HyperENTM: Evolving Scalable Neural Turing Machines through HyperNEAT

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Abstract

Recent developments within memory-augmented neural networks have solved sequential problems requiring long-term memory, which are intractable for traditional neural networks. However, current approaches still struggle to scale to large memory sizes and sequence lengths. In this paper we show how access to memory can be encoded geometrically through a HyperNEAT-based Neural Turing Machine (Hyper-ENTM). We demonstrate that using the indirect HyperNEAT encoding allows for training on small memory vectors in a bit-vector copy task and then applying the knowledge gained from such training to speed up training on larger size memory vectors. Additionally, we demonstrate that in some instances, networks trained to copy bit-vectors of size 9 can be scaled to sizes of 1,000 without further training. While the task in this paper is simple, these results could open up the problems amendable to networks with external memories to problems with larger memory vectors and theoretically unbounded memory sizes.

Introduction

Memory-augmented neural networks are a recent improvement on artificial neural networks (ANNs) that allow them to solve complex sequential tasks requiring long-term memory (Sukhbaatar et al. 2015; Graves et al. 2016; Graves, Wayne, and Danihelka 2014). Here we are particularly interested in Neural Turing Machines (NTM) (Graves, Wayne, and Danihelka 2014), which allow a network to use an external memory tape to read and write information during execution. This improvement enables the ANN to be trained in fewer iterations, for certain tasks, and also allows the network to change behaviour on the fly.

However, scaling to large memory sizes and sequence length is still challenging. Additionally, current algorithms have difficulties *extrapolating* information learned on smaller problem sizes to larger once, thereby bootstrapping from it. For example, in the copy tasks introduced by Graves et al. (2014) the goal is to store and later recall a sequence of bit vectors of a specific size. It would be desirable that a network trained on a certain bit vector size (e.g. 8 bits) would be able to scale to larger bit vector sizes without further training. However, current machine learning approaches often cannot transfer such knowledge.

Recently, Greve et al. (2016a) introduced an *evolvable* version of the NTM (ENTM), which did not rely on differen-

tiability and offered some unique advantages. First, in addition to the networks weights, the optimal neural architecture can be learned at the same time. Second, a hard memory attention mechanism is directly supported and the complete memory does not need to be accessed each time step. Third, a growing and theoretically infinite memory is now possible. Additionally, in contrast to the original NTM, the network was able to perfectly scale to very long sequence lengths. However, because it employed the direct genetic encoding NEAT, which means that every parameter of the network is described separately in its genotype, the approach had problems scaling to copy tasks with vectors of more than 8 bits.

To overcome these challenges, in this paper we combine the ENTM with the indirect Hypercube-based NeuroEvolution of Augmenting Topologies (HyperNEAT) encoding (Stanley, D'Ambrosio, and Gauci 2009). HyperNEAT provided a new perspective on evolving ANNs by showing that the pattern of weights across the connectivity of an ANN can be generated as a function of its geometry. HyperNEAT employs an indirect encoding called compositional pattern producing networks (CPPNs), which can compactly encode patterns with regularities such as symmetry, repetition, and repetition with variation (Stanley 2007). HyperNEAT exposed the fact that neuroevolution benefits from neurons that exist at locations within the space of the brain and that by placing neurons at locations, evolution can exploit topography (as opposed to just topology), which makes it possible to correlate the geometry of sensors with the geometry of the brain. While lacking in many ANNs, such geometry is a critical facet of natural brains (Sporns 2002). This insight allowed large ANNs with regularities in connectivity to evolve for high-dimensional problems.

In the new approach introduced in this paper, called *HyperENTM*, an evolved neural network generates the weights of a main model, *including how it connects to the external memory component*. Because HyperNEAT can learn the geometry of how the network should be connected to the external memory, it is possible to train a CPPN on a small bit vector sizes and then scale to larger bit vector sizes *without further training*.

While the task in this paper is simple it shows – for the first time – that access to an external memory can be indirectly encoded, an insight that could directly benefit indirectly encoded HyperNetworks training through gradient descent (Ha, Dai, and Le 2016) and could be applied to more complex problem by employing recent advances in Evolutionary Strategies (Salimans et al. 2017).

Backgorund

This section reviews NEAT, HyperNEAT, and Evolvable Neural Turing Machines, which are foundational to the approach introduced in this paper.

Neuroevolution of Augmenting Topologies

The HyperNEAT method that enables learning from geometry in this paper is an extension of the original NEAT algorithm that evolves ANNs through a *direct* encoding (Stanley and Miikkulainen 2002; Stanley and Miikkulainen 2004). It starts with a population of simple neural networks and then *complexifies* them over generations by adding new nodes and connections through mutation. By evolving networks in this way, the topology of the network does not need to be known a priori; NEAT searches through increasingly complex networks to find a suitable level of complexity.

The important feature of NEAT for the purpose of this paper is that it evolves *both* the topology and weights of a network. Because it starts simply and gradually adds complexity, it tends to find a solution network close to the minimal necessary size. The next section reviews the HyperNEAT extension to NEAT that is itself extended in this paper.

HyperNEAT

In direct encodings like NEAT, each part of the solution's representation maps to a single piece of structure in the final solution (Floreano, Dürr, and Mattiussi 2008). The significant disadvantage of this approach is that even when different parts of the solution are similar, they must be encoded and therefore discovered separately. Thus this paper employs an *indirect* encoding instead, which means that the description of the solution is compressed such that information can be reused. Indirect encodings are powerful because they allow solutions to be represented as a pattern of parameters, rather than requiring each parameter to be represented individually (Bongard 2002; Gauci and Stanley 2010; Hornby and Pollack 2002; Stanley and Miikkulainen 2003). HyperNEAT, reviewed in this section, is an indirect encoding extension of NEAT that is proven in a number of challenging domains that require discovering regularities (Clune et al. 2009; Gauci and Stanley 2010; Stanley, D'Ambrosio, and Gauci 2009). For a full description of HyperNEAT see (Gauci and Stanley 2010).

In HyperNEAT, NEAT is altered to evolve an indirect encoding called *compositional pattern producing networks* (CPPNs (Stanley 2007)) *instead* of ANNs. CPPNs, which are also networks, are designed to encode *compositions of functions*, wherein each function in the composition loosely corresponds to a useful regularity.

The appeal of this encoding is that it allows spatial patterns to be represented as networks of simple functions (i.e. CPPNs), which means that NEAT can evolve CPPNs just like ANNs. CPPNs are similar to ANNs, but they rely on



Figure 1: Hypercube-based Geometric Connectivity Pattern Interpretation. A collection nodes, called the *substrate*, is assigned coordinates that range from -1 to 1 in all dimensions. (1) Every potential connection in the substrate is queried to determine its presence and weight; the dark directed lines in the substrate depicted in the figure represent a sample of connections that are queried. (2) Internally, the CPPN (which is evolved) is a graph that determines which activation functions are connected. As in an ANN, the connections are weighted such that the output of a function is multiplied by the weight of its outgoing connection. For each query, the CPPN takes as input the positions of the two endpoints and (3) outputs the weight of the connection between them. Thus, CPPNs can produce regular patterns of connections in space.

more than one activation function (each representing a common regularity) and are an abstraction of biological development rather than of brains. The indirect CPPN encoding can compactly encode patterns with regularities such as symmetry, repetition, and repetition with variation (Stanley 2007). For example, simply by including a Gaussian function, which is symmetric, the output pattern can become symmetric. A periodic function such as sine creates segmentation through repetition. Most importantly, repetition with variation (e.g. such as the fingers of the human hand) is easily discovered by combining regular coordinate frames (e.g. sine and Gaussian) with irregular ones (e.g. the asymmetric x-axis). The potential for CPPNs to represent patterns with motifs reminiscent of patterns in natural organisms has been demonstrated in several studies (Secretan et al. 2008; Stanley 2007).

The main idea in HyperNEAT is that CPPNs can naturally encode *connectivity patterns* (Gauci and Stanley 2010; Stanley, D'Ambrosio, and Gauci 2009). That way, NEAT can evolve CPPNs that represent large-scale ANNs with their own symmetries and regularities.

Formally, CPPNs are *functions* of geometry (i.e. locations in space) that output connectivity patterns whose nodes are situated in n dimensions, where n is the number of dimensions in a Cartesian space. Consider a CPPN that takes four inputs labeled x_1, y_1, x_2 , and y_2 ; this point in fourdimensional space *also* denotes the connection between the two-dimensional points (x_1, y_1) and (x_2, y_2) , and the output of the CPPN for that input thereby represents the weight of that connection (Figure 1). By querying every possible connection among a pre-chosen set of points in this manner, a CPPN can produce an ANN, wherein each queried point is a neuron position. Because the connections are produced by a function of their endpoints, the final structure is produced with *knowledge* of its geometry.

In HyperNEAT, the experimenter defines both the location and role (i.e. hidden, input, or output) of each such node. As a rule of thumb, nodes are placed on the substrate to reflect the geometry of the task (Clune et al. 2009; Stanley, D'Ambrosio, and Gauci 2009). That way, the connectivity of the substrate is a function of the task structure. How to integrate this setup with an ANN that has an external memory component is an open question, which this paper tries to address.

Evolvable Neural Turing Machines (ENTM)

Based on the principles behind the NTM, the recently introduced ENTM uses NEAT to learn the topology and weights of the ANN controller (Greve, Jacobsen, and Risi 2016a). That way the topology of the network does not have to be defined a priori (as is the case in the original NTM setup) and the network can grow in response to the complexity of the task. As demonstrated by Greve et al., the ENTM often finds compact network topologies to solve a particular task, thereby avoiding searching through unnecessarily high-dimensional spaces. Additionally, the ENTM was able to solve a complex continual learning problem (Lüders et al. 2017). Because the network does not have to be differentiable, it can use hard attention and shift mechanisms, allowing it to generalize perfectly to longer sequences in a copy task. Additionally, a dynamic, theoretically unlimited tape size is now possible.

The ENTM has a single combined read/write head. The network emits a write vector w of size M, a write interpolation control input i, a content jump control input j, and three shift control inputs s_l , s_0 , and s_r (left shift, no shift, right shift). The size of the write vector M determines the size of each memory location on the tape. The write interpolation component allows blending between the write vector and the current tape values at the write position, where $M_h(t)$ is the content of the tape at the current head location h, at time step t, i_t is the write interpolation, and w_t is the write vector, all at time step t: $M_h(t) = M_h(t-1) \cdot (1-i_t) + w_t \cdot i_t$.

The content jump determines if the head should be moved to the location in memory that most closely resembles the write vector. A content jump is performed if the value of the control input exceeds 0.5. The similarity between write vector w and memory vector m is determined by: $s(w,m) = \frac{\sum_{i=1}^{M} |w_i - m_i|}{M}$. At each time step t, the following actions are performed in order: (1) Record the write vector w_t to the current head position h, interpolated with the existing content according to the write interpolation i_t . (2) If the content jump control input j_t is greater than 0.5, move the head to location on the tape most similar to the write vector w_t . (3) Shift the head one position left or right on the tape, or stay at the current location, according to the shift control inputs s_l , s_0 , and s_r . (4) Read and return the tape values at the new head position.

Approach: Hyper Neural Turing Machines (HyperENTM)

In the HyperENTM the CPPN does not only determine the connections between the task related ANN inputs and outputs but also how the information coming from the memory is integrated into the network and how information is written back to memory. Because HyperNEAT can learn the geometry of a task it should be able to learn the *geometric pattern* in the information written to and read from memory.

The following section details the HyperENTM approach on the copy task, which was first introduced by (Graves, Wayne, and Danihelka 2014). In the copy task the network is asked to store and later recall a sequence of bit vectors. At the start of the task the network receives a special input, which denotes the start of the input phase. Afterwards, the network receives the sequence of bit-vectors, one at a time. Once the sequence has been fully passed to the network it receives another special input, signaling the end of the input phase and the start of the output phase. For any subsequent time steps the network does not receive any input.

In summary, the network has the following inputs: *Start:* An input that is activated when the storing of numbers should begin. *Switch:* An input that is activated when the storing should stop and the network must start recalling the bit vectors instead. *Bit-vector input:* Before the switch input has been activated this input range is activated with the bits that are to be recited later. *Memory read input:* The memory vector that the TM read in the previous time step.

And following outputs: *Bit-vector output:* The bit vector that the network outputs to the environment. During the input phase this output is ignored. *Memory write output:* The memory vector that should be written to memory. *TM controls:* TM specific control outputs. Jump, interpolation, and three shift controls (left, stay, and right).

Copy Task Substrate

The substrate for the copy task is shown in Figure 2. The substrate is designed such that the bit-vector input nodes share x-coordinates with the memory vector write nodes and vice versa with memory vector read nodes and bit-vector output nodes. Furthermore, the switch input shares its x-coordinate with the jump output, thus encouraging the network to jump in memory when it should start reciting. In this paper, the size of the memory vector equals the bit vector size. Furthermore, none of the substrates contain hidden nodes as it has been shown that it is possible to solve even large versions of the problem without any hidden nodes (Greve, Jacobsen, and Risi 2016b).

Following Verbancsics and Stanley (2011), in addition to the CPPN output that determines the weights of each connection, each CPPN has an additional step-function output, called the *link-expression output* (LEO), which determines if a connections should be expressed. Potential connections are queried for each input on layers y = 1 and y = -1to each output on layers y = 1 and y = -1. The number of inputs and outputs on the y = -1 layer (Figure 2b) are scaled dependent on the size of the copy task bit vector. In the shown example the bit-vector size is three. Neurons are



Figure 2: The HyperENTM substrate for the copy task. All inputs are in z = 1 and all outputs in z = -1. Figure (a) shows all nodes in y = 1 which is the start/switch inputs and the tm controls. Notably the x-coordinate is the same for the switch input and the jump control output. Figure (b) shows the nodes in y = -1 which are the bit-vector and memory vector input and outputs. Bit-vector input nodes share x-coordinates with memory vector write nodes, while memory vector read nodes share x-coordinates.

uniformly distributed in the x interval [-1.0, -0.2] for bit vector inputs and memory write vector and in the interval [0.2, 1.0] for the memory read vector and bit vector output.

The CPPN has an additional output that determines the bias values for each nodes in the substrate. These values are determine through node-centric CPPN queries (i.e. both source and target neuron positions xyz are set to the location of the node whose bias should be determined).

Experiments

A total of three different approaches are evaluated on bitsizes of 1, 3, 5, and 9. **HyperNEAT** is compared to the direct **NEAT** encoding, and a **Seeded HyperNEAT** treatment that starts evolution with a CPPN seed that encourages locality on both the x- and y-coordinates (Figure 7a). A similar locality seed has been shown useful in HyperNEAT to encourage the evolution of modular networks (Verbancsics and Stanley 2011). This locality seed is then later adjusted by evolution (e.g. adding/removing nodes and connections and changing their weights).

The fitness function in this paper follows the one in the original ENTM paper (Greve, Jacobsen, and Risi 2016a). During training the network is given a sequence of random bit vectors, between 1 and 10 vectors long, and asked to recite it. The network is tasked to do this with 50 random sequences and assigned a normalized fitness. The network is evaluation the bit-vectors recited by the network are compared to those given to it during the input phase; for every bit-vector the network is given a score based on how close the output from the network corresponding to a specific bit was to the target. If the bit was within 0.25 of the target, the network is awarded a fitness of the difference between the actual output and the target output. Otherwise, the network is not awarded for that specific bit: $f = 1 - \frac{|x-x_t|}{0.25}$ if $|x-x_t| < 0.2$ and 0 otherwise. The fitness for any given bitvector is equal to the the sum of the fitness for each individual bit, normalized to the length of the bit-vector. Similarly,

the fitness for a complete sequence is the sum of the fitness for each bit-vector normalized to the length of the sequence. This results in a fitness score between 0 and 1. This fitness function rewards the network for gradually getting closer to the solution, but it does not actively reward the network for using the memory to store the inputs.

Experimental Parameters

For the NEAT experiments, offspring generation proportions are 50% sexual (crossover) and 50% asexual (mutation). Following (Lüders et al. 2017), we use 98.8% synapse weight mutation probability, 9% synapse addition probability, and 5% synapse removal probability. Node addition probability is set to 0.05%. The NEAT implementation SharpNEAT uses a complexity regulation strategy for the evolutionary process, which has proven to be quite impactful on our results. A threshold defines how complex the networks in the population can be (here defined as the number of genes in the genome and set to 10 in our experiments), before the algorithm switches to a simplifying phase, where it gradually reduces complexity.

For the HyperNEAT experiments the following parameters are used. Elitism proportion is 2%. Offspring generation proportions are 50% sexual (crossover) and 50% asexual (mutation). CPPN connection weights have a 98.8% probability of being changed, a 1% change of connection addition, and 0.1% change of node addition and node deletion. The activation functions available to new neurons in the CPPN are Linear, Gaussian, Sigmoid, and Sine, each with a 25% probability of being added. Both NEAT and HyperNEAT experiments run with a population size of 500 for a maximum of 10,000 generations or until a solution is found. The code is available from: https://github.com/kalanzai/ ENTM_CSharpPort.



Figure 3: Mean champion fitness for the different treatments and bit-sizes, averaged over 20 independent evolutionary runs.

Results

Figure 3 shows the mean champion fitness over 10,000 generations for each of the different approaches and bit vector sizes. While NEAT performs best on smaller bit vectors, as the size of the vector grows to 9 bits, the seeded HyperNEAT variant outperforms both NEAT and HyperNEAT. The numbers of solutions found (i.e. networks that reach a training score ≥ 0.999) in regards to the bit vector size are shown in Figure 4. For bit size 1 all approaches solve the problem equally well. However, as the size of the bit vector is increased the configurations using HyperNEAT and locality seed performs best and the only method that is able to find any solution for size 9.

Testing Performance. To determine how well the champions from the last generation generalize, they were tested on 100 random bit-vector sequences of a random lengths between 1 and 10 (Figure 5). On sizes 1 and 5 there is no statistical difference between either treatment (following a two-tailed Mann-Whitney U test). On size 3, NEAT performs significantly better than the seeded HyperNEAT (p < .00001). Finally, seeded HyperNEAT performs significantly better than NEAT on size 9 (p < .00001). The main conclusions are that (1) while NEAT performs best on smaller bit vectors it degrades rapidly with increased bit sizes, and (2) the seeded HyperNEAT variant is able to scale to larger sizes while maintaining performance better.

Generalizing to longer sequences. We also tested how many of the solutions, which were trained on bit sequences of length 10, generalize to sequences of length 100. The training and generalisation results are summarized in Ta-



Figure 4: The number of solutions found by each configuration for the four different bit vector sizes.



Figure 5: The mean performance of the champion networks from the last generation. NEAT does well on smaller sizes, but degenerates quickly as the size goes up.

ble 1, which shows the number of solutions for each of the three approaches, how many of those solutions generalized to sequences of length 100, and the average number of generations it took to find a solution. For all three methods, most solutions generalize perfectly to sequences that are longer than the sequences encountered during training.

Transfer Learning

To test the scalability of the Seeded HyperNEAT solutions, champion genomes from runs which found a solution for a given size were used as a seed for evolutionary runs of higher sizes. The specific runs and which seeds were used can be seen in Table 2, which also contains the number of solutions found, how many solutions generalized, and the average number of generations needed to find the solutions. Seeds denoted $X \rightarrow Y$ refer to champion genomes from a run of size Y which was seeded with a champion from a run of size X.

Because the number of solutions found varied between the different sizes (see Table 1), the scaling experiments were not run exactly 20 times. Instead, the number of runs was

Table 1: Generalisation Results. Shown are the number of solutions, the number of solutions that generalize, together with the average number of generations it took to find a solution and standard deviation.

	Size	#sol.	#gen	gens.	sd.
Seeded	1	20	20	1055.8	1147.4
HyperNEAT	3	5	5	4454.8	3395.8
	5	6	5	2695.5	2666.5
	9	8	5	1523.25	2004.1
HyperNEAT	1	20	20	1481.45	1670.8
	3	2	2	4395.5	388.2
	5	0	0	N/A	N/A
	9	0	0	N/A	N/A
NEAT	1	20	19	281	336.3
	3	19	19	2140.5	1594.4
	5	12	11	3213.4	2254.2
	9	0	0	N/A	N/A

Table 2: HyperNEAT Transfer Learning

Seed	Size	#sol	#general	gens.	sd.
3	5	12/20	6	434.1	574.6
3	9	16/20	2	1150.3	2935.9
5	9	23/24	11	58.9	129.2
$3 \rightarrow 5$	9	23/24	8	588	1992
5	17	18/20	12	258.9	301.3
9	17	24/24	12	89.3	235.9
$5 \rightarrow 9$	17	20/20	17	36.25	47.5
9	33	23/24	17	94	217
9→17	33	24/24	19	456.5	2002.4

the smallest number above or equal to 20 which allowed for each champion to be seeded an equal number of times, e.g. if there were 6 solutions 24 runs were made; 4 runs with the champion from each solution. Figure 6 shows a comparison of HyperNEAT seeded with the locality seed and seeded with champion genomes of smaller sizes on the size 9 problem. HyperNEAT yielded significantly better results when seeded with size 5 and $3\rightarrow$ 5 champions compared to starting with the locality seed (p < .001), but not when seeded with the champion from size 3.

Scaling without further training

The champions from runs which found a solution were tested for scaling to larger bit-vector sizes without further evolutionary training (i.e. new input and output nodes are created and queried by the CPPN; see copy task substrate section for details). Each genome was tested on 50 sequences of 100 random bit-vectors of size 1,000. Some of the champions found using only the LEO size 9 configuration scaled perfectly to a bit-size of 1,000 without further training, as seen in Table 3.

The main results is that it is possible to find CPPN that perfectly scale to any size. The fact that evolution with HyperNEAT performs significantly better, when seeded with a champion genome which solved a smaller size of the problem, together with the fact that evolution sometimes finds



Figure 6: Comparison of the size 9 problem with normal locality seed and with champion seeds from a smaller size.

Table 3: Scaling using LEO without further evolution

9 8 2	00	# which scaled to 100	# of champions	Size
		2	8	9
$9 \rightarrow 17$ 24 $7'$		7†	24	$9 \rightarrow 17$

[†] 6 of these can be traced back to the 2 champions from size 9 which scaled perfectly.

solutions which scale without further training, demonstrates that HyperNEAT can be used to scale the dimensionality of the bit-vector in the copy task domain.

Solution Example

Here we take a closer look at one of the champion genomes (trained on bit-vector size 9), which was able to scale perfectly to the size 1000 problem (Table 3). Figure 7 shows a visualization of the champion genome, as well as the locality seed from which it was evolved. The champion genome does resemble the seed but also evolved several additional connections that are necessary to solve the problem.

Figure 8 shows two different ANNs generated by the the same CPPN, which is shown in Figure 7b. It can be seen that for non-bias connections to be expressed, the source and destination nodes have to be located in the same position on both the x position and y layer in the substrate. These results suggest that the locality encouraging seed works as intended.

To further demonstrate the scalability of this evolved CPPN, memory usage for size 9 and 17 are shown in Figure 9. The output of the networks is shown at the top, followed by the input to the network. Next follows the difference between the given input and the output, i.e. how well the network recited the sequence given to it. The fourth section of the recording shows a heat map of the fitness score based on the bit-vector in that position, where red indicates a high fitness while blue indicates a low fitness.

Next follows the output from the network to the TM controller, followed by the *interpolation* output, and what was written to the memory tape. Finally, the recording shows the *jump* output from the network, the three different *shift* outputs, what read from the tape, and the position of the read/write head. As the recording shows, the network which



Figure 7: (a) The CPPN seed that is used to promote locality on the x and y axes. (b) A champion trained on the size 9 problem, which was able to scale without further evolution to size 1,000. Blue connections have a positive weight, while red connections have a negative weight.

solves the problem jumps exactly once when the *switch* input neuron is activated.

Conclusion

This paper showed that the indirect encoding HyperNEAT makes it feasible to train ENTMs with large memory vectors for a simple copy task, which would otherwise be infeasible to train with an direct encoding such as NEAT. Furthermore, starting with a CPPN seed that encouraged locality, it was possible to train solutions to the copy task that perfectly scale with the size of the bit vectors which should be memorized, without any further training. Lastly, we demonstrated that even solutions which do not scale perfectly can be used to shorten the number of generations needed to evolve a solution for bit-vectors of larger sizes. In the future it will be interesting to apply the approach to more complex domains, in which the geometry of the connectivity pattern to discover is more complex. Additionally, combining the presented approach with recent advances in Evolutionary Strategies (Salimans et al. 2017), which have been shown to allow evolution to scale to problems with extremely highdimensionality is a promising next step.

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Figure 8: Networks produced by the champion CPPN (Figure 7b) for bit sizes 3 (a) and 17 (b).

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Figure 9: Recordings of the activities for bit-sizes 9 (a) and 17 (b) networks. Both networks are produced by the same CPPN. See main text for details.

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