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Compositional Generalization in Transformers

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Abstract

Your English abstract here (mandatory if written in English and recommended otherwise).

Zusammenfassung

Hier die deutsche Zusammenfassung einfügen (notwendig).

Contents

1	Introduction	1
2	Background	3
2.1	Transformer	3
2.1.1	Elements	4
2.1.2	Encoder and Decoder Architectures	6
2.1.3	Recurrent and Looping Architectures	8
2.1.4	Positional Encoding Schemes	9
2.1.5	Training and Inference	10
2.2	Mechanistic Interpretability	11
2.3	Realizability	11
2.4	Deep Double Descent	11
3	Related Work	13
3.1	Learning Arithmetics with Transformers	13
3.2	Reasoning in Transformers	15
3.3	Compositional Learning	17
3.4	Generalization to Longer Sequence Lengths	18
4	Research Questions	21
5	Approach	23
6	Conclusion	25
A	Nomenclature	27
	Bibliography	29

List of Figures

2.1	(a) A single Transformer layer, consisting of multi-head self-attention, feed-forward network (MLP), and layer normalization. (b) A decoder-only transformer model. In the decoder, the self-attention mechanism has a causal mask to prevent attending to future tokens. . . .	7
2.2	(a) A block of multiple transformer layers used in the looped transformer. (b) Looped decoder-only transformer architecture. The input injection mechanism adds skip connections from the input sequence to the input of each block.	9
2.3	Training and inference processes for Transformers TODO TODO TODO TODO.	10

List of Tables

A.1 Table of nomenclature	27
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Chapter 1

Introduction

Chapter 2

Background

This chapter provides an in-depth overview of the Transformer architecture, focusing on its core components, different variants, positional encoding schemes, and the processes of training and inference.

Notation

\mathcal{V}	Vocabulary of input tokens.
n	Length of the input sequence.
b	Batch size for batched input sequences.
\mathbf{x}	Input sequence of tokens, $\mathbf{x} \in \mathcal{V}^n$
x_i	i -th token in the input sequence, $x_i \in \mathcal{V}$.
d	Dimensionality of the token embedding space.
\mathbf{e}_i	d -dimensional embedding vector of token x_i , $\mathbf{e}_i \in \mathbb{R}^d$.
\mathbf{E}	Embedding matrix, $\mathbf{E} \in \mathbb{R}^{ \mathcal{V} \times d}$.
\mathbf{H}	Matrix of a sequence of embedding vectors, $\mathbf{H} \in \mathbb{R}^{n \times d}$.
\mathbf{h}_i	i -th vector in the sequence of embeddings, $\mathbf{h}_i \in \mathbb{R}^d$.
\mathbf{O}	Output matrix from a Transformer layer, $\mathbf{O} \in \mathbb{R}^{n \times d}$.
\mathbf{Q}	Queries matrix, $\mathbf{Q} \in \mathbb{R}^{n \times d}$.
\mathbf{K}	Keys matrix, $\mathbf{K} \in \mathbb{R}^{n \times d}$.
\mathbf{V}	Values matrix, $\mathbf{V} \in \mathbb{R}^{n \times d}$.
θ	Model parameters (weights and biases).

2.1 Transformer

The Transformer architecture, introduced by Vaswani et al. (2017), performs sequence modeling by relying entirely on self-attention mechanism, instead of using convolution or recurrence.

Let \mathcal{V} denote the vocabulary of input tokens. While the tokens can represent

anything, in language modeling tasks they are usually learned subword units. In this work, however, a simple character tokenization scheme is used that is suitable for algorithmic tasks, so each token corresponds to a single character (letter, digit or symbol) in the sequence. An input sequence is represented as $\mathbf{x} = [x_1, x_2, \dots, x_n]$, where $x_i \in \mathcal{V}$ and n is the sequence length. Each token x_i is mapped to a d -dimensional embedding vector $\mathbf{e}_i \in \mathbb{R}^d$ using an embedding matrix $\mathbf{E} \in \mathbb{R}^{|\mathcal{V}| \times d}$. Thus, each row of \mathbf{E} corresponds to the embedding of a token in the vocabulary.

The input matrix to a Transformer layer is a sequence of vector embeddings (also called the *latent* or *hidden representation* for intermediate layer inputs), denoted $\mathbf{H} \in \mathbb{R}^{n \times d}$, where $\mathbf{H} = [\mathbf{h}_1^\top, \mathbf{h}_2^\top, \dots, \mathbf{h}_n^\top]^\top$. The output of a Transformer layer is also a sequence of vectors with the same sequence length, denoted $\mathbf{O} \in \mathbb{R}^{n \times d}$.

In practice, the inputs to the Transformer are batched, so the input has an additional dimension for the batch size, denoted b , with $\mathbf{H} \in \mathbb{R}^{b \times n \times d}$. This results in the first (batch) dimension being added throughout the intermediate representation and the output, but has no bearing on the description of the Transformer model.

2.1.1 Elements

The Transformer is composed of several key components to model dependencies in sequential data: multi-head attention, feed-forward networks, layer normalization, and residual connections. Informally, the attention mechanism transfers information *between* tokens, while the feed-forward networks process information *within* tokens. These components are stacked in each layer of the Transformer as shown in Figure 2.1 (a).

Attention Mechanism The attention mechanism (Bahdanau, Cho, and Bengio 2014) allows the model to weigh the relevance of different positions in the input sequence. For this purpose, it computes *queries*, *keys*, and *values* from the input embeddings and uses them to calculate attention scores. The output is a weighted sum of the values, where the weights are determined by the attention scores. The names “queries”, “keys”, and “values” are derived from the context of information retrieval, where the queries are the elements being searched for, the keys are the elements being searched, and the values are the elements being retrieved. In the context of the Transformer, intuitively, the query represents what the current token is “looking for” in the sequence, the keys represent what the token at a given position “offers” to the current token, and the values are the actual information that the current token “receives” from the other tokens.

First, the queries, keys, and values are computed as:

$$\begin{aligned}\mathbf{Q} &= \mathbf{H}\mathbf{W}^Q, \\ \mathbf{K} &= \mathbf{H}\mathbf{W}^K, \\ \mathbf{V} &= \mathbf{H}\mathbf{W}^V,\end{aligned}$$

where $\mathbf{W}^Q, \mathbf{W}^K, \mathbf{W}^V \in \mathbb{R}^{d \times d_k}$ are the weight matrices, and d_k is the dimension of the queries, keys, and values. In practice, the convention is to set $d_k = d$, which is

the case for the models in this work. Thus, $\mathbf{Q}, \mathbf{K}, \mathbf{V} \in \mathbb{R}^{n \times d}$.

Given queries \mathbf{Q} , keys \mathbf{K} , and values \mathbf{V} , the attention output is computed as:

$$\mathbf{O}_{\text{att}} = \text{Attention}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \text{softmax}\left(\frac{\mathbf{Q}\mathbf{K}^\top}{\sqrt{d}}\right) \mathbf{V}.$$

where the softmax function is applied along the last dimension, and is defined as:

$$\text{softmax}(\mathbf{x})_i = \frac{e^{x_i}}{\sum_j e^{x_j}}.$$

Note that the output of the attention mechanism has the same shape as the input, $\mathbf{O}_{\text{att}} \in \mathbb{R}^{n \times d}$.

Multi-Head Attention Multi-head attention extends the attention mechanism with multiple independent *heads* to allow the model to focus on information from different representation subspaces. So, instead of applying attention to the d -dimensional queries, keys, and values directly, they are projected into h different d_{head} -dimensional subspaces, where h is the number of heads. In this work, the head dimension d_{head} is set to d/h , so that the total dimensionality remains d . The outputs the heads are concatenated and linearly transformed to the original dimensionality:

$$\text{MultiHeadAttention}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \text{Concat}(\text{head}_1, \text{head}_2, \dots, \text{head}_h) \mathbf{W}^O,$$

where $\mathbf{W}^O \in \mathbb{R}^{d \times d}$ is the learned output weight matrix, and each head is computed as:

$$\text{head}_i = \text{Attention}(\mathbf{Q}\mathbf{W}_i^Q, \mathbf{K}\mathbf{W}_i^K, \mathbf{V}\mathbf{W}_i^V),$$

and $\mathbf{W}_i^Q, \mathbf{W}_i^K, \mathbf{W}_i^V \in \mathbb{R}^{d \times d_{\text{head}}}$ are the weight matrices for the i -th head.

Feed-Forward Networks Position-wise feed-forward networks (FFN), also called the Multi-layer Perceptron (MLP), are applied independently to each position in the sequence:

$$\text{FFN}(\mathbf{h}_i) = \sigma(\mathbf{h}_i \mathbf{W}_1 + \mathbf{b}_1) \mathbf{W}_2 + \mathbf{b}_2,$$

where $\mathbf{h}_i \in \mathbb{R}^d$ is the input vector, $\mathbf{W}_1 \in \mathbb{R}^{d \times d_{\text{ff}}}$, $\mathbf{W}_2 \in \mathbb{R}^{d_{\text{ff}} \times d}$, and σ is an activation function such as Rectified Linear Unit (ReLU).

Layer Normalization Layer normalization (Ba, Kiros, and Hinton 2016) is applied after each sub-layer over the last (feature) dimension. The LayerNorm function for a vector $v \in \mathbb{R}^d$ is defined as:

$$\text{LayerNorm}(v) = \frac{v - \mu}{\sigma} \gamma + \beta,$$

where the scale γ and bias vector β are learned scaling and shifting parameters, and μ and σ are the mean and standard deviation of v , computed as follows:

$$\mu = \frac{1}{d} \sum_{i=1}^d v_i,$$

$$\sigma = \sqrt{\frac{1}{d} \sum_{i=1}^d (v_i - \mu)^2}.$$

Residual Connections Residual connections (He et al. 2016) are usually applied to ease gradient flow and enable the training of deeper networks. In Transformer models, the residual connections are applied after each sub-layer (self-attention and MLP), followed by a layer normalization. Thus, the output of each sub-layer is:

$$\text{SubLayerOutput} = \text{LayerNorm}(\mathbf{x} + \text{SubLayer}(\mathbf{x})).$$

The residual connections-based view of the model also enables the concept of a *residual stream*, which is important in mechanistic interpretability. In this alternative view of the model, the residual connections are the main backbone of information flow through the model, with the sub-layers processing the hidden representation tensor \mathbf{H} and adding it back to the residual stream.

Block Structure The original Transformer introduced in Vaswani et al. 2017 consists of stacked encoder and decoder blocks, each containing multi-head attention and feed-forward networks, along with residual connections and layer normalization. However, different modified architectures have been proposed, such as the encoder-only BERT model (Devlin et al. 2019) and the decoder-only GPT model (Radford and Narasimhan 2018).

2.1.2 Encoder and Decoder Architectures

Encoder-Decoder The original Transformer model introduced by Vaswani et al. Vaswani et al. 2017 employs an encoder-decoder architecture. In this architecture, the encoder processes an input sequence $\mathbf{x} = (x_1, x_2, \dots, x_n)$ into a sequence of continuous representations $\mathbf{z} = (z_1, z_2, \dots, z_n)$. The decoder then generates an output sequence $\mathbf{y} = (y_1, y_2, \dots, y_m)$ by predicting the next token y_t based on the encoder's output and the previously generated tokens.

The encoder consists of a stack of N identical layers, each containing two sub-layers: a multi-head self-attention mechanism and a position-wise fully connected feed-forward network. The decoder has a similar structure but includes a third sub-layer: the *cross-attention*, also called *encoder-decoder attention*, where the queries come from the previous decoder layer, and the keys and values come from the output of the encoder. Hence, the difference between the self-attention and cross-attention mechanisms is that self-attention is usually applied to the same sequence,

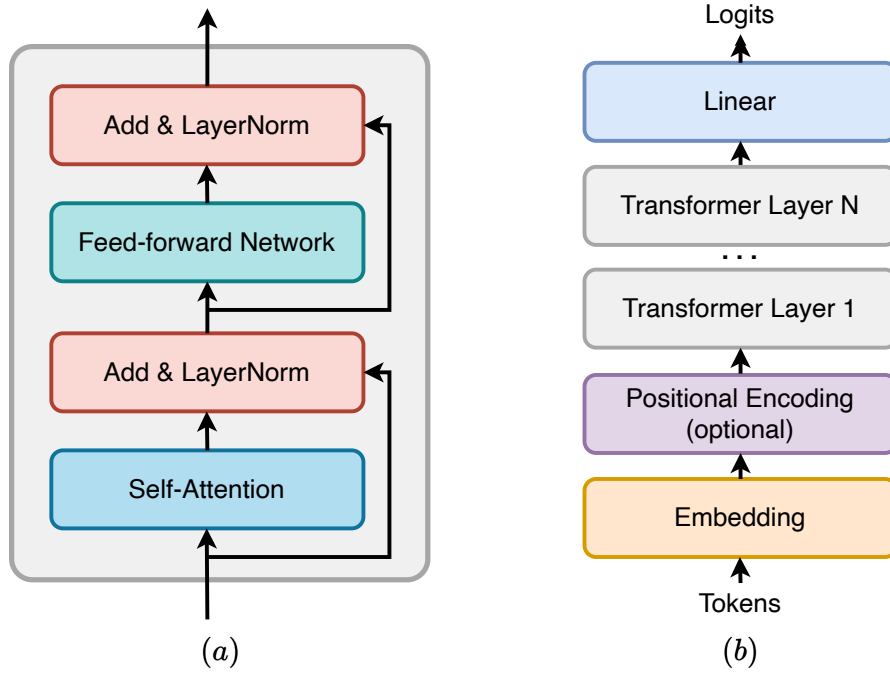


Figure 2.1: (a) A single Transformer layer, consisting of multi-head self-attention, feed-forward network (MLP), and layer normalization. (b) A decoder-only transformer model. In the decoder, the self-attention mechanism has a causal mask to prevent attending to future tokens.

while cross-attention is applied between two different sequences (e.g. one from the encoder, and one from the decoder). Moreover, the self-attention mechanism in the decoder has a causal mask to prevent attending to “future tokens”, ensuring output is generated autoregressively.

Encoder-only Encoder-only models focus exclusively on encoding the input sequence into a contextual representation without a decoder component. BERT (Bidirectional Encoder Representations from Transformers) Devlin et al. 2019 is a prominent example of this architecture. BERT utilizes a stack of Transformer encoder layers to produce deep bidirectional representations by jointly conditioning on both left and right context. This makes encoder-only models particularly well-suited for tasks that require a comprehensive understanding of the input, such as text classification, named entity recognition, and question answering.

These models are typically pre-trained on large unlabeled text corpora using self-supervised objectives like masked language modeling (MLM) and next sentence prediction (NSP). The pre-trained models can then be fine-tuned on specific downstream tasks.

Decoder-only Decoder-only models generate sequences based on prior tokens and are designed primarily for autoregressive language modeling and text generation tasks. GPT (Generative Pre-trained Transformer) Radford and Narasimhan

2018 is a canonical example of a decoder-only architecture. In these models, the Transformer decoder predicts the next token in a sequence by attending to the previous tokens without an encoder component. Recent research on language modeling has mostly focused on decoder-only models, since they can also be used on other language tasks through prompting, few-shot learning, and fine-tuning.

Decoder-only models are pre-trained on large text corpora to predict the next token, enabling them to generate coherent and contextually relevant text.

Encoder-Decoder vs. Decoder-Only Both model types are capable of autoregressive sequence generation and can be used for a wide range of tasks. The decoder-only models are favored in recent works due to them being simpler and having less inductive bias. However, encoder-decoder models are still widely used in machine translation, robotics, and multi-modal learning tasks. The additional structure in encoder-decoder models, as compared to using a decoder-only model with would-be encoder input sequence prepended to the decoder’s input can be summarized as:

- The input to the encoder passes through more layers (encoder layers) before reaching the decoder.
- It is assumed that input and output sequences are sufficiently different to justify using separate parameters for them (encoder and decoder).

In summary, the choice of Transformer architecture depends on the specific requirements of the task, though decoder-only models have been more widely used in recent research and are the focus of this work.

2.1.3 Recurrent and Looping Architectures

To enhance length generalization, some Transformers incorporate recurrence or looping mechanisms.

Universal Transformer The Universal Transformer Dehghani et al. 2018 introduces recurrence into the Transformer architecture by repeatedly applying the same transformer layers multiple times:

$$\mathbf{H}^{(t+1)} = \text{TransformerLayer}(\mathbf{H}^{(t)}),$$

where t denotes the iteration step. This enables the model to generalize better to sequences longer than those seen during training.

Looped Transformer Looped Transformers (Yang et al. 2023) extend the Transformer by incorporating iterative application of a block of transformer layers.

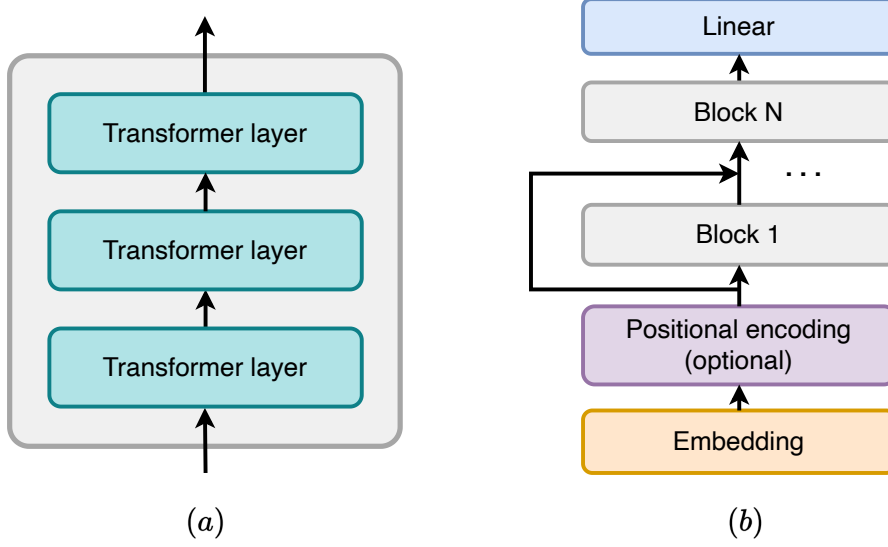


Figure 2.2: (a) A block of multiple transformer layers used in the looped transformer. (b) Looped decoder-only transformer architecture. The input injection mechanism adds skip connections from the input sequence to the input of each block.

2.1.4 Positional Encoding Schemes

Since the Transformer lacks inherent sequential order, positional encodings are added to input embeddings to provide position information. Though, several recent works have shown that the causal attention mechanism in a decoder-only transformer can also implicitly learn to encode positional information (Zuo and Guerzhoy 2024; Y. Zhou et al. 2024) in the absence of explicit positional encodings.

Sinusoidal Positional Encoding The original Transformer uses sinusoidal positional encodings Vaswani et al. 2017, defined as:

$$\mathbf{p}_{i,2k} = \sin\left(\frac{i}{10000^{2k/d}}\right),$$

$$\mathbf{p}_{i,2k+1} = \cos\left(\frac{i}{10000^{2k/d}}\right),$$

for position i and dimension k . These encodings allow the model to generalize to longer sequences by extrapolating the sinusoidal patterns.

Relative Position Representations Relative position representations Shaw, Uszkoreit, and Vaswani 2018 encode the relative distances between sequence elements directly into the attention mechanism. The attention scores are modified as:

$$e_{ij} = \frac{\mathbf{q}_i^\top \mathbf{k}_j + \mathbf{q}_i^\top \mathbf{a}_{i-j}^K + \mathbf{b}_{i-j}^Q{}^\top \mathbf{k}_j}{\sqrt{d_k}},$$

where \mathbf{a}_{i-j}^K and \mathbf{b}_{i-j}^Q are learned relative position embeddings.

Rotary Position Encoding (RoPE) RoPE Su et al. 2024 encodes positions using rotation matrices and incorporates relative position information into the self-attention mechanism. For each position i , the embedding is rotated by a position-dependent angle:

$$\mathbf{h}_i = \mathbf{e}_i \cdot \mathbf{R}(i),$$

where $\mathbf{R}(i)$ is a rotation matrix function of position i .

Randomized Positional Encodings Randomized positional encodings Ruoss et al. 2023 aim to improve length generalization by simulating longer sequences during training. They randomly select a subset of positions to represent the sequence, enhancing the model’s ability to handle sequences of unseen lengths.

Attention with Linear Biases (ALiBi) ALiBi Press, Smith, and Lewis 2021 introduces a linear bias to the attention scores based on the relative positions:

$$e_{ij} = \frac{\mathbf{q}_i^\top \mathbf{k}_j}{\sqrt{d_k}} + m \cdot |i - j|,$$

where m is a head-specific constant slope parameter. This bias encourages the model to focus on recent tokens and enables better extrapolation to longer sequences.

2.1.5 Training and Inference

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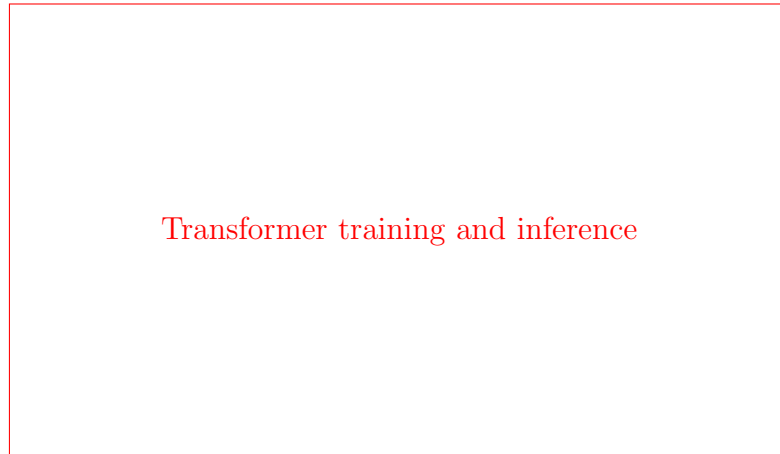


Figure 2.3: Training and inference processes for Transformers TODO TODO TODO TODO.

Training Training involves minimizing a loss function, typically the *cross-entropy loss* for language tasks, using an optimization algorithm like Stochastic Gradient Descent (SGD) or AdamW (Loshchilov and Hutter 2018). The model learns the parameters θ by backpropagating the loss through the network layers. The cross-entropy loss is defined as:

$$\mathcal{L} = -\frac{1}{b} \sum_{i=1}^b \sum_{j=1}^n \log p(x_{i,j} | x_{i,<j}),$$

where b is the batch size, n is the sequence length, and $p(x_{i,j} | x_{i,<j})$ is the probability of token $x_{i,j}$ given the previous tokens $x_{i,<j}$.

TODO: *describe answer-only loss*

Inference During inference, the trained model generates outputs by computing the forward pass through the network. For autoregressive models, techniques like beam search may be used to generate sequences.

2.2 Mechanistic Interpretability

Understanding how Transformers make decisions is crucial for interpretability and debugging. Key concepts include:

TODO: *expand*

Residual Stream The residual stream in a Transformer accumulates information across layers through residual connections. Analyzing this stream helps in understanding how information is propagated and transformed.

Activation Patching Activation patching involves replacing activations in a model with activations from a different context to study causal effects (Olsson et al. 2022). This technique can identify which components contribute to specific model behaviors.

Logit Lens The logit lens method inspects the logits (pre-softmax outputs) at different layers to interpret intermediate representations. It provides insights into how predictions evolve across layers.

Olsson et al. (2022) investigated "induction heads," attention heads that enable in-context learning by recognizing patterns like repeated sequences.

2.3 Realizability

2.4 Deep Double Descent

The phenomenon of *deep double descent* refers to the observation that increasing model capacity or training epochs can initially degrade performance before

TODO: *may rename, fix RASP/RASP-L and Ahuja and Mansouri paper*

improving it (Nakkiran et al. 2021). This challenges the traditional bias–variance trade-off, where increasing complexity always leads to overfitting.

Belkin et al. (2019) explored this phenomenon, showing that modern machine learning models can benefit from overparameterization, achieving better generalization even when they perfectly fit the training data.

Understanding deep double descent is important for training Transformers effectively, as it informs decisions about model size and training duration to optimize performance on tasks like integer addition.

ODO: *explain*
why I care about
this

Chapter 3

Related Work

In this chapter, a literature review is presented, focusing on the topics of transformers, learning arithmetic tasks, reasoning capabilities, compositional learning, and generalization to longer sequence lengths.

TODO: *rewr
summary*

3.1 Learning Arithmetics with Transformers

The ability of transformer models (Vaswani et al. 2017) to learn arithmetic operations such as integer addition has been a subject of significant research interest. Evaluations demonstrated that large pre-trained language models such as GPT-3 (Brown et al. 2020) can exhibit emergent capabilities across general-purpose tasks, including basic few-digit arithmetic, despite these tasks not being explicitly encoded by the unsupervised next-token prediction objective. However, even largest state-of-the-art models like GPT-4 (Achiam et al. 2023) struggle to robustly solve multi-digit addition and multiplication, especially when a larger number of digits are involved.

N. Lee et al. 2023 investigate how even small transformers, trained from random initialization, can efficiently learn arithmetic operations such as addition and multiplication. They show that training on chain-of-thought style data that includes intermediate step results significantly improves accuracy, sample complexity, and convergence speed, even in the absence of pretraining. This approach aligns with the experiments presented in this thesis on chain-of-thought training, where models are trained to output the steps involved in solving addition problems. One limitation of their work is that it limits each task to a fixed number of digits (e.g. 7 and 7 digit operands), using padding to ensure uniform input length. In contrast, this thesis extends the task to variable-length addition problems which is more difficult due to the need for models to learn to position-wise align digits as discussed in Chapter 4.

Understanding how transformers learn arithmetic tasks is further explored by Quirke and Barez 2023, who present an in-depth mechanistic analysis of a one-layer transformer model trained for integer addition. They reveal that the model processes the problem in a non-intuitive way: it divides the task into parallel,

digit-specific streams and employs distinct algorithms for different digit positions, merging the results in the MLP layer. This work also restricts the operands to a fixed length of 5 digits and employs padding, apart from restricting the model to a single layer.

Length generalization is a critical challenge in training transformers for arithmetic tasks that comes up in numerous research works. Jelassi et al. 2023 examine how transformers cope with learning basic integer arithmetic and generalizing to longer sequences than seen during training. They find that relative position embeddings enable length generalization for simple tasks such as addition, allowing models trained on 5-digit numbers to perform 15-digit sums. However, this method fails for multiplication, leading them to propose “train set priming” by adding a few (10 to 50) longer sequences to the training set. Despite showing interesting capabilities of learning from few examples, this defeats the purpose of *zero-shot* generalization to unseen lengths.

Similarly, Duan and Shi 2023 investigate the capabilities of transformers in learning arithmetic algorithms and introduce Attention Bias Calibration (ABC), a calibration stage that enables the model to automatically learn proper attention biases linked to relative position encoding mechanisms. Using ABC, they achieve robust length generalization on certain arithmetic tasks. Despite promising results, this work is limited due to the attention bias intervention being task-specific and the need for a modified training with 2 stages (first training to perfect interpolation accuracy to learn the attention biases, then training another model with extracted attention biases). Conversely, the main research interest in this domain lies in architectural modifications that apart from boosting algorithmic capabilities, also preserve or improve performance on other language tasks.

Recent work by McLeish et al. 2024 addresses the poor performance of transformers on arithmetic tasks by adding an embedding to each digit that encodes its position relative to the start of the number. This modification, along with architectural changes like input injection and recurrent layers, significantly improves performance, achieving up to 99% accuracy on 100-digit addition problems. As of now, this work represents the state-of-the-art in length generalization on integer addition, with test sequence lengths up to 6 times longer training sequence lengths (compared to previous SOTA of 2.5 times by Y. Zhou et al. 2024).

Investigations into the symbolic capabilities of large language models by Dave et al. 2024 and the arithmetic properties in the space of language model prompts by Krubiński 2023 further contribute to understanding how transformers process arithmetic operations and the challenges involved in symbolic reasoning tasks.

Mechanistic interpretability of transformers on arithmetic tasks is further explored by Nanda et al. 2022, who study the phenomenon of grokking in small transformer models trained on modular addition tasks. They fully reverse-engineer the learned algorithm and discover that the model implements a discrete Fourier transform and uses trigonometric identities to convert addition into rotations on a circle. Similarly, Zhong et al. 2023 investigate the mechanistic explanations of neural networks on modular addition tasks. They find that neural networks can discover multiple qualitatively different algorithms when trained on the same task,

ODO: expand on
these 2 papers

including known algorithms like the “Clock” algorithm (same as Nanda et al. 2022) and a novel “Pizza” algorithm. Unlike the focus of this thesis, which deals with integer addition where each digit is treated as a separate token, these works are limited to modular addition tasks where each number is a single token, i.e. 123 token instead of tokens for 1 , 2 , and 3 . This simplification allows for a detailed mechanistic understanding of the model but does not address the challenges associated with variable-length inputs and position-wise alignment of digits in full integer addition. Moreover, their primary concern is interpretability and understanding training dynamics, rather than improving length generalization or exploring failure modes in more complex arithmetic tasks.

In summary, the literature demonstrates that transformers can learn arithmetic tasks like integer addition, but challenges remain in achieving robust length generalization and understanding the underlying mechanisms by which these models perform arithmetic operations. These findings are directly relevant to the focus of this thesis, i. e. length generalization on integer addition and failure modes of transformers, since works either simplify the task to be modular addition ((Nanda et al. 2022), (Zhong et al. 2023)), fixed digit length ((N. Lee et al. 2023), (Quirke and Barez 2023)), or propose task-specific architectural modifications to improve performance ((McLeish et al. 2024)) whose performance on other language tasks is not explored.

3.2 Reasoning in Transformers

Transformers have shown remarkable abilities in reasoning tasks, particularly when employing techniques such as including a chain-of-thought (CoT) in the sequence instead of directly outputting an answer. Z. Li et al. 2024 provide a theoretical understanding of the power of chain-of-thought for decoder-only transformers, demonstrating that CoT empowers the model with the ability to perform inherently serial computation, which is otherwise lacking in transformers, especially for fewer layers. Intuitively, this is due to the fact that a CoT part in generated sequence allows the model to write out intermediate results and perform more computation before arriving at the final answer. This theoretical perspective also supports the experiments described in Chapter 5 involving chain-of-thought training to enhance the reasoning capabilities of models on arithmetic tasks.

Wang and D. Zhou 2024 explore the idea that chain-of-thought reasoning paths can be elicited from pre-trained language models by simply altering the decoding process, rather than relying on specific prompting techniques. Instead of decoding by taking the tokens with most activation (greedy decoding), they propose evaluating multiple possible first tokens, and then continue with greedy decoding for each of them. This results in multiple decoded sequences instead of a single answer sequence. They find that paths including a chain-of-thought part already frequently exist among these alternative sequences and that the presence of a CoT in the decoding path correlates with higher confidence in the model’s decoded answer. This work strengthens the argument that chain-of-thought reasoning is a powerful

mechanism for transformers to improve reasoning capabilities.

Another research direction is training the models to output a chain-of-thought sequence using bootstrapping from existing data and pre-trained models, without the need for curated CoT data. Zelikman, Wu, et al. 2022 propose the Self-Taught Reasoner (STaR) method to bootstrap reasoning capabilities using existing models and answer-only datasets. In STaR, a pre-trained LLM is encouraged to generate intermediate steps before answer using few-shot prompting, and it is assumed that if the resulting answer is correct, the generated CoT steps are also correct. Then, the model is fine-tuned on the generated CoT data. This method is shown to improve reasoning capabilities on various tasks, including arithmetic. Further extending the concept of self-generated reasoning, Zelikman, Harik, et al. 2024 introduce Quiet-STaR, where language models learn to generate “rationales” at each token to explain future text using reinforcement learning, thereby improving their predictions. This approach generalizes previous work on self-taught reasoning by Zelikman, Wu, et al. 2022, training the LLM to implicitly reason without explicit generation of a CoT trace, and can leverage unsupervised text datasets since the objective is not task-specific.

Goyal et al. 2024 propose training language models with “pause tokens”, allowing the model to perform more computation before outputting the next tokens. This method improves performance on reasoning tasks, including arithmetic. However, while it is tempting to think that the pause tokens implicitly perform a form of chain-of-thought reasoning, the authors do not explicitly analyze the internal reasoning processes of the model. Moreover, the pause tokens are not directly interpretable as distinct, structured intermediate steps, which is a key feature of chain-of-thought reasoning.

The limitations of transformers in performing counting tasks are highlighted by Yehudai et al. 2024, who focus on simple counting tasks involving counting the number of times a token appears in a string. They show that transformers can solve this task under certain conditions, such as when the dimension of the transformer state is linear in the context length. But in general this ability does not scale beyond this limit, based on the authors’ theoretical arguments for the observed limitations. While this work does not directly address arithmetic tasks, it provides insights into the limitations of transformers in handling a related counting task.

Understanding how transformers learn causal structures is investigated by Nichani, Damian, and J. D. Lee 2024, who introduce an in-context learning task requiring the learning of latent causal structures. They prove that gradient descent on a simplified two-layer transformer learns to solve this task by encoding the latent causal graph in the first attention layer, providing insights into the mechanisms by which transformers develop reasoning capabilities. However, this work is highly theoretical and does not directly address arithmetic tasks, nor other algorithmic or language tasks.

Overall, despite some theoretical results proving possibility of certain forms of reasoning, the literature does not show a robust solution that allows transformers to learn the generalizable algorithm for performing integer addition on an unbounded

number of digits, which is the main focus of this thesis. Moreover, even if theoretical possibility was to be established, it would still be of interest to interpret the learned algorithm in a higher-level, human-understandable form akin to Nanda et al. 2022.

3.3 Compositional Learning

Compositionality refers to the ability of models to understand and generate new combinations of known components.

The work of Hupkes et al. 2020 provides a theoretical framework for understanding compositional generalization in neural networks. They propose tests to investigate whether models systematically recombine known parts and rules, generalize to longer sequences, and favor rules over exceptions during training. This framework is relevant to our analysis of how transformers learn and generalize in arithmetic tasks.

TODO: cite Hupkes et al. 2020 and expand definition

Dziri et al. 2023 investigate the limits of transformers on compositional tasks, such as multi-digit multiplication and logic grid puzzles. They find that transformers tend to solve compositional tasks by reducing multi-step reasoning into *linearized subgraph matching* rather than developing systematic problem-solving skills, suggesting limitations in compositional generalization. Apart from suggesting an interesting description for how multi-step reasoning is realized on transformers, this work does not explore integer addition problems, instead focusing on 5 digit multiplication and logic puzzles.

Press, Zhang, et al. 2023 measure the compositionality gap in language models by evaluating how often models can correctly answer all sub-problems but fail to generate the overall solution. They find that as model size increases, single-hop question answering performance improves faster than multi-hop performance, indicating that while larger models have better factual recall, they do not necessarily improve in their ability to perform compositional reasoning. They propose methods like chain-of-thought and self-ask prompting to narrow the compositionality gap.

H. Zhou et al. 2023 propose the RASP-Generalization Conjecture, suggesting that transformers tend to length generalize on a task if it can be solved by a short program (in a domain-specific language describing the transformer architecture) that works for all input lengths. They use this framework to understand when and how transformers exhibit strong length generalization on algorithmic tasks, which is closely related to compositional learning.

In summary, while transformers have demonstrated some ability to perform compositional tasks, significant challenges remain in achieving systematic compositional generalization. These findings inform this thesis' focus on multi-task learning and understanding how models can be trained to perform compositional operations like digit alignment and modular sum, before correctly combining results from these sub-tasks into a final answer.

3.4 Generalization to Longer Sequence Lengths

Generalization to longer sequence lengths is a critical challenge in training transformers for tasks like integer addition. Positional encoding plays a significant role in length generalization. Kazemnejad et al. 2023 conduct a systematic empirical study comparing different positional encoding approaches, including Absolute Position Embedding (APE) (Vaswani et al. 2017), Relative position encoding (Shaw, Uszkoreit, and Vaswani 2018), ALiBi (Press, Smith, and Lewis 2021), Rotary position encoding (RoPE) (Su et al. 2024), and Transformers without positional encoding (NoPE). Interestingly, they find that explicit position embeddings are not essential for decoder-only transformers to generalize to longer sequences and that models without positional encoding outperform others in length generalization. The results of experiments conducted in this thesis are not consistent with these findings, observing much steeper performance drops on longer sequences when using NoPE, RoPE or APE.

Ruoss et al. 2023 introduce randomized positional encodings to boost length generalization of transformers. They demonstrate that their method allows transformers to generalize to sequences of unseen length by simulating the positions of longer sequences and randomly selecting an ordered subset to fit the sequence’s length. Experiments in this thesis also confirm that randomized positional encodings can improve length generalization on integer addition tasks. Moreover, experiments show that even without architectural changes, simply adding empty spaces to the input sequence can boost out-of-distribution accuracy for task lengths near to those encountered during training.

S. Li et al. 2024 propose a novel functional relative position encoding with progressive interpolation (FIRE) to improve transformer generalization to longer contexts. They theoretically show that FIRE can represent popular relative position encodings and empirically show that FIRE models have better generalization to longer contexts on both zero-shot language modeling and long text benchmarks.

The success of length generalization is also linked to data format and position encoding type. Y. Zhou et al. 2024 test the transformer’s ability to generalize using the two integer addition task. They show that transformers can achieve limited length generalization, but find that the performance depends on random weight initialization as well.

As mentioned in Section 3.1, McLeish et al. 2024 address length generalization by adding an embedding to each digit that encodes its position relative to the start of the number. This fix, along with architectural modifications, allows transformers to generalize to larger and more complex arithmetic problems, achieving state-of-the-art performance on addition tasks with longer sequences.

In this thesis’ experiments, different positional encodings and CoT training are explored to improve length generalization in integer addition tasks. The literature suggests that carefully designed positional encodings and data formatting can significantly impact the ability of transformers to generalize to longer sequences. Moreover, this work isolates the causes of failure in length generalization on integer addition, and proposes minimally invasive modifications to improve performance

on longer sequences.

Chapter 4

Research Questions

Research Questions

1. How do (smaller) transformers learn to compose sub-tasks for integer addition?
2. What architectural features or training strategies enhance compositional learning? (we want them to be applicable to other domains as well, at least not hurt in regular unsupervised text setting)
3. How do transformers generalize to larger sequences than seen during training?

Compositionality gap: difference between performance on subtasks and the full task. In our case full task is integer addition, with subtasks being digit-wise alignment, addition, and carry operations.

Experiments / Hypotheses

- RQ3: Models generalize to in-distribution sequence lengths but not OOD (longer or shorter) lengths.
 - Baseline performance.
 - Smaller 3×3 , 7×7 experiments, 1-19 digits and 18/20+ digits
 - Scratchpad can improve it to 18 and 20, not 21+
- RQ1: Sub-task decomposition: models decompose addition into:
 - digit-wise alignment
 - modular digit-wise addition
 - carry operations
 - Probing tasks for sub-task neural networks, saliency, etc. (TODO)
- RQ2: Positional embeddings are important for digit-wise addition and source of errors (e.g., alignment).

- Random spaces
 - Abacus
 - Relative pos encodings
- RQ1: Compositional learning strategies:
 - Simple to complex tasks (curriculum)
 - Multi-task learning (aux loss) (TODO)
- Error analysis: TODO for robustness.

Chapter 5

Approach

Chapter 6

Conclusion

Appendix A

Nomenclature

Symbol	Description
SOTA	State-of-the-art
MLP	Multi-layer perceptron
SGD	Stochastic gradient descent
FFNN	Feed-forward neural network
RNN	Recurrent neural network
GPT	Generative pre-trained transformer
BERT	Bidirectional encoder representations from transformers
T5	Text-to-text transfer transformer
LLM	Large language model
CoT	Chain-of-thought
OOD	Out-of-distribution

Table A.1: Table of nomenclature

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