Learnable activation functions

Does choice of activation function matter in smaller LMs?

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Abstract

The rapid expansion of large language models (LLMs) driven by the transformer architecture has introduced concerns about the lack of high-quality training data. This study investigates the role of activation functions in smaller-scale language models, specifically those with approximately 10million (M) parameters, to ensure sustained progress in LLM development despite data limitations. Activation functions, crucial for neural network performance, have evolved significantly, but comprehensive comparisons under consistent conditions remain scarce, especially for smaller parameter count models. This research systematically evaluates traditional and novel activation functions, including learnable variants, and introduces the Kolmogorov-Arnold Network (KAN) to language modeling. Using Hugging Face implementations of GPT-Neo and RoBERTa models, this study assesses performance impacts through the BabyLM evaluation pipeline. TODO: Add results and conclusions.

1 Introduction

The transformer architecture [18] has revolutionized the AI landscape and enabled the development of large language models (LLMs). However, as these models continue to grow in size. Current trends are forecasting running out of high-quality data required for optimal performance [19]. This limitation stimulates the initiative to explore the impact of architectural decisions on smaller models, which this project aims to investigate. By understanding how to optimize smaller models, we can ensure the progress of LLMs even with the projected lack of high-quality data.

The choice of activation functions has historically played a crucial role in the advancement of neural networks, such as the shift from Sigmoid activation functions to ReLU (Rectified Linear Unit), which significantly improved training speeds. As the era of large language models (LLMs) unfolded, the development of activation functions continued to evolve, resulting in over 400 documented activation functions [8]. Despite this progress, literature typically compares new activation functions against their immediate predecessors, leading to a gap in the literature: there is no comprehensive comparison of multiple activation functions under consistent conditions. This inconsistency is primarily due to variations in datasets and model sizes used in different studies, highlighting the need for a systematic evaluation. More specifically, with the trend of increasing model sizes, the investigation of the impact activation functions have on smaller models was left neglected. This research aims to address this gap by exploring the impact of activation functions on smaller-scale language models with around 10 million parameters.

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2 Background and related work

Activation functions are used to introduce non-linearity into neural networks, allowing them to model complex relationships in the data. They are applied to the nodes of the network and are essential for enabling the network to learn and perform a wide range of tasks, beyond what linear models can achieve.

The famous paper "Attention is All You Need" [18] used the state-of-the-art activation function at the time, ReLU. Since then, no significant improvements were made until the introduction of GELU, which quickly became the default activation function in most of the state-of-the-art LLMs [9]. The popularity of GELU stems from its ability to enhance model performance without introducing an efficiency overhead. Despite these advancements, continuous innovation leads to alternatives like GeGLU, noted for its effectiveness [17], also used in last year's winner of the BabyLM challenge [15]. However, a recently published paper suggests a return to ReLU [11], adding further confusion to the search for the optimal activation function. Fortunately, it also provides some clues that guide further exploration and motivate this research.

The paper suggests that suggests that the impact of activation functions diminishes as the model size increases, evident in models with over a billion parameters [11]. This also explains the initial move away from ReLU, since all the research on activation alternatives was done on models with the size of approximately 100 million parameters. Highlighting this finding further motivates the need to investigate activation functions in 10 million parameter models. The impact of activation functions is expected to be more significant in smaller models, and until now, decisions have been made with the trend of increasing model size in mind.

Furthermore, another gap appears in the research on activation functions with trainable parameters (adaptable activation functions). The possible explanation for this could be the trade-off between additional trainable parameters and performance. However, this was primarily studied in larger models. The only paper found on adaptive activation functions in LLMs is by Rajanand et al. [13], which found that adaptive activation functions outperform static ones in text-to-text machine translation [NOTE: add the exact numbers from the paper], a task closely related to language models. This suggests that adaptive activation functions could be beneficial for smaller models, but further research is needed to confirm this hypothesis. Given these insights, this research will explore the impact of various activation functions on smaller-scale language models with around 10 million parameters. Hypothesizing that at smaller scales, the choice of activation function is crucial, and having learnable parameters could be beneficial.

Kolmogorov-Arnold Networks (KAN) represent a recent development in neural network architecture, where activation functions are applied on edges instead of nodes [10]. This approach has been shown to outperform traditional neural networks in some tasks, particularly in scientific applications such as solving partial differential equations. However, at the time of this literature review, it has yet to be tested on language models. The primary benefit of KAN is the optimization of activation on each edge using splines. A spline is a piece-wise-defined polynomial function used in interpolation and approximation to create smooth curves through a

set of points [ADD REFERENCE]. With a spline on each edge, each edge can have its own custom activation function, trained separately and uniquely shaped. In contrast, adaptive activation functions have the same shape but different gradients. However, this comes with the drawback of an increased number of trainable parameters. This research will experiment with applying KAN to language modeling to assess its efficacy at smaller scales, filling the gap in the current literature.

3 Approach

Transformers comprise multiple layers, each crucial in processing input data and generating meaningful representations. Among these layers, the Feed-Forward Neural Network (FFN) layer typically consists of two linear transformations with an activation function in between, effectively forming a simple Multi-Layer Perceptron (MLP). This structure allows the default activation function to be switched out with different activation functions for testing, enabling a direct comparison of their performance while keeping everything else the same. To explore the effectiveness of various activation functions, I will modify existing implementations of prominent models like GPT-NEO and RoBERTa from the Hugging Face library.

3.1 Choosing activation functions

The activation functions to be evaluated are ReLU, SiLU, Swish, PReLU, GELU, GEGLU, learnable GELU, and learnable GEGLU. Additionally, the KAN network will be compared against all of these options.

GELU

Currently, the most popular activation function in LLMs is also used as the default activation function in the baseline models GPT-NEO and roBERTa. It is a smooth approximation of ReLU, originally defined as $\text{GELU}(x) = x \cdot \Phi(x)$, where $\Phi(x)$ is the Cumulative Distribution Function for the Gaussian Distribution. or optimization purposes, since calculating $\Phi(x)$ is computationally expensive, it is instead calculated with the tanh approximation as: $\text{GELU}(x) = 0.5x\left(1 + \tanh\left(\sqrt{\frac{2}{\pi}}\left(x + 0.044715x^3\right)\right)\right)$ [6]. This function will be used as a baseline for comparison with all other activations. [add figure of GELU]

ReLU and PReLU

ReLU was considered state-of-the-art at the time of the original transformer paper [18], but has since been surpassed by other activation functions. Baseline models are implemented using the PyTorch library, which provides an implementation for the ReLU activation function [RELU citation from docs], which will be used in this research.

$$\text{ReLU}(x) = \max(0, x)$$

This implementation will be used as a baseline for comparison with *PReLU* and *GELU*. The comparison with GELU is motivated by the findings of *I. Mirzadeh and Others* [11], which suggests that the use of ReLU is acceptable as the impact of activation functions diminishes with increasing model size. The objective is to determine how much worse (if at all) ReLU is compared to GELU when used with smaller models.

PReLU is a variant of ReLU that incorporates learnable parameters, allowing the activation function to adaptably learn the optimal slope for negative values. The PReLU function is available in the PyTorch library [pytorch citation]. It is mathematically defined as

$$\text{PReLU}(x) = \max(0, x) + a\min(0, x)$$

where a is a learnable parameter. It takes the *num_parameters* parameter which was set to *intermediate_size*. The objective is to evaluate whether adding a learnable parameter to ReLU can enhance performance and to measure the impact on training time. [ADD FIGURE OF RELU]

SiLU and Swish

SiLU was initially evaluated on LLMs in the original GELU paper [6] but was found to perform worse than the GELU activation function. It is defined as

$$\text{silu}(x) = x \cdot \sigma(x), \text{ where } \sigma(x) \text{ is the logistic sigmoid.}$$

PyTorch implementation of SiLU was used [cite pytorch silu]. It will be used only as a baseline comparison for the *Swish* activation function, which is its counterpart with learnable parameters, aiding the objective of exploring the impact of adding learnable parameters to activation functions.

Swish is a self-gated activation function that was proposed by *Ramachandran et al.* [14]. It is not available in the PyTorch library so it was implemented as proposed in the paper

$$\text{swish}(x) = x \cdot F.\text{silu}(\beta \cdot x)$$

where β is a learnable parameter. Using the idea seen in PyTorch PReLU implementation the *num_parameters* parameter, which determines the number of learnable parameters was added and set to *intermediate_size*. The objective is to evaluate whether the Swish activation function can outperform SiLU and to measure the impact of adding learnable parameters to activation functions.

[ADD FIGURE OF SILU]

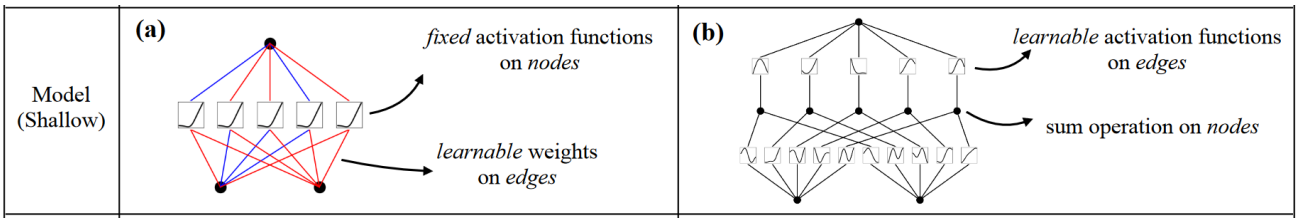

Figure 1: KAN vs MLP [3]

Learnable GELU

The GELU activation function will be parameterized with learnable parameters. The implementation will be based on the PyTorch GELU implementation with tanh approximation, which, out of the box, does not support learnable parameters. This approach appears to be novel, as no prior research has been found that explores the impact of adding learnable parameters to the GELU activation function. The new GELU activation function adds a learnable parameter as a scaling factor and is defined as follows:

$$0.5 \cdot \beta \cdot \text{input} \cdot \left(1.0 + \tanh\left(\sqrt{\frac{2.0}{\pi}} \cdot (\text{input} + 0.044715 \cdot \text{input}^3)\right)\right)$$

where β is a learnable parameter.

The *num_parameters* parameter was set to *intermediate_size* to determine the number of learnable parameters. The objective is to evaluate whether the learnable GELU activation function can outperform the standard GELU activation function and to measure the impact of adding learnable parameters to activation functions.

GEGLU and Learnable GEGLU

The *GEGLU* activation function is a variant of the GELU activation function that incorporates a gating mechanism as proposed by *Shazeer et al.* [17]. It promises to improve the performance of the GELU activation function by adding a gating mechanism. The GEGLU activation function was implemented as used by 2023 BabyLM winner [15] [12]:

```
class GeGLU(nn.Module):
 def forward(self, x):
     x, gate = x.chunk(2, dim=-1)
     x = x * F.gelu(gate, approximate='tanh')
     return x
```

Listing 1: Implementation of GeGLU

The *Learnable GEGLU* activation function is an enhanced variant of the GEGLU activation function, incorporating a learnable parameter following the same idea as Learnable GEGLU. This implementation extends the standard GEGLU by introducing a learnable scaling factor, making it a novel approach. The new Learnable GEGLU activation function is defined as follows:

```
def forward(self, input: Tensor) -> Tensor:
    x, gate = input.chunk(2, dim=-1)
    x = x * 0.5 * self.beta * gate * (1.0 +
        torch.tanh(math.sqrt(2.0 / math.pi) * (
        gate + 0.044715 * torch.pow(gate, 3.0)))
        )
    return x
```

Listing 2: Implementation of Learnable GeGLU

The objective is to first evaluate the performance of GeGLU compared to GELU, and then to evaluate the performance of Learnable GeGLU compared to GeGLU. The hypothesis is that Learnable GeGLU will be the best-performing activation function.

KAN-Network

The KAN network is a novel activation function that has shown promising results in the literature. The implementation of the KAN network is available but has shown to be problematic and slow. To address these issues, I will utilize an efficient-KAN implementation [1]. This approach requires careful selection of certain parameters, specifically the number of grid intervals (int) and the order of piecewise polynomials (k). Based on recommendations from the paper, I will set these parameters to 3 and 5, respectively. This configuration aims to balance performance and computational efficiency, ensuring that the KAN implementation is both effective and practical for the experiments. FFN layers from GPT-NEO and roBERTa both use MLPs in their implementation, which can be directly replaced with efficient-KAN implementation. As KAN network adds additional trainable parameters, the intermediate size for GPT-NEO was decreased to 256 and for roBERTa to 384 to keep the number of parameters around 10M as for other models.

The objective is to evaluate the performance of the KAN network compared to the other activation functions and to determine whether it is a viable alternative for LLMs.

4 Experimental setup

4.1 Research questions

Through the experiment, we aim to answer the following research questions:

- *Is the choice of activation function relevant to the performance of smaller models with 10M parameters?* We compared the pre-trained baseline models and models with *SiLU* and *ReLU* activation functions and compared the results of evaluation on BabyLM evaluation pipeline [22].

- *How does the addition of learnable parameters to the activation function improve the performance of the model?* We modified static activation functions to include learnable parameters, pre-trained them, and evaluated them on the BabyLM evaluation pipeline [22].
- *Do FFNs using KAN-networks outperform FFNs using MLP networks?* We used efficient-kan implementation of KAN-networks [1], pre-trained them and evaluated them on BabyLM evaluation pipeline [22].

4.2 Dataset

We used the TinyStoreis dataset for pre-training. It's a dataset of short stories, that contains words that a typical 4-year-old would likely understand, generated by GPT-3.5 and GPT-4. It has been shown that they can be used to train LMs that are around 10M parameters and can still generate coherent stories. [3].

4.3 Models

We used Hugging face implementations of GPTNeoForCausalLM [4] and RobertaForMaskedLM [5] models. GptNEO is GPT2-based decoder model, while roBERTa is based on Google's BERT model from 2018. We used these models as baselines for our experiments. The hyperparameters used for the models can be seen in table 1. The change in intermediate size for KAN-MLP implementnation was made due to increased number of learnable parameters in the activation function and the need to keep the total number of parameters in the model approximately constant. The final parameter counts shown in table 2.

4.4 Evaluation Setting and Metrics

Evaluation pipeline

We used the BabyLM evaluation pipeline [22] to evaluate the models. The pipeline consists of three components: BLiMP, GLUE and SuperGLUE. BLiMP is a benchmark for evaluating the linguistic capabilities of language models, consisting of 17 metrics, each specific in syntax, morphology or semantics. Models were evaluated zero-shot, by comparing the probabilities of the sequences in a minimal pair, under the assumption that the acceptable sequence will be considered more likely than its unacceptable counterpart. The final score was computed as an average of those 17 metrics. [23] [24]. GLUE and SuperGLUE are benchmarks for evaluating the performance of language models on a variety of natural language understanding tasks. GLUE consists of 9 tasks, while SuperGLUE consists of 8 tasks. The final score was computed as the average of the scores 7/9 GLUE tasks and 3/8 SuperGLUE tasks [21] [20].

Statistical significance testing

TODO: Make this section more reader friendly.

The following section justifies the choices made for the statistical significance testing, based and summarised from The Hitchhiker's Guide to Testing Statistical Significance in Natural Language Processing [2].

Since the distribution of the test statistic is not known, we had to choose approaches from non parametric family of approaches. Which is split in two categories. Sampling based tests and sampling free tests.

Sampling free tests are computationally less expensive but do not consider evaluation meausre values, only higher level statisics such as the number of cases in which each of the models perorms better than the other. Therefore they have less statistical power. Of those tests, Wilcoxon signed-rank test is the most powerful one as it makes use of ranking the differences between the test scores. Thats why we used it in our experiments. Its null hypothesis is that the differences are symmetrically distributed around zero. Absolute values of the differences are ranked and the sum of the ranks of the positive differences is compared to the sum of the ranks of the negative differences. The test is one-sided, as we are interested in the direction of the difference.

Sampling based tests compensate for the lack of distribution information with resampling. They are computationally more expensive, but can be less effective for smaller sets of results. We used bootstrapping as a sampling based test. It is a resampling method that involves drawing samples with replacement from the original results. These samples are used to approximate the distribution of the statistic. The p-value is calculated as the proportion of the samples in which the statisic is greater than the observed value. We used 1000 samples for bootstrapping in our experiments.

4.5 Hardware

All the models were trained and evaluated on a single NVIDIA A100 GPU with 4 CPUs and 24GB of memory on DelftBlue cluster.

5 Results

Results of evaluations on BLiMP and GLUE datasets are shown in Table 3. Training times for each model are shown in Table 4.

TODO: Highlight the most important results, add missing results.

Parameter	GPT Neo	RoBERTa
Embedding Parameters		
Vocab Size	10,000	10,000
Hidden Size	512	512
Max Position Embeddings	512	513
Blocks (Attention & FFN)		
Number of Layers	2	2
Attention Types	[[[”global”, ”local”], 1]]	N/A
Number of Attention Heads	4	4
Window Size	256	N/A
Intermediate Size	1024 (**256 for KAN-MLP**)	1024 (**384 for KAN-MLP**)

Table 1: Comparison of Parameters for GPT Neo and RoBERTa

Model Name	Number of Parameters
GPT with GELU (baseline)	9.0M
BERT with GELU (baseline)	9.0M
BERT with Learnable-GELU	9.0M
GPT with Learnable-GELU	9.0M
GPT with ReLU	9.0M
BERT with ReLU	9.0M
BERT with PReLU	9.0M
GPT with PReLU	9.0M
GPT with SiLU	9.0M
BERT with SiLU	9.0M
BERT with Swish	9.0M
GPT with Swish	9.0M
GPT with KAN MLP	11.0M
BERT with KAN MLP	11.0M

Table 2: Model Names and Number of Parameters

6 Discussion

TODO: Statistical significance analysis of results and discussion of application of findings.

- implications
- threats to validity
- future work

7 Conclusions and Future Work

TODO:

- brielfy repeat the RQs
- Discuss the the implications of results
- Suggest future research directions

8 Reponsible research

To prevent test set contamination, we pre-trained our models on datasets that were separate from those used for evaluation. This addresses an issue highlighted in recent works, where pre-training on test sets can artificially inflate performance metrics and call into question the validity of the results [16]. Ensuring distinct separation between training and evaluation datasets maintains the integrity of our findings and contributes to the reliability of our research.

In conducting this research, we ensured transparency and reproducibility by sharing the experimental setup under section 4. The datasets and models used are publicly available and can be found in the references. Furthermore, all the implemented code is available on GitHub? We adhered to scientific integrity by fabrication, and plagiarism, ensuring that everything reported accurately with proper citations.

TODO: Check this part: Guided by the Netherlands Code of Conduct for Research Integrity, we incorporated principles of honesty, transparency, and responsibility, ensuring our research practices align with the highest standards. We followed the educational and normative framework from chapters 2 and 3 of the Code, emphasizing good research practices that promote a responsible research environment [7].

Model	BLiMP	GLUE
BERT-Learnable-GELU-9.0M-2L-4H-512C-1024I	59.4%	57.1%
GPT-Learnable-GELU-9.0M-2L-4H-512C-1024	56.782%	67.62%
Same baselines		
GPT-9.0M-2L-4H-512C-1024I	55.6%	57.09%
BERT-9.0M-2L-4H-512C-1024I	49.1%	54.94%
Best baselines GLUE		
GPT-11.0M-3L-4H-512C-1024I-0	55.17%	60.2%
BERT-11.0M-3L-4H-512C-1024I	49.49%	55.41%
GPT-PReLU-9.0M-2L-4H-512C-1024I	57.0%	57.6%
BERT-PReLU-9.0M-2L-4H-512C-1024I	59.2%	56.1%
GPT-SiLU-9.0M-2L-4H-512C-1024I	56.3%	59.9%
GPT-ReLU-9.0M-2L-4H-512C-1024I	56.6%	59.9%
BERT-SiLU-9.0M-2L-4H-512C-1024I	58.3%	57.5%
BERT-ReLU-9.0M-2L-4H-512C-1024I	58.5%	57.2%
GPT-Swish-9.0M-2L-4H-512C-1024I	53.7%	57.6%
BERT-Swish-9.0M-2L-4H-512C-1024I	58.0%	57.8%
BERT-kan2-11.0M-2L-4H-512C-384I	56.69%	63.65%
KAN2-GPT-11.0M-2L-4H-512C-256I	63.43%	48.80%
Learnable GELU Seeds		
GPT-Learnable-GELU-seed4-9.0M-2L-4H-512C-1024I	56.0%	59.2%
GPT-Learnable-GELU-seed1-9.0M-2L-4H-512C-1024I	56.3%	58.8%
GPT-Learnable-GELU-seed2-9.0M-2L-4H-512C-1024I	57.4%	58.7%
BERT-Learnable-GELU-seed4-9.0M-2L-4H-512C-1024I	58.2%	57.0%
GPT-Learnable-GELU-seed5-9.0M-2L-4H-512C-1024I	58.3%	59.3%
GPT-Learnable-GELU-seed3-9.0M-2L-4H-512C-1024I	58.7%	59.6%
BERT-Learnable-GELU-seed3-9.0M-2L-4H-512C-1024I	59.0%	57.0%
BERT-Learnable-GELU-seed2-9.0M-2L-4H-512C-1024I	59.3%	59.7%
BERT-Learnable-GELU-seed5-9.0M-2L-4H-512C-1024I	59.8%	59.2%
BERT-Learnable-GELU-seed1-9.0M-2L-4H-512C-1024I	59.8%	56.2%

Table 3: Comparison of models across BLiMP and GLUE datasets

Model Name	Training Time
BERT-GeGlu	1h 48m 43s
GPT-GeGlu	1h 45m 35s
BERT-Learnable-GEGLU	1h 53m 16s
BERT-Learnable-GELU	1h 45m 39s
GPT-Learnable-GEGLU	1h 48m 19s
GPT-Learnable-GELU	1h 41m 19s
GPT-ReLU	2h 17m 4s
BERT-ReLU	2h 24m 46s
BERT-Swish	1h 43m 8s
GPT-Swish	1h 39m 22s
BERT-PReLU	1h 47m 27s
GPT-PReLU	1h 42m 28s
KAN2-GPT	3h 23m 35s
BERT-kan2	2h 52m 11s
BERT-kan	2h 19m
KAN-GPT	4h 23m 32s
GPT-SiLU	1h 39m 35s
BERT-SiLU	1h 45m 4s
GPT-base	1h 42m 26s
BERT-base	1h 45m 56s

Table 4: Model Names and Training Times

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