Task. Queries are displayed on the vertical axis in order of their appearance starting at the top. Keys are displayed on the horizontal axis starting from the left. Queries are only able to attend to themselves and preceding keys.

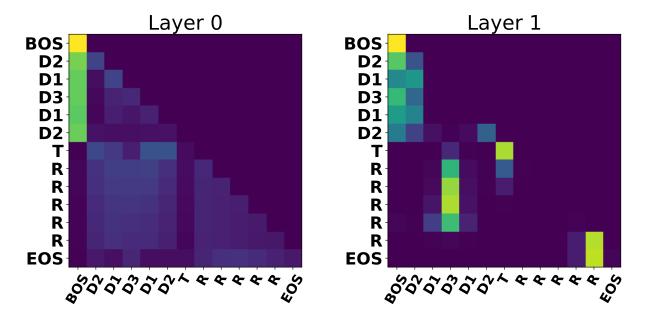


Figure 11: Attention weights for a single transformer with two layers using rotary positional encodings trained on the Variable-Length variant of the Multi-Object Task. Queries are displayed on the vertical axis in order of their appearance starting at the top. Keys are displayed on the horizontal axis starting from the left. Queries are only able to attend to themselves and preceding keys.

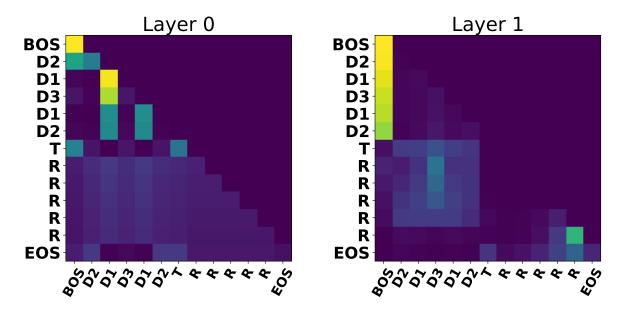


Figure 12: Attention weights for a single transformer model seed with two layers and no positional encodings (NoPE) trained on the Multi-Object Task. Queries are displayed on the vertical axis in order of their appearance starting at the top. Keys are displayed on the horizontal axis starting from the left. Queries are only able to attend to themselves and preceding keys.

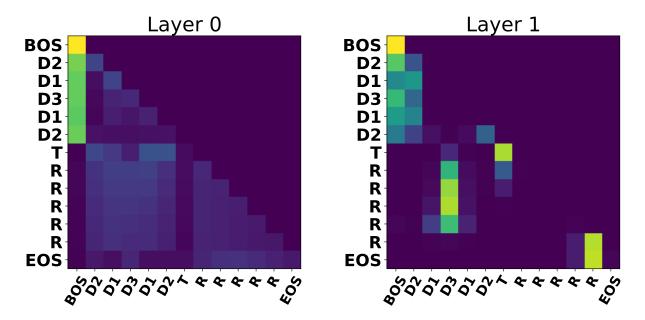


Figure 13: Attention weights for a single transformer with two layers using no positional encodings (NoPE) trained on the Variable-Length variant of the Multi-Object Task. Queries are displayed on the vertical axis in order of their appearance starting at the top. Keys are displayed on the horizontal axis starting from the left. Queries are only able to attend to themselves and preceding keys.

A.2 Model Details

All artificial neural network models were implemented and trained using PyTorch (Paszke et al., 2019) on Nvidia Titan X GPUs. Unless otherwise stated, all models used an embedding and hidden state size of 128 dimensions. To make the token predictions, each model used a two layer multi-layer perceptron (MLP) with GELU nonlinearities, with a hidden layer size of 4 times the hidden state dimensionality with 50% dropout on the hidden layer. The GRU and LSTM model variants each consisted of a single recurrent cell followed by the output MLP. Unless otherwise stated, the transformer architecture consisted of two layers using Rotary positional encodings (Su et al., 2023). Each model variant used the same learning rate scheduler, which consisted of the original transformer (Vaswani et al., 2017) scheduling of warmup followed by decay. We used 100 warmup steps, a maximum learning rate of 0.0001, a minimum of 1e-7, and a decay rate of 0.5. We used a batch size of 128, which caused each epoch to consist of 8 gradient update steps.

A.3 DAS Training Details

A.3.1 Rotation Matrix Training

To train the DAS rotation matrices, we applied PyTorch's default orthogonal parametrization to a square matrix of the same size as the model's state dimensionality. PyTorch creates the orthogonal matrix as the exponential of a skew symmetric matrix. In all experiments, we selected the number of dimensions to intervene upon as half of the dimensionality of the state. We chose this value after an initial hyperparameter search that showed the number of dimensions had little impact on performance (see Figure 8). We sample 10000 sequence pairs for the intervention training dataset. See Supplement A.3.3 for more details on intervention data construction and examples. We use a learning rate of 0.001 and a batch size of 512.

A.3.2 Symbolic Program Algorithms

Algorithm 1 One sequence step of the Up-Down Program

```
q \leftarrow \text{Count}
p \leftarrow \text{Phase}
y \leftarrow \text{input token}
if y == BOS then
                                                                           ▶ BOS is beginning of sequence token
   q \leftarrow 0, p \leftarrow 0
   return sample(D)
                                                                                            ⊳ sample a demo token
                                                                                         ▷ D is set of demo tokens
else if y \in D then
   q \leftarrow q + 1
   return sample(D)
else if y == T then

→ T is trigger token

   p \leftarrow 1
else if y == R then
                                                                                              ▷ R is response token
   q \leftarrow q - 1
end if
if (q == 0) \& (p == 1) then
   return EOS
                                                                                  end if
return R
```

Algorithm 2 One sequence step of the Up-Up Program

```
d \leftarrow \text{Demo Count}
r \leftarrow \text{Resp Count}
p \leftarrow \text{Phase}
y \leftarrow \text{input token}
if y == BOS then
                                                                                    ▷ BOS is beginning of sequence token
    d \leftarrow 0, r \leftarrow 0, p \leftarrow 0
    return sample(D)
                                                                                                      ⊳ sample a demo token
else if y \in D then
                                                                                                   ▷ D is set of demo tokens
    d \leftarrow d + 1
    return sample(D)
else if y == T then

→ T is trigger token

    p \leftarrow 1
else if y == R then
                                                                                                        \triangleright R is response token
    r \leftarrow r+1
end if
if (d == r) \& (p == 1) then
    return EOS
                                                                                           ▶ EOS is end of sequence token
end if
return R
```

Algorithm 3 One sequence step of the specific Ctx-Distr Program

```
v \leftarrow \text{list of previous values excluding the most recent step}
\ell \leftarrow \text{Input Value}
                                                                                   ▶ The value of the most recent token
p \leftarrow \text{Phase}
                                                               \triangleright 0 indicates the demo phase, 1 is the response phase
y \leftarrow \text{input token}
v.append(\ell)
s \leftarrow \text{SUM}(v)
if y == BOS then
                                                                                  ▷ BOS is beginning of sequence token
    \ell \leftarrow 0, p \leftarrow 0
    return sample(D)
                                                                                                    ⊳ sample a demo token
else if s \leq 0 and p == 1 then
                                                                                \triangleright Sum is 0 or less in the response phase
    return EOS
                                                                                          ▷ EOS is end of sequence token
else if y == T or y == R then
                                                                               ▷ T is trigger token, R is response token
    p \leftarrow 1
    \ell \leftarrow -1
    return R
else if y \in D then
                                                                                                 D is set of demo tokens
    \ell \leftarrow 1
end if
if p == 1 then
    return R
else
    return sample(D)
end if
```

A.3.3 DAS Intervention Data

Here we expand upon the intervention data used to train and test the DAS rotation matrices. We organize this section into programs, variables, and tasks. For each DAS training, we train a single orthonormal matrix and only create interventions that depend on a single variable from the corresponding program. To construct an intervention sample, we first sample a target sequence and a source squence and a positional index from each sequence. We limit positional indices to the demo and resp tokens. We then compute the values of each of the variables using the symbolic algorithm up to the positional index for both the target and source. The value of the variable of focus is then transferred from the source into the the target variable. We then continue the target sequence based on the new value. When the target sequence's counterfactual sequence begins in the demo phase, we uniformly sample the number of demo sequence steps before placing the trigger token such that the Count (or Demo Count) does not exceed the maximum count used in the task. We note that this makes the samples not strictly counterfactual in the definition used in the causal inference literature, but the desired effect is the same as the true counterfactual comes from the same distribution.

A.3.4 Up-Down Program Examples

Count Variable: Interventions attempt to transfer the representation corresponding to the difference between the number of resp tokens and demo tokens. Interventions are only performed at positional indices corresponding to demo or resp tokens.

$Multi\mbox{-}Object\ Examples$	1	2	3	4
Source Sequence	$BOS D_1$	$BOS D_2 D_1 D_1$	$BOS D_2 D_1 T R$	BOS D ₁ D ₃ T R R
Target Sequence	$BOS D_3 D_2$	$BOS D_2 T R$	$BOS D_1 D_2 D_1 T R$	$BOS D_2$
Original Labels	$D_2 D_3 T R R R R EOS$	EOS	R R EOS	$D_2 T R R EOS$
Counterfactual	$D_2 D_3 T R R R EOS$	R R R EOS	R EOS	$D_2 T R EOS$
$Single ext{-}Object\ Examples$	1	2	3	4
Source Sequence	BOS D	BOS D D D	BOS D D T R	BOS D D T R R
Target Sequence	BOS D D	BOS D T R	BOS D D D T R	BOS D
Original Labels	DDTRRRREOS	EOS	R R EOS	D T R R EOS
Counterfactual	DDTRRREOS	R R R EOS	R EOS	D T R EOS
$Same ext{-} Object\ Examples$	1	2	3	4
Source Sequence	BOS C	BOS C C C	BOS C C T C	BOS C C T C C
Target Sequence	BOS C C	BOS C T C	BOS C C C T C	BOS C
Original Labels	CCTCCCEOS	EOS	C C EOS	C T C C EOS
Counterfactual	CCTCCCEOS	C C C EOS	C EOS	C T C EOS

Phase Variable: Interventions transfer the representation corresponding to the Phase of the sequence (whether it is counting up or counting down). Interventions are only performed at positional indices corresponding to demo or resp tokens.

Multi-Object Examples	1	2	3	4
Source Sequence	$BOS D_1$	$BOS D_3 D_1 D_2$	$BOS D_2 D_1 T R$	BOS D ₂ D ₃ T R R
Target Sequence	$BOS D_2 D_1$	$BOS D_3 T R$	$BOS D_1 D_3 D_1 T R$	$BOS D_2$
Original Labels	$D_3 D_1 T R R R R EOS$	EOS	R R EOS	$D_1 T R R EOS$
Counterfactual	$D_3 D_1 T R R R R EOS$	$D_2 T R EOS$	R R EOS	R EOS
Single-Object Examples	1	2	3	4
Source Sequence	BOS D	BOS D D D	BOS D D T R	BOS D D T R R
Target Sequence	BOS D D	BOS D T R	BOS D D D T R	BOS D
Original Labels	DDTRRRREOS	EOS	R R EOS	D T R R EOS
Counterfactual	DDTRRRREOS	D T R EOS	R R EOS	R EOS
Same-Object Examples	1	2	3	4
Source Sequence	BOS C	BOS C C C	BOS C C T C	BOS C C T C C
Target Sequence	BOS C C	BOS C T C	BOS C C C T C	BOS C
Original Labels	CCTCCCEOS	EOS	C C EOS	C T C C EOS
Counterfactual	CCTCCCEOS	C T C EOS	C C EOS	C EOS

A.3.5 Up-Up Program Examples

Demo Count Variable: Interventions attempt to transfer the representation corresponding to the number of demo tokens in the sequence. Interventions are only performed at positional indices corresponding to demo or resp tokens. We remove training and evaluation samples in which the Demo Count is less than the Resp Count .

Multi-Object Examples	1	2	3	4
Source Sequence	$BOS D_1$	$BOS D_2 D_3 D_3$	$BOS D_2 D_1 T R R$	BOS D ₁ D ₃ T R R
Target Sequence	$BOS D_3 D_2$	$BOS D_2 D_2 D_3 T R R$	$BOS D_1 D_2 D_1 T R$	$BOS D_2$
Original Labels	T R R EOS	R EOS	R R EOS	$D_2 T R R EOS$
Counterfactual	T R EOS	R EOS	R EOS	$D_2 T R R R EOS$
Single-Object Examples	1	2	3	4
Source Sequence	BOS D	BOS D D D	BOS D D T R R	BOS D D T R R
Target Sequence	BOS D D	BOS D D D T R R	BOS D D D T R	BOS D
Original Labels	T R R EOS	R EOS	R R EOS	D T R R EOS
Counterfactual	T R EOS	R EOS	R EOS	DTRRREOS
Same-Object Examples	1	2	3	4
Source Sequence	BOS C	BOS C C C	BOS C C T C C	BOS C C T C C
Target Sequence	BOS C C	BOS C C C T C C	BOS C C C T C	BOS C
Original Labels	T C C EOS	C EOS	C C EOS	C T C C EOS
Counterfactual	T C EOS	C EOS	C EOS	C T C C C EOS

Resp Count Variable: Interventions attempt to transfer the representation corresponding to the number of response tokens in the sequence. Interventions are only performed at positional indices corresponding to demo or resp tokens. We remove samples from the training and evaluation sets that transfer a Resp Count greater than the Demo Count into the response phase.

Multi-Object Examples	1	2	3	4
Source Sequence	$BOS D_1 D_3 D_3$	$BOS D_2$	$BOS D_2 D_1 T R R$	BOS D ₁ D ₃ D ₃ T R R R
Target Sequence	$BOS D_3 D_2$	$BOS D_2 D_2 D_3 T R R$	$BOS D_1 D_2 D_1 T R$	$BOS D_2$
Original Labels	TRREOS	R EOS	R R EOS	$D_2 T R R EOS$
Counterfactual	T R R EOS	R R R EOS	R EOS	$D_2 T EOS$
Single-Object Examples	1	2	3	4
Source Sequence	BOS D D D	BOS D	BOS D D T R R	BOS D D D T R R R
Target Sequence	BOS D D	BOS D D D T R R	BOS D D D T R	BOS D
Original Labels	TRREOS	R EOS	R R EOS	DTRREOS
Counterfactual	T R R EOS	R R R EOS	R EOS	D T EOS
Same-Object Examples	1	2	3	4
Source Sequence	BOS C C C	BOS C	BOS C C T C C	BOSCCCTCC
Target Sequence	BOS C C	BOSCCCTCC	BOS C C C T C	BOS C
Original Labels	T C C EOS	C EOS	C C EOS	C T C C EOS
Counterfactual	T C C EOS	C C C EOS	C EOS	C T EOS
Counterfactual	TCCEOS	CCCEOS	CEOS	CTEOS

A.3.6 Ctx-Distr Program Examples

Anti-Markovian States: We perform these interventions directly by substituting the source hidden state into the target hidden state without using DAS. Each intervention examines whether the state encodes sufficient information to transfer the NN's behavior from the source sequence into the target sequence. If the NN uses a Markovian hidden state, then transferring the hidden state from one position to another should result in a corresponding transfer of behavior. In the case that the NN uses anti-Markovian states, then we would expect the model's behavior to be unchanged at token positions that did not receive interventions. Higher accuracies correspond to no behavioral transfer. Interventions are only performed at positional indices corresponding to non-terminal response tokens.

Multi-Object Examples	1	2	3	4
Source Sequence	$BOS D_1 D_3 T R R$	$BOS D_2 T R$	$BOS D_2 D_1 T R$	BOS D ₁ D ₃ D ₃ T R R
Target Sequence	$BOS D_3 D_2 T R$	$BOS D_2 D_2 D_3 T R$	$BOS D_1 D_2 T R R$	$BOS D_2 D_1 D_2 T R$
Original Label	R R EOS	R R R EOS	EOS	R R EOS
Counterfactual	R R EOS	R R R EOS	EOS	R R EOS
$Single ext{-}Object\ Examples$	1	2	3	4
Source Sequence	BOS D D T R R	BOS DT R	BOS D D D T R	BOS D D D T R R
Target Sequence	BOS D D T R	BOS D D D T R	BOS D D T R R	BOS D D D T R
Original Label	R R EOS	R R R EOS	EOS	R R EOS
Counterfactual	R R EOS	R R R EOS	EOS	R R EOS
Same-Object Examples	1	2	3	4
Source Sequence	BOS C C T C C	BOS CT C	BOS C C C T C	BOSCCCTCC
Target Sequence	BOS C C T C	BOS C C C T C	BOS C C T C C	BOS C C C T C
Original Label	C C EOS	C C C EOS	EOS	C C EOS
Counterfactual	C C EOS	C C C EOS	EOS	C C EOS

Input Value Variable: These interventions attempt to transfer the representation corresponding to the value with which the tokens contribute to the cumulative difference between the demo and resp tokens. A value of +1 is assigned to demo tokens, a value of -1 is assigned to resp tokens, and the algorithm stops when the sum of the values is equal to 0 in the resp phase. Interventions are only performed at positional indices corresponding to demo or resp tokens, and we restrict the number of demo tokens to be at least 2 when intervening on the demo phase. This latter restriction is to avoid cases where the cumulative value is negative.

$Multi ext{-}Object\ Examples$	1	2	3	4
Source Sequence	$BOS D_1$	$BOS D_2$	$BOS D_2 D_1 T R R$	BOS D ₁ D ₃ D ₃ T R R R
Target Sequence	$BOS D_3 D_2$	$BOS D_2 D_2 D_3 T R R$	$BOS D_1 D_2 D_1 T R$	$BOS D_2 D_1$
Original Labels	TRREOS	R EOS	R R EOS	$D_2 T R R R EOS$
Counterfactual	T R R EOS	R R R EOS	R R EOS	$D_2 T R EOS$
$Single ext{-}Object\ Examples$	1	2	3	4
Source Sequence	BOS D	BOS D	BOS D D T R R	BOS D D D T R R R
Target Sequence	BOS D D	BOS D D D T R R	BOS D D D T R	BOS D D
Original Labels	TRREOS	R EOS	R R EOS	DTRRREOS
Counterfactual	T R R EOS	R R R EOS	R R EOS	DTREOS
$Same ext{-} Object\ Examples$	1	2	3	4
Source Sequence	BOS C	BOS C	BOS C C T C C	BOSCCCTCC
Target Sequence	BOS C C	BOS C C C T C C	BOS C C C T C	BOS C C
Original Labels	T C C EOS	C EOS	C C EOS	C T C C C EOS
Counterfactual	T C C EOS	C C C EOS	C C EOS	C T C EOS

A.3.7 DAS Gradience Evaluation Data

The data used for Figures 4 (c) and (d) was constructed by sampling a single target sequence for every object count ranging from 1-20, and source sequences with object counts incrementing by 4 for each target sequence. Interventions were then constructed for each target count, source count pair within each sequence pair. This procedure was repeated for three times, each with a different number of steps in the demo phase before providing the trigger token. The number of continued demo steps was 1, 4, and 12 respectively.

A.4 Context Distributed Interventions

We detail in this section why our Ctx-Distr interchange interventions are sufficient to demonstrate that the transformers use a solution that re-references/recomputes the relevant information to solve the tasks at each step in the sequence. The hidden states in Layer 1 are a bottleneck at which a cumulative counting variable must exist if it were to use a strategy like the Up-Down or Up-Up programs. This is because the Attention Outputs of Layer 1 are the first activations that have had an opportunity to communicate across token positions. This means that the representations between the Residual Stream 1 of Layer 1 up to the Residual Stream 0 of Layer 2 cannot have read a cumulative state from the previous token position other than reading off the positional information from the previous positional encodings. The 2-layer architecture is then limited in that it has only one more opportunity to transfer information between positions—the attention mechanism in Layer 2. Thus, if a hidden state at time t were to have encoded a cumulative representation of the count that will be used by the model at time t+1, that cumulative representation must exist in the activation vectors between the Residual Stream 1 in Layer 1 and the Residual Stream 0 of Layer 2. If it is using such a cumulative representation, then when we perform a full activation swap in the Layer 1 hidden states then the resulting predictions should be influenced by the swap.

A.5 Variable-Length Task Variants

Here we include additional tasks to prevent the transformers with positional encodings from learning a solution that relies on reading out positional information. We introduce Variable-Length variants of each of the Multi-Object, Single-Object, and Same-Object tasks. In the Variable-Length versions, each token in the demo phase has a 0.2 probability of being sampled as a unique "void" token type, V, that should be ignored when determining the object quantity of the sequence. The number of demo tokens will still be equal to the object quantity when the trigger token is presented. We include these void tokens as a way to vary the length of the demo phase for a given object quantity, thus breaking correlations between positional information and object quantities. As an example, consider the possible sequence with a object quantity of 2: "BOS V D V V D T R R EOS".