CDF Normalization for Controlling the Distribution of Hidden Nodes

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Abstract

Batch Normalizaiton (BN) is a normalization method for deep neural networks that has been shown to accelerate training. While the effectiveness of BN is undisputed, the explanation of its effectiveness is still being studied. The original BN paper attributes the success of BN to reducing internal covariate shift, so we take this a step further and explicitly enforce a Gaussian distribution on hidden layer activations. This approach proves to be ineffective, demonstrating further that reducing internal covariate shift is not important for successful layer normalization.

1 Introduction

Deep Neural Networks have increased in popularity over the last several years, particular in fields like computer vision where the complexity of data requires deeper networks [8, 11, 13, 3]. Training these deep networks is challenging; many methods have been proposed to boost training performance, including optimization methods [12, 6], learning rate schedulers [9], and regularization methods [5]. One very popular regularization method is Batch Normalization (BN) [4], which standardizes the activations of convolutional and linear layers before applying an activation function. This simple normalization technique allows for more stable training with higher learning rates, and has become standard across many fields of deep learning.

In [4], BN's effectiveness is attributed to a reduction in internal covariate shift, which is defined as the shift in the distribution of layer activations due to changes in earlier layer's parameters during training. By making each activation have a constant learnable mean and variance, BN ensures that changes to network parameters earlier in the network do not effect the first and second moments of network activations later in the network. Further, the authors argue that the outputs of linear and convolution layers are "more Gaussian", in which case controlling the first and second moments of the output distributions actually control the whole distribution, since the distribution of Gaussian random variables is completely determined by the mean and variance.

However, the explanations for BN's effectiveness continue to be studied [10, 1]. Interestingly, in [10] the authors argue that BN accelerates training not because of a reduction in internal covariate shift, but because of a smoother loss landscape. To show this, the authors add random noise after BN to explicitly induce internal covariate shift, and they find that this "noisy" BN is just as effective as regular BN. Additionally, the authors find that adding such random noise without using BN prevents the network from training entirely. This suggests that reducing internal covariate shift is not actually why BN accelerates training, since training is accelerated even when internal covariate shift is present.

In this paper, we take a different approach than BN to further explore normalization techniques that reduce internal covariate shift. Instead of controlling just the mean and variance of activations, we explicitly enforce a standard Gaussian distribution upon activations. We do this by first applying an estimated cumulant distribution function (CDF) to each hidden layer activation, followed by transforming to a standard Gaussian distribution via the standard Gaussian inverse CDF. In theory,

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this would reduce internal covariate shift more than BN, since the inputs to subsequent layers are always enforced to follow the same distribution, not just the same mean and variance.

2 Method

In this section, we describe our method for transforming hidden layer activations to standard Gaussians, which we call CDF Normalization (CDFN). Consider a hidden layer matrix of activations X of size (N, d), where N is the mini-batch size and d is the hidden dimension. Let $X_1, \ldots, X_d$ be random variables representing the d hidden dimensions. Assume first that we have an estimate $\hat{F}_i, i = 1, \ldots, d$ for the CDFs of our random variables, then $\hat{F}_1(X_1), \ldots, \hat{F}_d(X_d)$ are approximately standard uniform random variables. Next, let Φ be the CDF of some other distribution (in our case, the standard Gaussian), then $\Phi^{-1}\left[\hat{F}_1(X_1)\right], \ldots, \Phi^{-1}\left[\hat{F}_d(X_d)\right]$ are all random variables with distributions given by Φ. This gives us a framework for approximately transforming data at this hidden layer to any distribution we desire.

We now turn our attention to how to calculate the CDF estimates $\hat{F}_1, \ldots, \hat{F}_d$. Following BN, it would be ideal to make our CDF estimates only using the current mini-batch so that gradient backpropagation accounts for the normalization. However, as we will discuss in section 4, this turns out to be challenging. Instead, we use a running collection of data from previous mini-batches to estimate the CDFs for the current mini-batch. We compute the empirical CDF using a running collection of n data samples, creating a step function, and we further linearly interpolate this step function to transform to a piece-wise linear function. This transformation creates a function whose gradient is not always 0, allowing for successful backpropagation of gradients. The process of linear interpolation is illustrated in Figure 3 in the Appendix. Lastly, the running collection of data is updated using a momentum parameter $m \in [n - N, n]$: sample m points from the current collection without replacement, and sample the remaining $n - m$ points from the current mini-batch. The overall CDFN process is summarized in Algorithm 1.

Algorithm 1: CDFN Procedure, done for each column of activations matrix X. For more details on Linear Interpolation step, see Figure 3

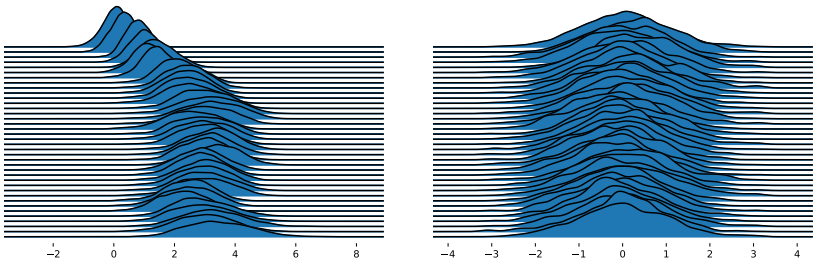
Input : Mini-batch column $x_1, \ldots, x_N$, running collection $y_1, \ldots, y_n$, momentum m
Output : Normalized mini-batched $x'_1, \ldots, x'_N$
ECDF$(a) = \frac{1}{n}\sum_{j=1}^{n} I(y_j \leq a)$
$\hat{F}(a) =$ LinInterp(ECDF(a))
for *j = 1, . . . , N* **do**
  $x'_j = \Phi^{-1}[\hat{F}(x_j)]$
end
$y_1, \ldots, y_n =$ sample$(y_1, \ldots, y_n, m) +$ sample$(x_1, \ldots, x_N, n - m)$
return $x'_1, \ldots, x'_N$

Note that we have described CDFN for two-dimensional hidden layers of size (N, d), yet hidden layers may be of higher dimensions, for example the output of a 2D convolution layer which is a four-dimensional tensor of size (N, C, H, W). In this case, CDFN is adapted similarly to BN: a CDF is estimated for each index of the second dimension (channel dimension) using values from all other dimensions.

3 Experiments

To test the CDFN procedure, we train a Convolutional Neural Network (CNN) on the CIFAR-10 image classification dataset [7]. Our CNN architecture is similar to a VGG style network [11]:

$$\begin{aligned}\text{ConvBlock}(3, 32) \rightarrow \text{ConvBlock}(32, 64) \rightarrow \text{MaxPool} \rightarrow \\ \text{ConvBlock}(64, 128) \rightarrow \text{ConvBlock}(128, 128) \rightarrow \text{MaxPool} \rightarrow \\ \text{ConvBlock}(128, 256) \rightarrow \text{ConvBlock}(256, 256) \rightarrow \text{MaxPool} \rightarrow \text{FinalLinear}\end{aligned}$$



(a) Before CDF Norm (b) After CDF Norm

Figure 1: Evolution of the distribution of one activation from the ConvBlock$(128, 256)$ layer before and after CDFN. Each horizontal line corresponds to one training iteration (mini-batch update), evolving from back to front.

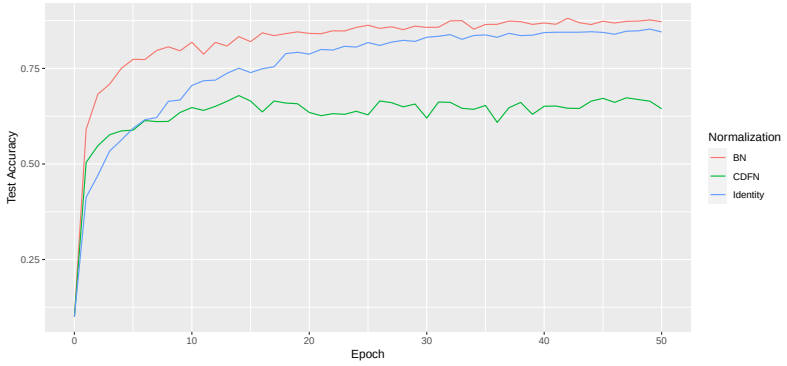


Figure 2: Test accuracies for different normalization techniques on the CIFAR-10 dataset.

A convolution block ConvBlock(n_{in}, n_{out}) is a sequential block with a 2D convolutional layer with n_{in} in channels, n_{out} out channels, 3×3 kernel size, and 1 padding, followed by a normalization layer and a ReLU activation. We choose this dataset and architecture in order to use a standard architecture which BN has been shown to be effective on. We train this network using the Adam optimizer [6] with a batch size of 128.

3.1 Reducing Internal Covariate Shift

The goal of using CDFN is to normalize the network in a way that reduces internal covariate shift, and thus we should check empirically that this is happening. For this, we train our CNN for 10 epochs, during which we keep track of the distribution of a random feature channel from the output of each convolutional layer before and after applying CDFN. The results of this experiment are shown in Figure 1. We see that even though the distribution of the activation is evolving during the training process, the CDFN normalization procedure is successfully transforming them to approximate Gaussian distributions that remain consistent through training. This supports the claim that CDFN is in fact greatly reducing internal covariate shift in the network.

3.2 Accuracy Results

Now that we know that CDFN does in fact eliminate internal covariate shift, we can access its performance. We do this by plotting the test accuracies for each epoch during training of our CIFAR-10 network with no normalization, BN, and CDFN. We use the same learning rate of 10^{-4} to maintain a fair convergence speed comparison even though we know BN allows for larger learning rates. The accuracies of such training runs are shown in Figure 2. As expected, BN converges faster while achieving similar final accuracy compared to using no normalization. On the other hand, while the initial convergence of CDFN is similar to using no normalization, the final accuracy achieved is much

lower, as CDFN achieves a final accuracy of less than 70% compared to final accuracies over 80% for the other two methods. All in all, we see that CDFN is not condusive to effective training.

4 Analysis

Even though BN and CDFN are both normalization techniques which standardize hidden layer activations, BN accelerates training while CDFN hinders training. What is different between BN and CDFN which leads to this severe difference in performance? One critical difference is that BN uses only the current mini-batch to perform normalization, while CDFN uses data from other mini-batches accululated through training. This difference is key, because using just the current mini-batch allows the normalization to flow through the gradient backpropagation. To illustrate this point, consider one column of the hidden layer activations matrix $\boldsymbol{x} = (x_1, \ldots, x_N)^T$. BN will transform this as

$$y = \text{BN}(\boldsymbol{x}) = \frac{\boldsymbol{x} - \mu_{\boldsymbol{x}}}{\sqrt{\sigma_{\boldsymbol{x}}^2 + \epsilon}}, \quad \mu_{\boldsymbol{x}} = \frac{1}{N}\sum_{i=1}^{N} x_i, \quad \sigma_{\boldsymbol{x}}^2 = \frac{1}{N}\sum_{i=1}^{N}(x_i - \mu_{\boldsymbol{x}})^2$$

During backpropagation, computing the gradient $\partial y / \partial \boldsymbol{x}$ takes into account the normalization step since both $\mu_{\boldsymbol{x}}$ and $\sigma_{\boldsymbol{x}}^2$ are functions of $\boldsymbol{x}$. Comparatively, CDFN does the transformation

$$y = \text{CDFN}(\boldsymbol{x}) = \Phi^{-1}\left[\hat{F}(\boldsymbol{x})\right]$$

where Φ and $\hat{F}$ are the standard Gaussian CDF and the approximated CDF respectively following Algorithm 1. When computing the gradient $\partial y / \partial \boldsymbol{x}$ here, we use the chain rule

$$\frac{\partial}{\partial \boldsymbol{x}} \Phi^{-1}\left[\hat{F}(\boldsymbol{x})\right] = \left(\Phi^{-1}\right)'\left(\hat{F}(\boldsymbol{x})\right) \cdot \hat{F}'(\boldsymbol{x})$$

The gradient of $\hat{F}$ with respect to $\boldsymbol{x}$ is simply some constant that does not depend on $\boldsymbol{x}$ since $\hat{F}$ is a piece-wise linear function formed from previous mini-batches independently of $\boldsymbol{x}$. Similarly, $\left(\Phi^{-1}\right)'\left(\hat{F}(\boldsymbol{x})\right)$ does not involve any other terms than $\boldsymbol{x}$ itself, so the gradient does not account for any normalization. Thus, it is possible that the optimizer will make gradient steps that are counteractive to the normalization from CDFN, similarly to the discussion about whitening in [4]. This provides both a potential reason why CDFN is not effective and also highlights how important it is for the normalization to flow through the gradient as in BN.

At this point, it is natural to wonder whether it is possible to adapt CDFN to use only the current mini-batch as in BN. It turns out that applying an estimated CDF from only the current mini-batch is challenging. The natural first attempt would be to compute the empirical CDF using the current mini-batch and proceed exactly as in CDFN. The problem is that applying an empirical CDF to the same data it is built on amounts to doing an argsort operation, and this operation is not differentiable. To get around this problem, we can "soften" the empirical CDF calculation so that it is differentiable. One way to do this is to replace the indicator functions in the empirical CDF with sigmoid functions centered at each point. This turns out to be too slow to be practical. Even computing a sum of sigmoids for a reasonably-sized subset of data points in a given mini-batch followed by linear interpolation is very slow and does not produce good results. Another potentially better approach would be to use some kind of soft rank function that is differentiable such as [2]. So far, we have discovered this to also work less effectively than using no normalization, and also to be too slow to be realistic when the soft ranking is over multiple dimensions as in CIFAR-10.

5 Conclusion

Batch Normalizaiton (BN) [4] has the effect of reducing internal covariate shift in neural networks, yet [10] demonstrates that the effectiveness of BN is not related to this reduction in internal covariate shift. We provide a normalization technique, CDF Normalization (CDFN), which reduces internal covariate shift even more than BN and yet hinders training. We argue that CDFN not using the current mini-batch for normalization disrupts gradient flow, and doing CDFN using only the current mini-batch is challenging. We leave it to future work to find more efficient and effective ways to perform CDFN-style normalization using only the current mini-batch.

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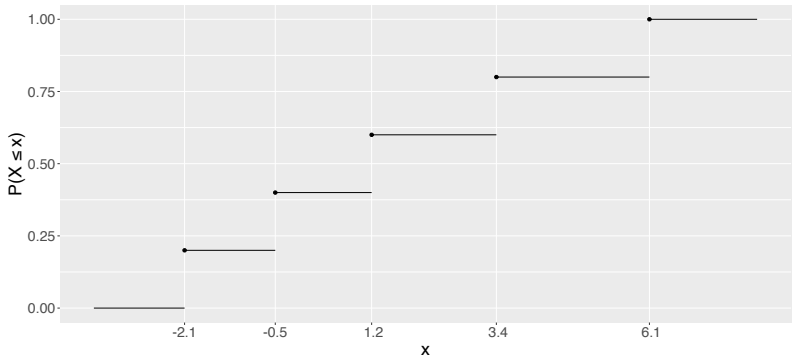
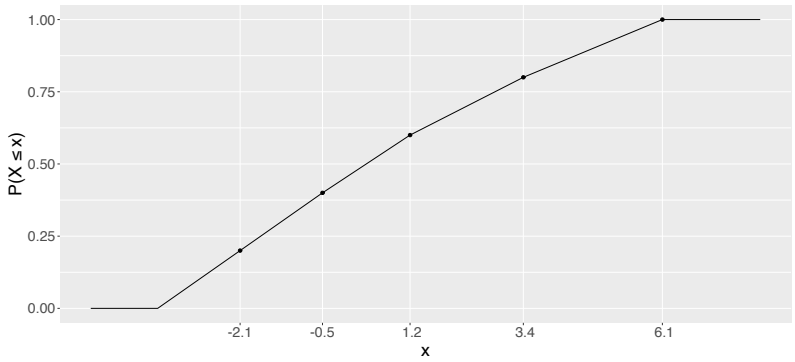


(a) Empirical CDF from sample



(b) Linear Interpolation of ECDF

Figure 3: Demonstration of Linear Interpolation from an empirical CDF. In a) a sample of $\{-2.1, -0.5, 1.2, 3.4, 6.1\}$ is used to construct the ECDF, which then is smoothed by linear interpolation in b). In practice, values after interpolation are truncated between [0.001, 0.999] to avoid infinities.

Appendix

In Figure 3, we demonstrate the process of generating a piece-wise linear function that estimates the CDF of a given data sample. In the example in the figure, we take the sample $S = \{-2.1, -0.5, 1.2, 3.4, 6.1\}$ and start by plotting the empirical CDF of this sample as the step function $a \mapsto \frac{1}{n} \sum_{s \in S} I(a \leq s)$. To perform linear interpolation of this step function, we simply build a piece-wise linear function connecting the jump points from the step function. After the last point, the function levels off at 1, while before the first point the function continues linearly down to 0 before leveling off. In practice, we take the additional step of truncating the function between 0.001 and 0.999 to avoid computing the inverse CDF of 0 or 1 during the following step when we convert from uniform to Gaussian distribution.