Automatically Composing Representation Transformations as a Means for Generalization

Michael Chang 1 Abhishek Gupta 1 Sergey Levine 1 Thomas L. Griffiths 1

Abstract

How can we build a learner that can capture the essence of what makes a hard problem more complex than a simple one, break the hard problem along characteristic lines into smaller problems it knows how to solve, and sequentially solve the smaller problems until the larger one is solved? To work towards this goal, we focus on learning to generalize in a particular family of problems that exhibit compositional and recursive structure: their solutions can be found by composing in sequence a set of reusable partial solutions. Our key idea is to recast the problem of generalization as a problem of learning algorithmic procedures: we can formulate a solution to this family as a sequential decision-making process over transformations between representations. Our formulation enables the learner to learn the structure and parameters of its own computation graph with sparse supervision, make analogies between problems by transforming one problem representation to another, and exploit modularity and reuse to scale to problems of varying complexity. Experiments on solving a variety of multilingual arithmetic problems demonstrate that our method discovers the hierarchical decomposition of a problem into its subproblems, generalizes out of distribution to unseen problem classes, and extrapolates to harder versions of the same problem, yielding a 10-fold reduction in sample complexity compared to a monolithic recurrent neural network.

1. Introduction

Teach a human to fish and feed them for a lifetime. For machines this is not so easy. Learning to generalize to harder problems from solving simpler ones is a difficult challenge in machine learning because the learner must discover regularities that cover a combinatorially large space of problems from only limited data. To make progress towards this goal, this paper focuses on a particular class of problems that exhibit compositional and recursive structure: their solutions can be found by composing in sequence a small set of reusable partial solutions. The key perspective of this paper is to recast the problem of generalization to a problem of learning algorithmic procedures over representation transformations: discovering the structure of a family of problems amounts to learning a set of reusable primitive transformations and their means of composition.

Approaches to this challenge generally have either assumed pre-specified transformations but learned the structure, often with dense supervision, or learned the transformations but pre-specified the structure (see Sec. 5). Pre-specifying one or the other is a major limitation to learning programs that can adapt to different types of data. The contribution of this paper is to propose a direction towards learning both the structure and transformations together with sparse supervision. We propose the compositional recursive learner (CRL), which learns both the structure and transformations of a modular recursive program that iteratively re-represents the input representation into more familiar representations it knows how to compute with.

Our approach is based on the following core ideas. The first core idea is that training on a distribution of composite problems can encourage the spontaneous specialization of reusable computational units that perform transformations between representations. Rather than learning to solve a new problem from scratch, a learner can make an analogy between the new problem and previously encountered problems and re-represent the new problem into one it knows how to solve. The second core idea is to treat the construction of a program as a sequential decision-making problem over these transformations. This formulation not only implements loops, recursion, composition, and selective attention, but enables metareasoning, where the learner dynamically customizes its program complexity to the problem instance. The third core idea is to operationalize the learner in differentiable programs by using reinforcement learning algorithms to solve the discrete optimization problem of se-
lecting which transformation to apply, while simultaneously learning the transformations with backpropagation.

Multilingual arithmetic problems are a challenging but minimal family of tasks that exhibit compositional and recursive properties (see Sec. 2). Understanding how to learn to decompose and exploit the structure of arithmetic is a first step towards solving any more complex domain, which would at least have the structure we study here in arithmetic. Our experiments on generalization to a completely unseen distribution of harder problems from only observing less than $3 \times 10^{-4}$ of the training distribution show that CRL outperforms baselines without recursive or compositional reusability in their structure, even when the baseline is pretrained on all of the primitive transformations of the dataset.

**Summary of contributions:** (1) To consider a learner whose primitive transformations and means of their composition match the structure of the problem distribution, we narrow the scope of problems to those that exhibit compositional and recursive structure, which we formalize in Sec. 2. (2) In Sec. 3 we propose a hypothesis that the emergence of primitive transformations can be encouraged by training on a distribution of composite problems. (3) We frame the problem of learning the structure of a program as a sequential decision-making problem over these transformations. These two pieces comprise the CRL framework. (4) To implement CRL in differentiable programs, we present a formalism for expressing the construction of a neural network in terms of an Markov decision process that generates computation graphs. (5) Our experimental findings in Sec. 4 highlight the limitations of monolithic static network architectures in generalizing to structurally similar but more complex problems than they have been trained on, providing evidence in favor of learners that dynamically re-program themselves, from a repertoire of learned reusable computational units, to the current problem they face.

**2. General Setup**

It would be impossible to generalize if the universe exhibited no regularities. Discovering and exploiting the structure in their world helps humans generalize make predictions and solve problems in new situations. We formalize the notion of compositional structure in terms of problems, describe the characteristics of these problems, and define the challenge of how to learn programs that reflect the structure of problems.

**Problems:** To solve a problem $P_i$ is to transform its input representation $x_i$ into its output representation $y_i$. $x_i$ and $y_i$ are associated with their respective types $t_x$ and $t_y$. In a translational problem, the input representation and the output representation differ (i.e. $t_x \neq t_y$). In a recursive problem, $x_i$ and $y_i$ are the same (i.e. $t_x = t_y$). Two problems $P_i$ and $P_j$ are of the same class if the types of their input representations and output representations match (i.e., $x_i = x_j$ and $y_i = y_j$). For clarity we focus on functions with one input and output; one can use currying to extend our analysis to functions with multiple inputs.

**Composite problems:** Problems can be compositions of other problems, which themselves can be composite. A composite problem $P_{a} = P_b \circ P_c$ means that the solution of $P_{a}$ can be found by first solving $P_c$, then solving $P_b$ with the output of $P_c$ as input. In this case, $P_{a}$ and $P_{b}$ are subproblems with respect to $P_{a}$. This imposes constraints on the types of the input and output representations, so $t_x = t_{x_a}$, $t_{x_b} = t_{y_c}$, and $t_{y_a} = t_{y_b}$ all hold, but $t_{x_a}$ need not be equal $t_{y_a}$. Note that translational problems can have both translational or recursive subproblems, and vice-versa. Therefore, all composite problems can be expressed as a composition of translational and recursive subproblems.

**Examples:** Towers of Hanoi is a recursive problem (where both $t_x$ and $t_y$ are disk configurations), as is arithmetic (where both $t_x$ and $t_y$ are expressions). Robot sensorimotor control is a translational problem with translational and recursive subproblems: sensorimotor control can be broken down into a recognition model (a translation problem between $t_x =$ pixels and $t_y =$ scene description), which itself is a composition of recursive problems (various image filters), and a control policy translating intermediate percepts to motor torques. Multimodal problems have different input and output types, but unimodal problems need not have the same type: translating French to English is a different class from translating French to Spanish.

**The goal:** Let $P$ be a set of composite problems that share a set of regularities. We want the learner to generalize to solve translational problems of unseen classes (e.g., the learner was trained to translate French to English and English to Spanish but not French to Spanish). We also want the learner to extrapolate to solve recursive problems that have higher complexity than it has seen (e.g., the learner was trained to solve up to 5-length arithmetic expressions but is tested on 10-length expressions).

**The challenge:** In general the internal compositional structure of problems is unknown. For a particular problem $P_i$, the learner only is given an input and the output type $(x_i, t_y)$ and is expected to produce output $y_i$. The only supervision signal it receives is its prediction error. The learner is trained on a set of problems $P_{\text{train}} \in P$ and tested on a disjoint set of problems $P_{\text{test}} \in P$. When data is limited, naïve approaches quickly overfit to $P_{\text{train}}$ and do not generalize to $P_{\text{test}}$. To solve translational problems the learner must learn to make an analogy between the new problem and previously encountered problems by re-representing the new problem into a class it is familiar with. To solve recursive problems, the learner must learn an algorithm to iteratively reduce the harder problem into simpler problems of the
same class. To do so, one powerful design strategy in constructing programs is to base the structure of the program on the structure of the system being modeled [1]; how does a learner automatically program itself to reflect the structure of each problem?

3. A Learner That Programs Itself

Learning both the structure and transformations of CRL from sparse supervision is challenging for several reasons. First, we need to encourage the “crystallization” of primitive transformations from data without any explicit feedback on what the transformations should be (Sec 3.1). Second, we need to learn how to compose these transformations to reflect the subproblem structure of the problems \( P \) without execution traces (Sec 3.2). Third, we need to learn the transformations themselves, but simultaneously learning both the primitives and the means of their composition is a difficult chicken-and-egg optimization problem because learning good transformations would make sense only if they are composed correctly, and vice versa (Sec 3.3).

3.1. Pattern-Matching over Problems via Analogy

If CRL is trained on a diverse distribution of composite problems that share enough structure, it may be able to distill out the individual structural components into specialized, modular computational units: atomic function operators that perform transformations between representations. Indeed, often it is easier to solve a problem \( P_b \) by making an analogy to a problem \( P_a \) that one already knows how to solve, rather than retraining to solve \( P_b \) from scratch [74, 76]. Transforming the type of input representation from \( t_{xa} \) to \( t_{xb} \) is one way of making such analogies. Therefore, if a learner hasn’t ever translated French to Spanish but knows how to translate French to English and English to Spanish, it can reduce the French to Spanish problem to a English to Spanish problem by transforming the French input to English input, which it knows how to compute with. If a learner hasn’t ever seen a 10-length arithmetic expression before, but it knows how to reduce an \( n \)-length expression to an \((n - 1)\)-length one, then it can iteratively reduce the 10-length expression down to a length it knows.

If we constrain the representational vocabulary and draw the boundaries of modularity via transformations between representations, we can encourage specialization to naturally emerge when the computational units do not know the global problem they are solving but can make local progress to iteratively re-represent the problem into a more familiar form. However, when there are shared subproblems across the composite family, we would hope CRL would learn reusable computational units that capture that subproblem structure in the family.

3.2. Learning the Structure of a Computation as a Sequential Decision-Making Process

A transformation between representations can be generalized as any computation which changes the state of a finite state machine to another. Learning how to apply computational units in sequence can then be formulated as a sequential decision-making problem, where the state space is the intermediate results produced by a program and the action space is the set of computations.

This kind of sequential decision problem can be formalized as a meta-level Markov decision process (MDP) [41], defined by a tuple \( (\mathcal{X}, \mathcal{F}, \mathcal{P}_{\text{meta}}, r, \gamma) \). \( \mathcal{X} \) is the set of information states (intermediate results of computation), \( \mathcal{F} \) is the set of computations, \( \mathcal{P}_{\text{meta}}(x_j, f_j, x_{j+1}) \) is the transition model that expresses the probability that at step \( j \) the computation \( f_j \) will change the information state from \( x_j \) to \( x_{j+1} \), \( \gamma \) is a discount factor. The goal of CRL is to select a series of computations \( f \) to iteratively transform the input \( x \) into its predicted output \( \hat{y} \). When CRL selects a special computation, the HALT signal, the current result is produced as output. The learner incurs a cost for every computation it executes and receives a terminal reward that reflects how its output \( \hat{y} \) matches the desired output \( y \). The computation cost and the HALT signal differentiate the meta-level MDP from a generic MDP, requiring CRL to balance program complexity and performance. The result is a program composed of a sequence of computations that customizes its complexity to the problem.

3.3. Learning the Transformations and their Means of Composition from Sparse Rewards

The meta-level MDP describes how to choose transformations, but not how to learn the form of the transformations themselves. We solve this problem by learning differentiable programs composed of neural networks, in which both the transformations and their composition are learned.

The implementation consists of a controller \( \pi(f|x, t_y) \), a set of functions \( f_k \in \mathcal{F} \), and an evaluator (Fig. 1). At step \( j \), the controller observes the intermediate state of computation \( x_j \) and the target output type \( t_y \). It selects a function \( f_k \) and a portion of \( x_j \) to operate on. The evaluator applies \( f_k \) to transform \( x_j \) into a new state of computation \( x_{j+1} \). When \( \pi \) selects HALT, a loss is computed by comparing the current state of computation with the desired output. The loss is backpropagated through the functions, which are trained with Adam [47]. The controller receives a sparse reward derived from the loss, incurs a cost for each computation, and is trained with proximal policy optimization [75].

The state space (excluding the initial state, which is CRL’s input) consists of the outputs of the functions, the action space consists of the functions themselves, and the transi-
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Figure 1. Compositional recursive learner (CRL): **top-left:** CRL is a cycle between a controller and evaluator: the controller selects a function $f$ given an intermediate representation $x$ and the evaluator applies $f$ on $x$ to create a new representation. **bottom-left:** CRL learns dynamically learns the structure of a program customized for its problem, and this program can be viewed as a finite state machine. **right:** A series of computations in the program is equivalent to a traversal through the Meta-MDP, where functions can be reused across different stages of computation, allowing for recursive computation.

The composition model is the evaluator. Unlike standard reinforcement learning problems, here the state space and action space can vary in dimensionality, as we show in our experiments. Moreover, as CRL trains, the function parameters change, so transition dynamics are non-stationary. To overcome these optimization difficulties, we draw from [20] and gradually grow the complexity of the problems during training such that learning more complex compositions are bootstrapped from transformations learned in the context of simple compositions earlier on (see Appx. C for intuition). Because the outputs of a function are the internal representations of the larger neural network, CRL simultaneously designs its own internal representation language and the transformations that convert between them. CRL’s states of computation are its internal representations, which may or may not correspond with the external representation given by the problem.

### 3.4. Discussion of Design Choices

Modularity and reuse of computational units are natural consequences of this framework. Such weight-sharing enables CRL to maximize knowledge it learns within and across problems under low data regimes. The computation graph that CRL constructs by its choices over functions is flexible enough to learn to reflect the true underlying compositional structure within a problem (although it need not to), thereby allowing CRL to make analogies transforming a larger problem into subproblems it knows how to solve. We need only a single controller that can learn to compose functions for a wide variety of problems; choosing when to terminate allows for metareasoning, extrapolation, and learning in an online setting where problems increasingly grow in complexity.

Our framework provides a language for describing a learner that designs itself: making the connection between programs, neural networks, and MDPs establishes the equivalence between computational units, functions, and representation transformations and opens opportunities to borrow tools from reinforcement learning and deep learning as a practical means for solving both the continuous and discrete optimization problems of respectively learning the transformations and their means composition. By explicitly attempting to discover and exploit the compositional structure of composite problems, we transform the generalization problem into a problem of learning algorithmic procedures over transformations between representations.

### 4. Experiments

Our experiments are aimed at evaluating the generalization, extrapolation, and compositional learning capabilities of CRL. Specifically: 1) Can we learn to solve problems which have recursive and compositional structure? 2) Does the structure of CRL allow us to learn how to solve these problems with significantly less data? 3) Can we generalize to harder problem instances, i.e. extrapolate? 4) Can we generalize to unseen problem classes using combinations of transformations learned from prior problems?
Domains: Multilingual arithmetic problems is a challenging but minimal domain that exhibits the compositional structure of problems we’d like to investigate: a) variable length inputs, b) variable problem complexity, c) reuse of subprocedures across problem, d) reuse of subprocedures within a single problem, e) a large combinatorial space created by composing together a small set of primitives using simple rules, f) a natural curriculum of easier (shorter) to harder (longer) problems g) diversity in the semantic roles of primitive components (e.g. operators like +, ×). For clarity, we use generalization to mean solving mathematically different problems with the same number of terms as in training and extrapolation to mean solving mathematically different problems with more terms than in training. We refer to generalization or extrapolation within a single window of 3 terms in the expression, and the reducer transforms to unseen length-10 expressions in the test set (within a single problem, e) a large combinatorial space created by composing together a small set of primitives using simple rules, f) a natural curriculum of easier (shorter) to harder (longer) problems g) diversity in the semantic roles of primitive components (e.g. operators like +, ×). For clarity, we use generalization to mean solving mathematically different problems with the same number of terms as in training and extrapolation to mean solving mathematically different problems with more terms than in training. We refer to generalization or extrapolation within a single window of 3 terms in the expression, and the reducer transforms to unseen length-10 expressions in the test set (within a single problem, e) a large combinatorial space created by composing together a small set of primitives using simple rules, f) a natural curriculum of easier (shorter) to harder (longer) problems g) diversity in the semantic roles of primitive components (e.g. operators like +, ×). For clarity, we use generalization to mean solving mathematically different problems with the same number of terms as in training and extrapolation to mean solving mathematically different problems with more terms than in training.

4.1. Generalization and Extrapolation In-Distribution: Numerical Math

This experiment addresses the recursive challenge. The input is a numerical arithmetic expression (e.g. 3 + 4 × 7) and the desired output (e.g. 1) is the evaluation of the expression modulo 10. The input and output have the same type. In our experiments we train on a curriculum of length-2 expressions to length-10 expressions, adding new expressions to an expanding dataset over the course of training in a lifelong learning fashion. The first challenge is to learn from this limited data (only 6510 training expressions) to generalize well to unseen length-10 expressions in the test set (∼ 214 possible). The second challenge is to extrapolate from this limited data to length-20 expressions (∼ 1029 possible).

Expressions are represented as sequences of one-hot vectors. The functions (“reducers”) used in CRL reduce a length k expression to a length k − 3 one: the controller chooses a window of 3 terms in the expression, and the reducer transforms that into a softmax distribution over a single term in the vocabulary. This process is repeated until the expression is reduced to one term, at which point the expression persists until the controller HALTS. Choosing to attend to a subset of the input is not domain-specific; this strategy is applicable in many settings [23, 57, 88]. We compare with an RNN architecture [19] directly trained to map input to output.

Results: Interestingly, though the RNN eventually generalizes to different 10-length expressions and extrapolates to 20-length expressions (yellow in Fig. 2) with 10 times more data as CRL, it completely overfits when given the same amount of data (gray). In contrast, CRL (red) does not overfit, generalizing significantly better to both the 10-length and 20-length test sets. We believe that the modular disentangled structure in CRL biases it to cleave the problem distribution at its joints, yielding this 10-fold reduction in sample complexity relative to the RNN.

Indeed, we found that the controller naturally learned windows centered around operators (e.g. 2 + 3 rather than ×4−), suggesting that it has discovered semantic role of these primitive two-term expressions by pattern-matching common structure across arithmetic expressions of different lengths. Note that CRL’s extrapolation accuracy here is not perfect compared to [14]: but what we believe is noteworthy is that CRL achieves such high extrapolation accuracy with only sparse supervision, without the step-by-step supervision on execution traces, the stack-based model of execution, and hardcoded transformations.

4.2. Generalization and Extrapolation Out-of-Distribution: Multilingual Math

This experiment addresses the translational challenge. Arithmetic expressions now come in m different types, each corresponding to a language that expresses it. An example input is three plus four times seven (the source language is English) and an example corresponding output is uno (the target language is Spanish). We arbitrarily chose m = 5 languages: English, Numerals, PigLatin, Reversed-English, Spanish. During training, each source language is seen with four target languages (and one held out for testing) and each target language is seen with four source languages (and one held out for testing). This is interesting and challenging because the test examples are outside the training distribution: the problems are not only mathematically different but from unseen language pairs.

The input is a tuple (x(s), t_y), where x is the arithmetic expression expressed in source language s, and t_y is the language the learner should output the answer in. To solve this problem, the learner must translate between types as well as solve the arithmetic problem – a strictly harder task than the numerical math experiment (Sec. 4.1). The problem space is increased by a factor of m^2 = 25, so the dataset is increased by an order of magnitude. In addition to reducers, our learner has a second type of function, a “translator”, which produces a length-k sequence of softmax distributions over the vocabulary from another length-k sequence.
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Figure 2. Numerical math task. We compare our learner with the RNN baseline. As a sanity check, we also compare with a version of our learner which has a hardcoded controller (HCC) and a learner which has hardcoded functions (HCF) (in which case the controller is restricted to select windows of 3 with an operator in the middle, but this is not the case in general). All models perform well on the training set. Only our method and its HCC, HCF modifications generalize to the testing and extrapolation set. The RNN requires 10 times more data to generalize to the testing and extrapolation set. For (b, c) we only show accuracy on the expressions with the maximum length of those added so far to the curriculum. “1e3” and “1e4” correspond to the order of magnitude of the number of samples in the dataset, of which 70% are used for training. 10, 50, and 90 percentiles are shown over 6 runs.

Here, the controller has access to $t_y$ at every step of computation, but the functions do not, forcing the functions to learn behaviors agnostic of the language pair and putting the burden of choosing how to generalizing to different input-output types on the controller. We again compare with an RNN, which receives $t_y$ concatenated with every element of $x^{(s)}$. The training and test sets are a curriculum of up to 5 terms and the extrapolation set is 10 terms.

Results: CRL (red in Fig. 3) generalizes and extrapolates consistently better in the low-data regime. As this task requires that the primitive transformations learned during training capture the regularities present in out-of-distribution language pairs, it is not surprising that CRL’s performance is more sensitive to parameter initialization than in the single-language case. Again we observe in that, while the RNN (purple) fails to generalize or extrapolate with the same amount of data as CRL, with 10 times more data the RNN (yellow) generalizes to the 5-terms test set, showing that data diversity helps monolithic neural networks generalize.

Limitations of monolithic RNNs: Even with 10 times more data, this time the RNN does not extrapolate to the 10-terms dataset, which exposes a limitation of monolithic
structure in RNNs related to that discussed in [52]. We hypothesized that although they are all learned, the existence of CRL’s attention mechanism and the topology of its reducers and translators may give it a domain-specific advantage over the RNN. To endow the RNN with domain-specific knowledge beforehand, we pre-trained the RNN (green and gray in Fig. 3) to 100% accuracy on auxiliary tasks of translating between numerical math to all other languages and of solving 3-term numerical math problems. We trained the pre-trained RNN on the multilingual task, shuffling in the auxiliary tasks with the multilingual training examples so it does not forget what it has been pre-trained on. This required quadrupling the hidden state of the RNN for it to have enough capacity to learn on the training+auxiliary set. Under these conditions the RNN still cannot extrapolate with 10 times more data, even though these auxiliary tasks give the RNN a nontrivial boost on the test set. This experiment suggests that solving problems with high-level symbolic compositionality may require a different direction of research for neural networks, not as monolithic function approximators but as disentangled modular differentiable programs that can be composed on the fly.

It is in the learner’s interest to generalize in a changing environment: All but the blue curve in Fig. 3 were models trained with a curriculum from length-2 to length-5 expressions. For CRL, the curriculum is updated every $10^5$ iterations, such that after $3 \cdot 10^5$ iterations all the training data has been added. Five observations are noteworthy. First, observing the initial consistent rise of the red training curve from 0 to $3 \cdot 10^5$ iterations shows CRL exhibits forward transfer [55] to expressions of longer length. Second, by the time length-5 expressions have been added, accuracy is nowhere near convergence (still around 20% for training and 15% for testing and extrapolation). It is only until around $1.5 \cdot 10^6$ iterations that the structure and transformations begin to really “crystallize” into some useful form. But despite training and generalization performance coming so late, our third observation is that the curriculum early on was crucial for the generalization performance more than a million iterations later: when CRL is directly trained only on 5-term expressions from the beginning without a curriculum (blue in Fig. 3), CRL does not generalize or extrapolate at all. Nevertheless, given that without a curriculum the CRL is trained on only $700 \times 20 = 1.4 \times 10^4$ length-5 expressions (of $\approx 2 \times 10^8$), our fourth observation that it is still able to learn at all having seen only $7 \times 10^{-5}$ of the training set shows that the CRL framework is a promising potential candidate for distilling out the hierarchical subproblem decomposition of a distribution of composite problems. The fifth observation is that while a changing problem distribution helps to encourage generalization, it alone is not enough: the RNNs with no modular disentangled structure are not able to generalize or extrapolate.

4.3. Qualitative Analysis

Because CRL dynamically composes itself to solve a particular problem, we can peek inside the learner to observe what functions it chooses, how it composes the functions together, and, if the functions are interpretable at convergence, what semantic role these functions play with respect to each other. Though the randomly initialized functions have no semantic meaning, as training progresses the functions gradually specialize such that after convergence the controller chooses a particular ordering of the functions given a new input expression. Fig. 4 elucidates how CRL makes analogies to re-represent an unseen problem into one that is more unfamiliar. Because the language pair is one it has not seen, the controller learns to route through expressions it does know how to work with to solve a new problem that it has never seen before. We believe that CRL’s generalization and extrapolation capability comes from the task-agnostic nature of its functions: only the controller must generalize, leaving the functions to learn transformations that the controller would commonly reuse across problems.

We see that CRL learns reducers that reduce to a particular language from any language, which result in intermediate hybrid-language expressions. Notably, after it has reduced the entire expression, it takes an additional step to translate the final term to a term in the target language, even though the term before translation is not in either the source or the target language. Indeed, we observe that the average number of moves during training was 3.9, during testing was 6.6, and during extrapolation was 15.4, showing that the controller reasons about its own computation, taking additional steps that it deems necessary to compose the tools that it has invented itself (the translators and reducers) to solve unseen problems (although it sometimes tries to HALT unnecessarily: see Appx. D.4). We originally expected that CRL would learn specialized translators that translated between every language pair, and specialized reducers that reduced expressions within a set of common languages, but were surprised that this did not happen: rather than learn reducers specific to both the input and output languages, the reducers tended to learn operations specific to the output language only. Upon further inspection, perhaps this is not surprising because of their nonlinear nature, but further work would be required to gain a deeper understanding.

5. Related Work

Our work is one of a small growing body of work bridging reformulation and metareasoning with deep learning; its emphasis on learning algorithmic procedures as a means for generalization departs from work that seeks to learn shared representations; it shows the benefit of hierarchical learning in low data regimes; it demonstrates a fully disentangled self-organizing neural network where both the transformations
Combinatorial generalization through metareasoning: To solve out-of-distribution problems, both metalearning and metareasoning approaches assume that the new problem shares regularities with previous problems but take different perspectives on how to exploit those regularities. The metalearning framework [70, 83] seeks to learn a learner that can learn quickly on the new problem. CRL departs from this paradigm by taking a metareasoning approach [41, 68], where the learner reasons about its own knowledge and computations to solve the new problem. Much recent metalearning work [6, 26, 27, 31, 37, 38, 53, 56, 60, 64, 79] focuses on domains where achieving zero-shot generalization is unclear and follow a common paradigm which assumes that the shared representation of monolithic architectures (with the exception of concurrent work [2]) can be shaped by the diversity of tasks in the training distribution as good initializations for future learning. But for combinatorial generalization, monolithic architectures may itself be a barrier to zero-shot generalization: our experiments suggest that such architectures are significantly less data efficient than compositional modular approaches. In these cases it may be possible to extract enough structure during training to generalize out-of-distribution without learning at all. Indeed, the monolithic/shared-representation paradigm can be improved in two complementary ways. The first, advocated in contemporaneous work [10], focuses on learning more structured representations of entities and relations with graph networks. The second, the focus of this paper, focuses on learning structured algorithmic procedures that can implement recursion and composition of partial solutions that operate on state representations. Instead of learning an algorithm to learn, the learner can learn an algorithm to reason: casting the generalization problem as an algorithm design problem is a growing hypothesis for the mechanism with which humans can generalize to new scenarios [15, 36, 54]. Our work is one of a small but growing community [32, 40, 61] linking metareasoning with deep learning.

Compositional neural program induction: Compositional approaches (as opposed to memory-augmented [6, 33–35, 45, 51, 80] or monolithic [46, 89] approaches for learning programs) to the challenge of discovering reusable primitive transformations and their means of composition generally fall into two categories. The first as-
sumes pre-specified transformations and learns the structure (from dense supervision on execution traces to sparse-rewards) [13, 14, 18, 22, 25, 28, 65, 87, 90]. The second learns the transformations but pre-specifies the structure [5, 21, 66]. These approaches are respectively analogous to our hardcoded-functions and hardcoded-controller ablations in Fig. 2. [89] noted the challenge of learning the individual operators and how to combine them; our paper can be considered a candidate to address this challenge. The closest work in this respect to ours is [29] which assumes a differentiable interpreter grounded in source code; we take a different perspective of learning algorithms through re-representations, which enables our method to adapt on-line to new problem classes. Our perspective comes with its own challenges; without grounding in source code, the concept of a for-loop is implicit in the controller, rather than an explicit concept that can exist independently of the data, which is desirable for constructing more complex programs.

**Self-organizing learners, disentanglement, hierarchical learning:** Research on self-organizing learners [20, 70, 72, 73] has so far been relatively theoretical; CRL is a synthesis of recent work in disentanglement and hierarchical learning that attempts to bring this old idea closer to reality. Just as the motivation behind disentangled representations [11, 17, 49, 82, 85] is to uncover the latent factors of variation, the motivation behind disentangled programs is to uncover the latent organization of a task. Finding such structure is important for generalization because it shields various parts of the representation or program from changing when one component changes. For example, [24, 42, 67] have begun to examine how to route through an fixed architecture to encapsulate computation, but the hard limitation that prevents fixed architectures from scaling to problems with complexity beyond that which they were trained is their limited number of computation steps. A parallel line of work runs through the hierarchical reinforcement learning (HRL) literature [9], with recent work [8, 27, 50, 58, 84] attempting to learn both lower-level policies as well as a higher-level policy that calls them. Several works have investigated the conditions in which hierarchy is useful for humans [12, 69, 77]; our experiments show that the hierarchical structure of CRL is more useful than the flat structure of the RNN for low-data compositional problems. The fast-weights (FW) literature [7, 71] is also related to the idea of selecting different weights at different steps of computation, but with a different motivation for learning context-dependent associative memory [3, 39, 44, 48, 86]. By combining adaptive computation time [32] with routing, CRL synthesizes all of these above ideas by dynamically composing learned reusable subnetworks together as fully disentangled programs, taking a step towards making the topology of the computation graph self-organizing as well.

### 6. Discussion

**Open Problems:** Although we have demonstrated on a representative family of problems the proof-of-concept of a learner that learns both the structure and transformations of its own computation to generalize and extrapolate to harder problems, this paper by no means has presented a complete solution; there are several directions in which the CRL formulation can be improved. From an optimization standpoint, the simultaneous optimization between discrete composition and continuous parameters presents an interesting challenge. Further work is required to reduce the variance in extrapolation accuracy, accelerate convergence, and reduce reliance on a curriculum. When the extrapolation task is too far out-of-distribution, the controller may get stuck in situations where it does not HALT for a much longer time than is required. From a representational standpoint, although CRL is a domain agnostic framework, we have so far demonstrated it in a setting where the representation is quite constrained; it is an open problem what the representation interface should be for other less symbolic tasks and how CRL scales to these problems. From an algorithmic standpoint, open problems include: how to incorporate external actions, how to generate computation graphs beyond a linear chain of functions, and how to infer the number of functions required for a family of problems.

**Conclusion:** We have considered learning to generalize and extrapolate with limited data to harder compositional problems than a learner has previously seen. We have taken steps toward this challenge by presenting a characterization, algorithm, and implementation of a learner that programs itself automatically to reflect the structure of the problem it faces. Our key ideas are (1) transforming representations with modular units of computation is a potential solution for decomposing problems in a way that reflects their subproblem structure; (2) learning the structure of a computation can be formulated as a sequential decision-making problem; (3) tools from reinforcement learning and deep learning can serve as a practical means for solving both the continuous and discrete optimization problems of respectively learning the transformations and their means of composition with sparse rewards. Our experiments support the core perspective of this paper: for compositional problems under low data regimes, casting the generalization problem as a problem of learning algorithmic procedures over representation transformations offers significant advantages over monolithic architectures that only rely on the diversity in the data to shape a shared representation. This work brings together ideas from various areas of research – reformulation, metareasoning, program induction, modularity, hierarchical reinforcement learning, self-organizing neural networks – to provide a proof-of-concept for learning general-purpose, compositional and recursive programs that design themselves and reason about their own computations.
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A. Data

**Numerical math:** The dataset contains arithmetic expressions of $k$ terms where the terms are integers $\in [0, 9]$ and the operators are $\in \{+,-,\cdot\}$. The number of possible problems is $(10^k)/(3^{k-1})$. The learner sees $5810/(2.04 \cdot 10^{14}) = 2.85 \cdot 10^{-11}$ of the training distribution. The number of possible problems in the extrapolation set is $(10^{20})(3^{19}) = 1.16 \cdot 10^{29}$. An input expression is a sequence of one-hot vectors of size 13.

| # Terms | Prob. Space | # Train Samples | Frac. of Prob. Space |
|---------|-------------|----------------|---------------------|
| 2       | $10^2(3^3) = 3 \cdot 10^2$ | 210 | $7 \cdot 10^{-1}$ |
| 3       | $10^3(3^3) = 9 \cdot 10^3$ | 700 | $7.78 \cdot 10^{-2}$ |
| 4       | $10^4(3^3) = 2.7 \cdot 10^4$ | 700 | $2.6 \cdot 10^{-3}$ |
| 5       | $10^5(3^3) = 8.1 \cdot 10^5$ | 700 | $8.64 \cdot 10^{-5}$ |
| 6       | $10^6(3^3) = 2.43 \cdot 10^6$ | 700 | $2.88 \cdot 10^{-6}$ |
| 7       | $10^7(3^3) = 7.29 \cdot 10^7$ | 700 | $9.60 \cdot 10^{-8}$ |
| 8       | $10^8(3^3) = 2.19 \cdot 10^8$ | 700 | $3.20 \cdot 10^{-9}$ |
| 9       | $10^9(3^3) = 6.56 \cdot 10^9$ | 700 | $1.07 \cdot 10^{-10}$ |
| 10      | $10^{10}(3^3) = 1.97 \cdot 10^{10}$ | 700 | $3.56 \cdot 10^{-12}$ |
| **Total** | $2.04 \cdot 10^{14}$ | **5810** | $2.85 \cdot 10^{-11}$ |

*Table 1. Numerical Arithmetic Dataset*

**Multilingual math:** The dataset contains arithmetic expressions of $k$ terms where the terms are integers $\in [0, 9]$ and the operators are $\in \{+,-,\cdot\}$, expressed in five different languages. With 5 choices for the source language and target language, the number of possible problems is $(10^k)/(3^{k-1})(5^2)$. In training, each source language is seen with 4 target languages and each target language is seen with 4 source languages: 20 pairs are seen in training and 5 pairs are held out for testing. The learner sees $46200/(1.68 \cdot 10^8) = 2.76 \cdot 10^{-4}$ of the training distribution. The entire space of possible problems in the extrapolation set is $(10^{10})(3^3)(5^2) = 4.92 \cdot 10^{15}$ out of which we draw samples from the 5 held-out language pairs ($(10^{10})(3^3)(5) = 9.84 \cdot 10^{14}$ possible). An input expression is a sequence of one-hot vectors of size $13 \times 5 + 1 = 66$ where the single additional element is a STOP token (for training the RNN).

| # Terms | Prob. Space | Train Prob. Space | # Train Samples | Frac. of Train Dist. | Frac. of Prob. Space |
|---------|-------------|-------------------|----------------|----------------------|---------------------|
| 2       | $(10^2)(3^3)/(25) = 7.5 \cdot 10^2$ | $(10^2)(3^3)/(20) = 6 \cdot 10^3$ | 210 \cdot 20 = $4.2 \cdot 10^3$ | $7 \cdot 10^{-1}$ | $5.6 \cdot 10^{-5}$ |
| 3       | $(10^3)(3^3)/(25) = 2.25 \cdot 10^3$ | $(10^3)(3^3)/(20) = 1.8 \cdot 10^4$ | 700 \cdot 20 = $1.4 \cdot 10^4$ | $7.78 \cdot 10^{-2}$ | $6.22 \cdot 10^{-5}$ |
| 4       | $(10^4)(3^3)/(25) = 6.75 \cdot 10^4$ | $(10^4)(3^3)/(20) = 5.4 \cdot 10^5$ | 700 \cdot 20 = $1.4 \cdot 10^4$ | $2.6 \cdot 10^{-3}$ | $2.07 \cdot 10^{-5}$ |
| 5       | $(10^5)(3^3)/(25) = 2.02 \cdot 10^5$ | $(10^5)(3^3)/(20) = 1.62 \cdot 10^6$ | 700 \cdot 20 = $1.4 \cdot 10^4$ | $8.64 \cdot 10^{-5}$ | $6.91 \cdot 10^{-5}$ |
| **Total** | $2.09 \cdot 10^9$ | $1.68 \cdot 10^8$ | **46200** | $2.76 \cdot 10^{-4}$ | $2.21 \cdot 10^{-4}$ |

*Table 2. Multilingual Arithmetic Dataset*

B. Learner Details

All models are implemented in PyTorch [62] and we will make the code and data available online.

B.1. Baselines

The RNN is implemented as a sequence-to-sequence [81] GRU. The routing networks (experimental comparison in Appx. D.1) implementation used the same hyperparameters as those for the best CRL model.

B.2. CRL

**Controller:** The controller consists of a policy network and a value function, each implemented as GRUs that read in the input expression. The value function outputs a value estimate for the current expression. For the numerical arithmetic task, the policy network first selects a reducer and then conditioned on that choice selects the location in the input expression to apply the reducer. For the multilingual arithmetic task, the policy first samples whether to halt, reduce, or translate, and then conditioned on that choice (if it doesn’t halt) it samples the reducer (along with an index to apply it) or translator.

**Functions:** The reducers are initialized as a two-layer feedforward network with ReLU non-linearities [59]. The translators are a linear weight matrices.
C. Experiment Details

Training procedure: The training procedure for the controller follows the standard Proximal Policy Optimization training procedure, where the learner samples a set of episodes, pushes them to a replay buffer, and every \( k \) episodes updates the controller based on the episodes collected. Independently, every \( k' \) episodes we consolidate those \( k' \) episodes into a batch and use it to train the functions. We found via a grid search \( k = 1024 \) and \( k' = 256 \). Through an informal search whose heuristic was performance on the training set, we settled on updating the curriculum of CRL every \( 10^5 \) iterations and updating the curriculum of the RNN every \( 5 \cdot 10^4 \) iterations.

Domain-specific nuances: In the case that HALT is called too early, CRL treats it as a no-op. Similarly, if a reduction operator is called when there is only one token in the expression, the learner also treats it as a no-op. There are other ways around this domain-specific nuance, such as to always halt whenever HALT is called but only do backpropagation from the loss if the expression has been fully reduced (otherwise it wouldn’t make sense to compute a loss on an expression that has not been fully reduced). The way we interpret these “invalid actions” is analogous to a standard practice in reinforcement learning of keeping an agent in the same state if it walks into a wall of a maze.

Symmetry breaking: We believe that the random initialization of the functions and the controller breaks the symmetry between the functions. For episodes 0 through \( k \) the controller still has the same random initial weights, and for episodes 0 through \( k' \) the functions still have the same random initial weights. Because of the initial randomness, the initial controller will select certain functions more than others for certain inputs; similarly initially certain functions will perform better than others for certain inputs. Therefore, after \( k \) iterations, the controller’s parameters will update in a direction that will make choosing the functions that luckily performed better for certain inputs more likely; similarly, after \( k' \) iterations, the functions’ parameters will update in a direction that will make them better for the inputs they have been given. So gradually, functions that initially were slightly better at certain inputs will become more specialized towards those inputs and they will also get selected more for those inputs.

Training objective: The objective of the composition of functions is to minimize the negative log likelihood of the correct answer to the arithmetic problem. The objective of the controller is to maximize reward. It receives a reward of 1 if the token with maximum log likelihood is that of the correct answer, 0 if not, and \(-0.01\) for every computation step it takes. The step penalty was found by a scale search over \{-1, -0.1, -0.01, -0.001\} and \(-0.01\) was a penalty that we found balanced accuracy and computation time to a reasonable degree during training. There is no explicit feedback on what the transformations should be and on how they are composed.

D. Additional Experiments

D.1. Ablation Study

![Routing Networks:](image)

Figure 5. Routing Networks: Routing Networks take significantly more iterations to train, showing that routing alone may not necessarily be enough for generalizing to new problems: reusing computational units within a computation provides a significant benefit. 10, 50, and 90 percentiles are shown over 6 runs.

We compare our approach to Routing Networks (RN) [67], which we can implement as an ablation of our method by fixing the number of computation steps and using a different controller per target language and per computation step. Figure 5 compares CRL with RN in the multilingual math domain. We observe that the assumptions that Routing Networks make for multitask classification do not necessarily hold for general compositional problems. For example, because RN uses a
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Figure 6. Variations: The minimum number of reducers and translators that can solve the multilingual math problems is 1 and \( m \) respectively, where \( m \) is the number of languages. This is on an extrapolation task, which has more terms and different language pairs.

(a, b): Four reducers and zero translators (red) is a pathological choice of functions that causes CRL to overfit, but it does not when translators are provided. (c) In the non-pathological cases, regardless of the number of functions, the learner metareasons about the resources it has to customize its computation to the problem. 10, 50, and 90 percentiles are shown over 6 runs.

D.2. Variations

Here we study the effect of varying the number of functions available to our learner. Fig. 6a, 6b highlights a particular pathological choice of functions that causes CRL to overfit. If CRL uses four reducers and zero translators (red), it is not surprising that it fails to generalize to the test set: recall that each source language is only seen with four target languages during training with one held out; each reducer can just learn to reduce to one of the four target languages. What is interesting though is that when we add five translators to the four reducers (blue), we see certain runs achieve 100% generalization, even though CRL need not use the translators at all in order to fit the training set. That the blue training curve is slightly faster than the red offers a possible explanation: it may be harder to find a program where each reducer can reduce any source language to their specialized target language, and easier to find programs that involve steps of re-representation (through these translators), where the solution to a new problem is found merely by re-representing that problem into a problem that learner is more familiar with. The four-reducers-five-translators could have overfitted completely like the four-reducers-zero-translators case, but it consistently does not.

Indeed, we find that when we vary the number of reducers in \( \{1, 3\} \) and the number of translators in \( \{5, 8\} \) in Fig. 6c, the extrapolation performance is consistent across the choices of different numbers of functions, suggesting that CRL is quite robust to the number of functions in non-pathological cases.

D.3. How far can we push extrapolation?

The extrapolation accuracy from 6 to 100 terms after training on a curriculum from 2 to 5 terms (46200 examples) on the multilingual arithmetic task (Sec. 4.2). The number of possible 100-term problems is \( (10^{100})(3^{99})(5^{2}) = 4.29 \cdot 10^{148} \) and CRL achieves about 60% accuracy on these problems; a random guess would be 10%.
D.4. Example executions

Here are two randomly selected execution traces from the numerical arithmetic extrapolation task (train on 10 terms, extrapolate to 20 terms), where CRL’s accuracy hovers around 80%. These expressions are derived from the internal representations of CRL, which are softmax distributions over the vocabulary (except for the first expression, which is one-hot because it is the input). The expressions here show the maximum value for each internal representation.

This is a successful execution. The input is $6 \times 1 + 3 - 4 + 6 \times 0 + 0 + 1 - 7 - 3 + 3 + 4 + 1 + 1 + 3 + 3 + 6 + 2 + 7$ and the correct answer is 3. Notice that the order in which controller applies its functions does not strictly follow the order of operations but respects the rules of order of operations: for example, it may decide to perform addition (A) before multiplication (B) if it doesn’t affect the final answer.

This is an unsuccessful execution. The input is $5 + 6 - 4 + 5 \times 7 \times 3 + 8 \times 0 \times 1 - 4 + 6 - 3 + 5 \times 3 + 6 - 0 - 4 - 6$ and the correct answer is 0. Notice that it tends to follow order of operations by doing multiplication first, although it does make mistakes (D), which in this case was the reason for its incorrect answer. Note that CRL never receives explicit feedback about its mistakes on what its functions learn to do or the order in which it applies them; it only receives a sparse reward signal at the very end. Although (C) was a calculation mistake, it turns out that it does not matter because the subexpression would be multiplied by 0 anyways.