Generalizing and Improving Weight Initialization

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Abstract

We propose a new weight initialization suited for arbitrary nonlinearities by generalizing previous weight initializations. The initialization corrects for the influence of dropout rates and an arbitrary nonlinearity’s influence on variance through simple corrective scalars. Consequently, this initialization does not require computing mini-batch statistics nor weight pre-initialization. This simple method enables improved accuracy over previous initializations, and it allows for training highly regularized neural networks where previous initializations lead to poor convergence.

1 Introduction

Weight initialization is one of many methods which greatly influence a neural network’s ability to learn. Guiding weight initialization research is the aim of a unit-variance neuron input distribution. This is because variance larger or smaller than one may cause activation outputs to explode or vanish. In order to achieve unit-variance, early attempts sought to adjust for a neuron’s fan-in [8]. More recent initializations correct for a neuron’s fan-out [2]. Meanwhile, some weight initializations compensate for the compressiveness of the ReLU nonlinearity (the ReLU’s tendency to reduce output variance) [3]. Indeed, [3] also shows that initializations without a specific, small corrective factor can render a neural network untrainable. To address this issue Batch Normalization reduces the role of weight initialization at the cost of up to 30% more computation [6]. A less computationally expensive solution is the LSUV weight initialization, yet this still requires computing batch statistics, a special forward pass, and makes no adjustment for backpropagation error signal variance [10]. Similarly, weight normalization uses a special feedforward pass and computes batch statistics [11]. The continued development of new weight initialization techniques vindicates its importance to neural networks.

We contribute a new weight initialization technique which includes a new correction factor for a layer’s dropout rate and adjusts for an arbitrary nonlinearity’s effect on the neuron output variance. All of this is obtained without computing batch statistics or adjustments to the forward pass, unlike recent methods to control variance [6] [10] [11]. By this new initialization, we enable faster and more accurate convergence. Beyond this, for networks with a very high dropout rate, some previous initializations produce networks performing worse than a simple logistic regression model; meanwhile, ours shows little difficulty coping with extreme dropout rates.

∗Work done while the author was at TTIC. Code available at github.com/hendrycks/init
2 Methods

In this section, we derive our new initialization by considering a neuron input distribution and its major sources of variance. We accomplish this by separately considering the feedforward and the backpropagation stages.

2.1 The Forward Pass

We use $\rho$ to denote the pointwise nonlinearity in each neural network layer. For simplicity, we use the term “neuron” to refer to an entry in a layer before applying $\rho$. Let us also call the input of the $l$-th layer $z^{l-1}$, and let the $n_{in} \times n_{out}$ weight matrix $W^l$ map from layer $l-1$ to $l$. Let an entry of this matrix be $w^l$. In our upcoming initialization, we initialize each column of $W^l$ on the unit hypersphere so that each column has an $\ell_2$ norm of 1. Now, if we assume that this network is trained with a dropout keep rate of $p$, we must scale the output of a layer by $1/p$. With that now specified, we conclude that neuron $i$ of layer $z^l$ has the variance

$$Var(z^l_i) = Var\left(\sum_{k=1}^{n_{in}} W^l_{ki} \rho(z^{l-1})_k / p\right)$$

$$= \frac{n_{in}p}{p^2} \Var(w^l \rho(z^{l-1}))$$

$$= \mathbb{E}[\rho(z^{l-1})^2]/p$$

because $\Var(w^l) = 1/n_{in}$, since we initialized $W^l$’s columns on the unit hypersphere. Knowing this variance allows us to adjust for the influence of an arbitrary nonlinearity and a desired dropout rate. In appendix A we empirically verify that a weight initialization with this forward correction allows for consistent input distribution variance throughout the layers of a 20-layer neural network for differing dropout rates.

2.2 Backpropagation

A similar analysis shows that if $L$ is our loss function and $\delta^l = \frac{\partial L}{\partial z^l}$, then

$$Var(\delta^l) = pm_{out} Var(w^{l+1} \delta^{l+1} \rho'(z^l)) = p\mathbb{E}[\rho'(z^l)^2].$$

In appendix B we empirically verify that this backward correction allows for consistent backpropagation error signal variance throughout the layers of a 20-layer neural network for differing dropout rates.

2.3 Our Initialization

We want that $Var(z^l) = 1$ and $Var(\delta^l) = Var(\delta^{l+1})$. To meet these different goals, we initialize our weights by adding these variances, while others take the arithmetic mean of these variances or ignore the backpropagation variance altogether [3, 2, 10]. Therefore, if $W^l$ has its columns sampled uniformly from the surface of a unit hypersphere, then our initialization is

$$W^l / \sqrt{\mathbb{E}[\rho(z^{l-1})^2]/p + p\mathbb{E}[\rho'(z^l)^2]}.$$

This initialization accounts for the influence of dropout rates and an arbitrary nonlinearity. Fortunately, we need only initialize a random standard Gaussian matrix and normalize its last dimension to generate $W^l$. Another strength of this initialization is that the expectations are similar to the values in Table 1 for standardized input data, so computing mini-batch statistics is needless for our initialization. Let us now see these new adjustments in action.
Table 1: Activation adjustment estimates for $z^{l-1}, z^l$ following a standard normal distribution.

| Activation       | $\mathbb{E}(\rho(z^l)^2)$ | $\mathbb{E}(\rho'(z^l)^2)$ |
|------------------|---------------------------|---------------------------|
| Identity         | 1                         | 1                         |
| ReLU             | 0.5                       | 0.5                       |
| GELU ($\mu = 0, \sigma = 1$) | 0.425 | 0.444 |
| tanh             | 0.394                     | 0.216                     |
| ELU ($\alpha = 1$) | 0.645 | 0.671 |

3 Experiments

In the experiments that follow, we utilize the MNIST dataset, a 10-class grayscale image dataset of handwritten digits, the Large Movie Review Dataset, a binary sentiment classification dataset, and the CIFAR-10 image dataset, a 10-class color image dataset. We use these data to compare our initialization with Xavier and He initialization across fully connected, recurrent, and convolutional architectures.

3.1 MNIST

Let us verify that this initialization competes with previous weight initialization schemes. To this end, we train a fully connected neural network with GELUs ($\mu = 0, \sigma = 1$), ReLUs, ELUs ($\alpha = 1$), and the tanh activation \[4, 1\]. Each 7-layer, 128 neuron wide neural network is trained for 50 epochs with a batch size of 128. We use the Adam optimizer and its suggested learning rate of $0.001$ \[7\]. We perform this task with no dropout, a dropout keep rate of 0.5, and a dropout keep rate of 0.3. Figure 1 shows that our initialization shows faster convergence at a dropout rate of 0.5 for activations like the ReLU and wide gains when the dropout keep rate decreases further.

3.2 MNIST with Extreme Regularization

We continue experimenting with MNIST but now with extreme regularization. For this experiment, we train a three-layer fully-connected network with hidden layers of width 4096 and GELU nonlinearities. To make the regularization extreme, we drop out 93.75% of the neurons so as to achieve an expected width of 256. Adam optimized the network for 50 epochs, tuning learning rate over \{10^{-3}, 10^{-4}, 10^{-5}\} for each initialization. In Table 2 we report the test error corresponding to the epoch with the best validation error across all learning rates and epochs. We found that other initializations demonstrated large dependency on the learning rate whereas ours was less sensitive to different learning rates. We find that our initialization works much better than the others in this setting, both during training and test.

| Initialization | Ours % | Xavier % | He % |
|----------------|--------|----------|------|
| Test Error     | 5.99   | 14.71    | 62.12|

Table 2: MNIST Classification Error. Test errors for networks trained when dropping out 3840 neurons (on average) of 4096 available neurons.
Figure 1: MNIST Classification Results. The first row is the training set log loss curves for the ReLU, the second row is for the tanh unit, the third the ELU, and the fourth the GELU. The leftmost column shows loss curves when there is no dropout, the middle when the dropout rate is 0.5, and rightmost is when the dropout preservation probability rate is 0.3. Each curve is a median of three runs.
3.3 Convolutional LSTM

Next, we classify sentiment with the Large Movie Review Dataset [9] using a convolutional LSTM architecture that convolves over the sentence and feeds the output into an LSTM. Due to the intricate architecture of a convolutional LSTM, and because our backpropagation variance analysis does not hold for backpropagation through time, this experiment then tests our initialization’s robustness under several violated assumptions. Now, using a filter length of 3, a 2 × 2 max pool, an embedding size of 128, a batch size of 30, two epochs, and an LSTM of dimension 70 with a ReLU output. We apply dropout (p = 0.7, p the keep rate) between the embedding and convolutional layer, and we apply dropout (p = 0.5) to the LSTM input. When an adjustment factor is unknown, we default to 0.5. As evident in Table 3, these schemes perform similarly, indicating that this initialization copes well with several breached assumptions.

| Initialization | Ours % | Xavier % | He % |
|----------------|--------|----------|------|
| Error          | 15.47  | 15.65    | 15.42|

Table 3: Large Movie Review Dataset. Test set error rates are an average of five runs.

3.4 CIFAR-10

Since VGG Net architectures [12] require considerable regularization and careful initialization, we use a variant of the architecture for our next initialization experiment. The VGG Net-like network has the stacks (2 × 3 × 64), (2 × 3 × 128), (3 × 3 × 256), (3 × 3 × 512), (3 × 3 × 512) followed by two fully-connected layers, each with 512 neurons. To regularize the deep network, we keep 60% of the neurons for every layer except the first two and last two layers, where we drop out no neurons and 50% of the neurons the first two and last two layers, respectively. Max pooling occurs after every stack, ReLU activations are applied on every neuron, and we decay the learning rate by 0.1 every 50 epochs all while training for 150 epochs with the Adam optimizer. We tuned over the learning rates \{10^{-3}, 10^{-4}, 10^{-5}\}. The results in Figure 2 demonstrate the importance of small corrective factors because the factors’ influence on neuron input variance changes exponentially as the network depth increases. While the networks still converge, failing to adjust for the dropout rate greatly hinders the performance of other initializations.

![Figure 2: CIFAR-10 VGG Net Results. Each training set log loss curve is selected from the best curve over the learning rates 10^{-3}, 10^{-4}, 10^{-5}.

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4 Discussion

In practice, if we lack an estimate for a nonlinearity adjustment factor, then 0.5 is a reasonable default. A justification for a 0.5 adjustment factor comes from connections to previous weight initializations. This is because if \( p = 1 \) and we default the adjustments to 0.5, our initialization is the “Xavier” initialization if we use vectors from within the unit hypercube rather than vectors on the unit hypersphere \([2]\). Knowing this connection, we can therefore generalize Xavier initialization to

\[
\text{Unif}[-1, 1] \times \sqrt{3} \sqrt{\frac{m_{\text{in}}}{p} \mathbb{E}[\rho(z_{l-1}^2)] + pm_{\text{out}} \mathbb{E}[\rho'(z_l)^2]}.
\]

Furthermore, we can optionally exclude the backpropagation variance term—in this case, if \( p = 1 \) and \( \rho \) is a ReLU, our initialization is He’s initialization if we use random normal weights \([3]\). Note that since \([3]\) considered a 0.5 corrective factor to account for the ReLU’s compressiveness (its tendency to reduce output variance), it is plausible that \( \mathbb{E}[\rho(z_{l-1}^2)] \) is a general adjustment for a nonlinearity’s compressiveness. Since most neural network nonlinearities are compressive, 0.5 is a reasonable default adjustment.

5 Conclusion

A simple modification to previous weight initializations shows marked improvements across different architectures, even when many adjustment factors are unknown. These improvements are most conspicuous when dropout is applied; indeed, for high dropout rates, previous weight initializations may not even converge to a competitive accuracy.

There are several plausible future directions starting from this result. For example, exploration into new nonlinearities that are not compressive is now more feasible, as our initialization would inhibit the neuron input variance from exploding. Furthermore, models with more parameters than data points are now easier to train if we combine very high dropout rates with our weight initialization. For one, this may improve generalizability of future networks. Further, this may help us better approximate biological learners; as Hinton \([5]\) suggests, they have more parameters than data points but use extreme regularization to successfully combat overfitting.

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[Note that the first and last hidden layers are adjacent to neurons which can be viewed as having an identity activation. For these, a 1.0 factor is more appropriate, but the practical difference is miniscule.]
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A  A Random Feedforward

We can encourage unit variance by dividing $W$, initialized on the unit hypersphere, by $\sqrt{\mathbb{E}(\rho(z^{l-1})^2)/p}$. Let us compare this correction to other initializations by feeding forward a random Gaussian matrix through 20 layers. Figure 3 shows the results of such an experiment, and in the experiment we use a ReLU activation function. Of course, as He initialization was designed specifically for the ReLU, it performs well when $p = 1$, but generates significant outliers when there is dropout. Only the unit hypersphere initialization with a $\sqrt{\mathbb{E}(\rho(z^{l-1})^2)/p}$ corrective term demonstrates stability when a feedforward does or does not use dropout.

Figure 3: A comparison of a unit hypersphere initialization with a forward correction, the Xavier initialization, and the He initialization. In particular, the range of values vary widely between each initialization, with exponential blowups and decay for He and Xavier initializations, respectively. Values set to zero by dropout are removed from the histograms.
B A Random Backpropagation

We can “feed backward” a random Gaussian matrix with standard deviation 0.01 and see how different initializations affect the distribution of error signals for each layer. Figure 4 shows the results when the backward correction factor is $pE[p'(z^2)]$. Again, we used the ReLU activation function due to its widespread use, so the He initialization performs considerably well.

Figure 4: A comparison of a unit hypersphere initialization with a backward correction, the Xavier initialization, and the He initialization. Values set to zero by dropout are removed from the histograms.