How Does Batch Normalization Help Binary Training?

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Abstract

Binary Neural Networks (BNNs) are difficult to train, and suffer from drop of accuracy. It appears in practice that BNNs fail to train in the absence of Batch Normalization (BatchNorm) layer. We find the main role of BatchNorm is to avoid exploding gradients in the case of BNNs. This finding suggests that the common initialization methods developed for full-precision networks are irrelevant to BNNs. We build a theoretical study on the role of BatchNorm in binary training, backed up by numerical experiments.

1 Introduction

Deep Neural Networks (DNNs) are complex and resources-hungry, preventing them from being deployed on edge devices. Binary Neural Networks (BNNs) (Hubara et al., 2018) are an attempt to alleviate these issues by adopting an extreme quantization scheme and constraint weight and activation to \([-1,+1]\). This extreme constraint often leads to under-fitting. Moreover, training networks with binary values does not match stochastic gradient descent mission, which is designed for continuous weight and activation. Consequently, BNNs suffer from an accuracy drop compared to their full-precision counterpart. Most of binary training in convolutional models include Batch Normalization (BatchNorm) layer (Ioffe and Szegedy, 2015). However, the BatchNorm layer is missing in most of recurrent networks, but Ardakani et al. (2019) report competitive quantized training by only adding BatchNorm to the gates. Here we argue why binary training without BatchNorm is infeasible.

It is natural to take a step back and wonder how important BatchNorm component is. We show that Glorot initialization (Glorot and Bengio, 2010) that protects gradients from explosion or vanishing is useless for BNNs, and this could be the reason why training BNNs using a pretrained model is preferred (Alizadeh et al., 2019). Briefly i) we show BNNs are insensitive to Glorot’s initialization parameters, so initializing weights from a distribution symmetric about zero and with an arbitrary variance is sufficient; ii) we demonstrate that BatchNorm prevents exploding gradient, and this make the common full-precision initialization schemes pointless; iii) we break down BatchNorm components to centering and scaling, and show only mini-batch centering is required; the scale can be fixed to a certain constant. We only perform experiments on CIFAR-10, but experiments on

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other data sets lead to the same conclusion.

2 Preliminaries

BNNs apply the sign function on full-precision values, only keeping the sign while discarding the magnitude. This allows up to 32× memory-wise compression and yields fast inference via XNOR-Popcount operation compared to float32-precision networks.

Let \( x \in \mathbb{R} \), the derivative of the sign function is required for backpropagation. An approximation, called the clipped straight-through estimator is \( \frac{\partial \text{sign}(x)}{\partial x} \approx 1_{[-1,1]}(x) \), where \( 1(.) \) is the indicator function.

A random variable taking binary values \( \{-1,1\} \) can be expressed as a transformed Bernoulli. The mathematical expectation and variance of this transformed Bernoulli variable \( \hat{x} \) is

\[
E(\hat{x}) = 2p - 1, \quad \text{Var}(\hat{x}) = 4p(1-p)
\]

As a consequence, the sum of such \( \hat{x} \)'s is a location-scale Binomial. The binary random variable \( \hat{x} \) is symmetric about zero if \( p = \frac{1}{2} \). The sum of \( K \) such binary variables is also symmetric about zero, but the variance evolves from 1 to \( K \). This property may require attention in initialization of binary networks, as the variance of such binary dot products need to be controlled.

It is well-known that BatchNorm facilitated neural networks training. A common intuition suggests BatchNorm matches input and output distribution in their first and second moments. There are two other clues among others: Ioffe and Szegedy (2015) claim that BatchNorm corrects covariate shift, and Santurkar et al. (2018) show BatchNorm bounds the gradient and makes the optimization smoother. None of these arguments work for BNNs! The role of BatchNorm is to prevent exploding gradient.

Suppose a mini batch of size \( B \) for a given neuron \( k \). Let \( \hat{\mu}_k, \hat{\sigma}_k \) be the mean and the standard deviation of the dot product, between inputs and weights, \( s_{kk}, b = 1, \ldots, B \). For a given layer \( l \), BatchNorm is defined as \( \text{BN}(s_{kk}) = z_{kk} = \gamma_k \hat{\sigma}_k + \beta_k \), where \( \hat{\sigma}_k = \frac{s_{kk} - \hat{\mu}_k}{\hat{\sigma}_k} \) is the standardized dot product and the pair \( (\gamma_k, \beta_k) \) is trainable, initialized with \((1,0)\).

Given the objective function \( L(.) \), BatchNorm parameters are trained in backpropagation

\[
\frac{\partial L}{\partial \beta_k} = \sum_{b=1}^{B} \frac{\partial L}{\partial z_{bb}} \quad \frac{\partial L}{\partial \gamma_k} = \sum_{b=1}^{B} \frac{\partial L}{\partial z_{bb}} \hat{\sigma}_k,
\]

For a given layer \( l \), it is easy to prove \( \frac{\partial L}{\partial s_{bb}} \) equals

\[
\frac{\gamma_k}{\hat{\sigma}_k} \left( -\frac{1}{B} \sum_{b'=1}^{B} \frac{\partial L}{\partial z_{bb'}} \hat{s}_{bb'} - \hat{\mu}_k \sum_{b'=1}^{B} \frac{\partial L}{\partial z_{bb'}} \hat{s}_{bb'} + \frac{\partial L}{\partial z_{bb}} \right).
\]

We follow the same assumptions as in Glorot and Bengio (2010), i.e. weights and activations are independent, and identically distributed (iid) and centred about zero. Formally, denote the dot product vector \( s^l_b \in \mathbb{R}^{K_l} \) of sample \( b \) in layer \( l \), with \( K_l \) neurons. Let \( f \) be the element-wise activation function, \( x_b \) be the input vector, \( W^l \in \mathbb{R}^{K_{l-1} \times K_l} \) with elements \( W^l = [w^l_{kk}] \) be the weights matrix; one may use simply \( w^l \) referring to an identically distributed elements of layer \( l \). It is easy to verify

\[
\frac{\partial L}{\partial s^l_{kk}} = f'(s^l_{kk}) \sum_{k'=1}^{K_{l+1}} u^l_{kk' k'+1} \frac{\partial L}{\partial s^l_{kk'}},
\]

\[
\frac{\partial L}{\partial w^l_{kk'}^l} = \sum_{b=1}^{B} s^l_{kk'} \frac{\partial L}{\partial s^l_{kk'}}.
\]

We assume that the feature element \( x \) and the weight element \( w \) are centred and iid, for a given neuron \( k = 1, \ldots, K_l \) at layer \( l \). We reserve \( k \) to index the current neuron and use \( k' \) for the previous or the next layer neuron depending on the context. One can show \( \text{Var}(s^l_{kk}) = \text{Var}(x) \prod_{l'=1}^{l-1} K_{l'} \text{Var}(w^{l'}) \), where \( \text{Var}(w^{l'}) \) is the variance of the weight in layer \( l' \). By applying similar mathematical mechanics, the variance of the
gradient for a neuron is
\[
\nabla (\frac{\partial L}{\partial s_{bk}^l}) = \nabla (\frac{\partial L}{\partial s^L}) \prod_{l'=l+1}^L K_{l'} \nabla (w^{l'}),
\]
which explodes or vanishes depending on \(\nabla(w^{l'})\). This is the main reason common full-precision initialization methods suggest \(\nabla(w^{l'}) = \frac{1}{K_l}\).

3 Effect of BatchNorm

We first question the role of BatchNorm in BNNs, and demonstrate that BatchNorm has a different role compared to the one it has in full-precision models. Most of BNNs contain BatchNorm layers, because they are infeasible to train without BatchNorm. BNNs use the sign activation, therefore the scale of input distribution has no effect on the forward pass, and only the location plays a role. This observation is enlightening: at inference time, a BatchNorm layer followed by sign is a threshold function. This motivates us to focus on centering more than scaling while initializing BNNs

\[
\text{sign}\{BN(s_{bk})\} = \begin{cases} +1 & \text{if } s_{bk} \geq |\mu_k - \frac{\hat{\delta}}{\gamma_k} \beta_k|, \\ -1 & \text{otherwise.} \end{cases}
\]

where \([\cdot]\) is the floor to integer. From (2) it is clear that controlling the variance has no fundamental effect on forward propagation if \(s_{bk}\) is symmetric about zero. The term \(b_k = \mu_k - \frac{\hat{\delta}}{\gamma_k} \beta_k\) can be regarded as as a new trainable parameter, thus BatchNorm layer can be replaced by adding biases to the network to compensate.

We are aware of dismissal of BatchNorm in forward pass but still BNNs do not converge in practice without BatchNorm. We suspect that BatchNorm layers help backpropagation and this is why only BNNs with BatchNorm converge.

4 BatchNorm and Initialization

In presence of BatchNorm layers, one may show that weights variance has no impact on the forward pass as the output will be normalized after passing through BatchNorm. In another word, for a given layer \(l\), \(\nabla(\text{BN}(s_{bk})) = \gamma_k^2\) for any full-precision network, BatchNorm affects backpropagation as

\[
\nabla (\frac{\partial L}{\partial s_{bk}^l}) = \left(\frac{\gamma_k}{B}\right)^2 (B^2 + 2B - 1 + \nabla(s_{bk}^2)) K_{l+1} \nabla (\frac{\partial L}{\partial s^{l+1}}),
\]

Setting \(\nabla(s^{l+1}) = \frac{1}{K_{l+1}}\) still does not stabilize the variance of the gradient. Gradients are stabilized only if \(\left(\frac{\gamma_k}{B}\right)^2 (B^2 + 2B - 1 + \nabla(s_{bk}^2)) \approx 1\). Moving from full precision weight \(w\) to binary weight \(\hat{w} = \text{sign}(w)\) changes the situation dramatically. In other words initializing with a symmetric distribution about zero with any variance gives \(\nabla(\hat{w}^{l+1}) = 1\), which does not cancel out the \(K_{l+1}\) in (3). Theorem 1 shows BatchNorm approximately cancels \(K_{l+1}\).

Theorem 1. Under common initialization assumptions, the gradient variance for BNNs without BatchNorm is

\[
\nabla (\frac{\partial L}{\partial s_{bk}^l}) = \nabla (\frac{\partial L}{\partial s^L}) \prod_{l'=l+1}^L K_{l'},
\]

and with BatchNorm is

\[
\nabla (\frac{\partial L}{\partial s_{bk}^l}) = \prod_{l'=l}^{l-1} K_{l'+1} \nabla (\frac{\partial L}{\partial s^L}) + o\left(\frac{1}{B^{1-\epsilon}}\right),
\]

for an arbitrary \(0 < \epsilon < 1\).

Proof of Theorem 1. The proof for BNNs without BatchNorm is trivial, so we only provide the proof for BNNs with BatchNorm. Here, \(s_{bk}^l\) refers to a binary dot product and \(\tilde{w}^l\) is a binary random variable representing the binary weight. We may suppose \(\nabla(s_{bk}^l) = \sigma_k^2 = K_{l-1}, \mu_k = 0\). One may prove \(\nabla \left(\frac{\partial L}{\partial s_{bk}^l}\right) = \left(\frac{\gamma_l}{B\sigma_k}\right)^2 (B^2 + 2B - 1 + \nabla(s_{bk}^2) K_{l+1} \nabla (\tilde{w}^{l+1}) \nabla (\frac{\partial L}{\partial s^{l+1}}))\). It is also possible to verify \(\nabla(s_{bk}^2)\) is bounded by \(K_{l-1} - 1\);
the proofs appear in Appendix. Suppose $\gamma^l_k = 1$ at initialization so
\[
\left( \frac{\gamma_k}{B\sigma^2_k} \right)^2 \{ B^2 + 2B - 1 + \mathbb{V}(\hat{s}_{bk}) \} = \left( \frac{1}{B\sqrt{K_{l-1}}} \right)^2 \{ B^2 + 2B - 1 + \mathbb{V}(\hat{s}_{bk}) \} = \frac{B^2 + 2B - 1 + \mathbb{V}(\hat{s}_{bk})}{K_{l-1}B^2} = \frac{1}{K_{l-1}} \left( 1 + o \left( \frac{1}{B^{1-\epsilon}} \right) \right) .
\]
Therefore,
\[
\mathbb{V} \left( \frac{\partial L}{\partial s_{lk}} \right) = \left( \frac{\gamma_k}{B\sigma^2_k} \right)^2 \{ B^2 + 2B - 1 + \mathbb{V}(\hat{s}_{bk}) \} K_{l+1} \mathbb{V}(\hat{w}^{l+1}) \mathbb{V} \left( \frac{\partial L}{\partial s^{l+1}} \right).
\]
After slight re-arrangement
\[
= \frac{K_{l+1}}{K_{l-1}} \left( 1 + o \left( \frac{1}{B^{1-\epsilon}} \right) \right) \mathbb{V} \left( \frac{\partial L}{\partial s^{l+1}} \right) = \mathbb{V} \left( \frac{\partial L}{\partial s^{l+1}} \right) \prod_{l'=l}^{L-1} \frac{K_{l'+1}}{K_{l'-1}} + o \left( \frac{1}{B^{1-\epsilon}} \right) .
\]

There are two implications of Theorem 1. i) BatchNorm corrects exploding gradients in BNNs as the layer width ratio $K_{l+1}/K_{l-1} \approx 1$ in common neural models. If this ratio diverges from unity binary training is problematic even with BatchNorm. ii) One may initialize the weights of a BNN from any distribution symmetric and centred about zero. We also demonstrate this analytical results are aligned with numerical experiments.

5 Experiments

We verify our analytical finding on the CIFAR-10 dataset (Krizhevsky, 2009) which consists of 50,000 training images and 10,000 test images. The images are $32 \times 32$ pixels with 3 channels. During training, we apply data augmentation by padding the images with 4 zeroes on each side, then we take a random crop of $32 \times 32$ and randomly flip them horizontally. At training and testing time, the inputs are normalized with $\mu = (0.4914, 0.4822, 0.4465)$, $\sigma = (0.247, 0.243, 0.261)$. In each model we evaluate on, the first convolution is kept in full-precision as well as the last linear classifier which is preceded by a ReLU activation. The models are trained with Adam (Kingma and Ba, 2014) and minimize the cross-entropy loss. We train a VGG-inspired architecture (Hubara et al., 2018), and a binarized ResNet-56 architecture (He et al., 2015) in which the sign function is applied on the input of a block instead of the output. It allows us to have a full-precision shortcut connection which limits the accuracy drop.

MobileNet-type architectures are designed for low-resource devices, and their binary training is quite challenging. This is why we also add a third model, MobileNet-v1 (Howard et al., 2017)\(^1\) which still holds the arguments and even improves accuracy compared to Glorot’s initialization.

For the VGG-inspired model the starting learning rate is $5 \times 10^{-3}$, otherwise it is $10^{-3}$. All models are trained for 150 epochs and their learning rate is divided by 10 at epochs 80, 120 and 140. We seek here to study how initialization from symmetric distributions with different variances affect the training of BNNs regarding the accuracy. As we showed earlier, the variance of the latent real-valued weights of BNNs do no impact variance of activation and variance of gradient. If we proceed with Glorot and Bengio (2010), latest layers that often include more parameters are initialized closer to the origin as their variance is a decreasing function of their number of neurons.

\(^1\)https://github.com/kuangliu/pytorch-cifar/blob/master/models/mobilenet.py
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Table 1: Effect of different variance values on best Top 1 accuracy, for binary quantized VGG, ResNet-56 (RN-56), and MobileNet version 1 (MN-v1) compared to Glorot’s initialization (G).

|        | \(\sigma^2\) | G 10^{-1} | G 10^{-2} | G 10^{-3} | G 10^{-4} |
|--------|---------------|-----------|-----------|-----------|-----------|
| VGG    | 90.5          | 90.4      | 90.7      | 90.6      | 90.6      |
| RN-56  | 88.5          | 86.9      | 88.5      | 88.8      | 88.1      |
| MN-v1  | 71.7          | 68.9      | 71.2      | 73.1      | 73.2      |

Table 1 gives the training results for the models initialized from a uniform distribution with mean zero and different constant variances. We observed a similar result for non-uniform distributions, such as Gaussian which confirms Glorot’s initialization is useless for BNNs. MobileNet-v1 is already a small efficient network, so is more sensitive to compression and suffers from a more severe accuracy drop. This is where the effect of different initialization variance is more visible: we see the largest accuracy gain by adjusting the initialization variance. We also tried to linearly increase and decrease the variance throughout the layers but the accuracy gain was marginal and we do not report them here. This confirms different variance across layers has no effect in training.

In a second study, we show scaling by \(\frac{1}{\sqrt{K_{l-1}}}\) solves gradient explosion and is the main role of BatchNorm in BNN training. As the scale does not impact the forward pass, it is interesting to see to what extent we can remove components of BatchNorm without causing too much accuracy loss. Computing the mean and variance estimates is burdensome especially on edge-device training methods such as federated learning (McMahan et al., 2017). We perform three experiments on binarized ResNet-56. In the first experiment, features are centred but we replace the variance of BatchNorm with constant scaling factor \(K_{l-1}\) and we adjust it by another version \((3K_{l-1})\) to match BatchNorm accuracy. In the second experiment, we only perform mean subtraction. In the third experiment, we replace BatchNorm layers with identity layers in the model, i.e. no BatchNorm in the network. We expect the second and the third experiment to suffer from exploding gradient and the first experiment to elevate the accuracy in a range similar to networks with BatchNorm, see Table 2.

As expected, “No BN” and “No Scale” do not converge, reaching 31.7%. However the accuracy reaches to 88.8% if the network has BatchNorm layers or 79.6% if properly scaled, confirming our analytical study. A network with BatchNorm is still ahead in terms of accuracy, as our assumptions of initialization regarding the distributions of weights and activations become inaccurate as training goes on. We may close the accuracy gap by tuning the scale, for instance \(\frac{1}{\sqrt{3K_{l-1}}}\). BatchNorm requires floating point operations, which are costly on low-resource devices, especially while training. We recommend to replace BatchNorm with a fixed scaling factor in the order of \(\frac{1}{\sqrt{K_{l-1}}}\) for such devices.

6 Conclusion

BNNs have a different behaviour compared to their full-precision counterpart and BatchNorm has a different role in binary networks. Binary network training requires BatchNorm to converge and we clarified why it is necessary: it prevents gradient explosion. As a biproduct of this study we found out full-precision initializa-
tion scheme is useless for BNNs. We can replace BatchNorm with a proper scaling, and we call for similar studies on more flexible fixed point quantization schemes, such as ternary, 4-bit, and 8-bit networks.

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