MATRIX MIXTURE OF EXPERTS IS THE BEST FAST FEED-FORWARD

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Paper under double-blind review

ABSTRACT

We dissect the recently introduced Fast Feed-Forward (FFF) neural network architecture and propose a matrix formulation of FFF that allows a unified perspective on FFF and Mixture of Experts (MoE) architectures. This formulation achieves, on average, nearly a 4x speedup in FFF inference on CPUs and 9x on GPUs, compared to the original formulation, for FFF depths up to 8. Additionally, it enables an almost 10% improvement in accuracy on the CIFAR-10 dataset (Krizhevsky et al.), while maintaining the same training time.

1 Introduction

Recent years have witnessed significant progress in the field of machine learning, marked by the development of increasingly complex and powerful models. One of the promising directions in this domain is the application of *Mixture of Experts* (MoE) methods (Jacobs et al. (1991); Fedus et al. (2022b;a); Jiang et al. (2024)).

The motivation behind employing MoE lies in addressing the challenges of scalability and efficiency in large neural networks. Modern machine learning tasks often require substantial computational resources. MoE techniques enable efficient allocation of computational resources by activating only those submodels that are most relevant for a given task. This approach reduces the overall computational overhead while maintaining high-quality predictions.

MoE was first introduced in "Adaptive Mixtures of Local Experts" by Jacobs et al. (1991). The central idea is a system comprising multiple models, each specializing in a subset of training data. Alongside these experts, a gating model is trained to determine the weights of each expert during inference.

Over time, the MoE concept has evolved, finding applications within the layers of deep neural networks, including large-scale language models (see Shazeer et al. (2017); Fedus et al. (2022b); Gale et al. (2022)). A version of MoE, *Hierarchical Mixture of Experts* (HMoE, first introduced by Jordan & Jacobs (1994)), dubbed *Fast Feed-Forward Networks* (FFF) in a namesake work by Belcak & Wattenhofer (2023b) gained not much attention and remains less explored than traditional MoE methods.

In this work, we present a matrix-based formulation of the FFF architecture that offers a unified parameterization with Mixture of Experts (MoE) models. This formulation results in a significant enhancement in efficiency, achieving nearly 4x faster inference on CPUs for networks with depths up to 8, and 9x faster on GPUs for depths up to 13. Furthermore, we observe a nearly 10% improvement in accuracy on the CIFAR-10 dataset, all while maintaining the same training time.

1.1 MIXTURE OF EXPERTS (MOE)

The primary concept of the MoE architecture involves partitioning a neural network layer (primarily fully connected) into independent blocks of neurons, called *experts*. A routing layer, also known as a *router*, precedes the experts and determines the subset of experts to be utilized at the inference time. The performance of the model is highly sensitive to the choice of the router. Recently, the most commonly employed mechanism for selecting experts involves calculating selection probabilities and using a weighted average over the selected experts:

$$R(i|\mathbf{x}) = \text{Softmax}(W\mathbf{x})_i \tag{1}$$

(2)

$$\mathbf{y} = \sum_{i \in \text{top-}k(R)} R(i|\mathbf{x}) f_i(\mathbf{x})$$

where $R(i|\mathbf{x})$ represents the probability of selecting the *i*-th expert, which is represented by the layer

For a MoE layer containing an equivalent total number of parameters as a dense fully connected layer, inference is faster because only a subset of experts is activated. The number of operations required during inference can be expressed as:

$$\mathcal{O}(K + E \times k)$$

where K is the total number of experts, $E=\frac{M}{K}$ is the size of each expert, M is the total parameter count of a layer, and k is the number of experts used during inference.

1.2 FAST FEED-FORWARD (FFF)

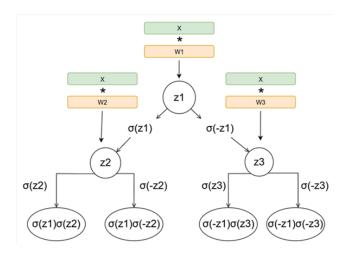


Figure 1: A diagram of a depth-2 tree in the FFF layer. The final layer provides probabilities for the leaves.

Belcak & Wattenhofer (2023b;a) introduced the FFF layer architecture. The primary idea is to achieve exponential acceleration during inference by selecting an expert from an exponentially large set and replacing the MoE router layer with a binary tree structure (see Figure 1).

Each node $i \in [1, 2^d - 1]$ in the tree contains a parameter vector $\mathbf{w}_i \in \mathbb{R}^n$. Based on the dot product between the input vector and the node's parameter vector, the probability of selecting the next parameter vector for one of the child nodes is computed as:

$$P(2i|\mathbf{x}, i) = \sigma(z_i) = \sigma(\mathbf{w}_i^{\mathsf{T}} \mathbf{x})$$
(3)

where $\sigma(x)=\frac{1}{1+e^{-x}}$. The probability of selecting the opposite child node is given by:

$$P(2i+1|\mathbf{x},i) = \sigma(-z_i) = 1 - \sigma(\mathbf{w}_i^{\mathsf{T}}\mathbf{x})$$
(4)

At the final level of the tree are the leaf nodes in, similar to the experts in MoE, henceforth referred to as experts. During training, data passes through all tree nodes, accumulating probabilities to form a distribution over the leaf nodes at the final layer. These probabilities are subsequently used to compute the weighted average:

$$\mathbb{E}_{i \sim R(i|\mathbf{x})}[f_i(\mathbf{x})] \tag{5}$$

where $R(i|\mathbf{x})$ denotes the probability of selecting leaf i, which is represented by the layer f_i .

During training, an FFF layer of depth $d = \log K$ uses all $\mathcal{O}(2^d \times E + 2^{d-1})$ parameters to compute the average, ensuring all experts are utilized. This approach enables a differentiable router, facilitating accurate gradient computation. However, it significantly increases computational costs during training (see Muqeeth et al. (2023)).

During inference, the FFF layer sequentially selects the most probable node at each level of the tree in a greedy manner, with the output of the selected leaf node serving as the final output vector. The computational complexity of this algorithm is logarithmic in the number of leaves, given by:

$$\mathcal{O}(d+E)$$

Thus, for an equivalent number of experts, FFF achieves exponential acceleration in search. However, this algorithm lacks parallelism, as each tree level must be computed sequentially.

2 COMMON PARAMETRIZATION FOR FFF AND MOE

2.1 LOGARITHMIC TRANSFORMATION

Consider the router in FFF, which represents the distribution of the selected experts $R(i|\mathbf{x})$. It is defined as follows:

$$R(i|\mathbf{x}) = \prod_{j \in \text{Path}(i)} P(j|\mathbf{x}, \lfloor \frac{j}{2} \rfloor)$$
 (6)

where Path(i) contains the indices of all nodes along the path from the root to the leaf i, and the probabilities P inside the product take the form of equations 3 or 4 depending on the parity of j, parameterized by weight vectors.

The logarithm of this distribution can be computed as:

$$\log R(i|\mathbf{x}) = \sum_{j \in \text{Path}(i)} a((-1)^j z_{\lfloor j/2 \rfloor}) \tag{7}$$

where a(x) is defined as:

$$a(x) = \log \sigma(x) = -\text{Softplus}(-x)$$
 (8)

In this equation, $(-1)^j$ indicates that for odd nodes, the probability is computed as the activation of an opposite value, as shown in equation 4. Expression in 7 represents a linear combination of activations from a subset of tree nodes. It can also be interpreted as a weighted sum of activations from all nodes¹, similar to the pre-activation in the next layer of a fully connected network for layers of size 2^{d-1} and 2^d .

2.2 LINEARITY

Since expression 7 is a linear combination, it can be represented in a matrix form. We can also convert this expression into probabilities by normalization. If $\mathbf{z}=(z_1,\ldots,z_{2^d-1})=W\mathbf{x}$, the expert distribution is expressed as:

$$R(i|\mathbf{x}) = \text{Softmax}(Ta(S\mathbf{z}))_i \tag{9}$$

¹The weights are 1 for the nodes on the path to the given leaf and 0 for all others.

where $T \in \mathbb{R}^{2^d \times 2(2^d-1)}$ is a matrix where $t_{ij}=1$ if $j \in \text{Path}(i)$ and 0 otherwise, and $S \in \mathbb{R}^{2(2^d-1)\times 2^d-1}$ contains ± 1 along the diagonal to account for the sign before the activation.

For example if FFF layer has depth d=2, then T and S are constructed as follows:

$$T = \begin{pmatrix} 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 \end{pmatrix} \quad S = \begin{pmatrix} 1 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & -1 \end{pmatrix}$$

Firstly, this formulation illustrates that the Fast Feed-Forward (FFF) architecture is a specific instance of a more general parameterization, given by $Ta(S\mathbf{z})$, where T, S, and a can be chosen arbitrarily. For example, the MoE model can be recovered by setting S=T=I (the identity matrix) and defining a(x)=x.

Secondly, this formulation clarifies the potential for parallelizing computations of the probabilities. However, a possible limitation of this approach is the challenge of storing these matrices in memory, especially when represented in their full form. Despite this, it is evident that the matrices are highly sparse, which allows for efficient storage using specialized data structures, such as the Compressed Sparse Row (CSR) format, to significantly reduce memory overhead while maintaining computational efficiency.

2.3 CHANGING THE ACTIVATION FUNCTION

Let us examine the activation function in the original FFF architecture in details. By removing the sign from the argument and flipping the signs of all weights at the nodes, we can construct an equivalent model. Additionally, the second sign in the Softplus function serves a critical purpose: it ensures that, during the transition to probabilities, the resulting values lie within the interval [0,1]. However, this second sign can be removed if appropriate normalization is applied at the end of the computation to achieve the same effect.

Given these considerations, we adopt the standard form of the activation function, a(x) = Softplus(x), as the default choice for the base FFF architecture.

With the flexibility to adjust our current parametrization, we further experiment with alternative activation functions within the model to explore their impact on performance.

3 EXPERIMENTS

To assess the impact of activation functions on the FFF architecture, we conducted experiments using the CIFAR-10 dataset Krizhevsky & Hinton (2009), chosen for its lightweight nature, which allows for rapid iteration across numerous model configurations. We trained several FFF models with varying depths, ranging from 1 to 4. For activation functions, we selected the following options: the baseline Softplus(x), a linear activation f(x) = x, and the ReLU function ReLU $(x) = \max(0, x)$.

3.1 Training Setup

The model architecture consists of a single FFF layer, configured with either 8 or 16 hidden neurons in each tree node. The experts are two-layer MLPs, also featuring 8 and 16 hidden neurons, respectively. Each model was trained for 8 epochs with a batch size of 128, using the Adam optimizer and a one-cycle learning rate schedule. The maximum learning rate was set to 8×10^{-4} to facilitate faster convergence.

3.2 RESULTS

The results demonstrated a consistent improvement in accuracy across all model sizes when ReLU or linear activation functions were used, compared to the baseline Softplus. An unexpected observation was that the absence of an activation function outperformed the baseline. This phenomenon

Activation	d=2.0	d=3.0	d=4.0
Linear	0.422	0.427	0.415
ReLU	0.422	0.403	0.404
Softplus	0.383	0.389	0.369

Table 1: Accuracy values for different activation functions across varying d values. Bold values indicate highest accuracy for each d value.

may be attributed to activation functions inhibiting the propagation of signals from features with negative contributions, thereby reducing the model's ability to select the appropriate expert effectively. Figure 2 presents the accuracy and loss trends for models with 8 hidden neurons, showcasing the performance dynamics across depths and activation functions. Additional plots for models with 16 hidden neurons are in the Appendix: A.

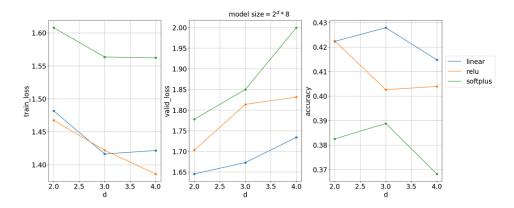


Figure 2: FFF loss on training and validation datasets, and validation accuracy for different model depth and activation functions.

The average change in relative model accuracy was analyzed for different activation functions. The baseline configuration, an FFF model with Softplus activation, represents the activation used in the original formulation. The average increase in accuracy, $\Delta A_{\rm avg}$, was calculated across various model depths. Notably, the ReLU activation function resulted in an average accuracy improvement of 6.9%, while the linear activation function achieved an even greater improvement of 9.8%. These results are summarized in Table 1.

4 BENCHMARKS

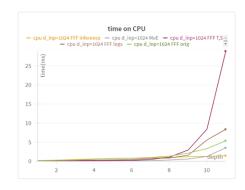
Benchmarking was conducted to evaluate the speed performance of FFF and MoE layers across different implementations. The number of hidden neurons for all models was chosen to be 1024. Tests involved three FFF variants and one MoE implementation.

The "FFF orig" implementation replicates the original training-mode FFF, sequentially computing probabilities layer by layer. "FFF inference" modifies this for inference, processing only one branch per layer based on the sign of a single dot product. "FFF logs" operates similarly to the original but uses logarithmic computations. "FFF T, S" optimizes the process using three matrix multiplications in dense configurations as detailed in 9.

The "MoE" implementation follows the standard Mixture of Experts structure, computing Softmax(Wx) via a single matrix multiplication. These variants were compared for computational efficiency and scalability.

4.1 Average speedup

The harmonic mean of time ratios between "FFF T,S" and "FFF orig" across depths, as shown in Figure 3, revealed a 3.5x speedup on CPUs up to depth 8, with performance degrading exponen-



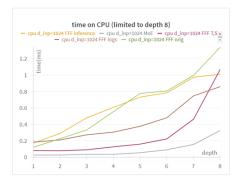


Figure 3: Performance comparison of the FFF layer in different implementations and MoE on CPU

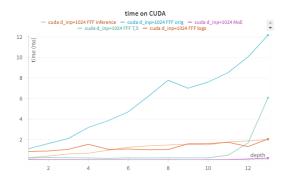


Figure 4: Performance comparison of the FFF layer in different implementations and MoE on GPU

tially due to dense matrix operations. On GPUs, as illustrated in Figure 4, "FFF T,S" achieved a 9x speedup over "FFF orig", while the classical "MoE" model remained 6.4x faster. Despite improvements, the results highlight the trade-off between computational efficiency and architectural complexity.

5 CONCLUSION

This work presents a matrix-based formulation of the FFF architecture, providing a unified view with MoE models. The approach achieves up to 4x and 9x faster inference on CPUs and GPUs for depths up to 8, while improving accuracy on CIFAR-10 by nearly 10%, driven by changes in the activation function. Benchmarking shows FFF T,S outperforms the original FFF but remains 6.4x slower than MoE on GPUs. FFF is efficient with more than 2^8 experts on CPU or 2^{13} on GPU; otherwise, MoE or the matrix formulation is preferable. These results highlight the scalability and efficiency of the proposed formulation.

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A ADDITIONAL RESULTS FOR MODELS WITH 16 HIDDEN NEURONS

This section presents the accuracy and loss plots for models with 16 hidden neurons in each tree node, corresponding to the experimental setup described in Section 3. These plots provide additional insights into the performance of different activation functions and model depths.

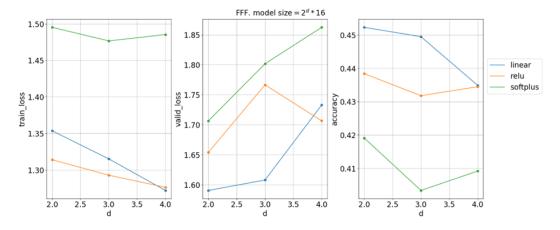


Figure 5: Accuracy and loss plots for models with 16 hidden neurons, across different activation functions and model depths.