

Investigating Recurrent Neural Network Memory Structures using Neuro-Evolution

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ABSTRACT

This paper presents a new algorithm, Evolutionary eXploration of Augmenting Memory Models (EXAMM), which is capable of evolving recurrent neural networks (RNNs) using a wide variety of memory structures, such as Δ -RNN, GRU, LSTM, MGU and UGRNN cells. EXAMM evolved RNNs to perform prediction of large-scale, real world time series data from the aviation and power industries. These data sets consist of very long time series (thousands of readings), each with a large number of potentially correlated and dependent parameters. Four different parameters were selected for prediction and EXAMM runs were performed using each memory cell type alone, each cell type and simple neurons, and with all possible memory cell types and simple neurons. Evolved RNN performance was measured using repeated k -fold cross validation, resulting in 2420 EXAMM runs which evolved 4,840,000 RNNs in ~24,200 CPU hours on a high performance computing cluster. Generalization of the evolved RNNs was examined statistically, providing findings that can help refine the design of RNN memory cells as well as inform future neuro-evolution algorithms.

CCS CONCEPTS

• Computing methodologies → Neural networks; Genetic algorithms;

KEYWORDS

Neuroevolution, Recurrent Neural Networks, Time Series Data

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1 INTRODUCTION

This work is motivated by a major open question in the field of artificial neural network (ANN) research: *What neural memory structures appear to be optimal for time-series prediction?* Conducting

such a search over ANN structures entails manual, primarily human-driven labor and activity. As more advances are made in the field, the number of possible architecture variations and modifications explodes combinatorially. This growing space combined with the limited, often simple heuristic local search that can be conducted by human experts means that efficiently finding architectures that generalize well while still maintaining low parameter complexity (given that regularization is important for most data sample sizes) makes for a nearly intractable search problem.

In natural biological systems, the process of evolution, over long time-spans, endows organisms with various inductive biases that allow them to adapt and learn their environment quickly and readily. It is thought that these inductive biases are what provide infants the ability to quickly learn complex pattern recognition/detection functions with limited data across various sensory modalities [14, 23], such as in visual and speech sensory domains. While artificial forms of evolution, such as the classical genetic algorithm [17], are significantly simplified from the actual evolutionary process that creates useful inductive biases to drive development and survival of organisms at large, these optimization procedures offer the chance to develop non-human centered ways of generating useful and even potentially optimal neural architectures.

The evolution of recurrent neural networks (RNNs) poses significant challenges above beyond the already challenging task of evolving feed forward and convolutional neural networks. RNNs are more challenging to train due to issues with exploding and vanishing gradients which occur when unrolling a RNN over long time series with the backpropagation through time (BPTT) algorithm [36]. Due to this issue, development of recurrent memory cells which can preserve memory and long term dependencies while alleviating the exploding and vanishing gradient problem has been an area of significant study [4, 5, 16, 26, 38]. Further, as in the case of time-varying data, input samples are strictly ordered in time and thus induce long-term dependencies that any useful stateful adaptive process/model must extract in order to generalize. The complexity of time-series tasks varies, entailing the prediction of a particular variable of interest over time or even constructing a full generative model of all the available variables, perhaps additionally involving other non-trivial tasks such as data imputation.

Due to these issues, RNNs for time series data prediction can require the use of a variety of memory cell structures in addition to recurrent connections spanning different time spans. To optimize within this large search space, Evolutionary eXploration of Augmenting Memory Models (EXAMM) integrates an extensible collection of different complex memory cell types with simple neuronal building blocks and recurrent connections of varying time spans.

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EXAMM was used to evolve RNNs with various cell types to predict time series data from two real-world, large-scale data sets. Results are particularly interesting in that while they show allowing selection from any of the available memory cell structures can provide very well performing networks in many test cases; it does come at the cost of reliability. Further, even small modifications to the neuro-evolutionary process, such as allowing simple neurons, can generally improve predictions, but they can also have unintended consequences – in some examples it meant the difference between a memory cell structure performing the best as opposed to the worst. The authors hope that these results can help guide not only the further development of neuro-evolution algorithms, but also help refine and inform the development of new memory cell structures and human designed RNNs.

2 EVOLVING RECURRENT NETWORKS

While neuro-evolution (applying evolutionary processes to the development of ANNs) has been used in searching the space of feed forward and even convolutional architectures for tasks involving static inputs [15, 22, 30–35, 37, 39], less effort has been put into exploring the evolution of recurrent memory structures that operate with complex time based data sequences and uncovering what forms and structures the neuro-evolutionary process finds.

Several methods for evolving NN topologies along with weights have been searched and deployed, with NeuroEvolution of Augmenting Topologies (NEAT) [32] perhaps being the most well-known. EXAMM differs from NEAT in that it includes more advanced node-level mutations (see Section 3.1.2), and utilizes Lamarckian weight initialization (see Section 3.2) along with backpropagation to evolve the weights as opposed to a simpler less efficient genetic strategy. Additionally, it has been developed with large-scale concurrency in mind, and utilizes an asynchronous steady state approach which has been shown to facilitate scalability to potentially millions of compute nodes [6].

Other recent work by Rawal and Miikkulainen has investigated an information maximization objective [28] strategy to evolve RNNs. This strategy essentially utilizes NEAT with Long Short Term Memory (LSTM) neurons instead of regular neurons. EXAMM provides a more in-depth study of the performance of possible recurrent cell types as it examines both simple neurons and four other cell structures beyond LSTMs. Rawal and Miikkulainen have also utilized tree-based encoding [29] to evolve recurrent cellular structures within fixed architectures built of layers of the evolved cell types. Combining this evolution of cell structure along with the overall RNN structure stands as interesting future work.

Ant colony optimization (ACO) has also been investigated as a way to select which connections should be utilized in RNNs and LSTM RNNs by Desell and ElSaid [9, 12, 13]. In particular, this ACO approach was shown to reduce the number of trainable connections in half while providing a significant improvement in predictions of engine vibration [12]. However, this approach works within a fixed RNN architecture and cannot evolve an overall RNN structure.

3 EXAMM

The EXAMM algorithm presented in this work expands on an earlier algorithms, EXALT [11] which can evolve RNNs with either

simple neurons or LSTM cells and EXACT which evolves convolutional neural networks for image classification [7, 8]. It further refines EXALT's mutation operations to reduce hyperparameters using statistical information from parental RNN genomes. Also, EXALT only used a single steady state population, and EXAMM expands on this to use islands, which have been shown by Alba and Tomassini to greatly improve performance of distributed evolutionary algorithms, potentially providing superlinear speedup [2]. A master process maintains each population of islands, and generates new RNNs from islands in a round robin manner to be trained upon request by workers. When a worker completes training a RNN, it is inserted into the island it was generated from if its fitness (mean squared error on the test data) is better than the worst in the island, and then the worst RNN in the island is removed. This asynchrony is particularly important as the generated RNNs will have different architectures, each taking a different amount of time to train. By having a master process control the population, workers can complete the training of the generated RNNs at whatever speed they can and the algorithm is naturally load balanced. This allows EXAMM to scale to the number of available processors, having a population size independent of processor availability, unlike synchronous parallel evolutionary strategies. The EXAMM codebase has a multithreaded implementation for multicore CPUs as well as an MPI [21] implementation for use on high performance computing resources.

3.1 Mutation and Recombination Operations

RNNs are evolved with edge-level operations, as done in NEAT, as well as with new high level node mutations as in EXALT and EXACT. Whereas NEAT only requires innovation numbers for new edges, EXAMM requires innovation numbers for both new nodes, new edges and new recurrent edges. The master process keeps track of all node, edge and recurrent edge innovations made, which are required to perform the crossover operation in linear time without a graph matching algorithm. Figures 1 and 2 display a visual walkthrough of all the mutation operations used by EXAMM. Nodes and edges selected to be modified are highlighted, and then new elements to the RNN are shown in green. Edge innovation numbers are not shown for clarity. Enabled edges are in black, disabled edges are in grey.

It should be noted that for the following operations, whenever an edge is added, unless otherwise specified, it is probabilistically selected to be a recurrent connection with the following recurrent probability: $p = \frac{n_{re}}{n_{ff} + n_{re}}$, where n_{re} is the number of enabled recurrent edges and n_{ff} is the number of enabled feed forward edges in the parent RNN. A recurrent connection will go back a randomly selected number of time steps with bound specified as search parameters (in this work, 1 to 10 time steps), allowing for recurrent connections of varying time spans. Any newly created node is selected uniformly at random as a simple neuron or from the memory cell types specified by the EXAMM run input parameters.

3.1.1 Edge Mutations:

Disable Edge. This operation randomly selects an enabled edge or recurrent edge in a RNN genome and disables it so that it is not used. The edge remains in the genome. As the *disable edge*

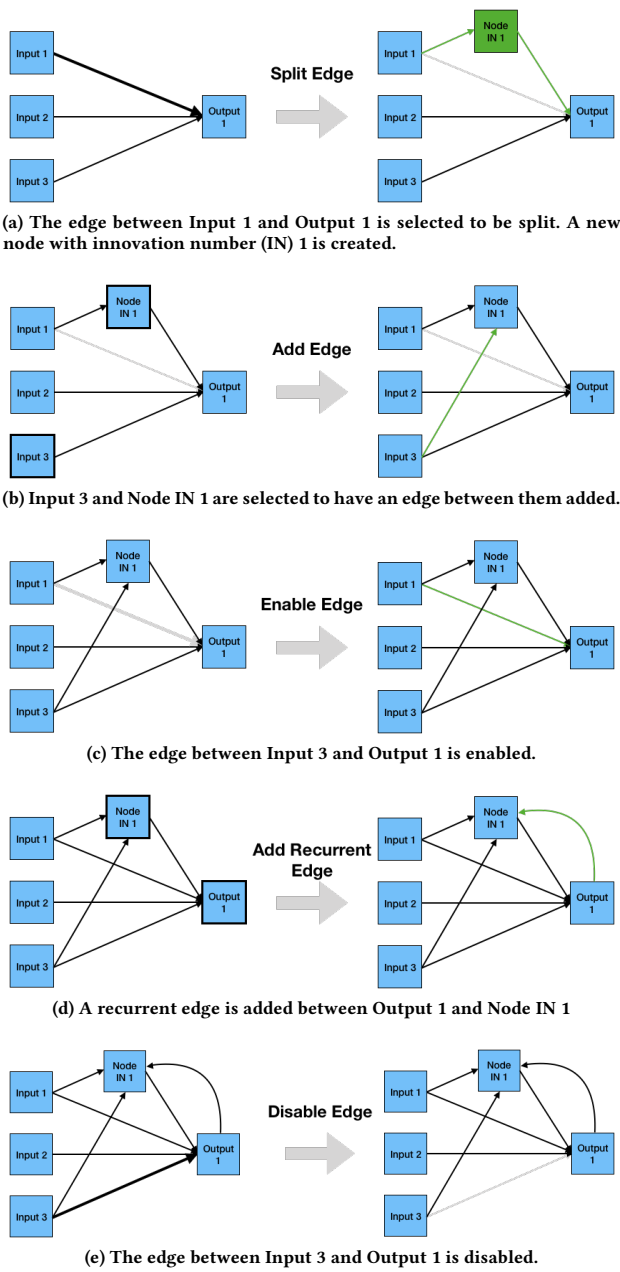


Figure 1: Edge mutation operations.

operation can potentially make an output node unreachable, after all mutation operations have been performed to generate a child RNN genome, if any output node is unreachable that RNN genome is discarded without training.

Enable Edge. If there are any disabled edges or recurrent edges in the RNN genome, this operation selects a disabled edge or recurrent edge at random and enables it.

Split Edge. This operation selects an enabled edge at random and disables it. It creates a new node and two new edges, and connects the input node of the split edge to the new node, and the new node to the output node of the split edge. If the split edge was recurrent, the new edges will also be recurrent (with the same time skip); otherwise they will be feed forward.

Add Edge. This operation selects two nodes n_1 and n_2 within the RNN Genome at random, such that $depth_{n_1} < depth_{n_2}$ and such that there is not already an edge between those nodes in this RNN Genome. Then it adds an edge from n_1 to n_2 .

Add Recurrent Edge. This operation selects two nodes n_1 and n_2 within the RNN Genome at random and then adds a recurrent edge from n_1 to n_2 , selecting a time span as described before. The same two nodes can be connected with multiple recurrent connections, each spanning different times; however it will not create a duplicate recurrent connection with the same time span.

3.1.2 Node Mutations:

Disable Node. This operation selects a random non-output node and disables it along with all of its incoming and outgoing edges. Note that this allows for input nodes to be dropped out, which can be useful when it is not previously known which input parameters are correlated to the output.

Enable Node. This operation selects a random disabled node and enables it along with all of its incoming and outgoing edges.

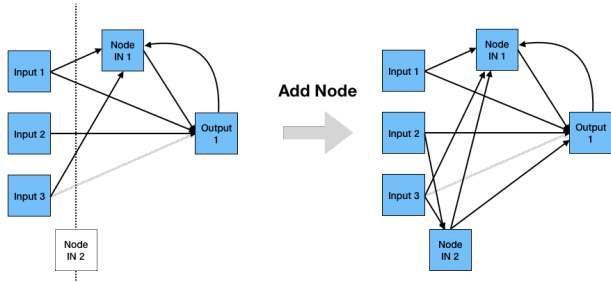
Add Node. This operation selects a random depth between 0 and 1, noninclusive. Given that the input node is always depth 0 and the output nodes are always depth 1, this depth will split the RNN in two. A new node is created at that depth, and the number of input and output edges and recurrent edges are generated using normal distributions with mean and variances equal to the mean and variances for the input/output edges and recurrent edges of all nodes in the parent RNN.

Split Node. This operation takes one non-input, non-output node at random and splits it. This node is disabled (as in the disable node operation) and two new nodes are created at the same depth as their parent. At least one input and one output edge are assigned to each of the new nodes, of a duplicate type from the parent, with the others being assigned randomly, ensuring that the newly created nodes have both inputs and outputs.

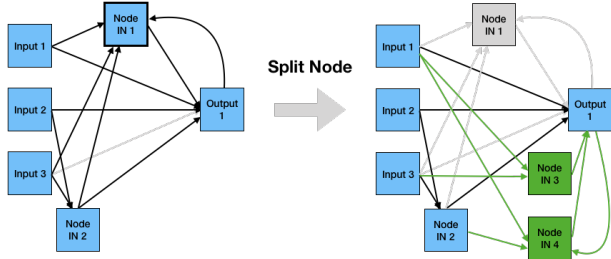
Merge Node. This operation takes two non-input, non-output nodes at random and combines them. Selected nodes are disabled (as in the disable node operation) and a new node is created at depth equal to the average of its parents. This node is connected to the inputs and outputs of its parents with a duplicate type from the parent; as input edges connected to lower depth nodes and output edges connect to greater depth nodes.

3.1.3 Other Operations:

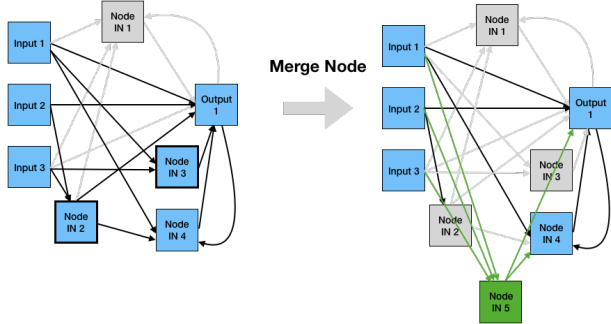
Crossover. creates a child RNN using all reachable nodes and edges from two parents. A node or edge is reachable if there is a path of enabled nodes and edges from an input node to it as well as a path of enabled nodes and edges from it to an output node, i.e., a node or edge is reachable if it actually affects the RNN. Crossover



(a) A node with IN 2 is selected to be added at a depth between the inputs & Node IN 1. Edges are randomly added to Input 2 and 3, and Node IN 1 and Output 1.



(b) Node IN 1 is selected to be split. It is disabled with its input/output edges. It is split into Nodes IN 3 and 4, which get half the inputs. Both have an output edge to Output 1 since there was only one output from Node IN 1.



(c) Node IN 2 and 3 are selected for a merger (input/output edges are disabled). Node IN 5 is created with edges between all their inputs/outputs.

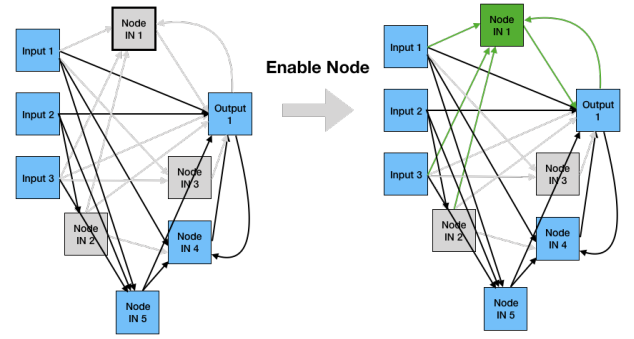
Figure 2: Node mutation operations.

can be done either within an island (*intra-island*) or between islands (*inter-island*). Inter-island crossover selects a random parent in the target island, and the best RNN from the other islands.

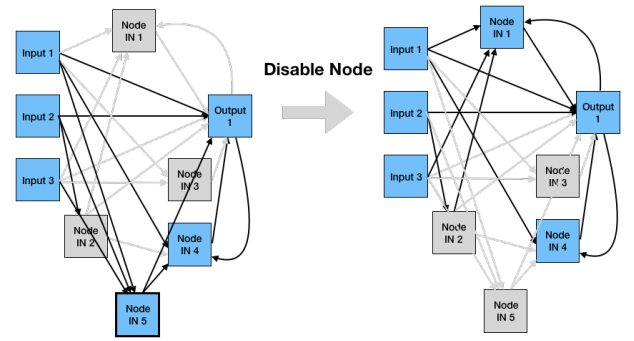
Clone. creates a copy of the parent genome, initialized to the same weights. This allows a particular genome to continue training in cases where further training may be more beneficial than performing a mutation or crossover.

3.2 Lamarckian Weight Initialization

For RNNs generated during population initialization, the weights are initialized uniformly at random between -0.5 and 0.5 . Biases and weights for new nodes and edges are initialized from a normal distribution based on the average, μ , and variance, σ^2 , of the parents'



(d) Node IN 1 is selected to be enabled, along with all its input and output edges.



(e) Node IN 5 is selected to be disabled, along with all its input and output edges.

Figure 2: Node mutation operations (continued).

weights. However, RNNs generated through mutation or crossover re-use parental weights, allowing the RNNs to train from where the parents are left off, i.e., “*Lamarckian*” weight initialization.

During crossover, in the case where an edge or node exists in both parents, the child weights are generated by recombining the parents’ weights. Given a random number $-0.5 \leq r \leq 1.5$, a child’s weight w_c is set to $w_c = r(w_{p2} - w_{p1}) + w_{p1}$, where w_{p1} is the weight from the more fit parent, and w_{p2} is the weight from the less fit parent. This allows the child weights to be set along a gradient calculated from the weights of the two parents.

This weight initialization strategy is particularly important as newly generated RNNs do not need to be completely retrained from scratch. In fact, the RNNs only need to be trained for a few epochs to investigate the benefits of newly added structures. In this work, the generated RNNs are only trained for 10 epochs (see Section 4.2), where training a static RNN structure from scratch may require hundreds or even thousands of epochs.

3.3 A Collection of Memory Cells

Node types vary in terms of complexity and with their design governing the form of the underlying memory structure. Simple neurons can be evolved into generalized versions of traditional Elman and Jordan neurons as EXAMM adds recurrent connections. Below describes how simple neurons can evolve to generalized Elman and Jordan neurons, as well as one complex cell, the Delta-RNN.

The Appendix describes all of the cell structures incorporated into EXAMM’s cell library, including the minimally gated unit (MGU) [38], the update-gated RNN (UGRNN) [5], the Gated Recurrent Unit (GRU) [4], and Long Short Term Memory (LSTM) [16].

Elman, Jordan and Arbitrary Recurrent Connections: In EXAMM, simple neurons are represented as traditional neurons with potentially both recurrent and feed forward inputs. I is the set of all nodes with a feed forward connection to simple neuron j while R is the set of all nodes with a recurrent connection to simple neuron j . At time step t , the output is a weighted summation of all feed forward inputs, where w_{ij} is the feed forward weight connecting node i to node j , plus a weighted summation of recurrent inputs, where v_{rjk} is the recurrent weight from node r at time step $t - k$ to the node j , where k is the time span of the recurrent connection. Thus the state function s for a computing a simple neuron is:¹

$$s_j(t) = \phi_s \left(\sum_{i \in I} w_{ij} \cdot s_i(t) + \sum_{r \in R, k} v_{rjk} \cdot s_r(t - k) \right)$$

The overall state is a linear combination of the projected input and an affine transformation of the vector summary of the past. The post-activation function, $\phi_s(\cdot)$, can be any differentiable element-wise function, however for the purposes of this work it was limited to the hyperbolic tangent, $\phi(v) = \tanh(v) = (e^{(2v)} - 1)/(e^{(2v)} + 1)$.

Elman-RNNs [10] connect recurrent nodes to themselves and potentially all other hidden nodes in the same layer. Jordan-RNNs [18] have recurrent connections from output node(s) to hidden node(s). EXAMM can evolve Elman connections when the *add recurrent edge* mutation adds a recurrent edge from a simple neuron back to itself, and Jordan connections when it adds a recurrent edge from an output to a simple neuron. It generalizes these structures by allowing varying time spans (Jordan and Elman network traditionally span only one time step) and arbitrary recurrent connections between from any pair of simple neurons or cells.

The Delta RNN (Δ -RNN) Cell: For models more complex than the simple RNN model, we looked to derive a vast set of gated neural architectures unified under a recent framework known as the Differential State Framework (DSF) [26]. A DSF neural model is essentially a composition of an inner function used to compute state proposals and an outer “mixing” function used to decide how much of a state proposal is incorporated into a slower moving state, *i.e.*, the longer term memory. These models are better equipped to handle the vanishing gradient problem induced by the difficulty of learning long-term dependencies over sequences [3]. Other models that can be derived under the DSF include the LSTM, the GRU, and the MGU [26]. One of the simplest DSF models is the Δ -RNN, which has been shown to perform competitively with more complex memory models in problems ranging from language modeling [25, 26] to image decoding [24]. With $\{\alpha, \beta_1, \beta_2, b_j, m\}$ as learnable coefficient scalars, the Δ -RNN state is defined as:

$$\begin{aligned} e_j^w &= \sum_{i \in I} w_{ij} \cdot s_i(t) + \sum_{r \in R, k} v_{rjk} \cdot s_r(t - k), & e_j^v &= m \cdot s_j(t - 1) \\ d_j^1 &= \alpha \cdot e_j^v \cdot e_j^w, & d_j^2 &= \beta_1 \cdot e_j^v + \beta_2 \cdot e_j^w, & r_j &= \sigma(e_j^w + b_j) \\ \tilde{s}_j(t) &= \phi_s(d_j^1 + d_j^2), & s_j(t) &= \Phi_s((1 - r_j) \cdot \tilde{s}_j(t) + r_j \cdot s_j(t - 1)) \end{aligned}$$

¹The bias is omitted for clarity and simplicity of presentation.

4 RESULTS

4.1 Open Data and Reproducibility

This work utilizes two data sets to benchmark the memory cells and RNNs evolved by EXAM. The first comes from a selection of 10 flights’ worth of data from the National General Aviation Flight Information Database (NGAFID) [1] and the other comes from a coal-fired power plant which has requested to remain anonymous. Both datasets are multivariate (26 and 12 parameters, respectively), non-seasonal, and the parameter recordings are not independent. They are very long – the aviation time series ranges from 1 to 3 hours of per-second data while the power plant data consists of 10 days of per-minute readings. EXAMM source code along with the data sets utilized have been made publicly available to facilitate reproducibility and further research in time series data prediction². To the authors’ knowledge, there are no other data sets of this type and at this scale publicly available.

RPM (rotations per minute) and *pitch* were selected as predictors from the aviation data since RPM is a product of engine activity, with other engine-related parameters correlated, and since pitch is directly influenced by pilot controls, thus particularly challenging to predict. *Main flame intensity* and *supplementary fuel flow* were selected as parameters of interest from the coal plant data. Similar to the choices from the NGAFID data, main flame intensity is mostly a product of conditions within the burner whereas supplementary fuel flow is more directly controlled by human operators.

4.2 Experimental Design

To better understand how the different memory cells performed in time series data prediction, multiple EXAMM runs were conducted that allowed different types of memory cells. The first set of runs (5) added cells of only a single, particular memory cell type, *i.e.*, either a Δ -RNN, GRU, LSTM, MGU, or UGRNN. The next set of runs (5) was nearly identical, except these allowed nodes to be simple neurons in addition to each particular memory cell type (such runs are appended with a *+simple* in the result tables). One final version was run where all cell types and simple neurons were allowed; resulting in 11 different EXAMM run types (such runs are labeled as *all* in the result tables). These different types of runs were done for each of the four prediction parameters (RPM, pitch, main flame intensity, and supplementary fuel flow). K -fold cross validation was done for each prediction parameter, with a fold size of 2. This resulted in 5 folds for the NGAFID data (as it had 10 flight data files), and 6 folds for the coal plant data (as it has 12 burner data files). Each fold and EXAMM setting run was repeated 10 times. In total, each of the 11 EXAMM run types was done 110 times (50 times for each NGAFID parameter k -fold validation and 60 times for each coal data parameter k -fold validation), for a total of 2,420 separate runs.

All neural networks were trained with backpropagation and stochastic gradient descent (SGD) using the same hyperparameters. SGD was run with a learning rate $\eta = 0.001$, utilizing Nesterov momentum with $mu = 0.9$. No dropout regularization was used since it has been shown in other work to reduce performance when training RNNs for time series prediction [12]. To prevent exploding

²URL removed due to the double blind review process.

gradients, gradient clipping (as described by Pascanu *et al.* [27]) was used when the norm of the gradient was above a threshold of 1.0. To improve performance for vanishing gradients, gradient boosting (the opposite of clipping) was used when the norm of the gradient was below a threshold of 0.05. The forget gate bias of the LSTM cells had 1.0 added to it as this has been shown to yield significant improvements in training time by Jozefowicz *et al.* [19]; otherwise weights were initialized as described in Section 3.2.

Each EXAMM run consisted of 10 islands, each with a population size of 5, and new RNNs were generated via intra-island crossover (at 20%), mutation (at 70%), and inter-island crossover (at 10%). All mutation operations (described in Section 3) except for *split edge* were utilized, as *split edge* can be recreated with the *add node* and *disable edge* operations. The 10 utilized mutation operations were performed each with a uniform 10% chance. Each EXAMM run generated 2000 RNNs, with each RNN being trained for 10 epochs. These runs were performed utilizing 20 processors in parallel, and on average required approximately 0.5 compute hours. In total, these results come from training over 4,840,000 RNNs, requiring ~24,200 CPU hours of compute time.

4.3 Evolved RNN Performance

Table 1 shows aggregated results for each of the 50 or 60 EXAMM runs done (5 or 6 folds, each with 10 repeats) that allowed only one of each memory cell type, along with the EXAMM runs that allowed for added nodes to be of all node types (*i.e.*, *all*). Table 2 further shows the aggregated results for runs which allowed both simple neurons and one particular cell type (*i.e.*, *+simple*).

These tables present the minimum, average, and maximum mean squared error (MSE) on average across the runs. Table 1 also shows the minimum, average, and maximum number of hidden nodes, which would be entirely of the one memory cell type, or of any memory cell type or simple neurons in the case of the *all* runs, as well as how the number of nodes correlate to the MSE. Similar statistics are shown for the numbers of feed forward edges and the numbers of recurrent edges. Note that as a lower MSE is better, a negative correlation means that having more nodes or edges was correlated to lower MSE. Table 2 also divides hidden nodes into counts for simple neurons and number of memory cell nodes for a certain run type. Top 2 best models (avg) scores are shown in **bold**.

The best found MSE scores across the four prediction parameters had a wide range, which could be expected due to varying complexities. As such, to properly rank performance of different run types a metric was needed. Table 4 orders the 11 different run types by how many standard deviations the results were from the mean for each prediction parameter. It also provides combined rankings, averaging the deviation from the mean across the four prediction parameters. Each of these tables are ordered from best to worst – a negative deviation from the mean is that many standard deviations less than the average MSE, and lower MSE is better.

The results of these experiments led to some interesting findings which the authors feel can help inform further development of neuro-evolution algorithms as well as RNN memory cells. Many of these findings can also serve as warnings to those looking to train well performing RNNs for time series prediction. We summarize the main takeaways from these results as follows:

No memory structure was truly the best: In the overall rankings (Table 4), the Δ -RNN, LSTM, and MGU cells seemed to have the highest rankings for best overall performance as well as average and worst case performance, with GRU cells being slightly behind. While UGRNN nodes did not do so well in the total ranking, it should be noted that when coupled with simple neurons, they did perform 2nd best for the best case for fuel flow, and were the best for the average case in predicting pitch. This highlights the importance of testing a wide selection of memory cell types when developing RNNs, as there is *no free lunch* in machine learning – each memory cell type had its own strengths and weaknesses. It is valuable to note that one of the simplest memory cell types, *i.e.*, the Δ -RNN, performs consistently and competitively with the more complicated, multi-gate LSTM (at the top of the rankings), which is consistent with a growing body of results [24–26].

Adding simple neurons generally helped - with some notable exceptions: When looking at the overall rankings, when simple neurons were added as an option to the neuro-evolution process, the networks performed better. The only exception to this was GRU cells, which tended to perform worse when simple neurons were allowed. These results may indicate that these memory cells lack the capability to track some kinds of dependencies which the additional simple neurons make up for; this means that there is potentially room to improve these cell structures to capture whatever the simple neurons were providing. Further examination of why the GRU cells performed worse with simple neurons compared to the other memory cells may help determine the cause of this and makes for an interesting direction for future RNN work.

Another very interesting finding was that utilizing simple neurons with MGU cells resulted in a dramatic improvement, bringing them from some of the worst rankings to some of the best rankings (*e.g.*, in the overall rankings for best found networks, MGU cells alone performed the worst while MGU with simple neurons performed the best). Other cell types (LSTM and Δ -RNN) showed less of an improvement. This finding may highlight that the MGU cells could stand to benefit from further development. This should serve as a warning to others developing neuro-evolution algorithms, in that even the rather simple change of allowing simple neurons can result in significant changes in RNN predictive ability. Selection of node and cell types for neuro-evolution should be done carefully.

Allowing all memory cells has risks and benefits: The authors had hoped that allowing the neuro-evolution process to simply select from all of the memory cell types would allow it to find and utilize whichever cells were most suited to the prediction problem. Unfortunately, this was not always the case. While using all memory cell types generally performed better than the mean on the best case, in the average and worst cases, it performed worse than the mean. This was most likely due to the fact that whenever a node was added to the network it could have been from any of the 6 types, so choosing from them uniformly at random ended up sometimes selecting the nodes not best to the task (as they improved the population, but not as well as another memory cell choice could have done). These results are backed up by Table 3, which shows the correlations between node types and MSE (again, a negative correlation means more of that cell type resulted in a lower/better

Flame Intensity (Power Plant Dataset)															
Run Type	MSE			Edges				Rec. Edges				Hidden Nodes			
	Min	Avg	Max	Min	Avg	Max	Corr.	Min	Avg	Max	Corr.	Min	Avg	Max	Corr.
all	0.000438215	0.00168176	0.00308112	11	28	64	-0.274	0	5.7	15	-0.147	11	16	22	-0.228
Δ-RNN	0.000419515	0.00164756	0.00365646	15	29	72	-0.163	1	6.3	16	-0.136	11	16	25	-0.251
GRU	0.000493313	0.00166337	0.0035205	11	28	56	-0.115	1	6.6	20	-0.101	12	16	21	0.109
LSTM	0.000460576	0.00174216	0.00386718	11	28	53	-0.187	0	7.9	26	-0.386	10	16	21	-0.241
MGU	0.000644687	0.00174361	0.00342526	8	27	49	-0.241	1	6.5	19	-0.127	13	16	21	-0.373
UGRNN	0.000531725	0.00166423	0.00399293	19	28	54	-0.215	1	6.9	25	-0.192	12	16	22	-0.209

Fuel Flow (Power Plant Dataset)															
Run Type	MSE			Edges				Rec. Edges				Hidden Nodes			
	Min	Avg	Max	Min	Avg	Max	Corr.	Min	Avg	Max	Corr.	Min	Avg	Max	Corr.
all	4.86288e-06	0.000134371	0.000293377	12	31	55	0.138	0	6.7	18	0.15	8	16	22	0.251
Δ-RNN	6.44047e-06	0.000140518	0.000306163	15	29	57	-0.0995	0	6.8	17	-0.264	12	16	22	-0.194
GRU	1.65072e-05	0.000131481	0.000289922	16	31	66	-0.193	0	6.6	29	-0.209	10	16	22	-0.146
LSTM	5.90673e-06	0.000121158	0.000262113	14	31	65	-0.0119	1	6.8	22	-0.028	11	16	23	0.0572
MGU	1.83369e-05	0.00013616	0.000281395	13	32	63	-0.235	0	6.7	17	-0.303	7	16	23	-0.141
UGRNN	6.08753e-06	0.000143734	0.000341757	10	29	78	0.0308	0	6.7	19	-0.0971	9	16	22	0.158

RPM (Aviation Dataset)															
Run Type	MSE			Edges				Rec. Edges				Hidden Nodes			
	Min	Avg	Max	Min	Avg	Max	Corr.	Min	Avg	Max	Corr.	Min	Avg	Max	Corr.
all	0.00410034	0.00725003	0.0142856	25	36	54	0.215	0	5.3	13	-0.133	24	29	33	0.0921
Δ-RNN	0.00247046	0.0066479	0.0132178	23	37	66	0.00237	0	4.8	16	-0.083	25	29	35	-0.00169
GRU	0.00221411	0.00684006	0.0108375	24	36	72	-0.207	0	5.9	16	-0.342	25	29	36	-0.262
LSTM	0.00323368	0.00736006	0.014325	24	35	46	0.018	0	4.7	14	-0.437	23	28	30	-0.14
MGU	0.00343788	0.00730802	0.0153965	28	38	57	0.057	0	5.3	14	-0.519	25	29	33	0.124
UGRNN	0.00307084	0.00716817	0.0116206	25	36	66	-0.277	0	5.3	15	-0.373	25	29	36	-0.315

Pitch (Aviation Dataset)															
Run Type	MSE			Edges				Rec. Edges				Hidden Nodes			
	Min	Avg	Max	Min	Avg	Max	Corr.	Min	Avg	Max	Corr.	Min	Avg	Max	Corr.
all	0.00101445	0.00347982	0.00582811	22	35	67	-0.132	0	3	10	-0.223	24	28	35	-0.109
Δ-RNN	0.00149607	0.00328248	0.00557884	24	35	49	0.0524	0	3.4	12	-0.114	23	28	32	0.104
GRU	0.00133482	0.00323731	0.00506138	22	34	54	-0.0691	0	3	11	-0.212	24	28	32	-0.113
LSTM	0.00114187	0.0033505	0.00558931	26	35	54	-0.147	0	3.5	9	-0.126	24	28	33	-0.117
MGU	0.00148457	0.00327753	0.00565053	26	35	51	0.0707	0	3.3	11	-0.388	25	28	32	0.0442
UGRNN	0.00117033	0.0033487	0.00559272	22	33	50	-0.0981	0	3	13	-0.165	23	28	32	-0.0133

Table 1: Statistics for RNNs Evolved With Individual Memory Cells and RNNs Evolved With All Memory Types.

Flame Intensity (Power Plant Dataset)																			
	MSE			Edges				Rec. Edges				Memory Cells				Simple Neurons			
Run Type	Min	Avg	Max	Min	Avg	Max	Corr.	Min	Avg	Max	Corr.	Min	Avg	Max	Corr.	Min	Avg	Max	Corr.
Δ-RNN+simple	0.00042112	0.0015147	0.0038971	12	27	62	-0.25	1	7.7	20	-0.222	0	1.9	7	-0.137	0	1.6	6	-0.238
GRU+simple	0.00068848	0.0016726	0.0039989	18	29	55	-0.23	0	7.1	17	-0.11	0	1.8	4	-0.133	0	1.9	6	-0.384
LSTM+simple	0.00046443	0.0015194	0.0032395	19	31	65	-0.21	1	7.3	18	-0.208	0	1.6	6	-0.27	0	2.2	7	0.0671
MGU+simple	0.00053109	0.0016088	0.003241	18	29	55	-0.19	0	7.8	21	-0.238	0	1.6	6	-0.00329	0	2	7	-0.213
UGRNN+simple	0.00043835	0.0016874	0.0041592	16	29	50	-0.31	1	6.2	16	-0.274	0	1.5	5	-0.349	0	2.4	6	-0.061
Fuel Flow (Power Plant Dataset)																			
	MSE			Edges				Rec. Edges				Memory Cells				Simple Neurons			
Run Type	Min	Avg	Max	Min	Avg	Max	Corr.	Min	Avg	Max	Corr.	Min	Avg	Max	Corr.	Min	Avg	Max	Corr.
Δ-RNN+simple	8.1558e-06	0.00012294	0.00026373	9	29	55	-0.12	0	6.4	15	-0.026	0	1.7	5	-0.2	0	1.8	6	-0.00871
GRU+simple	1.3193e-05	0.00013061	0.00028389	9	31	62	-0.17	0	6	21	0.00366	0	2.1	6	-0.196	0	1.8	6	0.0181
LSTM+simple	8.6606e-06	0.00013071	0.00025847	14	31	61	-0.098	0	6.5	22	-0.187	0	2.2	7	-0.0819	0	1.9	5	0.0817
MGU+simple	7.2707e-06	0.00012367	0.00028356	11	33	61	-0.072	1	6.8	26	-0.228	0	2.2	7	-0.107	0	2.1	8	-0.0846
UGRNN+simple	5.6189e-06	0.00014337	0.00030186	12	32	62	-0.15	0	6.1	15	-0.253	0	1.8	6	-0.0961	0	2.3	8	-0.102
RPM (Aviation Dataset)																			
	MSE			Edges				Rec. Edges				Memory Cells				Simple Neurons			
Run Type	Min	Avg	Max	Min	Avg	Max	Corr.	Min	Avg	Max	Corr.	Min	Avg	Max	Corr.	Min	Avg	Max	Corr.
Δ-RNN+simple	0.0029348	0.0069672	0.011182	25	36	48	-0.17	0	4.8	14	-0.496	0	0.88	3	0.0549	0	1.2	4	-0.142
GRU+simple	0.0039148	0.0070081	0.012816	29	38	63	-0.054	1	5.1	13	-0.049	0	1.2	4	-0.0963	0	1.3	5	0.0855
LSTM+simple	0.0027877	0.0063965	0.01091	27	37	60	-0.11	0	4.6	11	-0.5	0	1	3	-0.223	0	1.2	4	0.0936
MGU+simple	0.0024288	0.0065725	0.011325	24	36	44	0.051	0	5.6	13	-0.391	0	0.98	3	-0.0944	0	1.1	3	0.178
UGRNN+simple	0.0037114	0.0073811	0.012252	22	38	48	-0.11	0	4.3	10	-0.304	0	1.1	4	-0.00488	0	1.4	4	-0.0642
Pitch (Aviation Dataset)																			
	MSE			Edges				Rec. Edges				Memory Cells				Simple Neurons			
Run Type	Min	Avg	Max	Min	Avg	Max	Corr.	Min	Avg	Max	Corr.	Min	Avg	Max	Corr.	Min	Avg	Max	Corr.
Δ-RNN+simple	0.0015138	0.0032316	0.0053377	20	34	54	-0.14	0	2.6	8	-0.341	0	0.86	4	-0.00809	0	1.1	5	-0.168
GRU+simple	0.0011566	0.0032083	0.0067072	22	36	57	0.056	0	3.2	9	0.0472	0	0.98	4	0.042	0	1	3	-0.00732
LSTM+simple	0.0010335	0.0032365	0.005414	22	34	52	-0.25	0	2.9	10	-0.233	0	0.9	3	-0.176	0	0.98	4	-0.157
MGU+simple	0.0010133	0.0033326	0.0060865	25	35	53	-0.15	0	2.8	11	-0.307	0	0.88	3	-0.276	0	0.98	5	0.163
UGRNN+simple	0.0015551	0.0031352	0.0053126	22	34	52	0.1	0	3.1	8	-0.216	0	0.94	3	-0.063	0	1	4	0.181

Table 2: Statistics for RNNs Evolved With Simple Neurons and Memory Cells.

	Simple				LSTM				UGRNN				Δ -RNN				MGU				GRU			
Run Type	Min	Avg	Max	Corr	Min	Avg	Max	Corr	Min	Avg	Max	Corr	Min	Avg	Max	Corr	Min	Avg	Max	Corr	Min	Avg	Max	Corr
flame	0	0.6	3	0.044	0	0.5	3	-0.26	0	0.5	4	-0.11	0	0.5	2	-0.12	0	0.5	3	0.073	0	0.7	4	-0.17
fuel flow	0	0.8	3	0.0076	0	0.6	4	0.11	0	0.7	4	-0.061	0	0.6	4	-0.041	0	0.6	2	0.092	0	0.8	3	0.018
pitch	0	0.3	3	-0.017	0	0.3	3	-0.031	0	0.3	2	0.032	0	0.2	2	0.052	0	0.5	2	-0.036	0	0.3	2	-0.32
rpm	0	0.4	2	-0.14	0	0.4	2	0.24	0	0.3	2	-0.086	0	0.4	2	0.026	0	0.4	3	0.32	0	0.2	2	-0.16

Flame Intensity (Power Plant Dataset)					
Best Case		Avg. Case		Worst Case	
Δ -RNN	-0.92312	Δ -RNN+simple	-1.7775	all	-1.5404
Δ -RNN+simple	-0.90534	LSTM+simple	-1.7148	LSTM+simple	-1.5066
all	-0.71602	MGU+simple	-0.53749	MGU+simple	-1.1026
UGRNN+simple	-0.71451	Δ -RNN	-0.026901	MGU	-0.59787
LSTM	-0.46836	GRU	0.18143	GRU	-0.33703
LSTM+simple	-0.42565	UGRNN	0.19272	Δ -RNN	0.035348
GRU	-0.10578	GRU+simple	0.30281	LSTM	0.61246
MGU+simple	0.31264	all	0.42371	Δ -RNN+simple	0.69439
UGRNN	0.31964	UGRNN+simple	0.49785	UGRNN	0.9569
MGU	1.5708	LSTM	1.2196	GRU+simple	0.97318
GRU+simple	2.0557	MGU	1.2386	UGRNN+simple	1.4123
Fuel Flow (Power Plant Dataset)					
Best Case		Avg. Case		Worst Case	
all	-0.92643	LSTM	-1.4415	LSTM+simple	-1.2349
UGRNN+simple	-0.7644	Δ -RNN+simple	-1.2172	LSTM	-1.0818
LSTM	-0.70271	MGU+simple	-1.1255	Δ -RNN+simple	-1.014
UGRNN	-0.66396	GRU+simple	-0.25195	MGU	-0.27097
Δ -RNN	-0.58832	LSTM+simple	-0.23921	MGU+simple	-0.1799
MGU+simple	-0.41037	GRU	-0.14222	GRU+simple	-0.16598
Δ -RNN+simple	-0.22068	all	0.22163	GRU	0.087564
LSTM+simple	-0.1125	MGU	0.44679	all	0.42284
GRU+simple	0.55882	Δ -RNN	0.99531	UGRNN+simple	0.58938
GRU	1.5692	UGRNN+simple	1.3537	Δ -RNN	0.77052
MGU	1.9613	UGRNN	1.4002	UGRNN	2.2672
RPM (Aviation Dataset)					
Best Case		Avg. Case		Worst Case	
GRU	-1.444	LSTM+simple	-1.7472	GRU	-1.0958
MGU+simple	-1.1012	MGU+simple	-1.2299	LSTM+simple	-1.0499
Δ -RNN	-1.0347	Δ -RNN	-1.0081	Δ -RNN+simple	-0.87687
LSTM+simple	-0.52825	GRU	-0.4433	MGU+simple	-0.78566
Δ -RNN+simple	-0.29348	Δ -RNN+simple	-0.069508	UGRNN	-0.59783
UGRNN	-0.076276	GRU+simple	0.050686	UGRNN+simple	-0.19645
LSTM	0.18368	UGRNN	0.52115	GRU+simple	0.16258
MGU	0.50967	all	0.76179	Δ -RNN	0.41787
UGRNN+simple	0.9463	MGU	0.93224	all	1.0968
GRU+simple	1.271	LSTM	1.0852	LSTM	1.1219
all	1.5672	UGRNN+simple	1.147	MGU	1.8033
Pitch (Aviation Dataset)					
Best Case		Avg. Case		Worst Case	
MGU+simple	-1.1631	UGRNN+simple	-1.6163	GRU	-1.3295
all	-1.1577	GRU+simple	-0.82052	UGRNN+simple	-0.76284
LSTM+simple	-1.0698	Δ -RNN+simple	-0.56665	Δ -RNN+simple	-0.70622
LSTM	-0.5688	LSTM+simple	-0.51389	LSTM+simple	-0.53415
GRU+simple	-0.50079	GRU	-0.5047	Δ -RNN	-0.16235
UGRNN	-0.43726	MGU	-0.066984	LSTM	-0.13873
GRU	0.32298	Δ -RNN	-0.013118	UGRNN	-0.13104
MGU	1.0151	MGU+simple	0.53287	MGU	-0.00065639
Δ -RNN	1.0682	UGRNN	0.70761	all	0.39991
Δ -RNN+simple	1.1501	LSTM	0.72719	MGU+simple	0.98284
UGRNN+simple	1.3411	all	2.1345	GRU+simple	2.3828
Overall Combined					
Best Case		Avg. Case		Worst Case	
MGU+simple	-0.59051	LSTM+simple	-1.0538	LSTM+simple	-0.98141
LSTM+simple	-0.53405	Δ -RNN+simple	-0.90771	GRU	-0.6687
LSTM	-0.38905	MGU+simple	-0.59001	Δ -RNN+simple	-0.47566
Δ -RNN	-0.36948	GRU	-0.2272	MGU+simple	-0.27133
all	-0.30824	GRU+simple	-0.17974	all	0.047292
UGRNN	-0.21446	Δ -RNN	-0.013211	LSTM	0.12847
Δ -RNN+simple	-0.067358	UGRNN+simple	0.34556	MGU	0.23345
GRU	0.085614	LSTM	0.39761	UGRNN+simple	0.26059
UGRNN+simple	0.20212	MGU	0.63765	Δ -RNN	0.26535
GRU+simple	0.9212	UGRNN	0.70542	UGRNN	0.62381
MGU	1.2642	all	0.88541	GRU+simple	0.83814

Table 4: EXAMM Run Types Prediction Error Ranked By Standard Deviation From Mean.

the best: This last point raises some significant challenges for developing neuro-evolution algorithms. When looking at Table 3 and examining the memory cells types most correlated to improved performance against the memory cell types most frequently selected by EXAMM, meant that EXAMM was not selecting cell types that would produce the best performing RNNs. This may due to the fact that, in some cases, an RNN with a small number of well trained memory cells was sufficient to yield good predictions, and adding more cells to the network only served to confuse the predictions.

The implications of this are two fold: 1), running a neuro-evolution strategy allowing all memory cell types and then utilizing counts or correlations to select a single memory cell type for future runs may not produce the best results, and 2), dynamically tuning which memory cells are selected by a neuro-evolution strategy is more challenging since the process may not select the best cell types (e.g., when the network already has enough memory cells) – so this would at least need to be coupled with another strategy to determine when the network is “big enough”.

5 CONCLUSIONS AND FUTURE WORK

This work introduced a new neuro-evolution algorithm, Evolutionary eXploration of Augmenting Memory Models (EXAMM), for evolving recurrent neural architectures by directly incorporating powerful memory cells such as the Δ -RNN, MGU, GRU, LSTM and UGRNN units into the evolutionary process. EXAMM was evaluated on the task of predicting 4 different parameters from two large, real world time-series datasets. By using repeated k -fold cross validation and high performance computing, enough RNNs were evolved to be rigorously analyzed – a methodology the authors think should be highlighted as novel. Instead of utilizing them to outperform other algorithms on benchmarks, neuro-evolutionary processes can be used as selection methodologies, providing deeper insights into what neural structures perform best on certain tasks.

Key findings from this work show that a neuro-evolution strategy that selects from a wide number of memory cell structures can yield performant architectures. However, it does so at the expense of reliability in the average and worst cases. Furthermore, a simple modification to the evolutionary process, *i.e.*, allowing simple neurons, can have dramatic effects on network performance. In general, while this largely benefits most memory cells, outlier cases showed wide swings from worst to best and best to worst performance. The authors hope that these results will guide future memory cell development, as the addition of simple neurons dramatically improved MGU performance, but also decreased GRU performance. Understanding cases like that of the GRU could yield improvements in cell design. Results showed that cell selection does not necessarily correlate well to the best cell types for a particular problem, partly due to the fact that good cells may not necessarily require a large network. These results should serve as cautionary information for future development of neuro-evolution algorithms.

This paper opens up many avenues of future work. This includes extending EXAMM’s search process to allow cellular elements of the underlying neural model to be evolved (as in Rawal and Miikula [29]); evolving over a large set of post-activation functions; allowing for stochastic operations, *e.g.*, Bernoulli sampling; and incorporating operators such as convolution (to handle video sequences/time series) or its simple approximation, the perturbative operator [20]. Additional future work will involve various hyperparameter optimization strategies to dynamically determine RNN training metaparameters as well as what probabilities EXAMM uses to choose memory cell structures and what probabilities it uses for the mutation and recombination operators. Lastly, implementing even larger scale mutation operations, such as multi-node/layer mutations could potentially speed up EXAMM’s neuro-evolution process even further.

6 ACKNOWLEDGEMENTS

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7 APPENDIX

7.1 Memory Cell Types

There are various types of possible memory cells for EXAMM to select from, composing effectively an easily-extensible memory cell library. Since EXAMM operates with a focus on single unit processing elements we will present the formulation of each unit type from the same perspective (instead of the usual vectorized forms which deals with collections or layers of neuronal elements, as is done in other work).

The Long-Short Term Memory (LSTM): The LSTM [16] is one of the most commonly used gated neural model when modeling sequential data. The original motivation behind the LSTM was to implement the “constant error carousel” in order to mitigate the problem of vanishing gradients. This means that long-term memory can be explicitly represented with a separate cell state \mathbf{c}_t .

The LSTM state function (without any extensions, such as “peep-hole” connections) is implemented using the following equations:

$$\begin{aligned} f_j &= \sigma(\sum_{i \in I} w_{ij}^f \cdot s_i(t) + \sum_{r \in R, k} v_{rjk}^f \cdot s_r(t-k)) \\ i_j &= \sigma(\sum_{i \in I} w_{ij}^i \cdot s_i(t) + \sum_{r \in R, k} v_{rjk}^i \cdot s_r(t-k)) \\ \tilde{c}_j &= \tanh(\sum_{i \in I} w_{ij}^c \cdot s_i(t) + \sum_{r \in R, k} v_{rjk}^c \cdot s_r(t-k)) \\ o_j &= \sigma(\sum_{i \in I} w_{ij}^o \cdot s_i(t) + \sum_{r \in R, k} v_{rjk}^o \cdot s_r(t-k)) \\ c_j(t) &= f_j(t) \cdot c_j(t-1) + i_j \cdot \tilde{c}_j, \quad s_j(t) = o_j \cdot \phi_s(c_j(t)) \end{aligned}$$

where we depict the sharing of the transformation function’s output across the forget (\mathbf{f}_t), input (\mathbf{i}_t), cell-state proposal ($\tilde{\mathbf{c}}_t$), and output (\mathbf{o}_t) gates. The LSTM is by far the most parameter-hungry of the DSF models we explore.

The Gated Recurrent Unit (GRU): The Gated Recurrent Unit (GRU; [4]) can be viewed as an early attempt to simplify the LSTM. Among the changes made, the model fuses the LSTM input and forgets gates into a single gate, and merges the cell state and hidden state back together. The state function based on the GRU is calculated using the following equations:

$$z_j = \sigma(\sum_{i \in I} w_{ij}^z \cdot s_i(t) + \sum_{r \in R, k} v_{rjk}^z \cdot s_r(t-k)) \quad (1)$$

$$r_j = \sigma(\sum_{i \in I} w_{ij}^r \cdot s_i(t) + \sum_{r \in R, k} v_{rjk}^r \cdot s_r(t-k)) \quad (2)$$

$$\tilde{s}_j(t) = \phi_s(\sum_{i \in I} w_{ij}^s \cdot s_i(t) + \sum_{r \in R, k} v_{rjk}^s \cdot (r_j \cdot s_r(t-k))) \quad (3)$$

$$s_j(t) = z_j \cdot \tilde{s}_j + (1 - z_j) \cdot s_j(t-1) \quad (4)$$

nothing that $\phi_s(v) = \tanh(v)$.

The Minimally-Gated Unit (MGU): The MGU model is very similar in structure to the GRU, reducing number of required parameters by merging its reset and update gates into a single forget gate [38].

The state computation proceeds as follows:

$$f_j = \sigma(\sum_{i \in I} w_{ij}^f \cdot s_i(t) + \sum_{r \in R, k} v_{rjk}^f \cdot s_r(t-k)) \quad (5)$$

$$\tilde{s}_j(t) = \phi_s(\sum_{i \in I} w_{ij}^s \cdot s_i(t) + \sum_{r \in R, k} v_{rjk}^s \cdot (f_j \cdot s_r(t-k))) \quad (6)$$

$$s_j(t) = z_j \cdot \tilde{s}_j + (1 - z_j) \cdot s_j(t-1). \quad (7)$$

The Update-Gated RNN (UGRNN): The UGRNN [5] updates are defined in the following manner:

$$c_j = \phi_s(\sum_{i \in I} w_{ij}^c \cdot s_i(t) + \sum_{r \in R, k} v_{rjk}^c \cdot s_r(t-k)) \quad (8)$$

$$g_j = \sigma(\sum_{i \in I} w_{ij}^g \cdot s_i(t) + \sum_{r \in R, k} v_{rjk}^g \cdot s_r(t-k)) \quad (9)$$

$$s_j(t) = g_j \cdot s_j(t-1) + (1 - g_j) \cdot c_j. \quad (10)$$

The UGRNN, though more expensive than the Δ -RNN, is a simple model, essentially working like an Elman-RNN with a single update gate. This extra gate decides whether a hidden state is carried over from the previous time step or if the state should be updated.

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