Normalization of Neural Networks using Analytic Variance Propagation

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Abstract. We address the problem of estimating statistics of hidden units in a neural network using a method of analytic moment propagation. These statistics are useful for approximate whitening of the inputs in front of saturating non-linearities such as a sigmoid function. This is important for initialization of training and for reducing the accumulated scale and bias dependencies (compensating covariate shift), which presumably eases the learning. In batch normalization, which is currently a very widely applied technique, sample estimates of statistics of hidden units over a batch are used. The proposed estimation uses an analytic propagation of mean and variance of the training set through the network. The result depends on the network structure and its current weights but not on the specific batch input. The estimates are suitable for initialization and normalization, efficient to compute and independent of the batch size. The experimental verification well supports these claims. However, the method does not share the generalization properties of BN, to which our experiments give some additional insight.

1. Introduction

Batch normalization (BN) [5] is a widely applied method which is known to improve learning speed and performance of difficult networks. It is based on a whitening normalization that requires computing the mean and variance statistics of all activations over the training set. In [5] these statistics are approximated by those over a batch. Since [5], there have appeared a number of different normalization methods. A good overview is given in [2] who categorize current methods in three groups: methods based on sample statistics over different groups of hidden units [7, 17, 11], modifications of BN [12, 3, 4, 8] and methods normalizing weights instead of activations [13, 1, 19].

The proposed technique is a follow-up application of the work [16], where a feed-forward propagation of uncertainties (variances) in neural networks (NNs) is proposed, making NNs and Bayesian networks more alike. In this work we apply the idea of variance propagation to analyze standard networks. Namely, we are interested in estimating means and variances of activations in a given network provided basic statistics of the dataset. We show that the method [16] is suitable for this task, can be implemented very efficiently for CNNs and conduct a detailed experimental study.

The method is also related to normalization propagation [1] and deep information propagation [15] as will be discussed in §3.

1.1. Background

Normalization Methods Ioffe and Szegedy [5] proposed the following transformation to be applied in front of saturating non-linearities (such as logistic sigmoid):

$$X' = \frac{X - \mu}{\sigma} s + b,$$

where $s$ and $b$ are new parameters. Its purpose is twofold: 1) to make sure that the non-linearity on average receives a signal in a range where the output is not saturated and 2) to make the average scale and bias of activations controlled by local parameters $s$ and $b$ rather than by the cumulative effect of many layers.

The ideal whitening is achieved when $\mu = \mathbb{E}[X]$ and $\sigma^2 = \text{Var}[X]$ are the expectation statistics of $X$ over the dataset. While it is too costly to compute these expectations accurately for all hidden units in a deep network, they can be approximated in several ways. BN estimates $(\mu, \sigma^2)$ as sample statistics over a batch. Other estimates or approximations are possible. For example, layer normalization [7] uses sample statistics of different units across the spatial...
Weight Normalization (WN) [13], applied to the input $X = w^TZ$ can be viewed as setting $\mu = 0$ and $\sigma = \|w\|$ in (1). This choice indeed matches the expectations of $X$ when $Z$ has zero mean and unit variance [13]. Substituting, we obtain the formula $X' = w^T Z^'/\|w\| \cdot s + b$, which just normalizes the weight locally. The resulting variable $X'$ as well as a non-linear transform of it, $f(X')$, do not longer have a zero mean and unit variance (unless it is assumed that $s = 1$ and $b = 0$) and the chain of arguments breaks down. Despite such simplicity, WN has a positive effect on learning [13, 2]. These two techniques will be the baseline methods in our experiments.

**Invariances** Let $X$ be the output of a linear transform: $X = w^T Z + a$. Then $X'$ in (1) is invariant w.r.t. the bias $a$ and the scale of weights $\|w\|$. This holds true for the exact expectations $\mu$, $\sigma^2$ as well as for their estimates used by weight normalization, batch normalization and our method. The invariance to the bias is evident, it holds as soon as the estimate of $\mu$ satisfies the linearity of the expectation: $E[X] = w^T E[Z] + a$. The scale invariance follows from that the variance and its used estimates are 2-homogenous: $\text{Var}[\alpha w^T Z] = \alpha^2 \text{Var}[w^T Z]$. In this case there holds:

$$\frac{E[\alpha w^T Z]}{\sqrt{\text{Var}[\alpha w^T Z]}} = \frac{E[w^T Z]}{\sqrt{\text{Var}[w^T Z]}},$$

so the scale $\|w\|$ does not matter. For BN, the sample variance of $w^T Z$ expresses as $\langle \alpha w^T Z, C \rangle_F$, where $C = \frac{1}{n-1} \sum_i z_i z_i^T$ is the sample covariance matrix over a batch $\{z_i\}$, and $\langle \cdot, \cdot \rangle_F$ is the Frobenius inner product. This expression is 2-homogenous in $w$.

With these invariances we see that the new parameters $s$, $b$ in the expression (1) introduce back exactly the same number of degrees of freedom that are projected-out by the normalization. The difference is that the overall scale and bias are controlled now by the local parameters $s$, $b$ rather than by the cumulative effect of the preceding layers.

**Initialization** There are two ways to introduce a normalization: preserving the equivalence with the original network and resetting the scale and bias. In the first case, the new parameters $s$, $b$ in (1) are initialized as $s = \sigma$ and $b = \mu$, which makes (1) an identity. The network performance is preserved. This does not help to achieve a non-saturating regime discussed above but can be useful for further optimization of an already pretrained network.

In the second case, $s$ and $b$ are initialized, e.g., as $s = 1$ and $b = 0$. Starting from some initialization of network weights, such as random or orthogonal, this projecting initialization approximately compensates accumulated biases and scaling of linear and non-linear transforms and efficiently reinitializes the network to a point where non-linearities are not saturated on average. It makes the network training invariant to a scale-bias preprocessing transformation of the input images and the initial scale of the random weights. Converting the model back to the equivalent unnormalized form will preserve these properties and result in a good initialization point (e.g., [13]).

**Shortcomings of BN** Let us summarize the known issues / challenges with using BN in practice. The testing requires an up-to-date whole dataset statistics. This makes it more difficult to keep track of the training/validation error during the training. The application to recurrent networks is problematic: one has to unfold running statistics over recurrences. The computation overhead is not negligible: up to 25% according to [2]. The behavior is more stochastic than other methods [13] and destabilizing in GAN, where weight normalization performs better [19]. The batch size is a sensitive parameter affecting convergence and generalization properties [14, Fig. 7.38].

**2. Proposed Technique**

The proposed technique uses the same normalized form (1), but the mean and variance are estimated analytically rather than from a batch sample. The analytic method [16] is as follows. A basic neural network composes linear transforms and coordinate-wise non-linearities. Let us assume that $X$ is a vector-valued r.v. with components $X_i$ having statistics $\mu_i$ and $\sigma_i^2$. The statistics of a linear transform $Y = w^T X$ are given by

$$\mu' = E[Y] = w^T E[X] = w^T \mu,$$

$$\sigma'^2 = \sum_{ij} w_i w_j \text{Cov}[X] \approx \sum_i w_i^2 \sigma_i^2,$$

where $\text{Cov}[X]$ is the covariance matrix of $X$. The approximation of the covariance matrix by its diagonal is exact when $X_i$ are uncorrelated. The correlation of the outputs depends on the current weights $w$ and is zero when the weights are orthogonal. Note that random vectors are approximately orthogonal and therefore the assumption is plausible at least on initialization.
In order to treat non-linearities, let $X$ be a scalar r.v. with statistics $\mu$, $\sigma^2$ and $Y = f(X)$. One general method of variance estimation is to linearize $f$ around $\mu$ and apply the propagation in the linear case. However, this is only applicable to small variances, such that the linear approximation holds for all likely values of $X$. When we deal with statistics over a dataset, the variances should be assumed large. A more suitable approximation used in [16] computes expectations

$$
\mu' = \mathbb{E}[f(X)] = \int f(x)p(x)dx,
$$

$$
\sigma'^2 = \int f^2(x)p(x)dx - \mathbb{E}[f(X)]^2,
$$

assuming that $X$ is normally distributed: $X \sim \mathcal{N}(\mu, \sigma^2)$. This assumption is plausible when $X$ is a linear combination $X = w^T Z + a$, in which $Z_i$ are independent and weights are random. Empirically, this is a good approximation in many cases in practice\(^1\). This method is not a general one as it requires to compute integrals analytically, but for many cases of practical interest it is tractable. In particular it is the case for sigmoid $f(x) = 1/(1 + e^{-x})$ and ReLU($x$) = $\max(0, x)$ non-linearities and for $\max(x_1, x_2)$, which can be used to implement max-pooling and max-out, see [16, Table 2]. Let us illustrate the case for ReLU. Both integrals (4) can be taken (e.g., [16, §C.3]) and the result can be expressed as

$$
\mu' = \mu \Phi(a) + \sigma \phi(a) \tag{5a}
$$

$$
\sigma'^2 = \sigma^2 \mathcal{R}(a), \tag{5b}
$$

where $a = \mu/\sigma$, $\phi$ is the pdf of the standard normal distribution, $\Phi$ is its cdf and $\mathcal{R}(a) = a\phi(a) + (a^2+1)\Phi(a) - (a\Phi(a)+\phi(a))^2$. We see that both integrals express through functions of a single variable $a$. Even though they involve a non closed-form function $\Phi$, they can be accurately approximated. Fig. 1 illustrates this solution.

**Invariances** It is straightforward to see that linear propagating equations (3) satisfy the properties that $\mu'$ is linear and $\sigma'^2$ is 2-homogenous and therefore the scale-bias invariance holds.

\(^1\)There are variants of central limit theorem for non-i.i.d. and even weakly dependent variables https://en.wikipedia.org/wiki/Central_limit_theorem. See [18, Figs 2, 3] for experimental illustration of related assumptions in a network with dropout noise.

Figure 1: Propagation of uncertainty through ReLU (red). The black curve shows an example of input $X$: a normal pdf with mean $\mu = 3$, $\sigma = 1$ and support $\mu \pm 3\sigma$, amplified in value for visibility. The expectation of ReLU vs. the mean $\mu$ is shown as a blue curve. The std $\sigma'$ of ReLU is illustrated via the set $\mu' \pm 3\sigma'$ shown as shaded area. When the input $\sigma$ is different from 1 the plot in coordinates $\mu'/\sigma$ vs. $\mu/\sigma$ stays the same.

2.1. Efficiency

To compute statistics of all hidden units, the approximation can be applied layer-by-layer, propagating mean and variance. Let us consider a deep NN where normalization (1) is applied. The quantity

$$
\frac{X_i - \mu_i}{\sigma_i}, \tag{6}
$$

where $\mu$, $\sigma^2$ are statistics of $X$, has zero mean and unit variance. It implies that the computation of statistics in a normalized network decouples as follows:

- Start from the dataset statistics $(\mu^0, \sigma^0)$, which can be estimated prior to learning. They are commonly used for the initial data whitening transform. If such a whitening transform has been already applied we may assume $(\mu^0, \sigma^0) = (0, 1)$. Propagate the moments until the first normalization layer.

- Propagate from one normalization layer to the next one assuming the input statistics are $(0, 1)$.

The computation thus decouples in block of layers delimited by the normalization layers and the result of the normalization of such a block depends on the parameters only inside the block but not on any other parameters or data. Consider a network composed of blocks of the form (linear$(W^k)$, norm$(s^k, b^k)$, activation). Then the statistics for the normalization in block $k$ will depend only on parameters $W^k$, $s^{k-1}$, $b^{k-1}$.
Further on, to compute the normalization in a convolutional NN we do not need to work with spatial dimensions. The normalized input statistics \((0, 1)\) are the same over spatial dimensions and channels. The scale-bias parameters \(s, b\) are the same over spatial dimensions but not over channels. A convolutional filter \(W_{i,j,k}\) (per output channel) with \(i\) running over input channels and \(j, k\) over spatial dimensions, applied to a tensor which is constant across spatial dimensions, is equivalent to applying a linear transform \(w\) with components \(w_i = \sum_{j,k} W_{i,j,k}\) to a vector over channels. The propagation of the variance reduces similarly. The whole normalization is thus independent of the image and batch sizes and has a complexity similar to that of weight normalization.

**Initialization** In our case, just the initial statistics \((\mu^0, \sigma^0)\) are needed for the initialization. The equivalence-preserving initialization is exact for the whole dataset. In the projecting initialization, approximate expectations \(E[X_i]\) and \(\text{Var}[X_i]\) depend on the parameters of all layers down to the preceding normalization layer as explained above.

**Advantages** We see the following advantages compared to [5]. The proposed normalization has very little overhead for CNNs, also considering backpropagation. There is no dependency on batch size. The normalization is exactly the same during training and testing, we can easily convert between unnormalized and normalized forms while preserving the equivalence. Because the normalization decouples, there is no limitation to apply it in recurrent networks. The normalization is continuously differentiable and is non-stochastic. If dropout is applied during training, the normalization takes it into account analytically (dropout is a multiplication by a Bernoulli r.v. with known statistics, see details in [16]). Similar advantages hold for applying the method as initialization.

3. Related Work

Our method reduces to normalization propagation [1] when parameters \(s, b\) are not present. In this case the normalization results in centering of the ReLU non-linearity by a constant scale and bias as in [1]: when input statistics are \((0, 1)\) then so are the output statistics. A similar constant centering appears in self-normalizing networks [6]. Thus, as an initialization scheme, it is equivalent to [1, 6]. However, when the scale-bias parameters are enabled and varied, our method smoothly tracks the covariate shift, while [1] does not. Disabling scale and bias parameters as in [6] defines a different class of models with fewer degrees of freedom. Since scale-bias parameters may be different per channel, our normalization depends as well on the current weights \(w\). Further, note that applying dropout will change the statistics, which is taken into account in our method.

The technique [15] performs analysis of neural networks using mean field theory, which is related to our variance propagation. It allows to estimate quantities such as mean activations and even norms of gradients assuming that all weights are random. While they focus on asymptotic scenarios w.r.t. depth and address a limited family of architectures, the results are highly relevant for initialization methods.

Works [2, 13] discuss practical and theoretical properties of normalization schemes such as the effect of the reparametrization as a preconditioner, etc.

4. How (Not) to Make a Comparison

In our first attempt of comparing normalized and unnormalized training, we compare different methods with equal learning rate, initialized as recommended by the specific method. An example of such a comparison is shown in Fig. 2. It turns out to be rather uninformative and even misleading. First, we
are comparing training schemes starting at different points. Clearly, a better starting point gives an advantage [10, 13]. Thus, the effects of initialization and normalization are entangled. Second, comparing at equal learning rates is incorrect because the methods use different parametrization and thus efficiently rescale the descent steps differently, as explained below. Third, with limited training sets, NNs easily over-fit and the training cross-entropy loss can be made arbitrary close to zero while having poor generalization. To remedy this we will consider noise-augmented training sets.

To see the issue with the learning rate, consider what happens with the step size when a reparametrization is used. Let for example, \( \theta' = A \theta \) (a linear change of variables). The steepest descent in \( \theta \) for an objective \( f(\theta) \) has the form \( \theta^{t+1} := \theta^t - \alpha_t \nabla f(\theta^t) \). The steepest descent in \( \theta' \) for the minimization of \( f(\theta) = f(A^{-1} \theta') \) can be equivalently written as

\[
\theta^{t+1} = \theta^t - \alpha_t (A A^T)^{-1} \nabla f(\theta^t),
\]

i.e., as a preconditioned gradient descent (see e.g., [9, §8.7]). If we keep the learning rate the same, a method that minimizes \( f(2 \theta') \) results in a 4 times larger step size. Compared as in Fig. 2, it can be declared a “faster normalization scheme”. The issues applies to normalization schemes because a change of variables is involved and there is also a possibility, e.g., overestimate the variance.

The previous work [5] compared BN to the standard unnormalized training initialized differently and manually adjusting learning rate and other parameters. These issues are better addressed in [13], where BN, WN and an unnormalized network are all initialized with BN and a set of learning rates is tried for BN, WN and an unnormalized form for starting of other methods.

Normalizations are introduced with preserving the equivalence.

\[
\text{init} = \text{None}: \text{Initialize weights randomly, normalized as discussed above. } BN \text{ parameters are reduced with } \text{BN} \text{ for a function of a single variable (the learning rate) as detailed below. While it does not fully resolve the issue of a fair comparison, it is a method that can be used in practice and it does make the comparison more independent of trivial reparametrizations.}
\]

Implementation Details Our implementation in pytorch will be made publicly available.

To find the best learning rate \( lr \) we use the bounded Brent’s method\(^3\) to optimize the \( \log_{10} lr \) with bounds \([-6, -2]\) and a limit of 10 iterations. The objective is the running mean estimate of the stochastic loss in five epochs. The running mean uses exponential weights vanishing to 0.1 in 1 epoch.

Parameters We used batch size 128, Adam optimizer with learning rate \( lr \cdot 0.9^k \), where \( k \) is the epoch number (this gives a factor 10 reduction in 50 epochs). The initial learning rate \( lr \) is the parameter optimized as discussed above. BN parameters are

\(^2\)The gradient descent may however behave well in some cases. As explained in [13], due to scale-invariance the gradients of the main loss are orthogonal to \( w \) and the steps monotonously increase the norm \( ||w|| \). The regularization can be balancing this effect. However, a projection on the constrain \( ||w|| = 1 \) would be much simpler. Weight regularization of parameters \( s, b \) is also doubtful. Non-lineairities introduce an implicit scaling and bias depending on previous layers. Making \( ||b|| \) smaller does not necessarily make the total effective bias smaller, but instead can make it larger.

\(^3\)Available in scipy package
Figure 3: MNIST (no noise augmentation). Plots are grouped by the initialization method and show a running mean estimate of the stochastic batch-wise training objective vs. epochs. For all normalizations but BN this matches well with the training loss on the whole data set. For BN, its stochastic estimate deviates from its evaluation performance on the training set (shown as a Eval). In this task it is possible to bring the loss arbitrary close to zero, which AP2 normalization successfully does for all 3 inits – a clear case of overfitting.

Figure 4: Noisy MNIST: Training loss with different initializations.

the pytorch default ones: \( \epsilon = 10^{-5}, \text{momentum}^{4} = 0.1 \).

Datasets We used MNIST\(^{5}\) and CIFAR10\(^{6}\)

\(^{4}\)In pytorch this is the weight of the new data point, not of the previous estimate.

\(^{5}\)http://yann.lecun.com/exdb/mnist/

\(^{6}\)https://www.cs.toronto.edu/~kriz/cifar.html
datasets.

**MNIST** The initial dataset is augmented by random offsets in the range $[-2, 2]$ with zero padding. We tested a simple non-convolutional network with 6 hidden layers of logistic transform units, 20 in each (same as in [16]). Such network is already relatively hard to train with random initialization as seen in Fig. 3 (top), even when the best learning rate is chosen. BN starting from this initialization performs better but has problems with estimating the whole training set mean and variance. Its evaluation performance is very stochastic and does not match the training performance. With BN initialization, all methods succeed to train the network. It is seen that with optimized learning rates, their performance is much more similar than reported elsewhere. Here BN evaluation-mode performance is better than its batch performance. Finally, for AP2 initialization, standard network and weight normalization work well while BN oscillates despite that the automatically chosen learning rate is by an order of magnitude smaller than in the case of init=BN. It is interesting that with AP2 normalization, the learning objective is optimized well for all initializations. However, in this test scenario the model is overfitting, as can be seen from the validation loss and accuracy shown in Fig. 5, and therefore a better performance on the training loss is of little practical utility.

**Noisy-MNIST** The dataset is additionally augmented with Gaussian noise with variance 0.1. The results are shown in Fig. 7. The proposed normalization behaves well across all init points. BN achieves the overall best training objective, but the difference is not decisive, comparable to results of AP2 with other inits. The same holds for the validation accuracies in Fig. 8. BN has a significant generalization boost when using accumulated statistics (evaluation mode). This is an interesting phenomenon, perhaps related to boosting or ensemble techniques: the data-dependent (stochastic) normalization values are replaced with their running average counterparts (expectations).

**6. Conclusion**

In this work we explored an application of variance propagation [16] for computing normalization statistics. The resulting method has similar advantages as weight normalization: computation efficiency, continuous differentiability, data-independent plug-in/out capability, applicability to recurrent nets, etc. The procedure approximates the needed statistics in a clearly understood manner and is general in the sense that it can take into account different constructive elements of neural networks and their dependencies. We strove towards making experiments more objective by considering same initialization points and optimizing the learning rate. We observed that the remaining differences in the speed of different methods became much smaller than when compared naively, e.g., as in Fig. 2. It can be still observed that the proposed technique improves robustness to initialization points and achieves a lower training objective in many cases. It also gives a good initialization point to standard parametrization and weight normalization. It does not have the property of batch normalization to generalize (presumably due to stochasticity and averaging). The later however experienced a significant instability when applied to other initialization points in our tests.

We hypothesize that the proposed method may benefit from an orthogonal initialization because such initialization would make the uncorrelated inputs assumption exact. The role of the norm $||w||$, to which the normalized forms are invariant (but not their gradients!) is yet unclear.
AP2 is on par with BN.

conclusions about the speed of learning.

Figure 7: Noisy CIFAR-10: Training loss with different initializations. When the learning rate is optimized as proposed

Figure 5: MNIST: Validation loss and accuracies, BN-initialized training. BN shows less overfitting and better validation

accuracy. These results are consistent with [2, figure 3].

Figure 6: Noisy MNIST: Validation loss and accuracies, BN-initialized training. Here overfitting does not occur and

AP2 is on par with BN.

Figure 7: Noisy CIFAR-10: Training loss with different initializations. When the learning rate is optimized as proposed

in the paper, the differences between different init and normalization schemes are not so pronounced and we cannot make

collections about the speed of learning.

Figure 8: Noisy CIFAR-10: Validation accuracies corresponding to Fig. 7.
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