Compositional Generalization by Learning Analytical Expressions

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Abstract
Compositional generalization is a basic but essential intellective capability of human beings, which allows us to recombine known parts readily. However, existing neural network based models have been proven to be extremely deficient in such a capability. Inspired by work in cognition which argues compositionality can be captured by variable slots with symbolic functions, we present a refreshing view that connects a memory-augmented neural model with analytical expressions, to achieve compositional generalization. Our model consists of two cooperative neural modules Composer and Solver, fitting well with the cognitive argument while still being trained in an end-to-end manner via a hierarchical reinforcement learning algorithm. Experiments on a well-known benchmark SCAN demonstrate that our model seizes a great ability of compositional generalization, solving all challenges addressed by previous works with 100% accuracies.

1 Introduction
When using language, humans have a remarkable ability to recombine known parts to understand novel sentences they have never encountered before [8, 13, 12]. For example, once a person has learned the meanings of “walk”, “jump” and “walk twice”, it is effortless for him or her to understand the meaning of “jump twice”. This kind of ability relies on the compositionality of language. More formally, compositionality states such a phenomena, where the meaning of a complex expression (e.g. a sentence) is determined by the meanings of its constituents (e.g. the verb “jump” and the adverb “twice”) together with the way these constituents are combined (e.g. an adverb modifies a verb) [35]. Understanding compositionality in language is a basic but essential capacity for human beings, which is argued to be one of the key skills towards human-like machine intelligence [12, 26].

Recently, Lake and Baroni [20] made a step towards exploring and benchmarking the compositional generalization of neural networks. Compositional generalization is argued to be the ability to understand out-of-domain sentences, when the understanding requires leveraging the compositionality in language [30]. The test suite, their proposed Simplified version of the CommAI Navigation (SCAN) dataset, contains compositional navigation commands such as “walk twice” and corresponding action sequences WALK WALK. Such a task lies in the category of machine translation, and thus is expected to be well solved by current state-of-the-art translation models (e.g. sequence to sequence with attention [33, 3]). However, experiments on SCAN demonstrated that modern translation models dramatically fail to obtain a satisfactory performance on compositional generalization. For example,
although the meanings of “walk”, “walk twice” and “jump” have been seen, current models fail to generalize to understand “jump twice”. Subsequent works verified that it was not an isolated case, since convolutional encoder-decoder model and Transformer met the same problem [10]. There have been several attempts towards SCAN, but so far no neural based model can successfully solve all the compositional challenges on SCAN without extra resources [22, 19, 14].

In this paper, we propose a memory-augmented neural model to achieve the compositional generalization by Learning Analytical Expressions (LANE). Motivated by work in cognition which argues compositionality can be captured by variable slots with symbolic functions [4], our memory-augmented architecture is devised to contain two cooperative neural modules accordingly: Composer and Solver. Composer aims to find structured analytical expressions from unstructured sentences, while Solver focuses on understanding these expressions with accessing Memory (Sec. 3). These two modules are trained to learn analytical expressions together in an end-to-end manner via a hierarchical reinforcement learning algorithm (Sec. 4). Experiments on a well-known benchmark SCAN demonstrate that our model seizes a great ability of compositional generalization, reaching 100% accuracies in all tasks (Sec. 5). As far as we know, our model is the first neural model to pass all compositional challenges addressed by previous works on SCAN without extra resources. We will open-source our code upon acceptance, and we believe our work could shed light on the community.

2 Compositional Generalization Assessment

Since the study on compositional generalization of deep neural models is still in its infancy, the overwhelming majority of previous works employ artificial datasets to conduct assessment. As one of the most important benchmarks, the SCAN dataset is proposed to evaluate the compositional generalization ability of translation models [20]. As mentioned above, SCAN describes a simple navigation task that aims to translate compositional navigation sentences into executed action sequences. However, due to the open nature of compositional generalization, there is disagreement about which aspect should be addressed [35, 21, 16, 18]. To conduct a comprehensive assessment, we consider both systematicity and productivity, two important arguments for compositional generalization.

Systematicity evaluates if models can recombine known parts. To assess it, Lake and Baroni [20] proposed three tasks: (i) Add Jump. The pairs of train and test are split in terms of the primitive JUMP. All commands that contain, but are not exactly, the word “jump” form the test set. The rest forms the train set. (ii) Around Right. Any compositional command whose constitutes include “around right” is excluded from the train test. This task is proposed to evaluate whether the model can generalize the experience about “left” to “right”, especially on “around right”. (iii) Length. All commands with long outputs (i.e. output length is longer than 24), such as “around * twice * around” and “around * thrice”, are never seen in training, where ‘*’ indicates a wildcard. More recently, Keysers et al. [18] proposed another assessment, the distribution-based systematicity. It aims to measure the compositional generalization by using a setup where there is a large compound distribution divergence between train and test sets (Maximum Compound Divergence, MCD) [18].

Productivity is thought to be another key argument. It not only requires models to recombine known parts, but also evaluates if they can productively generalize to inputs beyond the length they have seen in training. It relates itself to the unboundedness of languages, which means languages license a theoretically infinite set of possible sentences [4]. To evaluate it, we re-create the SCAN dataset (SCAN-ext). Compared with SCAN using up to one “and” in a sentence, SCAN-ext roughly controls the distribution of input lengths by the number of “and” (e.g. “jump and walk twice and turn left”). Input sentences in the train set consist of at most 2 “and”, while the test set allows at most 9. Except for “and”, the generation of other parts follows the procedure in SCAN.

3 Methodology

In this section, we first show the intrinsic connection between language compositionality and analytical expressions. We then describe how these expressions are learned through our model.
3.1 Problem Statement

Cognitive scientists argue that the compositionality of language indeed constitutes an algebraic system, of the sort that can be captured by symbolic functions with variable slots [4, 12]. As an illustrative example, any adjective attached with a prefix “super-” can be regarded as applying a symbolic function (i.e. “super-adj”) on a variable slot (e.g. “good”), and will be mapped to a new adjective (e.g. “super-good”) [4]. Such a formulation frees the symbolic function from specific adjectives and makes it able to generalize on new adjectives (e.g. “super-bad”).

Taking a more complicated case from SCAN, as shown in Fig. 1, the understanding of “run opposite left after walk twice” can be regarded as a hierarchical application of symbolic functions. In Fig. 1, “$x$” and “$y$” are variables defined in the source domain, and “$X$” and “$Y$” are variables defined in the destination domain. We call a sequence of source domain variables or words (e.g. run) as a source analytical expression (SrcExp), and a sequence of destination domain variables or action words (e.g. RUN) as a destination analytical expression (DstExp). If there is no variable in an SrcExp (or DstExp), it is also a constant SrcExp (or DstExp). From bottom to up, each phrase marked blue represents an SrcExp which will be superseded by a source domain variable (e.g. $x$) when moving to the next hierarchy of understanding. These SrcExps can be recognized and translated into their corresponding DstExps by a set of symbolic functions. We call such SrcExps as recognizable SrcExps, and their corresponding DstExps as recognizable DstExps. By iterative recognizing and translating recognizable SrcExps, we can construct a tree hierarchy with a set of recognizable DstExps. By assigning values to the destination variables in recognizable DstExps recursively (dotted red arrows in Fig. 1), we can finally obtain a constant DstExp as the final resulted sequence.

It is well known that, variables are pieces of memory in computers, and a memory mechanism can be used to support variable-related operations. Thus we propose a memory-augmented neural model to achieve compositional generalization by automatically learning the above analytical expressions.

3.2 Model Design

Our model consists of three components: Composer, Solver and Memory. Composer accepts an SrcExp as input, and aims to find a recognizable SrcExp inside it. Solver first translates the recognizable SrcExp into a recognizable DstExp, and then assigns values to destination variables in the recognizable DstExp, obtaining a constant DstExp. Memory is designed to support variable-related operations in a differentiable manner [32]. The understanding of a sentence is an iterative procedure involving these three components, and below we take step $t$ as an example.

Composer Given an SrcExp $w^t$, Composer aims to find a recognizable SrcExp $\tilde{w}^t$. There are several ways to implement it, where we choose to gradually merge elements of $w^t$ until a recognizable SrcExp appears. For example, given “$x$ after $y$”, at first Composer merges “$x$” and “after”. Then it checks if “$x$ after” is a recognizable SrcExp. The answer for this case is NO, so Composer continues to merge “$x$ after” with “$y$”. Next, it checks if “$x$ after $y$” is a recognizable SrcExp. Fortunately, it is, and thus Composer triggers Solver to translate it. As indicated by the example, the overall procedure is iterative, and thus achieved by iteratively building a binary tree from bottom to up. That is to say, viewing elements of $w^t$ as nodes, Composer iteratively merges two neighboring nodes into a parent node at each layer (i.e. the merge process), and checks if the parent node represents a recognizable SrcExp (i.e. the check process).
The merge process is implemented by first enumerating all possible parent nodes of the current layer, and then selecting the one which has the highest merging score. Assuming \(i\)-th and \((i+1)\)-th node at layer \(l\) are represented by \(r^l_i\) and \(r^l_{i+1}\) respectively, their parent representation \(r^{l+1}_i\) can be obtained via a standard Tree-LSTM encoding \(r^l_i, r^l_{i+1}\) as input. As shown inside Composer in Fig. 2, given all parent node representations (blue neurons), Composer selects the parent node (solid lines with arrows) whose merging score is the maximum. In fact, the merging score measures the merging priority of \(r^l_{i+1}\) using a learnable query vector \(q\) by \(\langle q, r^l_{i+1}\rangle\), where \(\langle\cdot, \cdot\rangle\) represents the inner product. Once the parent node for layer \(l\) is determined, the check process is called.

The check process is to check if a parent node represents a recognizable SrcExp. Concretely, denoting \(r^l_{i+1}\) the parent node representation, an affine transformation is built based on it to obtain the probability \(p_c = \sigma(W_c r^l_{i+1} + b_c)\) where \(W_c\) and \(b_c\) are learned parameters and \(\sigma\) is the sigmoid function. \(p_c > 0.5\) means that the parent node represents a recognizable SrcExp, and thus Composer triggers Solver to translate it. Otherwise, the parent node and other unmerged nodes enter a new layer \(l+1\), based on which Composer restarts the merge process.

**Solver** Given a recognizable SrcExp \(\hat{w}\), Solver first translates it into a recognizable DstExp, and then obtains a constant DstExp \(\hat{d}\) via variable assignment through interacting with Memory. To achieve this, Solver is designed to be an LSTM-based sequence to sequence network with an attention mechanism [3]. It generates the recognizable DstExp via decoding step by step. At each step, Solver either generates an action word, or a destination variable. Using the recognizable DstExp as the skeleton, Solver obtains a constant DstExp by replacing each destination variable with its corresponding constant DstExp stored in Memory.

**Memory** There are a number of items in Memory, each of which contains a source vector (SrcVec), a destination vector (DesVec), and a value slot to temporarily store a constant DstExp. Here, the source vectors (yellow neurons) and destination vectors (red neurons) are learnable vectors, which are used to represent source variables (e.g. \(\$x, \$y\)) and destination variables (e.g. \(\$X, \$Y\)) respectively.

**Interaction** The understanding of a sentence takes several steps iteratively. At each step, Composer, Solver and Memory interact with each other. To illustrate the interaction clearly, Fig. 2 presents the overall procedure of our model at step \(t\) and \(t+1\) in detail (corresponding to step 5 and 6 in Fig. 1). Despite that variables are implemented by vectors, below we still call them variables for better illustration. At the beginning of step \(t\), an SrcExp \(\$x\ after \$y\ twice\) is fed into Composer. Then Composer finds a recognizable SrcExp \(\$y\ twice\) and sends it to Solver. Receiving \(\$y\ twice\), Solver first translates it into \(\$Y \$Y\). Using \(\$Y \$Y\) as the skeleton, Solver obtains \(\text{WALK} \ \text{WALK}\) by replacing \(\$Y\) with its corresponding constant DstExp \(\text{WALK}\) stored in Memory. Meanwhile, since \(\text{WALK}\) has been used, the value slot which stores \(\text{WALK}\) is set to be empty. Next, Solver applies for one item with an empty value slot in Memory, i.e. the item containing \(\$y\) and \(\$Y\), and then writes \(\text{WALK} \ \text{WALK}\) into its value slot. Finally, the recognizable SrcExp \(\$y\ twice\) in \(\hat{w}\) is superseded with \(\$Y\), producing \(\$x\ after \$y\) as the input for the next step. Such a procedure is repeated until the
We begin by introducing some preliminary formulations for our HRL algorithm. Denoting $s^t$ as the state at step $t$, it contains both $w^t$ and Memory. The action of Composer, denoted by $G^t$, is the recognizable SrcExp to be found at step $t$. Given $s^t$ as observation, the parameter of Composer $\theta$ defines a high-level policy $\pi_\theta(G^t | s^t)$. Once a high-level action $G^t$ is produced, the low-level agent Solver is triggered to react following a low-level policy conditioned on $G^t$. In this sense, the high-level action can be viewed as a sub-goal for the low-level agent. Denoting $a^t$ the action of Solver, the low-level policy $\pi_\varphi(a^t | G^t, s^t)$ is parameterized by the parameter of Solver $\varphi$. $a^t$ is the constant DstExp output by Solver at step $t$. More implementation details about $\pi_\theta$ and $\pi_\varphi$ can be found in the supplementary material.

### 4.1 Hierarchical Reinforcement Learning

We begin by introducing some preliminary formulations for our HRL algorithm. Denoting $s^t$ as the state at step $t$, it contains both $w^t$ and Memory. The action of Composer, denoted by $G^t$, is the recognizable SrcExp to be found at step $t$. Given $s^t$ as observation, the parameter of Composer $\theta$ defines a high-level policy $\pi_\theta(G^t | s^t)$. Once a high-level action $G^t$ is produced, the low-level agent Solver is triggered to react following a low-level policy conditioned on $G^t$. According to (i.e. step $T$) and predict the output action sequence, forming a trajectory $\tau = (s^1, a^1, \ldots, s^T, G^T, a^T)$. Once $\tau$ is determined, the reward is collected to optimize $\theta$ and $\varphi$ using policy gradient.

Denoting $R(\tau)$ as the reward of a trajectory $\tau$ (elaborated in Sec. 4.2), the training objective of our model is to maximize the expectation of rewards as:

$$
\max_{\theta, \varphi} J(\theta, \varphi) = \max_{\theta, \varphi} \mathbb{E}_{\tau \sim \pi_{\theta, \varphi}} R(\tau).
$$

Applying the likelihood ratio trick, $\theta$ and $\varphi$ can be optimized by ascending the following gradient:

$$
\nabla_{\theta, \varphi} J(\theta, \varphi) = \mathbb{E}_{\tau \sim \pi_{\theta, \varphi}} R(\tau) \nabla_{\theta, \varphi} \log \pi_{\theta, \varphi}(\tau).
$$

Expanding the above equation via the chain rule we can obtain:

$$
\nabla_{\theta, \varphi} J(\theta, \varphi) = \mathbb{E}_{\tau \sim \pi_{\theta, \varphi}} \sum_t R(\tau) \left[ \nabla_{\theta, \varphi} \log \pi_{\theta} (G^t | s^t) + \nabla_{\theta, \varphi} \log \pi_{\varphi} (a^t | G^t, s^t) \right].
$$

Considering the search space of $\tau$ is huge, the REINFORCE algorithm is leveraged to approximate Eq. 3 by sampling $\tau$ from $\pi_{\theta, \varphi}$ for $N$ times. Furthermore, the technique of subtracting a baseline $\hat{R}$ is employed to reduce variance, where the baseline is the mean reward over sampled $\tau$.

**Differential Update** Unlike standard Reinforcement Learning (RL) algorithms, we introduce a differential update strategy to optimize Composer and Solver via different learning rates. It is motivated by an intuition that actions of a high-level agent cannot be changed quickly. According to Eq. 3, simplifying $\mathbb{E}_{\tau \sim \pi_{\theta, \varphi}}$ as $\mathbb{E}$, the parameters of Composer and Solver are optimized as:

$$
\theta \leftarrow \theta + \alpha \cdot \mathbb{E} R(\tau) \sum_t \nabla_{\theta} \log \pi_{\theta} (G^t | s^t), \quad \varphi \leftarrow \varphi + \beta \cdot \mathbb{E} R(\tau) \sum_t \nabla_{\varphi} \log \pi_{\varphi} (a^t | G^t, s^t),
$$

where Solver’s learning rate $\beta$ is greater than Composer’s learning rate $\alpha$. In our experiments, the AdaDelta optimizer is employed to optimize our model, with $\alpha$ and $\beta$ as 0.1 and 1.0 respectively.
4.2 Reward Design

The design of the reward function is critical to an RL based algorithm. Bearing this in mind, we design our reward from two aspects: similarity and simplicity. It is worth noting that both rewards work globally, i.e., all actions share the same reward, as indicated by dotted lines in Fig. 3.

Similarity-based Reward  It is based on the similarity between the model’s output and the ground-truth. Since the output of our model is an action sequence, a kind of sequence similarity, the Intersection over Union (IoU) similarity, is employed as the similarity-based reward function. Given the sampled output $a^T$ and the ground-truth $o$, the similarity-based reward is computed by:

$$R_s(\tau) = \frac{|a^T \cap o|}{(|a^T| + |o| - |a^T \cap o|)},$$

where $a^T \cap o$ means the longest common substring between $a^T$ and $o$, and $|\cdot|$ represents the length of a sequence. Compared with exact matching, such a reward alleviates the reward sparsity issue.

Simplicity-based Reward  Inspired by Occam’s Razor principle that “the simplest solution is most likely the right one”, we try to encourage our model to have the fewest kinds of learned recognizable DstExps. In other words, we encourage the model to fully utilize variables and be more generalizable. Taking an illustration of “jump twice” $[\text{jump twice} \rightarrow \text{JUMP JUMP}]$ and $[\text{jump} \rightarrow \text{JUMP}, \text{\$x twice} \rightarrow \text{\$X \$X}]$ both result in correct outputs. Intuitively, the latter is more generalizable as it enables Solver to reuse learned recognizable DstExps, more in line with the Occam’s Razor principle. Concretely, when understanding a novel input “walk twice”, $\text{\$x twice} \rightarrow \text{\$X \$X}$ can be reused. Denoting $T^*$ as the number of steps where the recognizable DstExp only contains destination variables, we design a reward $R_a(\tau) = T^*/T$ as a measure of the simplicity. The final reward function $R(\tau)$ is a linear summation as $R(\tau) = R_s(\tau) + \gamma \cdot R_a(\tau)$, where $\gamma$ is a hyperparameter that is set as 0.5 in our experiments.

4.3 Curriculum Learning

One typical strategy for improving model generalization capacity is to use curriculum learning, which arranges examples from easy to hard in training [25, 1]. Motivated by it, we divide the training into different lessons according to the length of the input sequence. Our model starts training on the simplest lesson, and then the lesson complexity gradually increases. Besides, as done in literature [7], we accumulate training data from previous lessons to avoid catastrophic forgetting.

5 Experiments

In this section, we conduct a series of experiments to evaluate our model on various compositional tasks mentioned in Sec. 2. We then verify the importance of each component via a thorough ablation study. Finally we present two real cases to illustrate our model concretely. More implementation details of our model can be found in the supplementary material.

5.1 Experimental Setup

Task  Here we introduce Tasks used in our experiments. Systematicity is evaluated on Add Jump, Around Right and Length of SCAN [20], while distribution-based systematicity is assessed on MCD splits of SCAN [13]. MCD uses a nondeterministic algorithm to split examples into the train set and the test set. By using different random seeds, it introduces three tasks MCD1, MCD2, and MCD3. Productivity is evaluated on the SCAN-ext dataset. Besides them, we also conduct experiments on the Simple task of SCAN which requires no compositional generalization capacity, and the Limit task of MiniSCAN [21] which evaluates if models can learn compositional generalization when given limited (i.e. 14) training data. We follow previous works to split datasets for all tasks.

Baseline  We consider a range of state-of-the-art models on SCAN compositional tasks as our baselines. In terms of the usage of extra resources, we divide them into two groups: (i) No Extra Resources includes vanilla sequence to sequence with attention (Seq2Seq) [20, 24], convolutional sequence to sequence (CNN) [10], Transformer [37], Universal Transformer [9], Syntactic Attention [30] and Compositional Generalization for Primitive Substitutions (CGPS) [22], (ii) Using Extra Resources consists of Good Enough Compositional Data Augmentation (GECA) [2].
while a strong baseline CGPS shows a sharp drop. Furthermore, to the best of our knowledge, LA
perform perfectly, i.e. 100\% test accuracy on all tasks. Compared with state-of-the-art baselines without extra resources, LANE achieves significantly higher performance. Even in contrast to baselines with extra resources, LANE is highly competitive, suggesting that LANE is capable of learning human prior knowledge to some extent. Although program synthesis [28] also achieves perfect accuracies, it heavily depends on a predefined meta-grammar where decent task-related knowledge is encoded. As far as we know, LANE is the first neural model to pass all tasks without extra resources.

| Extra Resources | Model | Sample | Add Jump | Around Right | Length |
|-----------------|-------|--------|----------|--------------|--------|
| None            | Seq2Seq [20, 24] | 99.7 ± 0.3 | 1.2 | 2.5 ± 0.2 | 13.8 ± 0.5 |
|                 | CNN [10] | 100.0 ± 0.0 | 69.2 ± 0.2 | 56.7 ± 10.2 | 0.0 ± 0.0 |
|                 | Syntactic Attention [20] | 100.0 | 91.0 ± 27.4 | 28.9 ± 34.8 | 15.2 ± 0.7 |
|                 | CGPS [22] | 99.9 ± 0.1 | 98.8 ± 1.4 | 83.2 ± 13.2 | 20.3 ± 1.1 |
|                 | LANE (Ours) | 100.0 | 100.0 | 100.0 | 100.0 |

| Data Augmentation | Model | Limit |
|-------------------|-------|-------|
| GECA [2] | Human [21] | 84.3 |
| Meta Seq2Seq [19] | Seq2Seq | 2.5 |
| Equivariant Seq2seq [14] | CGPS | 76.0 |
| Program Synthesis [28] | Meta Seq2Seq | 100.0 |
| LANE (Ours) | LANE (Ours) | 100.0 |

5.2 Experimental Results

**Experiment 1: Systematicity on SCAN** As shown in Tab. 1, LANE achieves 100\% test accuracy on all tasks. Compared with state-of-the-art baselines without extra resources, LANE achieves significantly higher performance. Even in contrast to baselines with extra resources, LANE is highly competitive, suggesting that LANE is capable of learning human prior knowledge to some extent. Although program synthesis [28] also achieves perfect accuracies, it heavily depends on a predefined meta-grammar where decent task-related knowledge is encoded. As far as we know, LANE is the first neural model to pass all tasks without extra resources.

**Experiment 2: Distribution-based Systematicity on SCAN** LANE also achieves 100\% accuracy on the more challenging distribution-based systematicity tasks (see Tab. 2). By comparing Tab. 1 and Tab. 2, one can find LANE maintains a stable and perfect performance regardless of the task, while a strong baseline CGPS shows a sharp drop. Furthermore, to the best of our knowledge, LANE is also the first one to pass the assessment of distribution-based systematicity on SCAN.

**Experiment 3: Productivity** As shown in Fig. 4, there is a sharp divergence between input lengths of train and test set on SCAN-ext, suggesting it is a feasible benchmark for productivity. From the results (right), one can find that test accuracies of baselines are mainly ruled by the frequency of input lengths in the train set. In contrast, LANE maintains a perfect trend as the input length increases, indicating it has productive generalization capabilities. Furthermore, the trend suggests the potential of LANE on tackling inputs with unbounded length.

**Experiment 4: Compositional Generalization on MiniSCAN** Tab. 2 (right) shows the performance of various methods given limited training data, and LANE remains highly effective. Without extra resources such as permutation-based augmentation employed by Meta Seq2Seq, our model performs perfectly, i.e. 100\% on the Limit task. Compared with the human performance 84.3\% [21], to a certain extent, our model is close to the human ability at learning compositional generalization.
from few examples. However, it does not imply that either our model or Meta Seq2Seq triumphs over humans in terms of compositional generalization, as the Limit task is relatively simple.

5.3 Closer Analysis

We conduct a thorough ablation study in Tab. 3 to verify the effectiveness of each component. “w/o Composer” ablates the check process of Composer, making our model degenerate into a tree to sequence model, which employs a Tree-LSTM to build trees and encode input sequences dynamically. “w/o Curriculum Learning” means training our model on the full train set from the beginning. As the result shows, ablating each of above causes an enormous performance drop, indicating the necessity of Composer and the curriculum learning. “w/o Simplicity-based Reward”, which only considers the similarity-based reward, fails on several tasks such as Around Right. We attribute its failure to its inability to learn sufficiently general recognizable DstExps from the data. As for the differential update, we compare the results of several learning rate combinations in Fig. 5. As indicated, our designed differential update strategy is essential for successful convergence and high test accuracies. Meanwhile, LANE does not rely heavily on a particular combination of learning rates, suggesting its robustness. Last, we present learned tree structures of two real cases in Fig. 6. Observing that “twice” behaves differently under different contexts, it is non-trivial to produce such trees.

| Variant               | Simple | Add Jump | Length | Around Right | MCD1 | MCD2 | MCD3 |
|-----------------------|--------|----------|--------|--------------|------|------|------|
| w/o Composer          | 98.5 ± 0.6 | 0.0     | 11.1 ± 13.1 | 0.0        | 5.3 ± 2.4 | 0.7 ± 0.3 | 2.6 ± 0.9 |
| w/o Curriculum Learning | 0.0     | 0.0     | 0.0    | 0.0          | 0.0  | 0.0  | 0.0  |
| w/o Simplicity-based Reward | 100.0   | 100.0   | 100.0  | 0.0          | 100.0| 100.0| 78.8 ± 4.2 |

Figure 5: Accuracies on train set (left) and test set (right) under different learning rate combinations.

Figure 6: Learned tree structures in Composer of two real cases.

6 Related Work

The most related work is the line of exploring compositional generalization on neural networks, which has attracted a large attention on different topics in recent years. Under the topic of mathematical reasoning, Veldhoen et al. [35] explored the algebraic compositionality of neural networks via simple arithmetic expressions, and Saxton et al. [31] pushed the area forward by probing if the standard Seq2Seq model can resolve complex mathematical problems. Under the topic of logical inference, previous works devoted to testing the ability of neural networks on inferring logical relations between pairs of artificial language utterances [6,29]. Our work differently focuses more on the compositionality in languages, benchmarked by the SCAN compositional tasks [20].

As for the SCAN compositional tasks, there have been several attempts. Inspired by work in neuroscience which suggests a disjoint processing on syntactic and semantic, Russin et al. [30] proposed the Syntactic Attention model. Analogously, Li et al. [22] employed different representations for primitives and functions respectively (CGPS). Unlike their separate representations, our proposed Composer and Solver can be seen as separate at the module level. There are also some works which impose prior knowledge of compositionality via extra resources. Andreas [2] presented a data augmentation technique to enhance standard approaches (GECA). Lake [19] argued to achieve compositional generalization by meta learning, and thus they employed a Meta Seq2Seq model with
a memory mechanism. Regarding the memory mechanism, our work is similar to theirs. However, their training process, namely permutation training, requires handcrafted data augmentation. In a follow-up paper [28], they argued to generalize via the paradigm of program synthesis. Despite the nearly perfect performance, it also requires a predefined meta-grammar, where decent knowledge is encoded. Meanwhile, based on the group-equivariance theory, Gordon et al. [14] predefined local groups to enable models aware of equivariance between verbs or directions (Equivariant Seq2Seq). The biggest difference between our work and theirs is that we do not utilize any extra resource.

Our work is also related to those which apply RL on language. In this sense, using language as the abstraction for HRL [17] is the most related work. They proposed to use sentences as the sub-goal for the low-level policy in vision-based tasks, while we employ recognizable SrcExps as the sub-goal. In addition, the applications of RL on language involves topics such as natural language generation [11], conversational semantic parsing [23] and text classification [42].

7 Conclusion & Future Work

In this paper, we propose to achieve compositional generalization by learning analytical expressions. Motivated by work in cognition, we present a memory-augmented neural model which contains two cooperative neural modules Composer and Solver. These two modules are trained in an end-to-end manner via a hierarchical reinforcement learning algorithm. Experiments on a well-known benchmark demonstrate that our model solves all challenges addressed by previous works with 100% accuracies, surpassing existing baselines significantly. For future work, we plan to extend our model to a recently proposed compositional task CFQ [18] and more realistic applications.

Broader Impact

This work explores the topic of compositional generalization capacities in neural networks, which is a fundamental problem in artificial intelligence but not involved in real applications at now. Therefore, there will be no foreseeable societal consequences nor ethical aspects.

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As mentioned in Sec. 3, a Tree-LSTM \cite{li2015structured} model is employed to accomplish the merge process in Composer. Similar to LSTM, Tree-LSTM uses gate mechanisms to control the flow of information from child nodes to parent nodes. Meanwhile, it maintains a hidden state and a cell state analogously. Denoting $r^l_i$ as the node representation of $i$-th node at layer $l$, it consists of the hidden state vector $h^l_i$ and the cell state vector $c^l_i$. For any parent node, its node representation $r^l_i$ ($l > 1$) can be obtained by merging its left child node representation $r^{l-1}_{i-1} = (h^{l-1}_{i-1}, c^{l-1}_{i-1})$ and right child node representation $r^{l-1}_{i+1} = (h^{l-1}_{i+1}, c^{l-1}_{i+1})$ as:

$$
\begin{bmatrix}
\sigma \\
\sigma \\
e
\end{bmatrix}
\begin{bmatrix}
W_{\text{tree}} & \left[ h^{l-1}_{i-1} \right] + b_{\text{tree}} \\
\tanh
\end{bmatrix},
$$

where $W_{\text{tree}} \in \mathbb{R}^{5D_h \times 2D_h}$ is a learnable matrix, $b_{\text{tree}} \in \mathbb{R}^{5D_h}$ is a learnable vector, $\sigma$ and $\tanh$ are activation functions, and $\odot$ represents the element-wise product. As for leaf nodes, their representations $r^l_i$ ($l = 1$) can be obtained by applying leaf transformation on the embeddings of their corresponding elements $w^l_i$ (e.g. $\$x$, after) as:

$$
\begin{bmatrix}
h^l_i \\
c^l_i
\end{bmatrix}
= W_{\text{leaf}} \text{Emb}\left( w^l_i \right) + b_{\text{leaf}},
$$

where $W_{\text{leaf}} \in \mathbb{R}^{2D_h \times D_h}$ is a learnable matrix, $b_{\text{leaf}} \in \mathbb{R}^{2D_h}$ is a learnable vector, $w^l_i$ is the $i$-th element of $w^l$, and $\text{Emb}(w^l_i) \in \mathbb{R}^{D_h}$ represents the word embedding if $w^l_i$ is a word, otherwise the key vector of the source domain variable $w^l_i$.

\begin{itemize}
    \item **Details about Policy**
    
    In the following, we will explain the high-level policy $\pi_\theta$ and the low-level policy $\pi_\phi$ in detail. For the sake of clarity, we simplify $s^l$, $G^l$ and $a^l$ as $s$, $G$ and $a$, respectively.

    **High-level policy** Given $s$, the high-level agent picks $G$ according to the high-level policy $\pi_\theta( G | s )$ parameterized by $\theta$. As mentioned in Sec. 3, $G$ is obtained by applying in turn the merge and check process. Denoting the decisions made in the merge and check process at layer $l$ as $M_l$ and $C_l$, they

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are governed by parameters $\theta_M$ and $\theta_C$, respectively. A high-level action $G$ is indeed a sequence of $M$ and $C$ as $(M_1 C_1 \cdots M_L C_L)$, where $L$ represents the highest layer. Therefore, $\pi_\theta(G \mid s)$ is expanded as:

$$\pi_\theta (G = (M_1 C_1 \cdots M_L C_L) \mid s) = \prod_{l=1}^{L} \pi_{\theta,M} (M_l \mid s, M_{<l}, C_{<l}) \pi_{\theta,C} (C_l \mid s, M_{<l+1}, C_{<l}),$$  \hspace{1cm} (8)

where $\pi_{\theta,M}$ is implemented by a Tree-LSTM with a learnable query vector $q$ (mentioned in Sec. 3.2). Assuming there are $K$ parent node candidates for layer $l$, $M^l$ is a one-hot vector drawn from a $K$-dimensional categorical distribution $\pi_{\theta,M} (M_l \mid s, M_{<l}, C_{<l})$ with the weight $(p_1, \cdots, p_K)$. For the $k$-th parent node candidate, represented by $r_{k}^{l+1}$, its selection probability $p_k$ is computed by normalizing over all merging scores (mentioned in Sec. 3.2) as:

$$p_k = \frac{\exp (\langle q, r_k^{l+1} \rangle)}{\sum_{k=1}^{K} \exp (\langle q, r_k^{l+1} \rangle)}.$$  \hspace{1cm} (9)

As for $\pi_{\theta,C} (C_l \mid s, M_{<l+1}, C_{<l})$ in the check process, it follows a Bernoulli distribution with expectation $p_c^l = \sigma(W_{s}^{l+1} r_{k}^{l+1} + b_c)$, where $\theta_C = \{W_c, b_c\}$ are learned parameters. $p_c$ is indeed the trigger probability $p_c$ mentioned in Sec. 3.2.

**Low-level policy** When the high-level action $G$ is determined, the low-level agent is triggered to output $a$ according to the low-level policy $\pi_\varphi(a \mid G, s)$. The policy $\pi_\varphi(a \mid G, s)$ is implemented by an LSTM-based sequence to sequence network with an attention mechanism, i.e.,

$$\pi_\varphi(a = (a_1 \cdots a_M) \mid G, s) = \prod_{m=1}^{M} \pi_\varphi(a_m \mid G, s, a_{<m}),$$  \hspace{1cm} (10)

where $M$ is the number of decoding steps and $a_m$ represents an action word (e.g. **JUMP**), or a destination variable (e.g. $SY$) which will be replaced by its corresponding constant DstExp stored in Memory. At each decoding step, $a_m$ is sampled from a categorical distribution, whose sample space consists of all action words and destination variables with non-empty value slots.

**C Chain Rule Derivation**

Looking back to Eq. 8, the parameters $\theta$ and $\varphi$ can be optimized by ascending the following gradient:

$$\nabla_{\theta, \varphi} J(\theta, \varphi) = E_{\tau \sim \pi_\theta, \varphi} R(\tau) \nabla_{\theta, \varphi} \log \pi_{\theta, \varphi}(\tau),$$  \hspace{1cm} (11)

where the policy $\pi_{\theta, \varphi}$ can be further decomposed into a sequence of actions and state transitions:

$$\pi_{\theta, \varphi}(\tau) = p(s^1 G^1 a^1 \cdots s^T G^T a^T)$$

$$= p(s^1) \prod_{t=1}^{T} \pi_{\theta, \varphi}(a^t, G^t \mid s^t) p(s^{t+1} \mid s^t, G^t, a^t).$$  \hspace{1cm} (12)

Consider that the low-level action $a^t$ is conditioned on the high-level action $G^t$, which means that $\pi_{\theta, \varphi}(a^t, G^t \mid s^t) = \pi_\theta(G^t \mid s^t) \pi_\varphi(a^t \mid G^t, s^t)$, and thus $\pi_{\theta, \varphi}(\tau)$ can be expanded as:

$$\pi_{\theta, \varphi}(\tau) = p(s^1) \prod_{t=1}^{T} \pi_{\theta}(G^t \mid s^t) \pi_{\varphi}(a^t \mid G^t, s^t) p(s^{t+1} \mid s^t, G^t, a^t).$$  \hspace{1cm} (13)

Since the state at step $t + 1$ is fully determined by the state and actions at step $t$, not dependent on the policy parameters $\theta$ and $\varphi$, the gradients of $p(s^{t+1} \mid s^t, G^t, a^t)$ and $p(s^t)$ with respect to $\theta$ and $\varphi$ are 0. Therefore, $\nabla_{\theta, \varphi} J(\theta, \varphi)$ can be expanded as:

$$\nabla_{\theta, \varphi} J(\theta, \varphi) = E_{\tau \sim \pi_{\theta, \varphi}} R(\tau) \nabla_{\theta, \varphi} \log \pi_{\theta, \varphi}(\tau),$$

$$= E_{\tau \sim \pi_{\theta, \varphi}} R(\tau) \nabla_{\theta, \varphi} \sum_{t=1}^{T} \left[ \log \pi_{\theta}(G^t \mid s^t) + \log \pi_{\varphi}(a^t \mid G^t, s^t) \right],$$  \hspace{1cm} (14)

$$= E_{\tau \sim \pi_{\theta, \varphi}} R(\tau) \sum_{t=1}^{T} \left[ \nabla_{\theta, \varphi} \log \pi_{\theta}(G^t \mid s^t) + \nabla_{\theta, \varphi} \log \pi_{\varphi}(a^t \mid G^t, s^t) \right].$$
Table 4: The dataset splits for all tasks.

| Dataset | Simple | Add Jump | Around Right | Length | MCD (1/2/3) | Extend | MiniSCAN | Limit |
|---------|--------|----------|--------------|--------|-------------|--------|----------|-------|
| Train Size | 16728 | 14670 | 15225 | 16990 | 8365 | 20506 | 14 |
| Test Size | 4182 | 7706 | 4476 | 3920 | 1045 | 4000 | 8 |

D Implementation Details

Our model is implemented in PyTorch [29]. All experiments use the same hyperparameters. Dimensions of word embeddings, hidden states, key vectors and value vectors are set as 128. Hyperparameters $\gamma$ and $N$ are set as 0.5 and 10 respectively. All parameters are randomly initialized and updated via the AdaDelta [41] optimizer, with a learning rate of 0.1 for Composer and 1.0 for Solver. Meanwhile, as done in previous works [15], we introduce a regularization term to prevent our model from overfitting in the early stage of training. Its weight is set to 0.1 at the beginning, and exponentially anneals with a rate 0.5 as the lesson increases. The source code has been submitted as part of the supplementary material. As for data splits, we split each dataset into the train set and the test set for all tasks according to previous works. More details about train and test sizes can be seen in Tab. 4. More specifically, except for the task Limit, we further randomly take 20% training data as the development set to tune the hyperparameters, with the rest being the train set.