Leveraging Intermediate Neural Collapse with Simplex ETFs for Efficient Deep Neural Networks

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Abstract

Neural collapse is a phenomenon observed during the terminal phase of training when a neural network achieves zero training error, in which network activations, class means, and linear weights converge to a simplex equiangular tight frame (ETF), a set of vectors whose mutual distance within a subspace is maximized. Neural collapse has been theorized to contribute to neural network interpretability, robustness, and generalization, but utilization of neural collapse conditions in neural network training and regularization remains underexplored. Previous work has demonstrated that fixing the final layer of a neural network to a simplex ETF reduces the number of trainable weights without compromising the neural network's accuracy. Moreover, deep fully-connected networks exhibit neural collapse not only in the last layer, but on all layers beyond a given effective depth. We apply this knowledge to introduce two new training schemes: Adaptive-ETF, a generalized training framework in which we set all layers beyond effective depth to simplex ETFs, and ETF-Transformer, where the feed-forward network layers in a transformer block are set to simplex ETFs. We show that these modifications achieve similar training and testing performance to their baseline variants while using fewer learnable parameters.

1 Introduction

Steady advancements in machine learning over the past decade have enabled deep neural networks to achieve superhuman performance on many challenging real-world tasks, ranging from image classification to speech recognition and natural language modeling. However, the structure of these deep neural networks is highly complex. As such, neural networks have been largely regarded as black boxes. However, more recent work has shown that during the training process, neural networks tend to learn mathematically simple structures. One such example of this phenomenon is neural collapse.

Neural collapse (NC) is a phenomenon where all features learned by a neural network converge to their class means, the class means converge to last-layer linear classifier weights, and the feature means and weights of different classes are placed as far apart as possible, forming a simplex equiangular tight frame (ETF). NC was first documented by Papyan et. al. [4] during the terminal phase of training (TPT) of a deep neural network. During TPT, the training error of the network stays at zero, and the loss function is also pushed towards zero. Understanding and taking advantage of the neural collapse phenomenon is a large step towards designing neural networks with greater interpretability, robustness, and generalization capability.

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Contribution Previous work has largely focused on exploring neural collapse from a theoretical lens, documenting its occurrence and providing mathematical justifications for its existence. More recently, the concept of neural collapse has been extended to encompass intermediate neural network outputs as well, identifying a link with generalization bounds. [3] However, the effects of using simplex ETF during training with consideration for NC have been largely unexplored, especially in the domain of intermediate neural collapse.

In this paper, we investigate the use of simplex equiangular tight frames to mathematically constrain a neural network to observe neural collapse in final layers. A simplex ETF is a mathematical structure in a vector space $\mathbb{R}^C$ where C vectors are placed as far apart as possible in the space. We demonstrate that a fully-connected network with all layers beyond its effective depth (that is, all layers achieving intermediate neural collapse) set to a simplex ETF achieve the same train/test accuracy and effective depth as a vanilla MLP, demonstrating the feasibility of using intermediate-layer simplex ETFs during training to save on memory. We additionally demonstrate similar results in a transformer network: although neural collapse is not directly observed within fully-connected layers in transformer blocks, replacing fully-connected layers with simplex ETFs makes for faster training without significant loss to prediction accuracy.

2 Background: Neural Collapse

The task is a multiclass classification problem. We consider a distribution P over samples $(x, y) \in \mathcal{X} \times \mathcal{Y}_C$ where $\mathcal{X} \subset \mathbb{R}^d$ and $\mathcal{Y}_C = [C]$, and a deep neural network, which consists of a feature learner (all previous layers) $h(x) \in \mathbb{R}^k$ followed by a linear classifier of weights W and bias b; we can therefore consider the entire network itself as $g(x) = Wh(x) + b$. The regularized empirical objective function over i.i.d. observed dataset S using cross entropy loss ℓ is expressed as

$$\mathcal{L}_S^\lambda(g_W) := \frac{1}{|S|} \sum_{(x_i, y_i) \in S} \ell(g_W(x_i), y_i) + \lambda \|W\|_2^2.$$

There are four interconnected neural collapse conditions, stated below.[4]

2.1 (NC1) Variability collapse

The within-class variance of the features h go to zero, which means that all features collapse to class means.

$$\Sigma_W = \mathbb{E}_{i,c}[(h_{i,c} - \mu_c)(h_{i,c} - \mu_c)^\intercal] \to 0$$

2.2 (NC2) Convergence to Simplex Equiangular Tight Frame (ETF)

Over training, the vectors of the class means (in matrix $\dot{M}$) converge to having equal length, having the same angle between any pair of class means, and being maximally pairwise distant from each other.

$$\begin{aligned} &|\|\mu_c - \mu_G\|_2 - \|\mu_{c'} - \mu_G\|_2| \to 0, \\ &\left\langle \frac{\mu_c - \mu_G}{\|\mu_c - \mu_G\|_2}, \frac{\mu_{c'} - \mu_G}{\|\mu_{c'} - \mu_G\|_2} \right\rangle \to \frac{C}{C-1}\delta_{c,c'} - \frac{1}{C-1} \qquad \forall c, c' \end{aligned}$$

This is equivalent to the simplex equiangular tight frame (ETF) a well-studied structure in mathematics. The simplex ETF is described by the columns of the matrix

$$\dot{M} = \sqrt{\frac{C}{C-1}} P \left(I_C - \frac{1}{C} \mathbb{1}_C \mathbb{1}_C^\intercal \right)$$

where P forms the first C columns of an identity matrix of size k. [7]

2.3 (NC3) Convergence to self-duality

The class means and weights occupy dual vector spaces. In neural collapse, they converge to each other up to a rescaling.

$$\left\| \frac{W^\intercal}{\|W\|_F} - \frac{\dot{M}^\intercal}{\dot{M}\|_F} \right\| \to 0$$

2.4 (NC4) Simplfication to nearest class center (NCC)

For any data point, the classifier converges to choosing the class has the nearest training class mean in Euclidean distance.

$$\arg\max_{c'} < w_{c'}, h > + b_{c'} \to \arg\min_{c'} \|h - \mu_{c'}\|_2$$

Because the NC4 metric is most relevant to neural network intermediates, and because the equivalence of neural collapse conditions has been shown in [4], we use NCC accuracy to measure the degree of neural collapse for our experiments.

3 Related work: Simplex ETF and Effective Depth

Effective Depth Galanti et. al. [3] defines the notion of *effective depth* L_0 of a deep neural network as the minimum depth at which a deep neural network achieves NCC separability (NCC error $\leq \epsilon$). If the network does not achieve NCC separability, then $L_0 = L$. The minimal-depth hypothesis [3] states that there must exist some depth $L_0 \geq 1$ such that any network with depth greater than L_0 also achieves NCC separability. It follows that the NCC accuracy of layer L must be greater than or equal to the NCC accuracy of layer $L - 1$ for all layers $L \geq L_0$. Less strictly, ϵ-effective depth denotes the minimal depth of a network at which the NCC error is less than or equal to ϵ. ϵ-effective depth is the metric we use when evaluating effective depths of the neural networks in Section 4.

Simplex ETF for neural network training By NC2 and NC3, class means and linear classifiers both converge to a simplex ETF. Recent work by Zhu et. al. [7] has shown that if a network has exhibited neural collapse, then setting the final layer to be a simplex ETF allows for reduced parameters in the network while maintaining the same degree of accuracy as an otherwise equivalent model with a fully trainable final layer. This enables significantly reduced training-time memory usage.

Combining Effective Depth and Simplex ETF In this paper, we propose a training scheme that utilizes the simplex ETF framework for all layers past the ϵ-minimal depth of a given neural network. It has been previously demonstrated that a network where $L_0 \geq L$ with the final layer fixed to a simplex ETF achieves the same accuracy as an unconstrained network with the same architecture, using far less memory. Results from Galanti et. al. [3] show that overparameterized neural networks achieve NCC separability in not only the last layer, but in all layers between L_0 and the last layer. It follows that we can further extend the simplex ETF constraint to intermediate layers beyond the effective depth with no detriment to training. This demonstrates not only a method of training that saves on memory usage and number of learnable parameters, but also a link between NC2, NC3, and NC4 conditions that extends beyond the final layer of the neural network.

4 Experiments

Training We use the standardized Fashion-MNIST image dataset [6]. We use a cross-entropy loss function and train for 300 epochs with stochastic gradient decent, using weight decay 5e-4, momentum 0.9, and a learning rate schedule with initial learning rate 0.01, with decay factor 0.1 at epochs 60, 120, and 160. We use batch size 128 for all models.

Fashion-MNIST	# parameters	Train Accuracy	Test Accuracy
Baseline MLP	152586	98.02%	89.58%
Last layer ETF	151306	98.13%	89.44%
Last two layers ETF	134922	97.59%	89.20%
Last three layers ETF	118538	96.87%	88.50%
Adaptive ETF	-	98.09%	89.38%

Table 1: Best training and validation accuracy attained from MLP models.

Fashion-MNIST	# Parameters	Train Accuracy	Test Accuracy
Baseline ViT	9491978	93.91%	89.80%
Last layer ETF	9486858	93.89%	90.03%
Last layer + Last Block FC ETF	7389706	98.89%	90.06%
Last layer + Last 2 Blocks FC ETF	5292554	93.51%	89.97%
ETF-Transformer	3195402	93.23 %	89.78%

Table 2: Best training and validation accuracy attained from Vi-T model.

4.1 Intermediate Simplex ETF in Multilayered Perceptrons

We train and evaluate a 5-layer feedforward multi-layered perceptron with intermediate layers of width 128, ReLU activation, and batch normalization on intermediate layers. Figure 1 shows the compares of training the neural network without ETF constraints (baseline) to training the neural network while replacing the last 1, 2, and 3 layers with Simplex ETFs. The baseline results indicate that the network has an effective depth L_0 of 4. We observe that setting all layers past L_0 to simplex ETFs does not impact the train or test accuracy of the network.

Indeed, as can be seen in Figure 1, setting final layers to ETFs does not affect the final accuracy of the neural network, and the modified neural networks still have effective depths of 4. However, the behavior of the intermediate layers under more constrained conditions (last two or three layers ETF) differs from baseline. In addition to the final training and validation accuracy being lowered (Table 1), the last fully-connected layer before ETF layers exhibits lower NCC separability than other layers.

In both instances of over-constrained neural networks, the decrease in NCC separability is marked by a noticeable “phase change"— the NCC accuracy starts off high but decreases dramatically after the network accuracy improves past a certain point in training. This change does not affect the NCC separability of earlier layers, nor does it significantly affect train or test accuracy. Although this form of mode collapse is only observed in a heavily constrained neural network, it may hint towards underlying dynamics in neural network training that can affect feature representation and separability even in less constrained models. This suggests that similar mechanisms of mode collapse might occur subtly in standard networks, potentially impacting generalization and the interpretability of learned representations. Understanding this phenomenon could lead to better network designs and training strategies that preserve feature separability throughout the network layers.

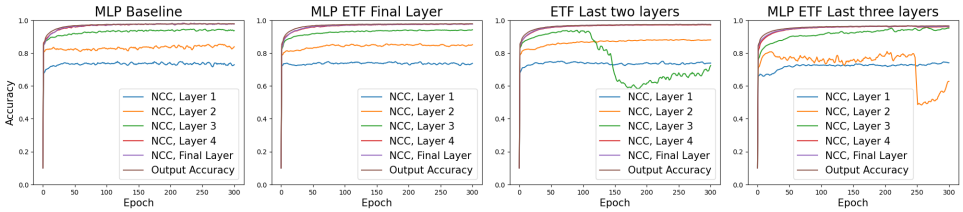

Figure 1: Training progress on baseline MLP compared to replacing the final layer, final two layers, and final three layers of the neural network with simplex ETFs.

New training scheme: Adaptive ETF Using results from training ETF-constrained MLPs, we observe that replaying layers beyond a fully-connected network's effective depth with simplex ETFs does not incur a penalty to train or test accuracy. This suggests a new training strategy, *Adaptive ETF*, that can be employed to greatly reduce memory usage in overparameterized neural networks. Given parameters ϵ, we fix a given layer of the neural network to a simplex ETF if its NCC error falls under ϵ. Figure 2 demonstrates this technique in use with $\epsilon = 0.1$. We clearly see that the model achieves the same train accuracy, test accuracy, and effective depth as a baseline network, demonstrating Adaptive ETF as a feasible training technique.

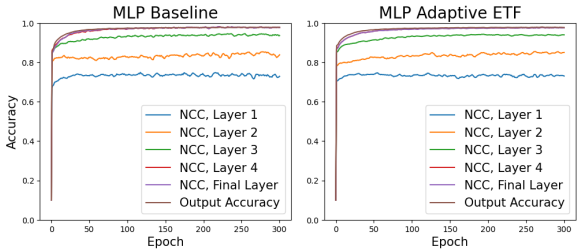

Figure 2: Training progress on baseline network compared to replacing feedforward layers with simplex ETFs beyond the effective depth.

4.2 Extension to Transformer Architectures: Introducing ETF-Transformer

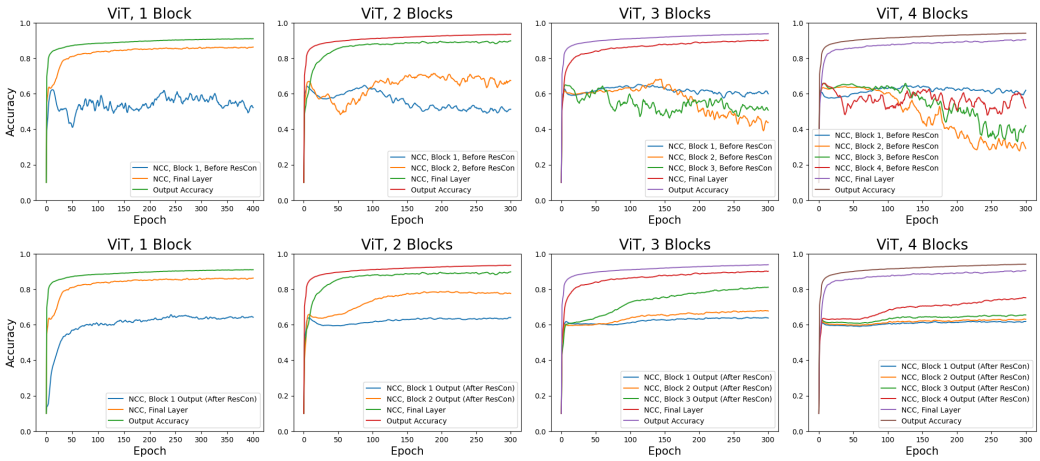

Figure 3: Comparison of training progress on vision transformers with 1 block, 2 blocks, 3 blocks, and 4 blocks.

In the previous sections, we have demonstrated the efficacy of using simplex ETFs to replace weights exhibiting neural collapse with fully-connected networks. However, many real-world tasks make use of more complicated models, such as transformers. We seek to translate as many of our insights as possible to these complicated models, even if the neural collapse phenomenon has not been as well-documented in these contexts.

To this end, we repeat our experiments on a visual transformer (ViT) model [2]. Each transformer block has 8 heads, an attention dimension of 64, and 2048 hidden units in the fully connected layer. We will investigate the effect of constraining the fully-connected layers in both the output and the transformer blocks to simplex ETFs.

As seen in Figure 3, the effective depth of the ViT model is always equal to one more than the number of blocks. That is, the notion of effective depth in MLPs does not carry over cleanly to transformers. NCC accuracy for intermediates after the residual connection is

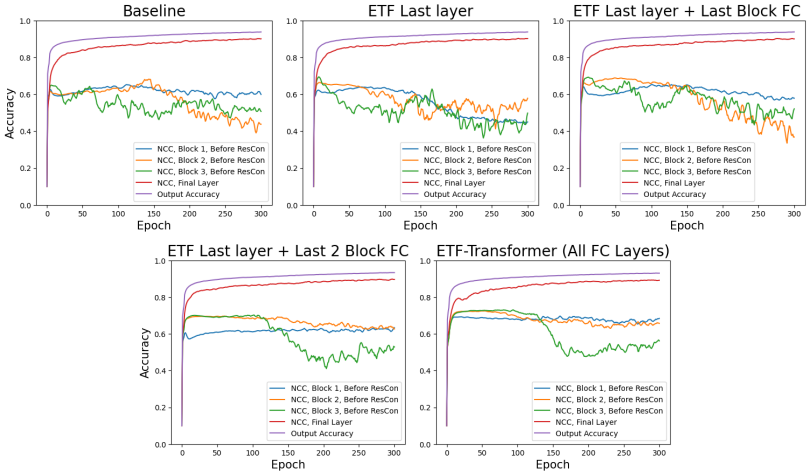

Figure 4: NCC for FC layers in transformer ETF architectures.

greater than for intermediates before the residual connection. This is consistent with the idea that NCC separability is achieved as a result of optimization rather than specifics of the neural network. However, it is important to note that the direct output of the FC layers (before residual connection) in the transformer architecture likely plays a similar role to the last non-ETF layer in the MLP network in Figure 1.

At the same time, experimental results show that constraining fully-connected layers to simplex ETFs does not significantly impact performance: Table 2 and Figure 4 show the accuracy and intermediate NCC results obtained on training a ViT model with 3 transformer blocks, constraining first the final layer, then the final layer plus the transformer FC layers in the last block, then the final layer plus the transformer FC layers in the last two blocks, and finally setting all FC layers outside of multi-head self attention to ETFs. Because we are able to set ETFs on all transformer blocks, we generalize this last training scheme as the *ETF-Transformer* approach. We note that due to the expressivity of the non-MLP components of the transformer model, the introduction of ETFs into ViT only slightly decrease the training accuracy and do not affect generalization.

5 Conclusion and Future Work

In this paper, we demonstrate the feasibility of using equiangular tight frames in training neural networks. Experiments show that when later layers $(L \geq L_0)$ are fixed to ETF, the network trains to the same accuracy as an unmodified network. This suggests a novel training scheme, Adaptive ETF, in which layers of the neural network are set to simplex ETFs once they achieve NCC separability. We demonstrate that Adaptive ETF achieves similar performance to an unmodified neural network on the Fashion-MNIST dataset.

We also demonstrate the strengths and limitations of carrying over the notion of simplex ETFs to transformers, using the ViT model. Even though neural collapse conditions are not as prevalent as in MLPs, we observe that setting feedforward layers to simplex ETFs in transformer blocks still results in a model that achieves similar accuracy to baseline,

This investigation opens up several new directions of research. First, the Adaptive-ETF technique and ETF-Transformer architecture can be applied to larger classification datasets, as well as datasets in different modalities such as natural language. Additionally, our experiments demonstrate that NC2 and NC3 can also be applied to intermediate layers, meaning that it is worthwile to revisit NCC-based generalization bounds [3] from the perspective of NC2 or NC3. Finally, our work yielded unexpected results when fixing early layers $(L < L_0)$ to simplex ETFs: the training accuracy decreased but the test accuracy stayed the same. This suggests an interesting avenue of exploration for using simplex ETFs in neural network regularization.

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