

# EXTENSIONS AND LIMITATIONS OF THE NEURAL GPU

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## ABSTRACT

The Neural GPU is a recent model that can learn algorithms such as multi-digit binary addition and binary multiplication in a way that generalizes to inputs of arbitrary length. We show that there are two simple ways of improving the performance of the Neural GPU: by carefully designing a curriculum, and by increasing model size. The latter requires a memory efficient implementation, as a naive implementation of the Neural GPU is memory intensive. We find that these techniques increase the set of algorithmic problems that can be solved by the Neural GPU: we have been able to learn to perform all the arithmetic operations (and generalize to arbitrarily long numbers) when the arguments are given in the decimal representation (which, surprisingly, has not been possible before). We have also been able to train the Neural GPU to evaluate long arithmetic expressions with multiple operands that require respecting the precedence order of the operands, although these have succeeded only in their binary representation, and not with perfect accuracy.

In addition, we gain insight into the Neural GPU by investigating its failure modes. We find that Neural GPUs that correctly generalize to arbitrarily long numbers still fail to compute the correct answer on highly-symmetric, atypical inputs: for example, a Neural GPU that achieves near-perfect generalization on decimal multiplication of up to 100-digit long numbers can fail on  $000000 \dots 002 \times 000000 \dots 002$  while succeeding at  $2 \times 2$ . These failure modes are reminiscent of adversarial examples.

## 1 INTRODUCTION

Deep Neural Networks (DNNs) are extremely useful for solving difficult pattern recognition tasks for two reasons: first, because they can compactly represent good solutions to difficult pattern recognition tasks; and second, because these good solutions can be found with stochastic gradient descent. It is not immediately obvious that a DNN should have the ability to represent solutions to such problems compactly. This is the case because the depth and width of DNNs allows them to simulate any parallel computer that runs for a modest number of steps, making it possible for the DNN to match the performance of *any* parallelizable statistical ML model by simply simulating it. This is one of the reasons DNNs are successful relative to other ML models.

DNNs are especially useful in the supervised learning setting, where the goal is achieve low test error over a given data distribution. Statistical learning theory (Vapnik, 2013) guarantees that this can be done by minimizing training error, as long as the training data is drawn from the same data distribution and when there is more training cases than parameters.

While the ability to achieve low test error on a specific data distribution is extremely useful in practice and has already enabled a wide range of practical applications, there is evidence that this ability does not fully capture the intuitive notion of pattern recognition. For example, the existence of adversarial examples, which are data cases that are nearly indistinguishable from real data cases that confuse all existing discriminative classifiers, suggests that supervised DNNs are substantially less robust than human pattern recognition. And indeed, we would expect a system that has fully “understood” the relevant visual (say) concepts to not be fooled by adversarial examples. Understanding and fixing this problem is an active area of research.

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Another domain where a mere low error on a specific data distribution seems unsatisfying is the domain of simple algorithms. Simple algorithms have a well-defined output for all conceivable inputs, so if we collect enough of input-output examples from a reasonably-chosen distribution where the outputs are computed by some (unknown) simple algorithm, a sufficiently good learning method ought to be able to infer the “true” algorithm: one that can perfectly generalize to all conceivable inputs, and not just the inputs that tend to occur in the training data distribution.

This problem lies at the core of *program induction*, an old field that has significant past work (Nordin, 1997; Liang et al., 2013; Wineberg & Oppacher, 1994; Solomonoff, 1964; Holland, 1992; Goldberg, 1989; Gomez et al., 2008). More recently, researchers have begun investigating this problem using the deep learning techniques of neural network function approximation and stochastic gradient descent (Graves et al., 2014; Zaremba & Sutskever, 2015; Kaiser & Sutskever, 2015; Kurach et al., 2015; Andrychowicz & Kurach, 2016). All these works have been able to learn algorithms that correctly generalize to inputs of much greater length than the training cases on some problems. The Neural GPU (Kaiser & Sutskever, 2015) is notable among these since it is the only model that has, thus far, been able to learn to correctly multiply integers of length much greater than it has been trained on.

The phenomenon of generalization to inputs that are outside the training distribution is poorly understood. The space of problems for which such generalization is possible has not been identified, and a detailed understanding of the causes of such generalization are missing as well. Given that the test inputs do not come from the training data distribution, we do not yet have a formal reason to believe that such out-of-distribution generalization should succeed.

In this paper, we attempt to better understand this generalization in the context of the Neural GPU. We empirically study the parameters that affect its probability of successfully generalizing to inputs much greater length, and also study its failures. We report three notable findings: first, that larger models can generalize on harder tasks; second, that very detailed curriculum can enable the training of otherwise un-trainable neural networks; and third, those models that achieve perfect generalization on longer test cases when they are drawn from the uniform distribution still fail on highly structured inputs. This suggests that these models fail to learn the “true algorithm” as well as we’ve hoped, and that additional research is required for to learn models that can generalize much better.

The code for this work can be found at <https://github.com/openai/ecprice-neural-gpu>.

## 2 RELATED WORK

The problem of learning algorithms from data has been investigated in the field of program synthesis (Nordin, 1997; Liang et al., 2013; Wineberg & Oppacher, 1994; Solomonoff, 1964) and genetic programming (Holland, 1992; Goldberg, 1989; Gomez et al., 2008). These approaches usually aim to directly produce the source code of an algorithm that solves the problem specified by the training data.

A recent approach to algorithm learning attempts to use the power of neural networks and their learning algorithm. Neural networks are inherently robust, and are capable of dealing with “imprecise” data (such as images or text) that can be difficult to handle in models that directly work with source code. There exist a number of neural network architecture that implement this idea: the Neural Turing Machine (NTM) (Graves et al., 2014), the standard LSTM (to some extent) (Zaremba & Sutskever, 2014), the Grid LSTM (Kalchbrenner et al., 2015), the Stack RNN (Joulin & Mikolov, 2015), the Neural DeQue (Grefenstette et al., 2015), the End-to-End Memory Networks (Sukhbaatar et al., 2015), the Hierarchical Attentive Memory (Andrychowicz & Kurach, 2016), and the Neural random-access machines (Kurach et al., 2015).

For a neural model to be able to learn an algorithm, it is essential that it is capable of running the necessary number of computational steps. Most of the above models have only been successfully used to learn algorithms that require a linear number of computational steps in the size of the input. While some models (Zaremba & Sutskever, 2015; Zaremba et al., 2015; Graves, 2016) can in principle learn the correct runtime for a given algorithm, in practice it has not been possible to learn algorithms requiring superlinear runtime, such as long integer multiplication. The only known

neural model that can solve tasks whose runtime is truly superlinear in the size of the input is the Neural GPU (Kaiser & Sutskever, 2015), which is the model that we investigate further in this paper.

The Grid LSTM (Kalchbrenner et al., 2015) is a powerful architecture that has been used to successfully learn 15-digit decimal addition. This model is similar to the Neural GPU – the main difference is that the Neural GPU is less recurrent. The Neural GPU has been shown to be able to generalize outside its training distribution, and while this has not been shown for the Grid LSTM, we believe that with appropriate modification, it should be capable of such generalization as well.

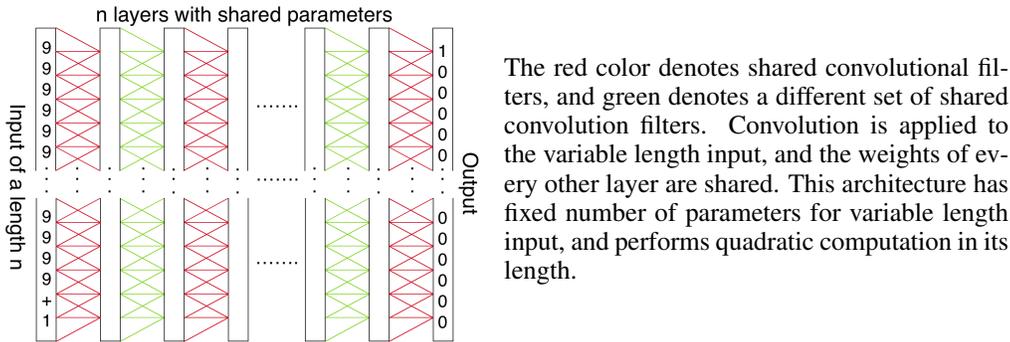


Figure 1: The Neural GPU.

Neural network models that are capable of learning and representing algorithms tend to be extremely deep and have an elaborate architecture, which makes the problem of minimizing their training error to be very challenging for stochastic gradient descent. To reduce the difficulty of the training problem, curriculum learning has been found to be critical. In particular, all the aforementioned models require a curriculum learning (Bengio et al., 2009; Zaremba & Sutskever, 2014) in order to successfully learn sophisticated functions, and the results in this paper are no different.

### 3 MODEL

The Neural GPU is an architecture developed by Kaiser & Sutskever (2015) that can learn algorithms such as binary multi-digit addition and multi-digit multiplication. The main idea of the Neural GPU is to build an architecture capable of performing the necessary computation for the task without being overly deep. By being less deep, the problem of minimizing its training error becomes easier. Tasks that require a super-linear number of computational operations (in the size of the input) cannot be solved by a neural architecture that can only perform a linear number computational operation. Table 1 lists the number of computational operations that can be performed by several different neural network architectures. In our notation, a feed forward network consumes input of a predefined, constant size  $O(1)$ , and performs a fixed number of computation operations (also  $O(1)$ ). Other architectures, such as classical convolution networks, also have a predefined input size ( $O(1)$ ), and process it with a constant  $O(1)$  number of computational operations. However, it is possible to apply the convolution operation to an input of variable size. This approach is sometimes used in object detection, where the same convolutional neural network is applied on images of variable size (Sermanet et al., 2013). Similarly, the recurrent neural network (RNN) is capable of processing inputs of variable length, where the amount of computation performed by the RNN is linear in the length of the sequence.

The Neural GPU architecture is the combination of a convolution on variable size inputs with a recurrent neural network as shown in Fig. 1. The Neural GPU consumes an input of a variable length  $n$ . It repeatedly applies several convolutional layers  $n$  times, where  $n$  is the length of the input; thus, the depth of the model is dependent on the length of the input. It performs  $O(n^2)$  operations for each input of the length  $O(n)$ . This is a desirable property, because now there is a possibility that the model could learn to represent algorithms whose runtime grows superlinearly in the size of the input, such as integer multiplication. Harder problems can require significantly more computational steps. While we could, in principle, unroll our models for an enormous number of

	Feed forward network	Classical CNN	CNN for detection	RNN	Neural Turing Machine	Grid LSTM	Neural GPU
Input Size	$O(1)$	$O(1)$	$O(n)$	$O(n)$	$O(n)$	$O(n)$	$O(n)$
Number of steps	$O(1)$	$O(1)$	$O(n)$	$O(n)$	$O(n)$	$O(n^2)$	$O(n^2)$

Table 1: This table compares the number of computational steps performed by various architectures as a function of their input size. In our notation,  $O(1)$  means that the number of steps (or the size of the input) are constant. In contrast,  $O(f(n))$  means that the input can be of variable length  $n$ , and that the number of steps grows as  $f(n)$  in the size of the input.

timesteps to make them capable of solving even NP-hard problems, it is exceedingly unlikely that gradient learning would succeed training models of such depth.

The architecture most similar to Neural GPU is the Grid LSTM (Kalchbrenner et al., 2015). It has been shown to learn 15 digit long decimal addition task, although it has not yet been shown to generalize to inputs of length greater than the training data.

To successfully train the Neural GPU, Kaiser & Sutskever (2015) used the following techniques:

- The architecture is that of a gated recurrent unit (GRU) through depth (Bahdanau et al., 2014).
- Tanh cutoff: the hyperbolic tangent activations used by the GRU are truncated once they reach a critical upper (and lower) bound. The hope is that this makes the results more “digital”.
- The use of Dropout (Srivastava et al., 2014).
- Instead of using the same weights at every pair of layers, the Neural GPU starts out by cycling through 6 independent sets of weights, which are gradually annealed to become identical as optimization progresses.
- Gradient noise: the original paper notes it as important, but the released code has this option disabled.

In this paper, we use all these techniques and analyze their importance Fig. 2. More details about the meaning of each modification are available in the original work (Kaiser & Sutskever, 2015).

## 4 IMPROVEMENTS TO THE NEURAL GPU

The performance obtained by the Neural GPU is very sensitive to the random seed used to produce the initialization and the order of the training data. For example, when we ran several identical models with different random seeds, we find, similarly to Kaiser & Sutskever (2015), that only a fraction of them generalizes to over 99% cases (where the test cases are of length much greater than the training cases, and the model is considered to have made an error when it mispredicts even one bit of the output vector). Such variability makes it hard to hill-climb in hyperparameter space. We address this problem by running  $\approx 15$  instances of the each model with different seeds on each of our 13 tasks. We measure the fraction of seeds that cause the model to surpass 99% accuracy on the (longer and out of distribution) test data. This fraction provides us with a reliable estimate of the quality of the hyperparameter configuration. Moreover, such measurements had to be done on several problems. Particular “tricks” often are effective just for a single problem, and damage performance on others.

Fig. 2 shows the success rate for a given size and model modification. We find that many model modifications help reduce training error but do not with generalization. Note that most changes to the model increase the success rate by no more than 10%, which is too small to be detected without the thorough experimental framework that we’ve outlined above.

Our experiments in Fig. 2 show that the simplest way to increase performance is to increase the size of the model. The rows of Table 2 consistently show that larger models are more likely to generalize. In contrast, smaller models are often unable to minimize training error. For example, we were not able to achieve 0% training error when models with 128 and 256 filters are trained on decimal multiplication task (left Fig. 3), while the larger models with 512 filters achieve 0% training

# Filters	Training data			Test data		
	24	128	256	24	128	256
Classical Neural GPU	70%	99%	100%	41%	53%	53%
without tanh cutoff	58%	99%		29%	45%	
without dropout	83%	100%		35%	46%	
one independent copy of weights	67%	77%		44%	62%	
with noise on gradients	72%	100%		43%	53%	
with batch-normalization	85%	100%		26%	24%	
with resnet instead of GRU	20%	91%		16%	18%	

Figure 2: Generalization of training error of Neural GPU is highly dependent on initialization seed. Table measures fraction seeds achieved error  $< 1\%$ . Each entry of this matrix involves running experiments with 15 different seeds on 13 different tasks.

error (although they do not generalize to long test inputs since curriculum was not used). It is not self-evident that larger model would generalize better, but the empirical results are clear. We suspect that the over-parameterization of the model makes the optimization task easier.

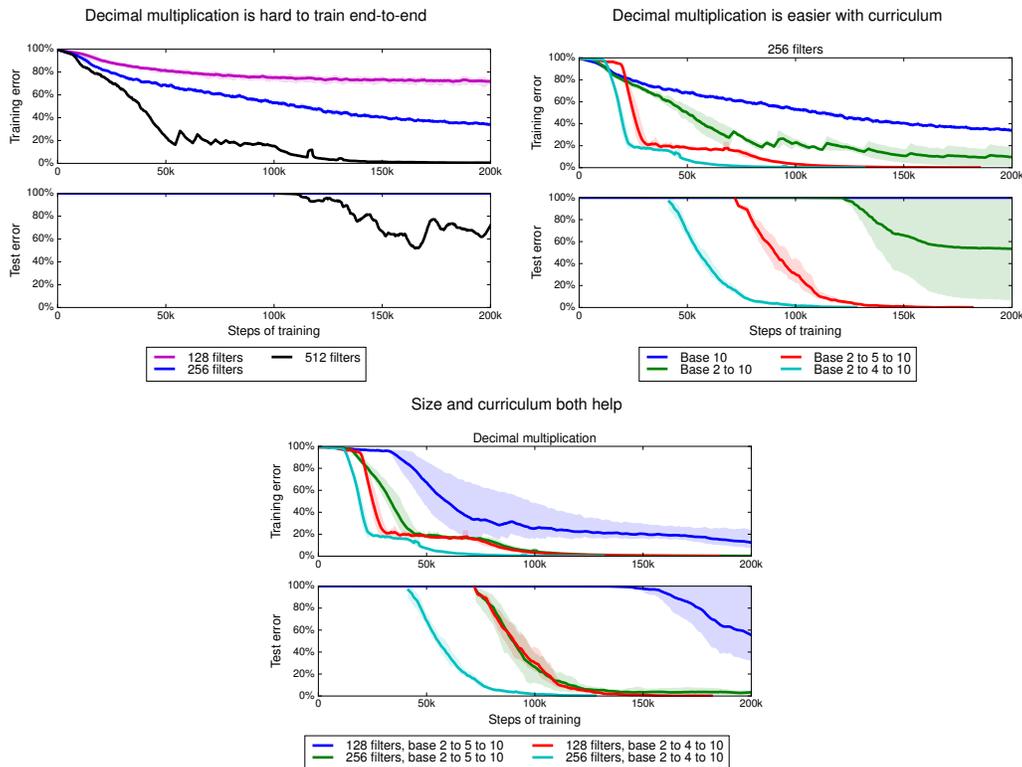


Figure 3: Training (top) and test error (bottom) on the decimal multiplication task. (First) models of different sizes trained without curriculum. Only very large models can successfully optimize the training error, and none are able to generalize. (Second) variable-sized models trained with curriculum over different bases. For instance, we find that a medium-sized model generalizes to much longer test cases on decimal multiplication if it is first trained on binary multiplication and then on quaternary multiplication, before being trained on decimal multiplication. (Third) the best results are achieved when we apply curriculum on models with large numbers of filters. We find that training a model first on binary numbers, then 4-ary, then decimal works significantly better than training it on binary numbers, then 5-ary, then decimal. The difference is comparable to the difference between 128 and 256 filters.

Running models with 512 filters is challenging, because they do not fit into the memory of the GPU on the problems that we have been exploring. In the implementation used for the experiments in this paper, a Neural GPU with 128 filters does not fit into GPU memory (12 GB) due to its large number

of activations. To train larger models, we used several techniques for reducing the model’s memory footprint. First, instead of unrolling the graph, we used TensorFlow’s symbolic `tf.while_loop`, which can store intermediate activations on CPU thanks to the `swap_memory` option (implemented in tensorflow (Abadi, 2015)). Second, we have decreased the batch size, which further lowered the memory footprint. A third way would be to use the methods described by Martens & Sutskever (2012); Gruslys et al. (2016), however we have not experimented with them.

Curriculum \ # filters	128	256	512
10	Fails	Fails	Struggles
2 → 10	Fails	Struggles	Struggles
2 → 5 → 10	Struggles	Works	Works
2 → 4 → 10	Works	Works	Works

Table 2: The table summarizes the setting where the Neural GPU succeeds to learn decimal multiplication. It is essential to use a large model and to use a high-quality curriculum. The curriculum column indicates the base in which training took place; i.e.  $2 \rightarrow 4 \rightarrow 10$  means that we have started training in the binary base, then we moved to quaternary base, and finally to the decimal.

In its current form, the Neural GPU cannot reliably learn to solve hard tasks such as decimal multiplication from examples (although sporadically it does). We find that an elaborate curriculum is necessary in order to learn such problems reliably, and to solve harder tasks. Our curriculum involves starting with short examples first, and solving intermediate task on the way to solve the target task. For instance, a curriculum for decimal multiplication could consist of first learning multiplication in base 2, then base 4, and finally base 10. The second plot in Fig. 3 shows the training and test error for models trained with curriculum. The third plot in Fig. 3 presents results for different curriculum types and model sizes. Table 2 summarizes the success rates for different model sizes, and curriculum.

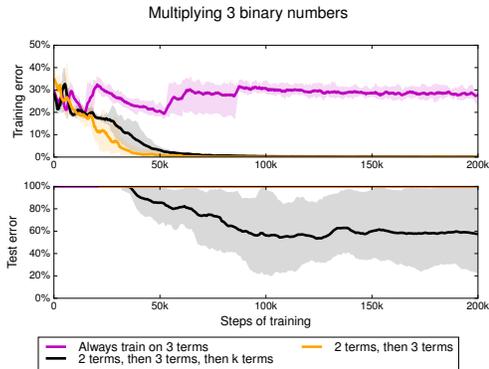


Figure 4: Influence of curriculum on 3-numbers multiplication task.

We have obtained other notable results on the 3-numbers multiplication task (Fig. 4). We were not able to reach perfect error when training on such this task without a curriculum. We found that training on multiplication of 2 numbers and then moving to multiplication of 3 numbers improved performance. However, such model doesn’t generalize. The best performance on the 3-numbers multiplication is achieved when each training instance consists  $l$  numbers, where  $l$  is randomly chosen between 1 and  $\lfloor \frac{n-1}{2} \rfloor$ , where  $n$  is the length of a single number.

Another experiment is to train a model on sequences of arithmetic operations with multiple numbers. We train on expressions of length 41, and test on expressions of length 201. When using the binary representation, our model is able to correctly solve 30% of length-201 expressions, where as always we count success only when the whole number is predicted correctly. For an example of successful generalization, the model successfully evaluated the expression `001110111001/1+10-10*0/1/1*111/10*010+0/010011-10/10101*0+ 010/1*00-110*1*0/1/101000- 00000+ 000-1+ 1-1011111*010-010/0011111011-010-1100-0/0010000*01*0010000+ 0111110+ 00001+10/10*111111111-10*10-1*11111+01` (whose value is `10100001011`). Fig. 5 summarizes this result.

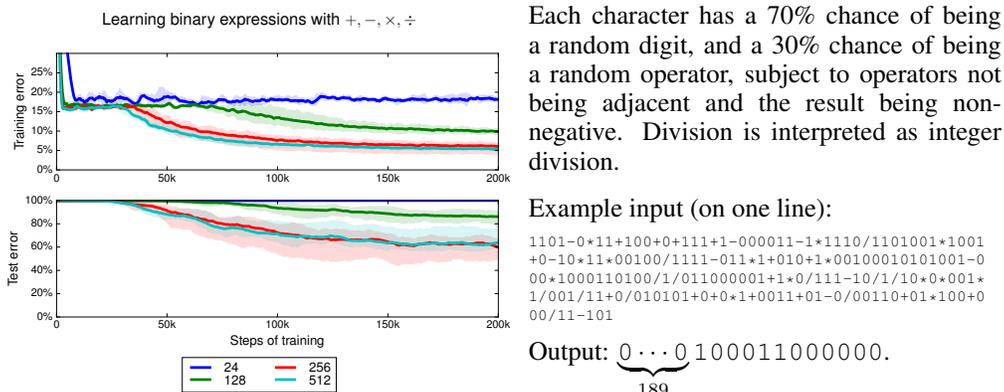


Figure 5: Task of learning binary arithmetic on multiple numbers simultaneously using the operators +, -, ×, ÷.

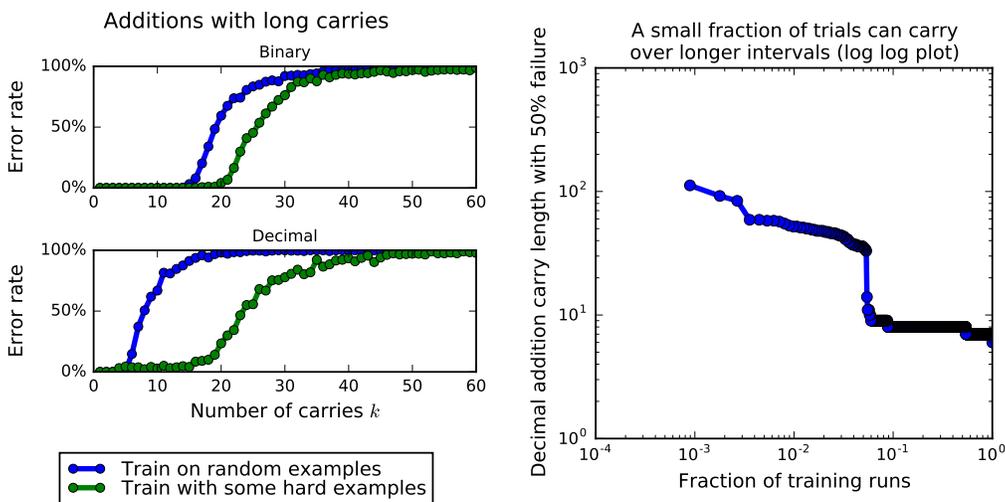


Figure 6: Left: while trained models for addition work on random inputs, they do not reliably work on inputs containing long carry sequences. Right: occasional training runs yield models that carry over somewhat longer sequences.

## 5 GENERALIZATION

Integer addition is a well defined algorithm, so knowledge of its operation is sufficient to add arbitrary numbers. Our trained model generalize perfectly to > 99% of uniformly random test cases of much greater length (having a single digit error in the whole 100-digit number is considered an error). However, we found that it fails on a much larger fraction of “structured” examples. For example, it fails on cases that involve carrying a digit for many steps.

The probability that a bit is to be carried  $k$  times, on uniformly random binary inputs, is  $2^{-k}$ . Training and testing on random examples will thus not notice failure to carry more than about 20 bits. We find that the model typically fails to generalize on test cases that require more than 20 steps of carry, as shown in Fig. 6. Similarly, with decimal addition, the chance of carrying  $k$  digits is  $10^{-k}$  and most trained models stop working reliably after 6 digits.

Introducing “hard” training instances with long carries does not solve this issue. Our training instances involve 20-digit numbers, so they can only carry for 20 digits. Indeed, we find that the trained model will usually answer length-20 carry inputs correctly, but not length-30.

The above behavior holds for most trained models, but as in Kaiser & Sutskever (2015) we find that training the Neural GPU with different random seeds will occasionally find models that generalize better. We trained a decimal addition model with 1121 different seeds, and measure for each model the number of carries at which the error rate crosses 50%. As shown on the right of Fig. 6, the distribution is bimodal: 94% of models have a threshold between 7 and 9 digits, while almost the entire remainder (5.5%) have a threshold of at least length 33. These “successful” models seem to follow roughly a power law distribution: 5% are at least 33, 1% are at least 52, and our best performing model worked up to a carry of length 112. If this behavior is indeed a power law, it is not a very promising way to find highly-generalizing models: a rough extrapolation suggests generalizing to 1000 digits would require 200 million trials.

We observe similar generalization issues with multiplication. A model that has < 1% error on two random 100-digit long decimal examples fails much more often on very symmetric numbers and on numbers that requires to carry for many steps (we test it by verifying performance on numbers that multiply to  $b^{100}$  or  $b^{100} - 1$ ). It also failed much more often on multiplying single digit numbers when they are prepended with many zeros (Table 3); one random trained model failed on 38 of the 100 possible pairs of single-digit numbers.

Left Operand	Right Operand	Observed value	Is prediction correct ?
Single digit examples			
1	1	1	✓
2	1	2	✓
2	2	4	✓
2	3	6	✓
2	4	8	✓
3	3	6	✓
3	5	15	✓
Single digit examples with prepended zeros			
$\underbrace{0 \dots 0}_{99} 1$	$\underbrace{0 \dots 0}_{99} 1$	$\underbrace{0 \dots 0}_{199} 1$	✓
$\underbrace{0 \dots 0}_{99} 2$	$\underbrace{0 \dots 0}_{99} 1$	$0 \dots 0 0176666666666885 \underbrace{0 \dots 0}_{40} 07$	✗
$\underbrace{0 \dots 0}_{99} 2$	$\underbrace{0 \dots 0}_{99} 2$	$0 \dots 0 022333333333770 \underbrace{0 \dots 0}_{40} 14$	✗
$\underbrace{0 \dots 0}_{99} 2$	$\underbrace{0 \dots 0}_{99} 3$	$0 \dots 0 066000000000655 \underbrace{0 \dots 0}_{40} 21$	✗
$\underbrace{0 \dots 0}_{99} 2$	$\underbrace{0 \dots 0}_{99} 4$	$0 \dots 0 075166666667540 \underbrace{0 \dots 0}_{40} 28$	✗
$\underbrace{0 \dots 0}_{99} 3$	$\underbrace{0 \dots 0}_{99} 3$	$\underbrace{0 \dots 0}_{199} 9$	✓
$\underbrace{0 \dots 0}_{99} 3$	$\underbrace{0 \dots 0}_{99} 5$	$\underbrace{0 \dots 0}_{198} 15$	✓

Table 3: Neural GPU generalizes well to random 100-digit examples. However, it might fail to multiply single digit examples with large number of prepended zeros. Models trained on different seeds suffer on different examples with prepended zeros. Therefore, problem is removable by model averaging. However, they all consistently fail on examples that require carrying for many steps.

The multiplication model also fails on highly regular cases. The outputs of the multiplication model are similar to the correct answer, however it seems that the model made a mistake in the middle of the computation. For instance, we took two numbers that multiply to  $10^{180} - 1$ . Such a number is full of nines. However, model predicted:  $10^{180} + 10^{103} - 1$  instead. The predicted number differs on 78 positions, because it has many zeros instead of nines; at some point, it starts to guess that it is getting a carry. Moreover, the model has trouble with very structured expressions, such as  $111111111 \times 111111111$ . It fails for any number of ones above 8.

## 6 GLOBAL OPERATION

The Neural GPU is a cellular automaton, which is a Turing complete computational model (Chopard & Droz, 1998; Wolfram, 1984). However, the automaton is often computationally inefficient compared to the von Neumann architecture. It is difficult for a cellular automaton to move data globally as the entirety of its computation operates locally at each step. We wanted to understand the importance of globally moving data around for solving algorithmic tasks.

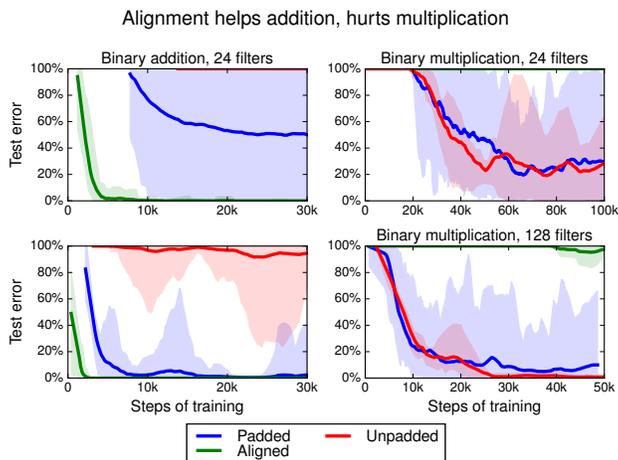


Figure 7: This figure shows the importance of input argument alignment on performance on the addition and the multiplication tasks. We find that alignment is beneficial to addition, but detrimental to multiplication. Note that these experiments were conducted with a small neural GPU that had only 24 filters, so its generalization error is not as strong as that of the larger models. However, the overall patterns tend to carry over from small models to large ones.

In principle, the Neural GPU could be made more powerful by adding a global operation in each of its layers. We have briefly tried to include an attention mechanism that has the ability to easily shift rectangles of data to locations specified by the model, but we were not able to improve empirical results. We skip these experiments here, and instead investigate a simpler form of this question.

Given that the Neural GPU cannot easily move information across long distances, it is conceivable that having both arguments concatenated would hurt its performance. We therefore experimented with several input representations, as described below:

- Padded: 12345+00067
- Unpadded: 12345+67
- Aligned:  $\begin{array}{r} 12345 \\ +00067 \end{array}$

Could we manually align data in a way that helps to solve a task? This could indicate that an architectural modification that performs a global operation is needed. And indeed, we found that the addition task on aligned numbers has higher success rate than on concatenated numbers, and addition on unpadded numbers is the hardest one (Fig. 7, left).

However, we observe the opposite outcome for the multiplication task (Fig. 7, right). Empirically, aligning numbers for multiplication makes the task more difficult. These results suggest that an architectural modification that makes it easy to move the data globally need not provide an improvement on all problems.

## 7 CONCLUSION

In this paper, we investigated the generalization ability of the Neural GPU. We have discovered that larger Neural GPUs generalize better, and provided examples of several curriculums that made it possible for the Neural GPU to solve tasks that it was not able to solve before. Finally, we showed that its generalization is incomplete, as while it has successfully generalized to longer inputs, there still exist highly structured test cases that cause the model to fail.

It is desirable to develop learning methods that can learn algorithms that achieve perfect generalization. One way of moving forward is to investigate ways in which the model can benefit from additional sources of information that are not present in the task itself.

## 8 ACKNOWLEDGMENT

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