Is Feature Diversity Necessary in Neural Network Initialization?

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Abstract

Standard practice in training neural networks involves initializing the weights in an independent fashion. The results of recent work suggest that feature "diversity" at initialization plays an important role in training the network. However, other initialization schemes with reduced feature diversity have also been shown to be viable. In this work, we conduct a series of experiments aimed at elucidating the importance of feature diversity at initialization. We show that a complete lack of diversity is harmful to training, but its effects can be counteracted by a relatively small addition of noise - even the noise in standard non-deterministic GPU computations is sufficient. Furthermore, we construct a deep convolutional network with identical features at initialization and almost all of the weights initialized at 0 that can be trained to reach accuracy matching its standard-initialized counterpart.

1 Introduction And Related Work

Random, independent initialization of weights in deep neural networks [DNNs] is a common practice across numerous architectures and machine learning tasks [6, 11, 10]. Common initialization schemes [4, 5] are generally motivated by ensuring that the variance of the neurons does not grow rapidly with depth at initialization. Empirically, it has been established that the method used to initialize the weights of each layer can have a significant effect on the accuracy of the trained model.

The recently proposed "lottery ticket hypothesis" [2, 3] suggests a new explanation of why the initial values of weights in the network play such a vital rule in the training process. After showing that sparse networks could be trained as well as dense networks if certain subsets of the weights were initialized with the same values, the authors suggests that neural networks contain trainable sub-networks, characterized by their unique architecture and initialization. By training the dense neural network, one can learn and extract the sparse sub-network. This approach therefore views the initialization process as a "gamble". Initializing the network with constant values, in this context, would be equivalent to buying several Lottery Tickets with the same numbers on them.

While this may indicate that feature diversity is an important property of the network initialization, there are counterexamples as well. Calculations of signal propagation in random neural networks [8, 9], applied in [12] to convolutional networks, led the authors to suggest the Delta Orthogonal initialization, which they have used to successfully train a 10,000 layers neural network to classify CIFAR-10 images. While this initialization was shown to provide the optimal signal propagation, it stands out as being relatively sparse, with only a single non-zero value per convolution filter at initialization. When studying residual neural networks (without batch normalization) following the same approach, as was done in [13], it was shown that signal propagation is optimized when the entire signal passes through the residual connection at initialization, and this is achievable by simply initializing all weights that can be bypassed to zero. This approach is also supported by [14], where the authors suggests the Fixup initialization in which the final layer of the residual block (a block which can be bypassed by a single skip connection) is initialized to zero. The Fixup initialization
allows successful training of residual neural networks without the need to use batch normalization even on complex data sets. We find the success of those initializations to be in some contradiction with the "lottery ticket hypothesis".

In this work, we attempt to take the idea that feature diversity may not be necessary, as suggested by the initialization schemes proposed above, to the extreme. We do this by designing and studying neural networks where all the weights in each layer are initialized to a constant, single value, which can often be 0. We investigate whether such a networks are trainable, and whether initializations which lack "diversity" in initial features have negative effects on the training process.

2 Replicated features

When considering a deep neural network classifier, the neurons in each hidden layer can be regarded as representing a feature, extracted from the input by the preceding computational logic in the network. The consecutive logic in the network uses the features to classify the input to the (hopefully) correct label. [7] shows how classification accuracy improves as the number of features increases, even when said features are selected randomly and not optimized as in the case of standard back-propagation.

It is clear that having more than a single neuron representing the same feature in our final trained model is redundant — a group of neurons that are identical for all inputs will not contribute to a successful classification. We therefore ask the question: given that our network was initialized so the same neurons in a layer represent the same feature, will they diverge and contribute to the model accuracy during the training process?

To answer this question, we consider a 2-layer fully connected neural network:

\[
X \in \mathbb{R}^d, W_1 \in \mathbb{R}^{N \times d}, W_2 \in \mathbb{R}^{\text{classes} \times N} \\
h(X, W_1) = \text{Relu}(W_1 X) \\
f(X, W_1, W_2) = \text{SoftMax}(W_2 h(x, W_1))
\]

where we initialize the neural network as follow: the weight matrix \(W_2\) is initialized using the standard He initialization [5], and for each number of features \(K\), we initialize the temporary matrices \(\tilde{W}_1 \in \mathbb{R}^{K \times d}\) using the He initialization, and initialize \(W_1\) using \(r = \frac{N}{K}\) replications of \(\tilde{W}_1\), so

\[
\forall i, W_1[i, :] = \tilde{W}_1[i \mod K, :](1 - \lambda) + \lambda \tilde{W}_1[i, :].
\]

where \(\lambda\) is a parameter simulating noise. For \(\lambda = 0, K > 1\), this would result in each row in \(W_1\) being repeated \(r\) times at initialization (and consequently, the same also applies to each hidden layer neuron).

We identify two main possible causes for initially identical neurons to diverge during training: First, stochastic operations can result similar rows in \(W_1\) receiving different gradient updates. The most commonly used operation that would achieve this is dropout, which will randomly mask neurons, so some neurons may freeze while their "replicas" change. The second cause is back-propagation itself:

Even when not using dropout, the gradient of \(W_1\) will be: \(\frac{dL}{dW_{1,j}} = \frac{dL}{dh_j} \frac{dW_{1,j}}{dh_j} \frac{dh_j}{dX_j}\) and since \(\frac{dL}{dh_j}\) depends on the corresponding column \((W^T_2)_i\) (which is random at initialization), the update gradient may be different for each row. We check the effect of features diverging due to back-propagation, by training the neural network over the MNIST dataset, while changing the width the network \(N\) and the number of unique features at initialization. The training was done with standard SGD, learning rate of 0.1, with test accuracy measured after 7500 training steps and 30 seeds per sample. Results of this experiment are displayed in Figure 1.

3 Training a deep convolutional network with identical features at initialization

In this section, we train a deep convolutional neural network with a symmetric initialization that results in identical features at all layers, which we refer to as Constnet. We show that despite the relatively limited variety of distinct sub-networks at initialization (many sub-networks will be initially identical due to the induced symmetry), the network we come up with is, with some limitations, trainable, and its test accuracy matches that of a similar network with standard initialization. The code
Figure 1: Test error of a 2-layers fully connected network. In the left panel the hidden layer features were initialized so the same random feature is represented $K$ times. In the right panel, the weights were initialized similarly but a small i.i.d. component was added to the initialization of each weight in the matrix $W_1$. The number of features upon initialization is evidently the strongest indicator of the network success in our experiment. Increasing the hidden layer width without the addition of new features at the start of the training can significantly improve performance in the case of smaller networks, but this effect saturates quickly. Surprisingly, our results even indicate that wider networks without additional new initial features perform worse when the hidden layer becomes too big. For a $\lambda = 0.01$, the effect of the replicated features vanishes completely. Figure 3 in the Appendix details the error bars of the noiseless results.

Figure 2: Hidden layer width vs. test error for replicating this experiment, and more, is available at: https://github.com/yanivbl6/fixup. It is based on the code-base of [14].

The Constnet architecture is based on the ResNet [6] and its adaptation with Fixup [14]. Our main modification is that each skip connection only bypasses a single convolutional layer, unlike the standard ResNet where two layers are skipped.

We initialized the network as follows:

a. First, we set the final fully-connected layer to zero.

b. Next, the weights in layers bypassed by a residual connections are set to zero as well, as in the case of Fixup (we only have a single layer in each residual block so the Fixup initialization becomes trivial).

c. Finally, inspired by the Delta Orthogonal initialization [12], we initialize all values in the first convolution so only the middle weight in each filter has non-zero value, and set the middle weight to a constant, forcing symmetry between all channels (input and output).

We start by applying this initialization on the first layer convolution and then extend it to the $1 \times 1$ convolutions used to widen the network as well. We note that even though the Fixup initialization allows discarding the batch normalization operations while maintaining the model accuracy, our network does contain batch normalization as it proved to be more robust to changes in hyperparameters (mainly learning rate and mixup’s $\alpha$ parameter).

To reiterate - almost all the weights in Constnet are initialized at 0, and all the non-zero weights are initialized to an identical value per layer. We train our model on the CIFAR-10 and CIFAR-100 datasets. We use standard SGD with momentum, 12 residual layers with a $\times 10$ network widening after every 4 layers, a learning rate of 0.1. Since our entire network is now symmetrical, we rely on some other mechanism aside from initialization to break symmetry. In our experiments, the stochasticity introduced by standard GPU computations and floating point errors was sufficient to break symmetry. Another convenient mechanism for introducing stochasticity in a controlled way is Dropout. The results of this experiment, with various values of dropout, are shown in Table 1 in the appendix. As expected in the case of no dropout (and when floating point errors are eliminated by

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1This is essential in preventing vanishing gradients when initializing weights to 0.

2Specifically - by default the NVIDIA cuDNN library performs non-deterministic parallelized addition operations that, combined with floating point error, introduce enough stochasticity so as to break symmetry.
using CUDNN in deterministic mode), the initial symmetry could not be broken and training did not occur at all.

Our results show that even with low dropout rate (0.01), the test accuracy achieved by a network initialized with identical features at all layers is unchanged from that of a network trained using standard initialization (both networks achieving accuracy above 95%). These results can be seen in Figure 2.

4 Discussion and Future Work

Our results suggest that feature diversity at initialization may not be essential in neural network training. As long as the correct architecture is used, the network can still be trained to break the initial symmetry and produce equally good results even when the initial features are not diverse and are in fact identical.

One interesting direction of future work is to examine the lottery ticket hypothesis in this context. Can a neural network be efficiently pruned to produce a sparse network, even when the initialization has identical features in all the layers?

Another advantage of training a network with most of the weights initialized at zero is that this could provide a way to train a network that is sparse throughout training (instead of training a dense network and then pruning it). With proper regularization and/or an application of a sparsity-inducing operator such as the Prox operator [1] one could potentially train a Constnet in a way that most of the weights remain at zero throughout training and only some minimal necessary subset has large magnitude.

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Appendix

Figure 3: Results of the figure 1, with detailed error bars.

| Drop Rate | Constant Initialization | Test Accuracy [%] |
|-----------|-------------------------|-------------------|
|           | (a)                     | (b)               | (c) | (d) |                     |
| 0.01      | ✓                       | ✓                 | ✓   | ✓   | 95.2                |
| 0.15      | ✓                       | ✓                 | ✓   | ✓   | 95.5                |
| 0.1       | ✓                       | ✓                 | ✓   | ✓   | 95.3                |
| 0.01      | ✓                       | ✓                 | ✓   | ✓   | 95.3                |
| 0.00      | ✓                       | ✓                 | ✓   | ✓   | 95.0                |
| 0.1       | ✓                       | ✓                 | ✓   | ✓   | 95.2                |
| 0.01      | ✓                       | ✓                 | ✓   | ✓   | 95.3                |
| 0.00      | ✓                       | ✓                 | ✓   | ✓   | 10.0*               |

Table 1: Results of training a Resnet-like network with varying initializations and drop-rates after 200 epochs. The different initialization parts are: (a) Whether the weights on the convolution in the residual blocks is set to zero. (b) Whether the final FC layer weights are set to zero. (c) Whether the initial convolution is symmetrical and constant for all input and output channels. (d) Whether the weights of the \( (1, 1) \) convolutions used to adjust the dimensions when widening the residual blocks is initialized with a single constant. *Non-deterministic GPU computations (which are the default when using the NVIDIA cuDNN library) enable training with (a-d) enabled and no dropout, leading to similar performance to a standard random initialization.