### Memorize or generalize?
### Searching for a compositional RNN in a haystack

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**Abstract**

Neural networks are very powerful learning systems, but they do not readily generalize from one task to the other. This is partly due to the fact that they do not learn in a compositional way, that is, by discovering skills that are shared by different tasks, and recombining them to solve new problems. In this paper, we explore the compositional generalization capabilities of recurrent neural networks (RNNs). We first propose the *lookup table composition* domain as a simple setup to test compositional behaviour and show that it is theoretically possible for a standard RNN to learn to behave compositionally in this domain when trained with standard gradient descent and provided with additional supervision. We then remove this additional supervision and perform a search over a large number of model initializations to investigate the proportion of RNNs that can still converge to a compositional solution. We discover that a small but non-negligible proportion of RNNs do reach partial compositional solutions even without special architectural constraints. This suggests that a combination of gradient descent and evolutionary strategies directly favouring the minority models that developed more compositional approaches might suffice to lead standard RNNs towards compositional solutions.

1. **Introduction**

The last few years have seen the re-emergence of neural networks as incredibly effective all-purpose learning systems (LeCun et al., 2015). However, neural networks still need to be specialized to specific tasks, with little or no cross-task transfer, and they require huge amounts of training data to perform well (Lake et al., 2017). One reason for these limitations is that they are not able to perform compositional learning, that is, to discover and store skills that are common across problems, and to re-combine them in a hierarchical fashion to solve new challenges (Schmidhuber, 1990). The ability to perform compositional learning would provide better generalization and therefore result in a reduction of sample complexity of learning algorithms. Further down the road, compositional methods might be key ingredients in the formulation of full-fledged, general-purpose lifelong learning systems.

In stark contrast to neural networks, compositional abilities – as it is generally agreed – are a core aspect of human cognition (Minsky, 1986; Fodor & Pylyshyn, 1988; Fodor & Lepore, 2002; Lake et al., 2017). Direct evidence for the claim that humans are compositional learners was provided by Schulz et al. (2016), who explored human intuitions about functions through extrapolation and completion experiments, and concluded that these intuitions are best described as compositional.\textsuperscript{1} Strikingly, Piantadosi & Aslin (2016) have shown that 3.5-4.5 year olds generalize function composition above chance even when they have not been trained on the composition process itself.

In view of the clear advantages of compositional learning, there has been a growing interest in equipping neural networks with compositional abilities (the literature is partly reviewed in Section 5). As opposed to that line of research, in this paper we explore the compositional generalization capabilities of standard recurrent neural networks (RNNs, Elman, 1990) without any special architectural constraints.

We first introduce the *lookup table composition* domain as a simple and highly flexible setup to test compositional behaviour (Sections 2 and 3). We then analytically sketch how an RNN can represent and compose functions, and demonstrate that it can learn this behaviour if explicit supervision is provided on its hidden layer (Section 4.1). Finally, we attempt to let RNNs discover a compositional solution to our

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\textsuperscript{1}Specifically, the authors show that participants “prefer compositional over non-compositional function extrapolations, that samples from the human prior over functions are best described by a compositional model, and that people perceive compositional functions as more predictable than their non-compositional but otherwise similar counterparts.” (Schulz et al., 2016)
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sets of tasks via standard example-driven gradient-descent-based training (Section 4.2) and examine what proportion of the trained models do discover such a solution.

While an average training run does not converge to a RNN that behaves compositionally, in a large random search over initializations a (partially) compositional solution is discovered in a small but non-negligible number of cases. Interestingly, convergence to a compositional solution was not determined by the initialization of the model, but rather by seemingly minor random factors such as order of task presentations and weight updates. All in all, our results suggest that a combination of gradient descent and evolutionary strategies directly favouring the minority models that developed more compositional approaches might lead to inducing compositional RNNs without special architectural constraints.

2. Composing table lookup functions

The ability to discover and apply function composition is a natural starting point to test the compositional skills of a learning system. Mastering function composition increases the expressivity of a system: It is only through function composition that a system could handle recursion, allowing it to process an infinite number of objects through finite means. This “combinatorial infinity” property can be observed in language (e.g., in the power to construct sentences of unbounded length by multiple clause embedding, Hauser et al., 2002) and other cognitive domains (e.g., planning or mathematical reasoning).

Since our focus is on composition itself, rather than on the ability of the learning system to solve sophisticated primitive tasks, we consider a set of tasks that only require rote memorization, namely the table lookup tasks. For all possible bit strings of a fixed length, a table lookup function is an arbitrary bijective mapping of the string set onto itself. For example, there are 8 possible 3 bit strings, and consequently 8! = 40,320 distinct mapping tables, as each possible permutation of the string set corresponds to one distinct output assignment (see for example mapping tables $g$ and $c$ in Table 1).

As the table lookup functions share domain and co-domain, the output of any function is a well-formed input for any other function, and thus we can generate an infinite number of new functions by composition. For example, if $g(000) = 110$, $g(010) = 001$, $c(001) = 000$ and $c(010) = 101$, we can apply function compositions such as $cg(000) = 101$, $gg(000) = 001$, $cgc(001) = 101$, and so forth.

In an attempt to make the presence of composition more explicit, we require our models to produce, as output of a composed table lookup, the output of the intermediate steps as well.\(^2\) This is illustrated for compositions of two 3-bit string tables in Table 1.

An important advantage of the table lookup tasks is the clear separation of atomic and composed tasks, which allows for a straightforward evaluation of compositional behaviour on part of the learning system. Let us consider a learning system that has mastered the mappings $g$ and $c$ and has been presented with several input-output pairs of the composed function $cg$. If it behaves compositionally and if it understands that the mapping $cg$ is a composition of the two underlying mappings $g$ and $c$, it should have no trouble in producing the correct output for unseen inputs of this composed mapping, i.e., it should be able to perform zero-shot generalization.

3. Compositional table lookups as sequence-to-sequence learning

We approach the lookup table tasks from the perspective of character-level sequence-to-sequence learning (Sutskever et al., 2014). Figure 1a shows an example of a single episode in which the network reads the input «NCg:001.», which represents the atomic task $g(001)$. The network starts producing the output, «110.», as soon as the dot character signals the end of the input string. The output is considered correct if the output string consists of the correct outcome of function application specified on input, and if the output string is terminated with a dot. Similarly, Figure 1b shows a sample episode of function composition $cg(001)$.\(^3\) The

\(^2\) Results are however stable if, instead, we only request models to produce the final output.

\(^3\) Note that we present the function codes in order of application to the network. In this example, «gc» requires applying lookup $g$ before $c$. 

| Atomic $g$ | Atomic $c$ |
|----------------|----------------|
| 000 → 010 | 000 → 100 |
| 001 → 110 | 001 → 000 |
| 010 → 001 | 010 → 101 |

Table 1. Examples of two atomic 3-bit lookup tasks $g$ and $c$ and their composition $cg$. Note that the output of the composition includes the output of the intermediate step (in this case, of applying function $g$).
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The model used in the experiments is a neural network with two hidden layers: a recurrent LSTM (Hochreiter & Schmidhuber, 1997) layer with 60 units (restricted to 29 units for the experiment in Section 4.1) and a sigmoid layer with 10 units (Figure 2). The input layer of the model consists of concatenated one-hot vector encodings of the input character (or a space « » when the whole prompt has been read) and the output character of the previous step. This architecture is motivated by the compositional solution we propose in Section 4.1 below. The input vocabulary of the network consists of characters «P», «N», «C» specifying the type of task (atomic or composed), lookup table codes «a», «b» through «h», bits «0» and «1», punctuation marks «:» and «.», and space « ». The output layer is a softmax layer with three units for the three possible output characters «0», «1», and «.». At each step the output character with the highest score is selected.

The model and training were implemented in PyTorch. The Adam algorithm (Kingma & Ba, 2014) was used for optimization. Other details of the training procedures are described separately for the two experiments in sections 4.1 and 4.2 below.

4. Experiments

4.1. Experiment 1: Can an RNN encode a compositional solution through a finite-state automaton?

In the first experiment, we tested whether there exist such weights of a character-level RNN that give place to a model demonstrating compositional behaviour. If this were the case, it would show that in principle a RNN of the described architecture can achieve strong generalization capabilities and produce correct outputs for unseen inputs of known composed functions.

If we limit ourselves to a specific maximum number of lookup tables of finite length bit strings and a maximum number of possible composition steps, a simple approach to model lookup table compositions is through finite-state automata (FSA). Instead of producing the weights directly by hand, we designed an encoding scheme for the recurrent layer that represents the state of such an automaton and we directly supervised the output of this layer to conform to this scheme. Once this encoding scheme has been learned, we proceeded to training the mapping from state representations to output characters.

The state of the FSA solving lookup table compositions needs to encode the following pieces of information: a (finite) stack of atomic tasks to perform, the input bit string for the current task, an index into the output string, and the bits produced so far for the current task (as they form the input string of the following task). Such state information can be represented by the recurrent layer in the form of a binary code. Specifically in our case, the units of the hidden layer are divided into the following segments (Figure 2):

- segment A (8 units) encodes the current atomic task (out of 8) using one-hot encoding,
- segment B (8 units) encodes the following atomic task (if any) using one-hot encoding; segments A and B represent the "call" stack,
- segment C (6 units) encodes the input bit string using three one-hot vectors of size 2 units,
- segment D (3 units) represents an index into the output string, i.e., it encodes which bit (index) of the output string should be output (none, first, second, or third),
- segment E (4 units) stores the characters output on previous steps of the current mapping task (two one-hot vectors, each of size 2).

This encoding consists of a total of 29 units. Note that the hidden layer only records the information provided by the input string and does not encode the actual characters to output; in particular, it does not remember the lookup tables, as this is left to a separate sigmoid unit layer and to the output layer. The units of the sigmoid layer have non-zero weights only on connections from segments A (task), C (input), and D (output index), as these are the only segments directly affecting which character should be output at each step.

As an example, let us consider the input «PCgc:001.». All units of the recurrent layer output values of approximately zero at the beginning of the episode. As the network reads the input, appropriate units change their output from zero to values close to one. Specifically, after reading the third character «g», the seventh unit of segment A starts to output value 1, as g is the first mapping to be performed. After reading the next character, «c», the third unit of segment B activates, since the second mapping to perform is c. Next, the input string is encoded in segment C. Finally, as the network reads the dot character, the first unit of segment D activates, signaling that the network should produce the first output bit of the first mapping g(001). On the next step, this first output bit is “stored” in segment E and the second
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Figure 1. Compositional table lookups as sequence-to-sequence learning (refer to Table 1 for the lookup tables).

Figure 2. Model architecture. The LSTM layer is further subdivided into 5 segments in Experiment 1; see Section 4.1 for further details on the segments.

Training and evaluation The weights of this network are trained in two phases, as the encoding scheme needs to be learned prior to the mapping of state representations to output characters. In the first phase, the network learns to set the right transitions between recurrent layer states in the presence of specific input. For this, we generated random pairs of input-output strings of the correct form for both atomic and composed tasks. For each input-output pair (or episode) we furthermore generated a sequence of binary vectors of length 29 representing the target values of the recurrent layer at each time step using the encoding scheme described above. We used these vectors as direct supervision on the output of the recurrent layer (using mean-squared error loss) and trained the weights of input-to-hidden and recurrent connections with stochastic gradient descent and backpropagation through time, updating the weights after each episode for a total of 1,000k training episodes. In the second phase, we proceeded to train the mappings from recurrent layer state representations to output characters (using cross-entropy loss). In this step, we froze the weights of input-to-hidden and recurrent connections and only trained the connections between the recurrent and sigmoid layers and from the sigmoid to the output layer. We generated a random task set consisting of 8 atomic 3-bit tasks. We sampled 1,000k episodes from the atomic tasks, and trained the network using stochastic gradient descent, updating the weights after each episode. Note that there is no need for training on composed tasks as the ability to produce correct output strings for composed tasks should follow automatically once the atomic tasks are learned, thanks to (1) the specific pre-training of recurrent layer transitions in the first phase of training, and (2) the connections between the two hidden layers. The final network was evaluated on all possible inputs to the 8 atomic and the 64 associated composed tasks.

Results The trained network produces correct output across both atomic and composed tasks in 96% of the cases. Note that the network has not seen any composed tasks during training and its generalization capabilities are purely due to the transition logic of the recurrent layer and the connectivity between the two hidden layers. This experimental result confirms that the weight-space of a RNN can implement the specific compositional FSA solution that we sketched above, and can learn it when provided with direct supervision on the structure of the automaton. However, the results do not imply that the devised binary encoding is a natural solution to the problem, nor that a RNN can in practice discover a compositional solution when provided with input/output examples as the only training signal. These questions are pursued in the following section.
4.2. Experiment 2: Search for a compositional RNN over model initializations

To investigate the proportion of RNNs that converge to a compositional solution when training on input/output examples only, we run a large random search over model initializations, train the networks with standard cross-entropy loss and gradient descent on a set of atomic and composed tasks, and then test them on zero-shot compositional generalization, to check if any of the RNNs in the batch discovered a compositional solution, this time without any external guidance.\footnote{We also explored a pure search-based approach where networks are randomly initialized (in the same range specified below) and directly tested without further training. No network of this sort behaves better than chance level.}

**Training** We generated a random task set of 8 atomic 3-bit lookup tasks and the corresponding 64 pairwise compositions. 50k models with the same architecture as in the previous experiment were trained in two phases, at first with episodes drawn from atomic tasks only (1,000k training episodes) and later with tasks sampled across both atomic and composed tasks (further 1,000k episodes). For each composed task, we withheld two input strings that were used for evaluation (see below). Each model was initialized with random weights drawn from a uniform distribution \( U(-0.1, 0.1) \) and with zero biases, and was trained with backpropagation through time. We used the cross-entropy loss and updated the weights after each episode (stochastic gradient descent). The training of each model was performed asynchronously on 40 CPUs in parallel. As shown in Figure 3, by the end of the first phase most of the models mastered all atomic tasks and, by the end of the second, they further mastered all composed tasks when fed seen inputs.

**Evaluation** We evaluate the compositionality of trained models by their zero-shot generalization to withheld inputs on composed tasks. In our case, we test the models on \( 2 \times 64 = 128 \) unseen composed task-input combinations, and report the percentage of correctly answered test items as generalization performance.

**Baselines** We evaluated several random baselines. The simplest one, random-output, produces output strings by randomly sampling from the set of the three possible output characters «0», «1», and «?». As learning the expected form of the output sequence (three bits and a dot character for atomic tasks, six bits and a dot for composed tasks) is relatively easy for a network, we also evaluated baseline random-wellformed-output, which randomly samples six bits and appends the dot for all test items. Lastly, we evaluated baseline random-task-code, which is equivalent to the model employed in the experiment, but whose training

![](image307x549to530x725)

**Figure 3.** Average success rate (percentage of correct outputs in the most recent 100 episodes) during atomic (first 1,000k episodes) and atomic-composed lookup training (second 1,000k episodes). For this figure, we generated five random task sets of 8 atomic and 64 composed tasks, and trained 10 randomly initialized networks on each task set. The success rate shown is averaged across these \( 5 \times 10 \) networks.

input strings for composed tasks (such as «PCcf:010») were altered so that there is no consistent relation between the task codes («CF») and the underlying tasks. This last baseline is meant to capture any kind of statistical biases in the task set (such as shared input-output mapping pairs for a subset of inputs across two lookup tables) that would not be captured by a fully random baseline. Baselines random-output and random-wellformed-output were evaluated 10k times on the test dataset, while baseline random-task-codes was evaluated for 1k trained models.

**Results** Figure 4 shows the overall distribution of the 50k runs in terms of generalization performance. For comparison, Figure 5 shows the baseline random-task-codes generalization performance distribution across 1k runs of models, and Table 2 shows average generalization performance for all baselines. Most runs in Figure 4 show performance well above the baselines, but they are far from successful at generalization. However, we also observe a tail of models that do generalize very well: \( \approx 2\% \) models reach zero-shot accuracy \( > 80\% \), and 0.75% models reach zero-shot accuracy \( > 90\% \), while no baseline model ever achieves performance anywhere close to these levels. We thus conclude that RNNs trained with standard gradient descent methods on a task involving composition can, occasionally, discover a compositional solution that allows them to generalize zero-shot. The chances to randomly stumble upon such a RNN are, however, quite slim.

The first follow-up question we ask is whether the compositional RNNs learned to parse the “language” of the
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Figure 4. Generalization performance of the 50k models trained in the search experiment.

| Generalization performance (%) |
|--------------------------------|
| RNN                            | 19.60     |
| Baselines                      |           |
| - random-output                | 0.00      |
| - random-wellformed-output     | 0.01      |
| - random-task-codes            | 4.56      |

Table 2. Average generalization performance in the random RNN search and for all three baselines.

Figure 5. Generalization performance of the 1K models of baseline random-task-codes.

Figure 6. Distribution of generalization performance of 5k models trained with consistent but shuffled task prompts for composed tasks.

Figure 6 suggests that obfuscating the prompts so that it is no longer possible to identify the atomic tasks involved in a compositional operation (e.g., «db» consistently cues the composition of tasks a and h) does not affect the overall performance curve. Thus, even for the RNNs that converged to a compositional solution, the latter is associated to arbitrary codes that must be memorized, rather than to a decompositional analysis of the prompts.  

Next, we inquire about the importance of the curriculum we used in the main experiment, where we started by teaching the model how to perform atomic lookups, and later added compositional tasks. Figure 7 suggests that, when training on composed tasks only, a larger number of models drop to baseline level on generalization, but on the other hand there is also a considerably larger proportion of models that learn to generalize correctly (5.55% of 7k trained models with zero-shot accuracy > 90%). Together with the previous experiment, this suggests that it is not only the case that successful models fail to relate atomic and composed task codes. They are also most probably failing to exploit their knowledge of atomic tasks when solving composed tasks. Success at zero-shot generalization of models trained solely on composed tasks suggests that the models are inducing their own representation of the atomic lookups while learning the composed tasks, rather than exploiting prompts, and thus interpret, say, the «gc» sequence as an instruction to apply lookup table g followed by lookup table c. This is a stronger form of compositionality, akin to the one we encounter in natural language, where string composition mirrors meaning composition (Montague, 1970). The network did not generalize well to these tasks, which confirms it is not learning to decode prompt structure (data not shown).

8This observation is supported by additional experiments in which the network was trained with a subset of composed tasks and tested on unseen composed tasks. The network did not generalize well to these tasks, which confirms it is not learning to decode prompt structure (data not shown).
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Figure 7. Distribution of generalization performance of 7k models trained with composed tasks only.

Figure 8. Distribution of generalization performance of 1k re-runs with an initialization that originally led to perfect generalization.

Finally, we test whether it is the different initializations and their properties that lead some models to generalize better than others. In Figure 8, we report the distribution of 1k re-runs with one of the most successful initializations in the random search experiment. In Figure 9, we report the same distribution for one of the worst initializations in the original experiment. Surprisingly, the figures suggest that initializations have no effect on the odds to converge to a successful model. Evidently, the determining factor is the (random) order in which tasks are presented and weights updated during training.

5. Related work

The idea of statistical learning systems, and more specifically neural networks capable of skill composition has been around for a long time, particularly in the domain of reinforcement learning, where it is natural to frame higher-level tasks as hierarchical compositions of simpler actions (Schmidhuber, 1990; Sutton et al., 1999; Barto & Mahadevan, 2003; Taylor & Stone, 2009). In this domain, composition almost always consists in temporally concatenating sequences of actions, and thus lacks the recursive properties of proper function composition discussed in Section 2.

As early as Singh (1992), a standard approach to neural-network-based composition has been to structure the network into a set of modules that are trained to solve specific tasks, plus a controller or gating system that learns which module to call at each point in time. The modular approach has recently been greatly extended, and applied to problems, such as visual question answering, that require proper function composition (Andreas et al., 2016; 2017; Hu et al., 2017; Johnson et al., 2017). While the tasks tackled by these models are much more complex than table lookup composition, the models themselves must make strong a priori assumptions about the structure of the controller, the set of modules and how they can be combined. They moreover require direct supervision on the module sequence to be applied, or some degree of hand-coding of module functionality. For these reasons, it is difficult to see how such approaches could scale up to genuine lifelong learning scenarios, where one is faced with an open-ended set of new skills to be acquired.

A very promising recent work (Sahni et al., 2017) focuses on skill composition. In the proposed architecture, separate skill networks produce embeddings that are then (possibly recursively) composed by a differentiable composition function. Still, the system requires separate training of the skill networks and composition function.

Finally, compositional skills of sequence-to-sequence recur-
rent networks have been recently evaluated in the framework of a simple compositional navigation environment, showing that RNNs fail when generalization requires systematic compositional skills (Lake & Baroni, 2017).

### 6. Discussion

We have studied the question of whether a recurrent neural network (RNN) can learn to solve a function composition task compositionally, that is, by storing the constituent functions, and combining them to solve new problems in a zero-shot fashion.

In the specific table-lookup domain we considered, we find that it is theoretically possible for a RNN to learn to behave compositionally in the sense above, at least up to a finite number of compositions. Moreover, a large random search shows that a certain proportion of RNNs converged to a compositional solution as indicated by their successful generalization to unseen inputs of composed tasks that is well above chance levels. These seem, however, to perform a weaker form of composition that does not rely on analyzing the composed task prompts, suggesting that networks represent the latter as single undecomposable units that index specific atomic or composed tasks.

Our results show that initializations, at least in the range explored in our experiments, have very little effect on the final performance of the networks, suggesting instead that seemingly minor random factors such as order of task presentations and weight updates determine whether the path taken by the model is memorization-based or compositional.

In future research, we would like first of all to gain a better understanding of the compositional strategies induced by the best models. One approach to do this is through extracting FSAs from learned RNNs (Giles et al., 1992; Weiss et al., 2017), i.e., the opposite of the FSA-into-RNN process that has been carried out in Section 4.1.

Second, we would like to devise new training regimes leading RNNs to fully compositional solutions in more stable ways. One key insight here is that our current training regime does not explicitly reward zero-shot generalization, which is only evaluated at test time for models that have been trained with standard cross-entropy-based gradient descent on a large number of repetitive examples. Gradient-based techniques are hard to apply to a generalization objective, which cannot be naturally formulated in differentiable terms. Thus, in our following experiments we plan to switch to more flexible evolutionary techniques, using zero-shot generalization on held-out compositions as our fitness criterion. Switching to an evolutionary approach also opens up interesting possibilities in terms of neural network plasticity, and we would like to explore architectures that grow larger during training, as they might encourage more modular structures that in turn should favour compositionality (Soltoggio et al., 2017). At the same time, with the huge power afforded by these methods come more difficulties in making them converge. We informally experimented with the popular NEAT algorithm (Stanley & Miikkulainen, 2002) applied to our lookup tables, but we were not able to get it to solve even the atomic tasks.

Third, future work should take advantage of the full potentials of the table lookup domain. These include testing the generalization to more compositions, working with longer bit strings, and testing the comprehension of the prompt “language” by evaluating on zero-shot compositions instead of zero-shot inputs only. Finally, we would like to explore to what extent results obtained in this domain generalize to other compositional problems (for example, in language).

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