Penetrating the "Grokking" Phenomenon

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Abstract

This article is concerned about the Grokking phenomenon in the learning of modular addition. Starting from transformer models with AdamW optimizer, we perform experiments investigate the effect of training fraction on the training and validation accuracy. Other model structures, optimizers and regularization techniques are considered. We also explore Grokking in multivariate modular addition. Lastly, we adopt the Grokfast algorithm and provide a possible explanation of Grokking. The code of our experiments can be accessed at our github repository.

Keywords Grokking; modular addition; Grokfast; transformer; Adam

1 Introduction

In machine learning, the "Grokking" phenomenon refers to a sudden, unexpected breakthrough in the model's learning process, typically occurring when the model reaches a very low training error. It often appears as a sudden, dramatic improvement in performance after a period of seemingly slow learning. This phenomenon is particularly surprising because, before grokking, the model might have struggled with overfitting or faced training challenges, and after grokking, it generally performs exceptionally well. In short, grokking is when a model "suddenly gets it" and improves significantly, often exceeding expectations, see, for example, [1], [2], [3], [4] and [5].

In this paper, we aim to investigate the Grokking phenomenon in the learning of modular addition. We will replicate some results in [1] via various models, optimizers and regularization techniques. After that, some discussion on Grokking is provided.

2 The problem and data

Formally, we want to explore the learning of (binary) modular addition

$$(x, y) \mapsto x + y \bmod p, \quad \text{for } x, y \in \mathbb{Z}_p.$$

Each token "x", "$+$", "y", "$=$" and the outcome "$x + y \bmod p$" is embedded into a one-hot vector with length $p + 2$. Here the dimension $p + 2$ is due to the additional tokens "$+$" and "$=$", which are embedded as $(0, \ldots, 1, 0)_{1\times(p+2)}$ and $(0, \ldots, 0, 1)_{1\times(p+2)}$ repectively. Here is a toy example of $p = 3$. Let $x = 1$, $y = 2$, then "x", "$+$", "y", "$=$" and "$x + y \bmod p$" (i.e. "0") are encoded as $(0, 1, 0, 0, 0)$, $(0, 0, 0, 1, 0)$, $(0, 0, 1, 0, 0)$, $(0, 0, 0, 0, 1)$ and $(1, 0, 0, 0, 0)$, respectively. The size of total data is p^2. We choose $p = 97$ here and afterwards without loss of generality, while larger p corresponds a harder problem.

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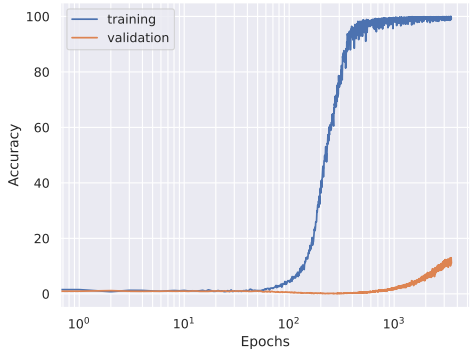
3 Experiments

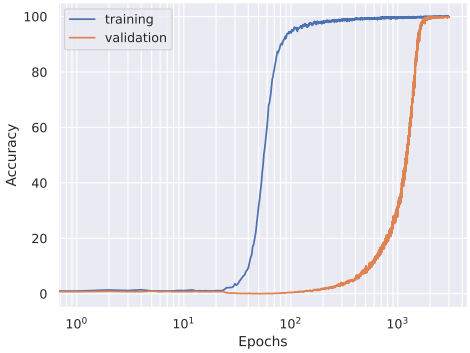
3.1 Grokking for transformer models

We first study the impact of the fraction of training set $\alpha \in (0, 1)$ on the Grokking phenomenon for transformer models using the AdamW optimizer with weight decay 0.05 and learning rate 10^{-3}. Specifically, the transformer model used has 2 layers and 4 attention heads. The embedding dimension is 128, and the batchsize set as 256. Figure 1 plots the relationship the training/validation accuracy and the number of epochs corresponding to $\alpha \in \{0.3, 0.4, 0.5, 0.7\}$. The Grokking phenomenon does occur such that both training and validation accuracy rise quickly after a long while of slow learning, and the validation accuracy starts to rise after the training one begins.

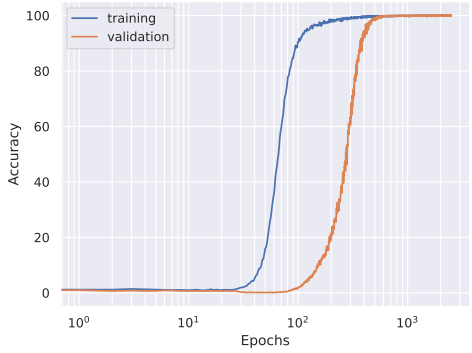
The effects of training fraction α can also be found from the four pictures. On the one hand, larger α leads to faster Grokking. For instance, when $\alpha = 0.3$, it takes more than 10^3 epochs before the validation accuracy starts to rise, whereas, in comparison, it only takes about 100 epochs when $\alpha = 0.5$. On the other hand, the gap between the training and validation accuracy is narrowed with the increase of α. A notable evidence is that when α reaches 0.7, the two accuracy curves seem to rise simultaneously.



(a) Training and validation accuracy with $\alpha = 0.3$



(b) Training and validation accuracy with $\alpha = 0.4$



(c) Training and validation accuracy with $\alpha = 0.5$

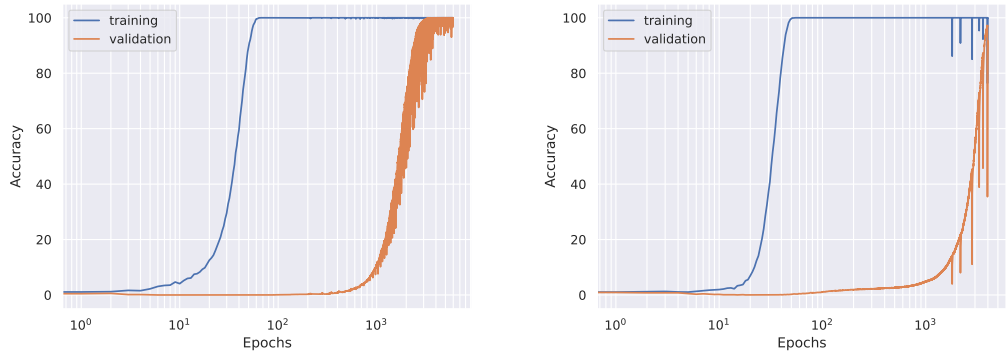
(d) Training and validation accuracy with $\alpha = 0.7$

Figure 1: Grokking phenomenon on transformer model with different training fraction α

3.2 Grokking with other network achitectures

In order to investigate the Grokking on other models, we perform the same experiments with MLP and LSTM. The MLP and LSTM both have two hidden layers of dimension 512. The batchsize dimension and the learning rate mainly follow the settings in Section 3.1 for the convenience of comparison. The training and validation accuracy for MLP and LSTM with $\alpha = 0.5$ are displayed in Figure 2.

The Grokking phenomenon also appears in the two models we consider. In contrast to transformer models with the same $\alpha = 0.5$ in Figure 1c, it takes fewer epochs before the training accuracy begins to rise, while it is the opposite case for validation accuracy. Moreover, the validation accuracy of these two models increases with significant fluctuations, indicating unstable generalization ability.



(a) Training and validation accuracy of MLP with $\alpha = 0.5$

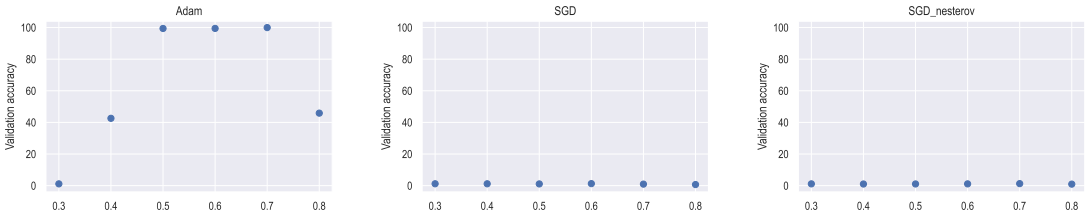
(b) Training and validation accuracy of LSTM with $\alpha = 0.5$

Figure 2: Grokking phenomenon on MLP and LSTM with $\alpha = 0.5$

3.3 The effects of different optimizers and regularization techniques

In this section, we will focus on the impact of optimizers and regularization techniques on Grokking for transformer models. For optimizers, we consider SGD and SGD with Nesterov momentum (where we set the momentum parameter as 0.9) as competitors against Adam. The maximum validation accuracy with different training fraction α within an optimization budget of 8000 steps with batch size 256 is plotted in Figure 3.

It is shown that in contrast with Adam, the validation accuracy with SGD and SGD nesterov remains at a relatively low level within the optimization budget we consider for each α. This is mainly because Adam can quickly adapt and adjust parameters in the early stages of training, it typically converges to a better solution faster than SGD. Besides, Adam has better adaptability to gradient noise and sparse gradients, making the training process more stable.



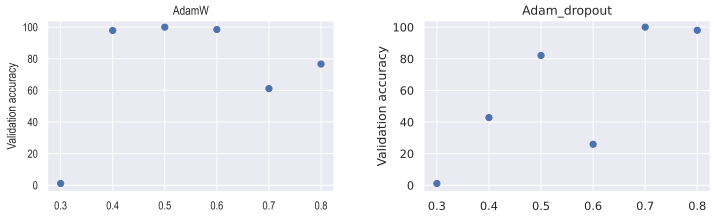
(a) Adam

(b) SGD

(c) SGD nesterov

Figure 3: The maximum validation accuracy with different optimizers within an optimization budget of 8000 steps

For the regularization techniques, we consider weight decay of 0.05 (i.e, AdamW) and dropout (with probability 0.1) for transformer models with Adam optimizer. The corresponding results can be found in Figure 4. Compared with Adam in Figure 3a, AdamW (Figure 4a) improves the validation accuracy at $\alpha = 0.3$ and 0.8, while Adam with dropout (Figure 4b) performs better at $\alpha = 0.8$ but worse at $\alpha = 0.5$ and 0.6.



(a) AdamW (b) Adam with dropout

Figure 4: The maximum validation accuracy with different regularization techniques within an optimization budget of 8000 steps

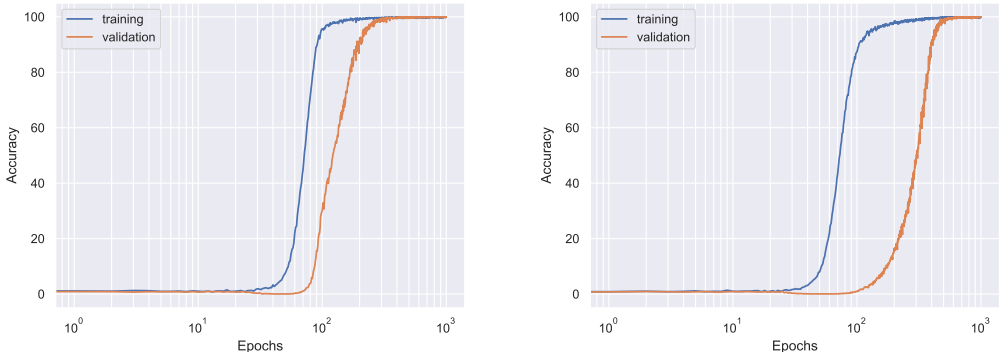
In addition, we also conider the Grokfast algorithm introduced by [2], which is detailed as Algorithm 1. Grokfast can simultaneously implement momentum, weight decay, and the filtering. In our experiments, the initial parameters window size w and scalar factor λ are set according to the values in [2]. Figure plots 5 the training and validation accuracy with Grokfast. In fact, Grokfast without filter (Figure 5b) is analogous to AdamW, and the filter (Figure 5a) accelerates the generalization.

Algorithm 1: GROKFAST

Param: window size w, scalar factor λ.
Input: initial parameters θ_0, stochastic objective function $f(\theta)$, optimizer's parameter update $u(g,t)$ from gradient g at timestep t.
begin: $t \leftarrow 0$; $Q \leftarrow$ Queue(capacity = w);
while θ_t *not converged* **do**

$t \leftarrow t+1$;
$g_t \leftarrow \nabla_\theta f(\theta_{t-1})$; // Calculate gradients
Insert(Q, g_t) ; // Insert gradients to Q
$\hat{g}_t \leftarrow g_t + \lambda \cdot \text{Avg}(Q)$; // Filter gradients
$\hat{u}_t \leftarrow u(\hat{g}_t, t)$; // Calculate update
$\theta_t \leftarrow \theta_{t-1} + \hat{u}_t$; // Update parameters

end while.



(a) Grokfast with fliter (b) Grokfast without fliter

Figure 5: Training and validation accuracy with Grokfast for $\alpha = 0.5$

3.4 A harder problem: multivariate modular addition

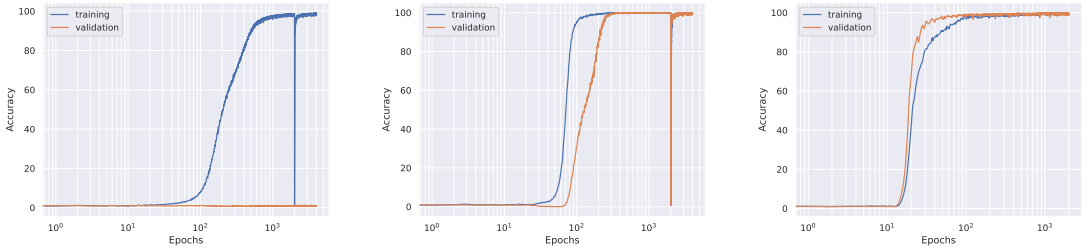
In this section we consider the learning of multivariate modular addition as an extention. Specifically, the problem is

$$(x_1, \ldots, x_K) \mapsto \left(\sum_{k=1}^{K} x_k \right) \mod p,$$

where $x_k \in [p]$ for $k = 1, \ldots, K$. Our goal is to find the influence of the dimension K on the Grokking phenomenon. We use the same transformer model as set in Section 3.1. To start, we first consider the case $K = 3$.

Figure 6 shows the training and validation accuracy with and without pretraining. We pretrain the model on $K = 2$ data for 2000 epochs, and then use a $K = 3$ dataset of size 10^4 to train another 2000 epochs. Figures 6b shows the accuracy of total 4000 epochs, while 6c shows the last 2000 epochs after pretraining. In order to conduct a fair comparision, for unpretrained model we used two different $K = 3$ dataset of size 10^4 and train the model on each dataset for 2000 epochs.

For unpretrained models, we do not see Grokking for the validation accuracy within the range of epochs in Figure 6a, while the training accuracy does grok (the breakpoint is a checkpoint, and so is the breakpoint in Figure 6b). On the contrary, for pretrained models, we can see the Grokking phonomenon within fewer epochs for both training and validation accuracy, see Figures 6b and 6c. Besides, when $K = 2$ is pretrained, the validation accuracy even groks faster than the training accuracy. Therefore, the pretraining of smaller K will be helpful for the learning of larger K.



(a) Training and validation accuracy without pretrained

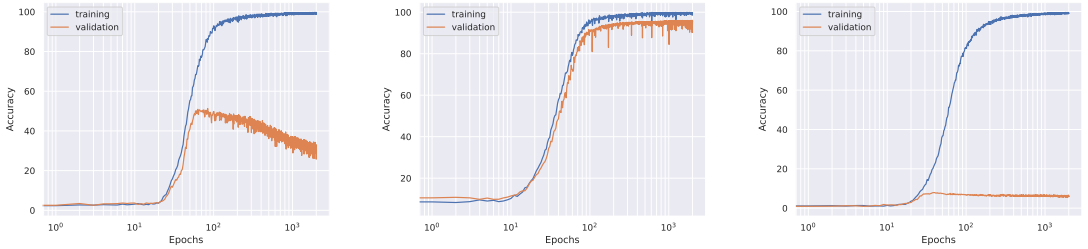
(b) Training and validation accuracy with $K = 2$ pretrained

(c) Training and validation accuracy after pretraining

Figure 6: Grokking phenomenon on transformer model with $K = 3$

Based on the above findings, we perform experiments for $K = 4, 5, 6$ with $K = 2$ pretrained. The results are displayed in Figure 7. Compared with Figure 6c, the training accuracy still groks even though a little bit later than $K = 3$. However, the validation accuracy shows unstable performance: when $K = 4$ (see Figure 7a), it rises to about 0.5 and then gradually decreases; when $K = 6$ (see Figure 7c), it does not grok within the range of epochs plotted. This implies the "curse of dimension" such that the larger K corresponds to a harder task to learn and generalize.

We found that when $K = 4$, the performance is rather strange. We conjecture that there are some similar structures of $K = 2$ and $K = 4$, the model learns this structure at first instead of correct modular addition.



(a) Training and validation accuracy with $K = 4$

(b) Training and validation accuracy with $K = 5$

(c) Training and validation accuracy with $K = 6$

Figure 7: Grokking phenomenon on transformer model with larger K based on pretrained $K = 2$

4 Explanation of Grokking

In this section, we will provide some explanations for the Grokking phenomenon. These explanations are mainly based on two aspects: the principle of acceleration achieved by the Grokfast algorithm and the existing theories that explain the Grokking phenomenon at different stages.

4.1 Difficulty in learning the low-frequency part of parameters

According to the experimental results of the Grokfast algorithm, the occurrence of the Grokking phenomenon is significantly faster than that without using Grokfast. The gap between the reduction of training error and the improvement of generalization accuracy has narrowed significantly, indicating the success of the Grokfast algorithm in accelerating the Grokking phenomenon.

The Grokfast algorithm incorporates an update that amplifies the low-frequency components of the gradient after gradient updates, while maintaining the rest of the updates unchanged. Therefore, its success illustrates an important reason for the Grokking phenomenon: the low-frequency components of parameters are difficult to learn. During the initial stages of training, the high-frequency components of parameters are quickly learned, and these components are sufficient for the model to fit the data on the training set, as the amplitude of the high-frequency components of parameters is larger, allowing them to represent existing data well. However, when generalizing across the entire dataset, the high-frequency components of parameters cannot fit the low-frequency components of data on the validation set well. They can only represent data that is not on the training set very roughly, making it difficult to improve generalization accuracy.

In the process of generalization, the model is actually learning the low-frequency part of the parameters to more accurately fit the validation set. Grokfast enables the model to learn the low-frequency part of the parameters more quickly, which makes the generalization of the model faster compared to attain high accuracy on the training set. Therefore, an important reason for the Grokking phenomenon is the difficulty in learning the low-frequency part of parameters.

4.2 Existing theoretical explanations at different stages

According to [5], the large initialization induces a very strong early phase implicit bias towards kernel predictors, but over time, it decays and competes with a late phase implicit bias towards min-norm/max-margin predictors induced by the small weight decay, resulting in a transition that turns out to be proven sharp in between.

Briefly, the phenomenon of rapid learning on the training set in the early stages is similar to the behavior of kernel predictors, while the phenomenon of gradual generalization in the later stages can be explained by min-norm or max-margin predictors caused by the small weight decay. The occurrence of the Grokking phenomenon is based on the sharp transformation between these two stages, and the characteristics of each stage conform to the properties of existing models.Specifically, the effectiveness of kernel predictors is closely related to the choice of kernel, which can easily lead to overfitting, while min-norm or max-margin predictors have stronger robustness and generalization ability. They have a regularization structure, thus they learn slower but have less generalization error. This explanation corresponds precisely to the two stages of the Grokking phenomenon.

In terms of kernel rigime, [3] provides a more systematic explanation. The paper points out that, the dichotomy between early kernel regime and late feature learning triggered by weak implicit or explicit regularization seems to be the most promising theory to explain grokking.

The paper also proves that, a wide variety of architectures all fail to generalize in the initial phase of training,because networks in the kernel regime can only generalize if trained on at least a constant fraction of all possible data points. If this property is not satisfied by the training set, then the Grokking phenomenon may not even occur.

In addition, the paper demonstrates that networks with appropriate regularization can generalize with many few samples. This highlights the importance of regularization in the Grokking phenomenon, which plays a crucial role in later generalization.

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