GATING MECHANISMS UNDERLYING SEQUENCE-TO-SEQUENCE WORKING MEMORY

ABSTRACT

Working memory is the process by which a system temporarily stores information across a necessary duration. Memory retention and manipulation of discrete sequences are fundamental building blocks for the underlying computation required to perform working memory tasks. Recurrent neural networks (RNNs) have proven themselves to be powerful tools for such problems, as they, through training, bring rise to the dynamical behavior necessary to enact these computations over many time-steps. As of yet, the means by which these learned internal structures of the network result in a desired set of outputs remains broadly elusive. Furthermore, what *is* known is often difficult to extrapolate from due to a task specific formalism. In this work, we analyze an RNN, trained perfectly on a discrete sequence working memory task, in fine detail. We explain the learned mechanisms by which this network holds memory and extracts information from memory, and how gating is a natural architectural component to achieve these structures. A synthetic solution to a simplified variant of the working memory task is realized. We then explore how these results can be extrapolated to alternative tasks.

1 INTRODUCTION

Recurrent neural networks (RNNs), by construction, transform stimuli across multiple time-points to produce nonlinear working memory representations that can be used to solve complex tasks (Elman, 1990; Hochreiter & Schmidhuber, 1997; Mante et al., 2013). Memorization and manipulation of discrete sequences of elements are a common low level requirement to many broad families of such problems (Hochreiter & Schmidhuber, 1997; Jordan et al., 2021; Yang et al., 2019). However, a full understanding of how the underlying dynamics learned by these networks accurately bring rise to the necessary computations remains an open area of research (Sussillo & Barak, 2013). That is, from a dynamical system's point of view (Guckenheimer & Holmes, 1983; Jordan et al., 2021), how does the network's internal phase-flow and attractor structures, brought forth by training, play a part in the found solution to the desired task? Furthermore, many of the known properties of trained RNNs' learned dynamical mechanisms are specific to individual problems (Henaff et al., 2016; Jarne, 2020; Ichikawa & Kaneko, 2021). Therefore, due to their narrow formalism, such attributes are often difficult to extrapolate to alternative tasks of the same family. It has been demonstrated that the underlying attractor structures of RNNs successfully trained on an individual task are often

Figure 1: Superimposed trajectories for hidden-state neurons $82 - 84$ across one thousand trials of VDCM, from a perfectly trained GRU, demonstrating slow manifold dynamics during the delay period of each trial. These three dimensions are representative of all 250 in the RNN.

similar, if not topologically equivalent, across networks, regardless of architecture, initialization, and hyper-parameters (Maheswaranathan et al., 2019). However, one would also expect commonalities between the underlying structures of RNNs trained on similar, but none the less, different tasks (Flesch et al., 2021; Yang et al., 2019) – a research feat not yet well explored.

To better train and interpret the solutions found by RNN models we require a finer grain analysis, where results can be broadened to very general classes of problems. In this way, found mechanisms can be identified, studied, and synthetically recreated to be made more understandable. Moreover, the synthetic realization of dynamical mechanisms, inspired by those obtained through gradient based optimization, can be combined and extrapolated from to form synthetic RNN solutions to related tasks.

We surgically analyze a single RNN trained on a discrete sequence working memory task. The network performs with no mistakes on a sufficiently sized validation set of trials. Inspired by the behavior discovered in the network, we design and experimentally validate a synthetic solution to a simplified version of the same task, realizable in relatively low dimensions. We then discuss how such findings apply to networks trained on different but mechanistically similar tasks, including a sequence-to-sequence translation task.

2 VARIABLE DELAY COPY MEMORY TASK AND RNN MODEL

In choosing an appropriate task, we look at *copy memory*; a standard benchmark to evaluate a neural network's ability to accurately recall information seen many time-steps in the past (Hochreiter & Schmidhuber, 1997; Henaff et al., 2016; Arjovsky et al., 2016). Let $A = \{a_i\}_{i=1}^K$ be a set of K symbols. We then pick $S, T \in \mathbb{N}$. The input is a vector of categories, length $T + 2S$, where each entry is one-hot encoded. Each trial of the task consists of three phases, of length S, T, and S respectively. During the first phase (encoding), the network is presented with with S entries uniformly sampled from $\{a_i\}_{i=1}^K$, to be remembered sequentially. During the second phase (delay period), the network is fed $T - 1$ inputs of a_{K+1}, a *blank* category, indicating no important information is entering the network. At the final time-step of the second phase $S + T$, a delimiter a_{K+2} is input to the network, indicating that the RNN should output the original S entries of input in the same order by which they appeared in the first phase of the trial beginning at the next time-step (third phase – decoding). During these last S time-steps, the inputs are all set to the blank category a_{K+1}. During the first $T + S$ time-steps (encoding and delay period), the network should output a_{K+1}. The task is to minimize the average cross-entropy of the outputs at every time-step. As such, the networks should remember a sequence of S elements for T time-steps.

Henaff, Szlam, and LeCun developed and experimentally verified a synthetic solution to this task (Henaff et al., 2016). However, if we allow T to vary from trial to trial, the underlying dynamical mechanisms allowing the RNN to properly enact the computation remains elusive. We will refer to this task as *variable delay copy memory* (VDCM), as coined by (Henaff et al., 2016). We successfully trained a GRU network (Cho et al., 2014), by novel means (*Anonymous*), with a linear readout on VDCM, such that it performs perfectly on all the test trials. For each trial we set $K = 8$, $S = 10$, and $T \sim \mathcal{U}(100, 101, ..., 120)$. The model used is represented as follows:

$$\boldsymbol{z}_t = \sigma(\mathbf{W}_z \boldsymbol{x}_t + \boldsymbol{b}_{iz} + \mathbf{U}_z \boldsymbol{h}_{t-1} + \boldsymbol{b}_{hz}) \tag{1}$$

$$\boldsymbol{r}_t = \sigma(\mathbf{W}_r \boldsymbol{x}_t + \boldsymbol{b}_{ir} + \mathbf{U}_r \boldsymbol{h}_{t-1} + \boldsymbol{b}_{hr}) \tag{2}$$

$$\boldsymbol{h}_t = (1 - \boldsymbol{z}_t) \odot \tanh(\mathbf{W}_h \boldsymbol{x}_t + \boldsymbol{b}_{ih} + \boldsymbol{r}_t(\mathbf{U}_h \boldsymbol{h}_{t-1} + \boldsymbol{b}_{hh})) + \boldsymbol{z}_t \odot \boldsymbol{h}_{t-1} \tag{3}$$

$$\boldsymbol{y}_t = \mathbf{V}_{out} \boldsymbol{h}_t + \boldsymbol{b}_{out} \tag{4}$$

$$y_{choice} = \arg\max([\boldsymbol{y}_t]_m), m \in [0, 1, ..., K] \subset \mathbb{N} \cup \{0\} \tag{5}$$

where $\boldsymbol{h}_t \in \mathbb{R}^d$, $d = 250$, $\boldsymbol{x}_t \in \mathbb{R}^{K+2}$, $\mathbf{W}_z, \mathbf{W}_r, \mathbf{W}_h \in \mathbb{R}^{d \times S}$ and $\mathbf{U}_z, \mathbf{U}_r, \mathbf{U}_h \in \mathbb{R}^{d \times d}$ are the parameter matrices, $\boldsymbol{b}_{iz}, \boldsymbol{b}_{ir}, \boldsymbol{b}_{ih}, \boldsymbol{b}_{hz}, \boldsymbol{b}_{hr}, \boldsymbol{b}_{hh} \in \mathbb{R}^d$ are bias vectors, $\odot$ represents element-wise multiplication, and $\sigma(\boldsymbol{z}) = 1/(1 + e^{-\boldsymbol{z}})$ is the element-wise logistic sigmoid function. For the linear readout $\boldsymbol{y}_t \in \mathbb{R}^{K+1}$, $\boldsymbol{b}_{out} \in \mathbb{R}^{S-1}$ and $\mathbf{V}_{out} \in \mathbb{R}^{(S-1) \times d}$. y_{choice} is taken as the largest element of $\boldsymbol{y}_t$ at each time-step, and represents the chosen class readout.

3   ENCODING ON SLOW MANIFOLDS

The computations required for VDCM fall into two main parts. The first is the memory structure. How does the GRU retain information about the elements presented to the network at each of the ten encoding time-steps? The second is memory recall. How does the GRU pull stored information from memory in the correct order? In this section we will focus on the former, and explain the structure by which our trained RNN enacts to properly encode inputted information.

Fig. 1 demonstrates the behavior of hidden-state neurons $82 - 84$ of the trained GRU network, while performing VDCM. The trajectory of these selected neurons across one thousand trials are superimposed, clearly indicating the three segments of the task. If we look at the delay period, beginning at $t = 11$, we notice that the neural activity appears to be near constant across each trial. We note that the selection of neurons shown in Fig. 1 are representative of the behavior of every neuron in the network. What is of primary interest are the neurons that significantly vary trial to trail, such as neurons 82 and 83. These varying neurons indicate the existence of a slow manifold, an observation in line with recent research (Ghazizadeh & Ching, 2021). In the GRU architecture, such behavior results from either an approximation of a pseudo-line attractor (Jordan et al., 2021) (effectively orthogonal to the projection of the constant drive at the input during the delay period), or from the influence of the update gate z_t (Cho et al., 2014). If we look at the update gate for dimensions with analogous behavior to 82 and 83, what we find is that, during the delay period, most demonstrate a value close to 1 for z_t. Such activity simplifies the RNN's hidden-state equation to the following approximate form:

$$[\boldsymbol{h}_t]_i \approx [\boldsymbol{h}_{t-1}]_i \tag{6}$$

where i indexes the neurons with a high update-gate during the delay period. As such, the network retains near perfect memory of the past in these directions. We assert that this is the primary mechanism for maintaining memory for VDCM in our trained network, as pseudo-line attractors are finely tuned (Jordan et al., 2021), and therefore difficult to implement.

Figure 2:   Cartoon representation of how an encoded element can be represented on a slow manifold. **Left:** if we have a slow manifold (blue), the state of the system lies on a specific region of this manifold. That region, when mapped to the output $\boldsymbol{y}_t$, will ensure that the a specified dimension in the output space has the largest dimension (green circle). Due to the implementation of the *argmax* function (or the functionally equivalent *softmax*) for VCDM, the largest element in readout will be chosen as the class. **Right:**   the projection to each readout dimension is linear, and as such can be thought of as the superposition of K hyperplanes, shown in black. These hyperplanes can be arranged such that a segment exists where each element can be chosen.

Given that we know the mechanism being used to encode information, the next step is to dive into the low level details of how exactly this computation is being enacted. We trained this network to be able to encode 8^{10} possible sequences, $K = 8$ elements to choose from at each time-step, across $S = 10$ time-steps. We hypothesize that such a computation can be implemented by carefully placing each trajectory on a high dimensional slow manifold, where the manifold is segmented to associate specific regions with each possible readout element. Due to the implementation of the

argmax function for VCDM, the largest element in the readout vector will be chosen as the class. A cartoon representation of such a regime is depicted in Fig. 2, where we can place the hyperplanes representing the projection to each readout dimension in such a way that there exists a region for each projection to obtain the largest value among the set of all readout hyperplanes.

If this is true, how is the slow manifold organized? We implemented a perturbation based experiment, where we compare the network response to random input sequences with carefully crafted perturbations at the beginning of the delay period of those sequences. If we can alter the readout of some decoding phase time-step q to a desired element p by altering a subset of neurons at $t = 11$ and letting that change propagate throughout the trial, it suggests those neurons are primarily responsible for encoding that time-step / element pair. We want to show that we can do this consistently across test trials. The algorithm we developed to determine such a manifold mapping is detailed in appendix A. The results of the algorithm on our trained network are displayed in Fig. 3. The average

Figure 3: Results for using our algorithm to map out the structure of the slow-manifold in our trained RNN. **Top:** probability of a *successful* perturbation at the beginning of the delay period ($t = 11$) for each possible element across each encoding time-step. *Success* indicates that the neurons perturbed successfully altered the appropriate decoding time-step readout to the desired element without altering the readouts at any other time-step. **Bottom:** number of neurons used for each perturbation. All pairs of time-steps and elements required at least 5 neurons.

success rate across all pairs was 96.3%. We interpret the neurons used to alter each of the test trials for a given q and p as tuned to that encoding time-step / element pair. We note that only 73 of the 250 neurons in the network *may* be used to encode memory. We can reorder these 73 neurons by their *center of mass* with respect to the 80 possible combinations of q and p, where we sweep through all values p can take on for $q = 1$, then $q = 2$, etc. Fig. 4 (Left) depicts such a reordering, revealing a block-like structure. We see that a nonempty set of neurons account for every element at each specific time-step q. The plot is colored by the expected value that neuron (row) takes when presented with a specific element at a given time-step (column). All neurons belonging to one of these subsets behave differently depending on what element is presented at that time-step, as indicated by color along each row, suggesting further structure to each region of the slow manifold.

Let's consider the neurons primarily tuned to a single time-step; the neurons tuned to (encoding) time-step 9, for example. We can use principal component analysis (PCA) to visualize the activity of these neurons in a low dimension (Bishop, 2006). We project the activity from each of the perturbed neurons across the set of test trials at $t = 11$ to a 2D PC subspace as demonstrated in Fig. 4 (Right). We see that the set of data points for each color forms eight distinct clusters, one for each possible element inputted to the network at $t = 9$. Each cluster demonstrates variability in a single direction, indicated by the blue arrow. Since there is no noise during VDCM, as this task is deterministic, the only source for this variability is the influence of the elements presented to the network at all time-steps before $t = 9$. This suggests that not only are the neurons primarily tuned to $t = 9$ not fully decoupled from the neurons tuned to other time-steps, but also that the network allocated at least one direction to these disruptions.

However, this observation brings about an important point regarding the directions in the 250D GRU associated with encoding elements inputted at $t = 9$. While PCA brings about the dimensions with the highest variability across trials, it does not indicate which dimensions are most crucial for enacting the computation. While insightful in understanding how training structured the sub-mechanisms that make up each mechanism in the task, this direction allocated to noise may not be used to indicate class during the decoding portion of the task. In the following section, we will dive into the second major computation required for VDCM, decoding. It will be shown that analysis of decoding will enable us to better understand the mechanism used for encoding. For all other encoding time-steps, plots analogous to Fig. 4 (right) can be found in appendix B.

Figure 4: **Left:** the 73 neurons exhibiting slow manifold dynamics during the delay period. Every eight columns corresponds to the different elements that can be given at a specific encoding time-step. Matrix elements displayed in white indicate that the corresponding neuron (row) do not respond to changes in these element / time-step pairs. Further color indicates the expected value that neuron takes when a given element is input at the corresponding time-step. **Right:** PCA projection of the activity of the neurons tuned to encode information from $t = 9$ (green strip on the left) at the beginning of the delay period ($t = 11$). The activity at $t = 11$ for each trial is plotted as a data point colored by which element was presented to the network at $t = 9$. The background coloring indicates what class is most likely to be readout at the 9th step of decoding, if this PC space was projected back up to the hidden subspace of neurons tuned to time-step 9 at $t = 11$, replacing them.

4 DECODING AND THE ROLE OF GATING

How does information from memory get readout in the desired order? The readout at each time-step is determined by equation 4 and equation 5. The linear readout matrix $\mathbf{V}_{out}$ and readout bias vector $\boldsymbol{b}_{out}$ separate the hidden-state space $\boldsymbol{h}_t$ into classification regions with linear decision boundaries. Prior to receiving the readout signal at the end of the delay period, the network remains in a regime where only the delimiter symbol "8" is outputted. The readout signal perturbs the hidden-state of the network into a *decoding subspace*, where some means of telling time (i.e a *clock*) must activate. Decoding the first element of the sequence is easy enough, as the network needs only to perturb the hidden-state to a region where the neurons tuned to encoding the first time-step of each trial are dominant in readout. But then how does the network properly output the remaining elements of the input sequence? The most natural means to enact this behavior is built into the GRU architecture, as the added gates, $\boldsymbol{z}_t$ and $\boldsymbol{r}_t$, act to *forget* or *reset* information stored in the hidden-state. If some neuron, of index ρ, in the network has corresponding update-gate and reset-gate values close to zero, the evolution of that neuron can be approximated as follows:

$$[\boldsymbol{h}_t]_\rho \approx \tanh([\mathbf{W}_h]_\rho \cdot \boldsymbol{x}_t + [\boldsymbol{b}_{ih}]_\rho) \tag{7}$$

where $[\mathbf{W}_h]_\rho$ indicates row ρ of $\mathbf{W}_h$. Therefore, the network loses all information previously stored in this dimension of the system. Moreover, the neuron associated with this direction is overwritten by the input $\boldsymbol{x}_t$.

We want to analyze our trained GRU network to see if the decoding regime exploits this behavior. Prior to doing this, it is important to define what exactly is meant for a neuron to be "reset." We will define the metric $\kappa = \overline{(1 - [z_t]_\rho)(1 - [r_t]_\rho)} \in [0, 1]$, where the overhead bar represents a sample mean. If a neuron ρ is to forget all previous information held within it $(1 - [z_t]_\rho)(1 - [r_t]_\rho) \approx 1$. The closer to zero this term is, the more information from previous steps is retained. We ran 1000 randomly generated input sequences through the network and determined κ for every neuron at each decoding time-step. We can then determine a threshold ζ, where neurons with $\kappa > \zeta$ at a given time-step are considered "reset." We chose $\zeta = 0.255$, and detail our reasoning in appendix C.

Using this threshold we can reorder the neurons of the network by which decoding time-step each is reset after for the first time (i.e. the first time $\kappa > \zeta$ holds after the readout signal is presented). Fig.

5 (Left) depicts this reordering, allowing us to visualize κ for each neuron using our choice of ζ. We notice a clear staircase pattern, indicating the existence of a non-empty set of neurons that reset for the first time after every time-step of decoding. Furthermore, due to the methods used to obtain our value of ζ, it is assured that at least one neuron in each of these sets is tuned to the equivalent time-step during the encoding phase of each trial.

Figure 5: **Left:** mean activity of our defined metric $\kappa = \overline{(1 - [z_t]_\rho)(1 - [r_t]_\rho)}$ for each neuron when we line up the decoding phases across trials. We reordered the neurons such that those which "reset" at time-step 1 of decoding are on top, followed by those which "reset" for the first time at time-step 2, etc. Doing so reveals the demonstrated staircase pattern, indicating that there exists a distinct set of neurons which are reset at each step of the decoding phase. **Right:** a recoloring of Fig. 4, indicating at what time-step each neuron active in memory retention during the delay period is reset in the decoding phase. We note that every time-step of encoding has at least one corresponding neuron that is appropriately reset at the equivalent step of decoding, with the exception of those tuned to $t = 3$.

We can recolor Fig. 4 (left) by which time-step of decoding each of the 73 neurons involved in encoding are reset after. This is demonstrated in Fig. 5 (Right). For the set of neurons tuned to each time-step of the encoding phase, at least one neuron is reset after its corresponding decoding time-step. This isn't a surprise, as we ensured this was the case when choosing ζ. However, what is surprising is that for each set of neurons, with the exception of $t = 3$, at least one neuron exists that is tuned to every element of its corresponding time-step. Therefore, this regime demonstrates a near complete picture of the most important neurons responsible for performing VDCM. We say *important* to indicate that these neurons are the primary carriers of information (i.e. hold memory) throughout each trial of the task, while the others play a more supporting role; either managing internal mechanisms for telling time during the encoding/decoding phases of the task or fine tuning the discussed dynamical mechanisms, such as the direction allocated for noise demonstrated in Fig. 4 (right). Furthermore, our analysis suggests that the system is, for the most part, canonical in its encoding and decoding mechanisms. This is a result of the GRU architecture, as both gates are canonical in their functionality, meaning information is maintained or reset in the directions of individual neurons (Cho et al., 2014).

5 SOLUTION TO THE $K = 2$ CASE OF VDCM

Given what we know about the inner functionality of our trained network, we would like to develop a complete solution for performing VDCM based off of found behavior. The solution should layout a specific set of parameters for the GRU network. No training will be required and the internal dynamical behavior must be highly interpretable. We will incorporate a slow manifold to encode the input sequence. Furthermore, we will design an appropriate readout projection and sequentially reset the neurons allocated to memory as to output each element of the sequence in the desired order. This will be done with a separately designed clock mechanism, which will be used for determining the number of time-steps which have passed during both the encoding and decoding phases of each trial.

We restrict our solution to the $K = 2$ case of VDCM, such that each sequence to be encoded is a binary string of length S. Any information expressible as a binary string of elements can be encoded and later decoded in this context, with 2^S different states achievable with a single network of $2(S+1)$ neurons, as we shall demonstrate below. Furthermore, this allows for a more pedagogical approach in our presentation, as our goal is to build a deep intuition for these mechanisms and demonstrate a proof of concept in extrapolation. As we'll see, only one neuron is needed to hold memory from a given time-step in the $K = 2$ case of this problem. Fig. 6 (left) depicts a schematic representation of our solution. For easy visualization, Fig. 6 (right) illustrates the decoding mechanism for the $S = K = 2$ case.

Figure 6: **Left:** Schematic representation of the synthetic solution to VDCM for arbitrary S and $K = 2$, where elements are notated as either A or B. The system acts in one of two modes, either encoding or decoding. During the encoding phase of each trial, elements to be remembered are presented to the network, setting the values of the first S neurons (a slow manifold) sequentially, as dictated by an internal clock. After the first S time-steps, the system switches out of the encoding mode into decoding. The clock is not reactivated until the readout signal is given, which will begin resetting the values of the S neurons allocated to memory to zero, again sequentially. Done properly, the network will readout the encoded elements in their original order. **Right:** An example of the memory structure for the $S = K = 2$ case of our solution. The decision boundary separates the $h_1 - h_2$ plane into regions associated with each element. Four subregions exist, where information can be encoded such that each of the four possible sequences can be readout.

We begin by reiterating what each dimension of our input $\boldsymbol{x}_t \in \mathbb{R}^4$ describes. x_1 and x_2 are the two possible sequence elements, A and B respectively, x_3 is the blank symbol and x_4 is the readout signal. All unspecified parameter matrices and bias vectors only contain zeros in their entries. Fig. 7 depicts a complete picture of all nonzero parameter matrices and bias vectors used in our synthetic solution. From this, we can further define each subcomponent. We allocate S neurons initialized at zero to memory, and $S + 1$ neurons, all initialized at -1 except for the second to last, which is initialized at 1, to the clock. Furthermore we allocate one neuron initialized at -1 to a switch. The switch will determine if the system is finished encoding or not, by saturating near -1 (low) or 1 (high). We also choose two parameters, α and β, such that $\alpha \gg \beta \gg 0$. $\alpha = 10$ and $\beta = 3$ has worked well for us. All unspecified subcomponent entries are considered to be zero.

Starting from the upper left, λ_{11} encodes information directly into memory. Each row i of λ_{11} is $\begin{bmatrix} r^{-i} & -(r^{-i}) \end{bmatrix}$. We chose $r = 3$. The larger r is, the greater in value S can be while maintaining perfect accuracy on the task. λ_{21} ensures the clock doesn't indicate two simultaneous time-steps during the encoding phase. Every element in the last two rows of λ_{21} are $-\alpha$. The submatrix $\lambda_{31} = \begin{bmatrix} -\alpha & -\alpha \end{bmatrix}$ holds the switch low during the encoding phase. The last row of λ_{22} is $\begin{bmatrix} -\alpha & \alpha \end{bmatrix}$, ensuring the clock remains deactivated during the delay period and reactivates upon receiving the readout signal. $\lambda_{32} = \begin{bmatrix} \alpha & \alpha \end{bmatrix}$ keeps the switch high after the encoding phase.

In regards to the hidden-state dynamics, H_{22} has α for every entry along the super-diagonal. This is the clock mechanism, which works in isolation, causing the clock neurons to sequentially rise from a low to a high value. Every entry of the bias sub-blocks F_2 and F_3 are set to $-\beta$. F_2 ensures that

Figure 7: Nonzero parameter matrices and bias vectors used in our synthetic solution to VDCM. Each is broken up into subcomponents, where nonzero subcomponents are denoted in gray. The dimensions of each subcomponent are depicted in blue. The functional connectivity of each block matrix can be obtained by the purple and red labeling. For example, consider $\mathbf{V}_{out}$, which takes part in the readout projection from the hidden-state. Whether an A or a B is outputted is dependent only on the hidden-state dimensions allocated to memory.

after a neuron allocated to the clock takes on a high value, it will be brought back to a low value at the next time-step. We chose $\beta \ll \alpha$ to ensure that neurons multiplied by α can overcome the functional effects of those multiplied by β. Similarly, F_3 keeps the neuron allocated to the switch low during the encoding phase. The entries $\sum_{j=0}^{S-1}(S-j)$ for each j column of G_{12} are all α, and act to sequentially reset each of the S neurons allocated to memory after each time-step dictated by the clock during the decoding phase. Every entry of F_1 is β, as to ensure the reset-gate for each neuron in memory is kept high prior to decoding, thereby retaining memory.

The primary component to readout from memory is J_{11}. The first row of J_{11} is $[1 \quad 0 \quad 1 \quad 0\dots]$, always alternating. The second row takes a similar structure and is $[0 \quad -1 \quad 0 \quad -1\dots]$, again alternating. In conjunction with the placement of the encoded information on the slow manifold, as defined by the two geometric series which make up the columns of λ_{11}, this ensures that information encoded at earlier time-steps takes precedence until reset. Fig. 6 (right) depicts the resultant decision boundary when $S = 2$. All but the far right entry of J_{22} is $-\alpha$, $J_{23} = -\alpha$, and $C_2 = \frac{3-2S}{2}\alpha$. These ensure that, unless both the switch is high and the clock is activated, only the blank symbol will be outputted. Thus completes our synthetic solution to the $K = 2$ case for VDCM. We validated this solution on the same test set of trials used for our traditionally trained network, and it performs with perfect accuracy. Examples of the hidden-state dynamics for the $S = 2$ and $S = 10$ cases are depicted in Fig. 8, and the code to generate these plots are in the supplementary material.

6 DISCUSSION

We've identified and analyzed a set of underlying dynamical mechanisms which enact the computations necessary to perfectly perform VDCM, a sequence-to-sequence working memory task, with a GRU network architecture. The internal dynamical behavior of the RNN constitutes the execution of both an encoding mechanism, where information can then be held indefinitely in memory, and a decoding mechanism, which makes use of and deletes information held in memory for accurate readout. The encoding regime stores information on a slow manifold, which makes up a subspace of the hidden-state space of the system. Regions of this manifold are tuned to specific time-steps of the encoding period, where subregions within each region are structured to differentiate between what input was presented to the network at the time-step the region was tuned to. The decoding mechanism deletes information sequentially from memory, allowing data stored at later time-steps to take precedence in the readout. Both of these mechanisms take advantage of gating to behave properly. We then detailed out a synthetic solution to the $K = 2$ case of VDCM and demonstrated its functionality. In this section, we want to convince the reader that this analysis does not so narrowly apply only to RNNs trained on VDCM, but on alternative tasks as well.

The mechanisms realized in our synthetic solution can be applied in a variety of different contexts, so long as the mechanistic function required of each is retained across tasks. Consider the parity

Figure 8: Hidden-state trajectories for 1000 superimposed trials of VDCM using our synthetic solution, for both the $S = 2$ case (left) and the $S = 10$ case (right). Neurons fall into one of three functional categories. S neurons are allocated to holding memory. $S + 1$ neurons create the clock, which indicates what time-step of encoding or decoding is present, and one neuron is allocated to a switch. When *low*, the switch indicates the trial is in its encoding phase. When *high*, the trial has finished encoding. A high switch in conjunction with the readout signal begins the decoding phase.

bit problem (Wegener & Pruim, 2005). The RNN is given a binary string of length S and has to simultaneously output a binary string, indicating if the number of 1's presented to the network is *even* or *odd*. Unaltered, this task only requires an XOR operation between the input and output at the previous time-step. This suggests the need of a memory structure (or buffer) that holds one piece of information – the last element outputted. However, if we change the task so that the RNN needs to readout the desired binary sequence arbitrarily long after then entire input sequence has been presented, then the task is nearly identical to VDCM (Fig. 9 (middle)). The one caveat is that the information encoded in memory is not the input itself, but the output from the XOR operation of the input and information about the last element stored in memory. Let's construct another task; a

Figure 9: Schematic representation of the mechanistic connectivity of the processes and structures used to accurately perform VDCM, modified parity bit, and a binary character translation task. **Left:** input is encoded in memory, which is self sustaining, and is later decoded and outputted. **Middle:** nearly identical to VDCM, but what is encoded is the output of an XOR operation between the input and the previous encoded value in memory. **Right:** same as VDCM, but memory must undergo a nonlinear computation prior to decoding.

sequence-to-sequence translation task with a binary character language and a variable delay between receiving the input binary sequence and needing to output a desired binary sequence. Suppose that if the input sequence ends in a 1, the desired output sequence is the input sequence in reverse order, beginning with the last element seen. Furthermore, if the sequence ends in a 0, the desired output sequence is the input sequence with all the bits flipped – every 0 becomes a 1 and vice versa. Such a task is also nearly identical to VDCM. The memory structure can be made the same, but must undergo some nonlinear computation prior or during each decoding time-step (Fig. 9 (right)). We were unable to train an RNN on this latter task by any conventional means (appendix D), suggesting a need for more sophisticated training methods which leverage the dynamical behavior required of the RNN to complete the task. We leave this to future work, and note this result as an important example of why the work done in this manuscript is important for RNNs when performing more sophisticated tasks.

REFERENCES

Martin Arjovsky, Amar Shah, and Yoshua Bengio. Unitary evolution recurrent neural networks. In *Proceedings of the 33rd International Conference on International Conference on Machine Learning - Volume 48*, ICML'16, pp. 1120–1128, New York, NY, USA, June 2016. JMLR.org.

Christopher M. Bishop. *Pattern Recognition and Machine Learning (Information Science and Statistics)*. Springer-Verlag, Berlin, Heidelberg, 2006. ISBN 0387310738.

Kyunghyun Cho, Bart van Merrienboer, Caglar Gulcehre, Dzmitry Bahdanau, Fethi Bougares, Holger Schwenk, and Yoshua Bengio. Learning Phrase Representations using RNN Encoder–Decoder for Statistical Machine Translation. In *Proceedings of the 2014 Conference on Empirical Methods in Natural Language Processing (EMNLP)*, pp. 1724–1734, Doha, Qatar, 2014. Association for Computational Linguistics. doi: 10.3115/v1/D14-1179. URL http://aclweb.org/anthology/D14-1179.

Jeffrey L. Elman. Finding structure in time. *Cognitive Science*, 14(2):179–211, April 1990. ISSN 0364-0213. doi: 10.1016/0364-0213(90)90002-E. URL https://www.sciencedirect.com/science/article/pii/036402139090002E.

Timo Flesch, Keno Juechems, Tsvetomira Dumbalska, Andrew Saxe, and Christopher Summerfield. Rich and lazy learning of task representations in brains and neural networks. *bioRxiv*, 2021. doi: 10.1101/2021.04.23.441128. URL https://www.biorxiv.org/content/early/2021/04/23/2021.04.23.441128.

Elham Ghazizadeh and ShiNung Ching. Slow manifolds within network dynamics encode working memory efficiently and robustly. *PLOS Computational Biology*, 17(9):1–20, 09 2021. doi: 10.1371/journal.pcbi.1009366. URL https://doi.org/10.1371/journal.pcbi.1009366.

John Guckenheimer and P. J. Holmes. *Nonlinear Oscillations, Dynamical Systems, and Bifurcations of Vector Fields*. Applied Mathematical Sciences. Springer-Verlag, New York, 1983. ISBN 978-0-387-90819-9. doi: 10.1007/978-1-4612-1140-2. URL https://www.springer.com/gp/book/9780387908199.

Mikael Henaff, Arthur Szlam, and Yann LeCun. Recurrent Orthogonal Networks and Long-Memory Tasks. In *International Conference on Machine Learning*, pp. 2034–2042. PMLR, June 2016. URL https://proceedings.mlr.press/v48/henaff16.html. ISSN: 1938-7228.

Sepp Hochreiter and Jürgen Schmidhuber. Long Short-Term Memory. *Neural Computation*, 9 (8):1735–1780, November 1997. ISSN 0899-7667. doi: 10.1162/neco.1997.9.8.1735. URL https://doi.org/10.1162/neco.1997.9.8.1735.

Kohei Ichikawa and Kunihiko Kaneko. Short term memory by transient oscillatory dynamics in recurrent neural networks. *arXiv:2010.15308*, August 2021. URL http://arxiv.org/abs/2010.15308. arXiv: 2010.15308.

Cecilia Jarne. The dynamics of Recurrent Neural Networks trained for temporal tasks and the eigenvalue spectrum. *arXiv:2005.13074*, June 2020. URL http://arxiv.org/abs/2005.13074. arXiv: 2005.13074.

Ian D. Jordan, Piotr Aleksander Sokół, and Il Memming Park. Gated Recurrent Units Viewed Through the Lens of Continuous Time Dynamical Systems. *Frontiers in Computational Neuroscience*, 15:67, 2021. ISSN 1662-5188. doi: 10.3389/fncom.2021.678158. URL https://www.frontiersin.org/article/10.3389/fncom.2021.678158.

Richard Liaw, Eric Liang, Robert Nishihara, Philipp Moritz, Joseph E Gonzalez, and Ion Stoica. Tune: A research platform for distributed model selection and training. *arXiv preprint arXiv:1807.05118*, 2018.

Niru Maheswaranathan, Alex Williams, Matthew Golub, Surya Ganguli, and David Sussillo. Universality and individuality in neural dynamics across large populations of recurrent networks. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d'Alché-Buc, E. Fox, and R. Garnett (eds.), *Advances in Neural Information Processing Systems*, volume 32. Curran Associates, Inc., 2019. URL `https://proceedings.neurips.cc/paper/2019/file/5f5d472067f77b5c88f69f1bcfda1e08-Paper.pdf`.

Valerio Mante, David Sussillo, Krishna V. Shenoy, and William T. Newsome. Context-dependent computation by recurrent dynamics in prefrontal cortex. *Nature*, 503(7474):78–84, November 2013. ISSN 1476-4687. doi: 10.1038/nature12742. URL `https://www.nature.com/articles/nature12742`.

David Sussillo and Omri Barak. Opening the black box: low-dimensional dynamics in high-dimensional recurrent neural networks. *Neural Computation*, 25(3):626–649, March 2013. ISSN 1530-888X. doi: 10.1162/NECO_a_00409.

Anonymous. Quasi-periodic attractors carry stable gradients.

Ingo Wegener and R. Pruim. *Complexity Theory: Exploring the Limits of Efficient Algorithms*. Springer-Verlag, Berlin, Heidelberg, 2005. ISBN 3540210458.

Guangyu Robert Yang, Madhura R. Joglekar, H. Francis Song, William T. Newsome, and Xiao-Jing Wang. Task representations in neural networks trained to perform many cognitive tasks. *Nature Neuroscience*, 22(2):297–306, February 2019. ISSN 1097-6256, 1546-1726. doi: 10.1038/s41593-018-0310-2. URL `http://www.nature.com/articles/s41593-018-0310-2`.

A   SLOW MANIFOLD MAPPING

Algorithm 1: Slow Manifold Map

1: **procedure** MAP(S, K)
2:     $Q \leftarrow \{0, 1, ..., S - 1\}$ ▷ time-steps
3:     $P \leftarrow \{0, 1, ..., K - 1\}$ ▷ available symbols
4:     **for** each element i of Q **do**
5:         **for** each element j of P **do**
6:             $q \leftarrow Q_i$
7:             $p \leftarrow P_i$
8:             **for** N iterations **do**   ▷ we chose $N \leftarrow 1000$
9:                 Generate γ ▷ random input sequence to the RNN where $\gamma_q \neq p$
10:                $\nu \leftarrow \gamma$
11:                $\nu_q \leftarrow p$
12:                Run both γ and ν through the RNN and save the hidden-states of each at $t = S$
13:                Record which k neurons are sufficiently different ▷ threshold of 10^{-3} was used
14:            Approximate $\mathbb{E}[\boldsymbol{h}_k]$ when ν is inputted to the RNN $\forall k$
15:            **for** M iteration **do**   ▷ we chose $M \leftarrow 1000$ and $n \leftarrow 4$
16:                Generate $\tilde{\gamma}$ ▷ random input sequence to the RNN where $\tilde{\gamma}_q \neq p$
17:                Run $\tilde{\gamma}$ through the RNN, but alter $\boldsymbol{h}_k = \mathbb{E}[\boldsymbol{h}_k]$ for the n most frequently recorded
                   neurons at $t = S$ during the forward pass
18:                **if** $y_{choice} = p$ at step q of decoding and all other outputs are correct **then**
19:                    record that this iteration was a *success*
20:            **if** number of successes is less than M and $n \leq n_{max}$ **then** ▷ we chose $n_{max} \leftarrow 15$
21:                $n \leftarrow n + 1$
22:                **go to** 15
23:            **else if** $n > n_{max}$ **then**
24:                Disregard all but the n recorded neurons for n which gave the most successes
25:            **else**
26:                Disregard all but the n recorded neurons
        return The remaining values for each set of recorded neurons for all qp-pairs

---

B   ALL PCA PLOTS

Figure 10: Equivalent plots to Fig. 4 (Right), for each set of neurons used to encode each additional time-step during the encoding phase of VDCM.

C   RESET THRESHOLD

We'd like our threshold ζ to be relatively low (i.e close to zero), where κ exhibits little variance about ζ. Furthermore, we need to ensure that a nonempty set of neurons exists for each set of neurons tuned to each encoding time-step, such that each is reset for the first time during the correct decoding time-step. For example, if a neuron is tuned to encode information presented at $t = 5$, then when the decoding period of the trial begins, the neuron should remain "not-reset" up until the fifth time-step of readout, where it will then properly reset. This will also indicate which neurons described in section 3 are most important for holding onto memory at each encoding time-step. Fig. 11 further details our reasoning for a choice of ζ, which we set to 0.255.

Figure 11: Plot indicating how we chose a threshold ζ on κ, where values under this threshold are considered "not-reset", and those above are considered "reset." **Top:** histogram showing the sample mean values of κ each neuron takes across all steps of the decoding phase, over one thousand trials. Notice the bimodal distribution, as this metric for most neurons is usually close to zero or one. The green curve represents the standard deviation of the average values of κ for each bin of the histogram. We want to pick a ζ with relatively low variance to ensure that individual neurons do not cross back and forth over the threshold trial to trial. **Bottom:** For varying κ, white indicates values of ζ where no neurons tuned to a given time-step in the encoding phase are shown to reset by our analysis. We want our threshold to not only be small, but to contain at least one neuron for each encoding time-step to be reset appropriately.

D   TRAINING RESULTS

Hyper-parameters were chosen using Bayesian optimization (Ax https://ax.dev/ from the Ray Tune library) (Liaw et al., 2018) with validation likelihood used as the decision criterion. Specific values for the learning rate, learning rate scheduler, learning rate decay factor and gradient clipping were chosen over 100 iterations of the tuning algorithm All models were trained using Adam, with a batch size of 200; models used for hyper parameter optimization were trained for at most 100 epochs, while the models that were ultimately chosen were trained for a fixed 200 epochs. Standard cross-entropy loss was used as the loss functional. Unless implied otherwise by the name, models were initialized using the default method in PyTorch, which internally samples from a uniform distribution $\mathcal{U}(-\frac{1}{\sqrt{N}}, \frac{1}{\sqrt{N}})$ with N being the number of hidden units.

Figure 12: Test performance for trained RNNs on VDCM. Colors indicate mean activity of each architecture and initialization strategy used (10 networks each). The shaded region about each curve depicts the variance across networks. **Left:** cross-entropy loss across epochs. **Middle:** traditional network accuracy. **Right:** depicts what fraction of test trials the network outputted the sequence with no mistakes. Notice that no network other than GRU got close to learning VDCM.

Figure 13: Test performance for trained RNNs on a modified parity bit task. Colors indicate mean activity of each architecture and initialization strategy used (10 networks each). The shaded region about each curve depicts the variance across networks. **Left:** cross-entropy loss across epochs. **Middle:** traditional network accuracy. **Right:** depicts what fraction of test trials the network outputted the sequence with no mistakes. LSTM does manage to learn this task.

Figure 14: Test performance for trained RNNs on a binary character translation task. Colors indicate mean activity of each architecture and initialization strategy used (10 networks each). The shaded region about each curve depicts the variance across networks. **Left:** cross-entropy loss across epochs. **Middle:** traditional network accuracy. **Right:** depicts what fraction of test trials the network outputted the sequence with no mistakes. LSTM learns this task the best, but is still unable to consistently output entire the desired sequences with no mistakes.