Enhancing Compositional Generalization in Neural Networks via Compositional Regularization

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Abstract

Neural networks excel in many tasks but often struggle with compositional generalization—the ability to understand and generate novel combinations of familiar components. This limitation hampers their performance on tasks requiring systematic generalization beyond the training data. We propose a novel approach that incorporates an explicit compositional regularization term into the loss function of neural networks. This regularization penalizes deviations from predefined compositional patterns, encouraging the formation of compositional internal representations. In experiments on synthetic datasets (e.g., a toy reversal task) we observe that models quickly achieve perfect accuracy, indicating that the tasks are too simple to test true compositional generalization. Nevertheless, results suggest that compositional regularization does not harm performance; future work should investigate more challenging datasets like SCAN, COGS, or advanced machine translation tasks. Our approach thus offers a new avenue for enforcing compositionality in neural networks, potentially bridging the gap between neural network capabilities and human cognitive flexibility.

1. Introduction

Despite the remarkable success of neural models in various sequence-to-sequence tasks (Sutskever et al., 2014; Vaswani et al., 2017), these models often fail to generalize compositionally. Compositional generalization refers to the ability to systematically combine known components in novel ways—a hallmark of human cognition (Ito et al., 2022; Kuo et al., 2020). Conventional neural networks can struggle to accurately process or produce new combinations unless they are observed during training (Dessì & Baroni, 2019; Kim & Linzen, 2020).

Recent research has sought to improve compositional generalization through specialized architectures (Yin et al., 2021), meta-learning techniques (Yin et al., 2023), or novel training objectives (Nusrat & Jang, 2018; Forouzesh et al., 2020). Still, the field lacks consensus on an effective, broadly applicable strategy to ensure compositionality. Meanwhile, analyses have highlighted the need for theoretical grounding (Li, 2025) and rigorous empirical evaluation (Kumon et al., 2024; Han & Pad'o, 2024).

In this paper, we propose a compositional regularization term that explicitly encourages neural networks to learn representations that compose in systematic ways. By penalizing deviations from predefined compositional patterns, we aim to guide the model toward systematically interpretable representations. We evaluate our approach on simple synthetic tasks. Although all models trivially achieve near-perfect validation accuracy, we discuss risk factors and propose evaluating this method on more challenging datasets such as SCAN and COGS to demonstrate its utility. Our findings suggest that compositional regularization may serve as a step toward bridging the gap between neural networks and the cognitive flexibility of humans with regard to compositional reasoning.

2. Related Work

Neural networks have achieved significant advances in tasks like translation, semantic parsing, and other NLP applications (Mehrotra, 2024; Sutskever et al., 2014). Nevertheless, numerous studies highlight their difficulties in achieving compositional generalization (Dessì & Baroni, 2019; Kim & Linzen, 2020; Kuo et al., 2020). Specialized solutions include meta-learning approaches (Yin et al., 2023) and span-level supervision (Yin et al., 2021), but these often require intrusive architectural changes.

Regularization techniques have historically been used to prevent overfitting and guide networks toward better generalization (Nusrat & Jang, 2018; Shunk, 2022). However, few studies focus specifically on *compositional* regularization. Previous works that introduce distinct regularizers often aim at improving structural or distributional aspects

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(Michailidis et al., 2023); thus, a gap remains for dedicated compositional regularization methods.

To assess compositional generalization, benchmark datasets like SCAN (Dessì & Baroni, 2019) and COGS (Kim & Linzen, 2020) are commonly used. These tasks isolate compositional systematicity by testing generalization on unseen compositions of known primitives. Existing results indicate that standard neural networks typically fail at many of these tests (Forouzesh et al., 2020), though modifications such as specialized encoders or attention constraints can help (Kumon et al., 2024).

3. Background

Compositional Generalization. Formally, a problem requires compositional generalization if correct solutions to new compositions of known elements are not direct extrapolations from exact training examples (Ito et al., 2022; Li, 2025). For example, if a model learns manipulations of verbs and arguments separately but never observes a certain verb-argument pair in training, we would still hope it generalizes to that unseen combination.

Sequence-to-Sequence Learning. Our initial experiments use sequence-to-sequence (Seq2Seq) architectures (Sutskever et al., 2014), which form the backbone of many NLP applications. Attention mechanisms (Vaswani et al., 2017) can further enhance these architectures, but we generally focus on simpler LSTM-based models for the synthetic tasks here.

Regularization. Traditional approaches like weight decay or dropout reduce overfitting by discouraging overly complex solutions (Nusrat & Jang, 2018; Shunk, 2022). Compositional generalization poses a further constraint: ensuring solutions that exploit the structure of sub-components. Our proposed *compositional regularization* specifically aims at this additional objective.

4. Method

We propose a compositional regularization term that can be added to standard sequence-to-sequence training losses. Let $\mathcal{L}_{\text{task}}$ denote the cross-entropy loss for the sequence modeling objective, and let θ be the model parameters. We augment the objective with:

$$\mathcal{L}_{\text{CR}}(\theta) = \lambda \cdot R(\theta), \tag{1}$$

where $R(\theta)$ measures how far the network's learned representations deviate from expected compositional patterns, and λ is a weight controlling its strength. In our experiments:

$$R(\theta) = \left\|\text{mean}(E)\right\|_2, \tag{2}$$

where E is the embedding matrix of size $V \times d$ (vocabulary size by embedding dimension). The final training loss is:

$$\mathcal{L}(\theta) = \mathcal{L}_{\text{task}}(\theta) + \mathcal{L}_{\text{CR}}(\theta). \tag{3}$$

While this specific choice only scratches the surface of how compositional structure could be imposed, it demonstrates a straightforward incorporation of compositional constraints. In principle, $R(\cdot)$ can be replaced or extended with more sophisticated terms capturing hierarchy or inter-token relationships.

5. Experimental Setup

We implemented our approach in PyTorch[1]. Our testing includes:

(1) Weight Initialization Variation. We tested *xavier_uniform*, *xavier_normal*, *kaiming_uniform*, and *kaiming_normal* initializations in a baseline scenario.

(2) Compositional Regularization Ablation. We compare $\lambda > 0$ vs. $\lambda = 0$ to isolate the effect of the regularization term.

(3) Embedding Dimension Ablation. Using embedding sizes 128, 64, and 32 to observe whether dimension influences learning with or without our regularization.

(4) Sequence Length Variation. Synthetic tasks with sequence lengths 3, 5, 7, and 10.

In all cases, the dataset is a simple sequence reversal task. Inputs are integers from a small vocabulary, and outputs are reversed copies. The tasks proved too simple: all models quickly approached 100% validation accuracy regardless of regularization or hyperparameters, highlighting the need for more challenging benchmarks to demonstrate compositional generalization.

6. Experiments

Baseline (Weight Initialization). We systematically varied weight initialization strategies. As shown in Figure 1, each strategy converges quickly to near-perfect accuracy. We also plot the corresponding training loss curves (Figure 2) and find similarly rapid convergence.

Removing Compositional Regularization. We compared $\lambda > 0$ (with regularization) vs. $\lambda = 0$ (no regularization). Figure 3 shows that both converge similarly in this simple dataset. Although the regularization does not degrade performance, it also does not reveal an advantage under such easy conditions.

Effect of Embedding Dimension. We tested embedding

[1] Code snippets appear in the Appendix.

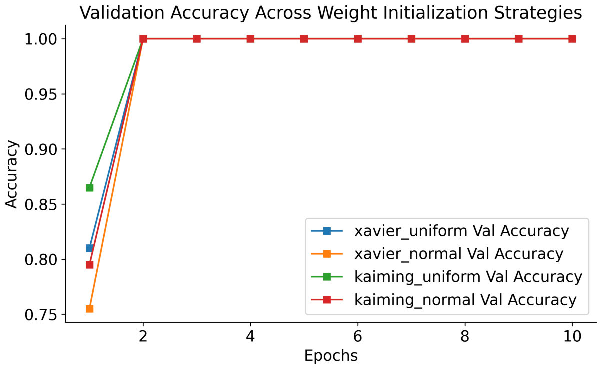

Figure 1. Validation Accuracy Across Weight Initialization Strategies (Simple Reversal Task). All curves reach 1.0 in a few epochs.

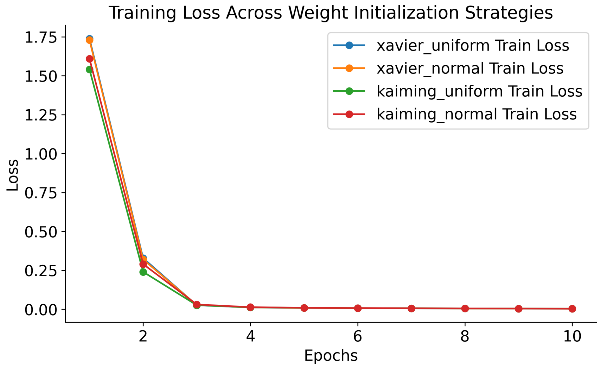

Figure 2. Training Loss Across Weight Initialization Strategies. Again, all methods converge rapidly to near-zero loss.

dimensions 128, 64, and 32. All reached 100% validation quickly. As Figures 4 and 5 show, training/validation curves exhibit a similar pattern of fast convergence, again illustrating that these tasks are insufficiently challenging to highlight compositional generalization.

Sequence Length Variation. We varied sequence lengths (3, 5, 7, 10). The model still attains 1.0 accuracy with little or no difference in final performance. See Figures 6 and 7.

Summary. Across all ablations, the synthetic reversal tasks do not expose any difficulty requiring systematic compositional thinking. Our compositional regularizer does not harm performance and thus remains a candidate for further testing on more challenging compositional tasks.

7. Conclusion

We introduced a compositional regularization term for neural networks, aiming to encourage systematically compositional internal representations. While experiments on a simple reversal task showed no detriment in performance, they also failed to reveal concrete advantages of compositional regularization in such a simple setting. Future work should evaluate our approach on more challenging datasets designed to test compositional generalization, such as SCAN (Dessì & Baroni, 2019) or COGS (Kim & Linzen, 2020), as well as machine translation tasks (Kumon et al., 2024; Han & Pad'o, 2024). We hypothesize that, under more demanding compositional scenarios, penalizing deviations from compositional patterns can improve systematic generalization and help bridge the gap between neural networks and human-like compositional reasoning.

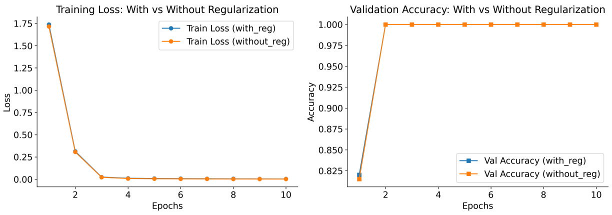

Figure 3. Training Loss (left) and Validation Accuracy (right), with vs. without Compositional Regularization. Both quickly plateau at ideal performance in this trivial task.

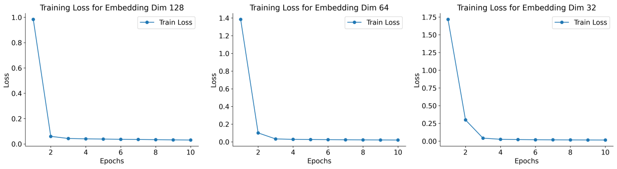

Figure 4. Training Loss for Different Embedding Dimensions. All converge rapidly.

Impact Statement

Our work aims to improve the ability of neural networks to generalize systematically by embedding compositional principles directly into the training objective. While the current experiments are inconclusive, if successful on more complex tasks, this approach could reduce the need for large training datasets and potentially lead to models that generalize more reliably to novel scenarios. We see minimal direct risk associated with our proposed method, though any machine learning model can be misapplied or deployed in contexts where human supervision and caution are still warranted.

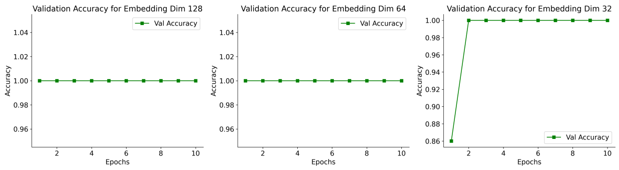

Figure 5. Validation Accuracy for Different Embedding Dimensions (Synthetic Reversal). Perfect accuracy is achieved quickly.

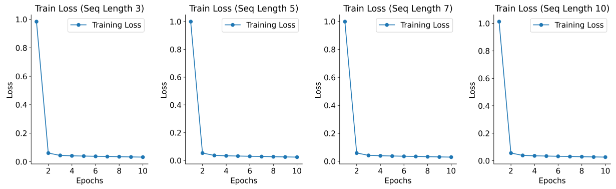

Figure 6. Training Loss with Sequence Length Variation. Despite differences in sequence length, training converges to near-zero.

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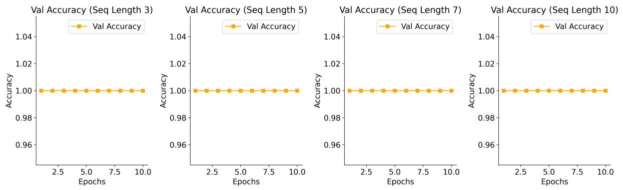

Figure 7. Validation Accuracy with Sequence Length Variation. All quickly reach 1.0, indicating that the task is too simple.

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Supplementary Material

A. Code Snippets and Extended Plots

We include here additional code and extended figures illustrating the results across multiple seeds and slightly varying hyperparameters. Due to the simplicity of the synthetic tasks, the results are largely consistent: near-perfect accuracy is reached rapidly.

A.1. Additional Synthetic Datasets

Below is a sample generator for synthetic data:

```
import numpy as np

def create_synthetic_data(data_size=1000, seq_length=5, vocab_size=10):
    """
    Create random sequences of integers in [1, vocab_size),
    with reversed outputs as a simple toy task.
    """
    np.random.seed(42)
    inputs = np.random.randint(1, vocab_size, size=(data_size, seq_length))
    outputs = np.fliplr(inputs).copy()
    return inputs, outputs
```

A.2. Compositional Loss Example

```
import torch
import torch.nn as nn

def compositional_loss(output, target, model, lambda_reg=0.01):
    """
    Cross-entropy + regularization penalty for compositional structure.
    """
    ce_loss = nn.CrossEntropyLoss()(output.transpose(1, 2), target)
    embeddings = model.embedding.weight
    mean_embedding = embeddings.mean(dim=0)
    reg_loss = lambda_reg * torch.norm(mean_embedding, p=2)
    return ce_loss + reg_loss
```

A.3. Extra Visuals

For completeness, we also generated additional figures that summarize synthetic dataset performance for multiple seeds, minor architectural adjustments, and so forth. These produce qualitatively similar conclusions, reinforcing that the tasks are too simple to demonstrate gains from compositional regularization.

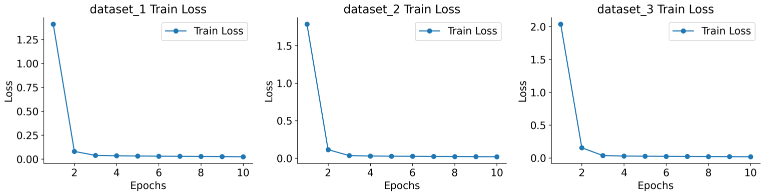

Figure 8. Sample training loss (per epoch) across different synthetic datasets. Convergence remains quick and complete.

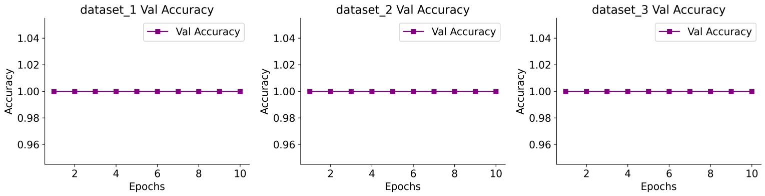

Figure 9. Sample validation accuracy across different synthetic datasets, consistently saturating at 1.0.