Initialization Of Deep Networks Case of Rectifiers

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Mathematics Behind Neural Network Weights Initialization - Part Three: In this third of a three part series of posts, we will attempt to go through the weight initialization algorithms as developed by various researchers taking into account influences derived from the evolution of neural network architecture and the activation function in particular.

Introduction

Recent success in deep networks can be credited to the use of non-saturated activation function Rectified Linear unit (RReLu) which has replaced its saturated counterpart (e.g. sigmoid, tanh). Benefits associated with the ReLu activation function include:

- Ability to mitigate the exploding or vanishing gradient problem; this largely due to the fact that for all inputs into the activation function of values grater than 0, the gradient is always 1 (constant gradient)
- The constant gradient of ReLu activations results in faster learning. This helps expedite convergence of the training procedure yielding better better solutions than sigmoidlike units
- Unlike the sigmoidlike units (such as sigmoid or tanh activations) ReLu activations does not involve computing of an an exponent which is a factor that results to a faster training and evaluation times.
- Producing sparse representations with true zeros. All inputs into the activation function of values less than or equal to 0, results in an output value of 0. Sparse representations are considered more valuable

Xavier and Bengio (2010) [2] had earlier on proposed the “Xavier” initialization, a method whose derivation was based on the assumption that the activations are linear. This assumption however is invalid for ReLu and PReLu. He, Kaiming, et al. 2015 [1] later on derived a robust initialization method that particularly considers the rectifier nonlinearities.

In this article we discuss the algorithm put forward by He, Kaiming, et al. 2015 [1].

Notation

1. k is the side length of a convolutional kernel. (also the spatial filter size of the layer)
2. c is the channel number. (also input channel)
3. n is the number of connections of a response ($n = k \times k \times c \implies k^2c$)
4. $\mathbf{x}$ is the co-located $k \times k$ pixels in c inputs channels. ($\mathbf{x} = (k^2c) \times 1$)
5. W is the matrix where d is the total number number of filters. Every row of W i.e $(d_1, d_2, \cdots, d_d)$ represents the weights of a filter. ($W = d \times n$)
6. $\mathbf{b}$ is the vector of biases.
7. $\mathbf{y}$ is the response pixel of the output map
8. l is used to index the layers
9. $f(\cdot)$ is the activation function
10. $\mathbf{x} = f(\mathbf{y}_{l-1})$
11. $c = d_{l-1}$
12. $\mathbf{y}_l = W_l\mathbf{x}_l + \mathbf{b}_l$

Forward Propagation Case

Considerations made here include:

- The initialized elements in W_l be mutually independent and share the same distribution.
- The elements in $\mathbf{x}_l$ are mutually independent and share the same distribution.
- $\mathbf{x}_l$ and W_l are independent of each other.

The variance of y_l can be given by:

$$Var[y_l] = n_l Var[w_l x_l], \tag{1}$$

where y_l, w_l, x_l represent random variables of each element in $\mathbf{y}_l, W_l, \mathbf{x}_l$. Let w_l have a zero mean, then the variance of the product of independent variables gives us:

$$Var[y_l] = n_l Var[w_l] E[x_l^2]. \tag{2}$$

Lets look at how the Eqn. (2) above is arrived at:-

For random variables $\mathbf{x}_l$ and W_l, independent of each other, we can use basic properties of expectation to show that:

$$Var[w_l x_l] = E[w_l^2]E[x_l^2] - \overbrace{[E[x_l]]^2[E[w_l]]^2}^{\bigstar}, \tag{A}$$

From Eqn. (2) above, we let w_l have a zero mean $\implies E[w_l] = [E[w_l]]^2 = 0$. This means that in Eqn. (A), $\bigstar$ evaluates to zero. We are then left with:

$$Var[w_l x_l] = E[w_l^2]E[x_l^2], \tag{B}$$

Using the formula for variance $Var[w_l] = E[w_l^2] - [E[w_l]]^2$ and the fact that $E[w_l] = 0$ we come to the conclusion that $Var[w_l] = E[w_l^2]$.

With this conclusion we can replace $E[w_l^2]$ in Eqn. (B) with $Var[w_l]$ to obtain the following Eqn.:

$$Var[w_l x_l] = Var[w_l]E[x_l^2], \tag{C}$$

By substituting Eqn. (C) into Eqn. (1) we obtain:

$$Var[y_l] = n_l Var[w_l]E[x_l^2]. \tag{2}$$

In Eqn. (2) it is well worth noting that $E[x_l^2]$ is the expectation of the square of x_l and cannot resolve to $Var[x_l]$ i.e $E[x_l^2] \neq Var[x_l]$ as we did above for w_l unless x_l has zero mean.

The effect of ReLu activation is such that $x_l = max(0, y_{l-1})$ and thus it does not have zero mean. For this reason the conclusion here is different compared to the initialization style in [2].

We can also observe here that despite the mean of x_l i.e $E[x_l]$ being non zero, the product of the two means $E[x_l]$ and $E[w_l]$ will lead to a zero mean since $E[w_l] = 0$ as shown in the Eqn. below:

$$E[y_l] = E[w_l x_l] = E[x_l]E[w_l] = 0.$$

If we let w_{l-1} have a symmetric distribution around zero and $b_{l-1} = 0$, then from our observation above y_{l-1} has zero mean and a symmetric distribution around zero. This leads to $E[x_l^2] = \frac{1}{2}Var[y_{l-1}]$ when $f(\cdot)$ is ReLu. Putting this in Eqn. (2), we obtain:

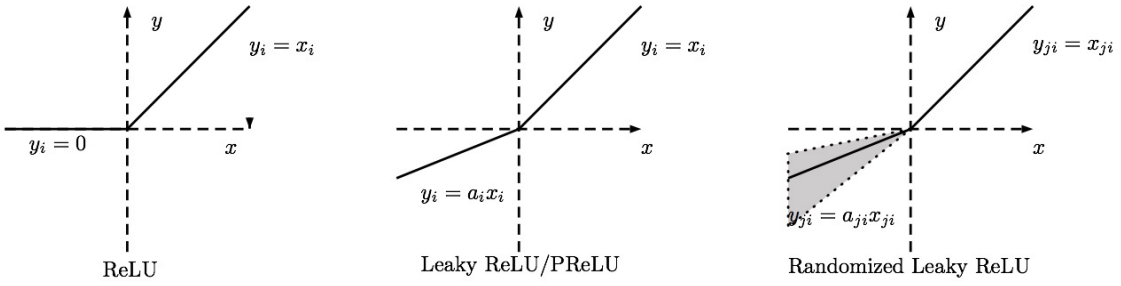
$$Var[y_l] = n_l Var[w_l]\frac{1}{2}Var[y_{l-1}]. \tag{3}$$

With L layers put together, we have:

$$Var[y_L] = Var[y_1]\left(\prod_{l=1}^{L}\frac{1}{2}n_l Var[w_l]\right). \tag{4}$$

The product in Eqn. (4) is key to the initialization design.

Lets take some time to explain the effect of ReLu activation as seen in Eqn. (3).



For the family of rectified linear (ReL) shown illustrated in the diagram above, we have a generic activation function defined as follows:

$$f(y_i) = \begin{cases} y_i, & \text{if } y_i > 0 \\ a_i y_i, & \text{if } y_i \leq 0 \end{cases} \tag{5}$$

In the activation function (5) above, y_i is the input of the nonlinear activation f on the ith channel, and a_i is the coefficient controlling the slope of the negative part. i in a_i indicates that we allow the nonlinear activation to vary on different channels.

The variations of rectified linear (ReL) take the following forms:

1. **ReLu**: obtained when $a_i = 0$. The resultant activation function is of the form $f(y_i) = max(0, y_i)$
2. **PReLu**: Parametric ReLu - obtained when a_i is a learnable parameter. The resultant activation function is of the form $f(y_i) = max(0, y_i) + a_i min(0, y_i)$
3. **LReLu**: Leaky ReLu - obtained when $a_i = 0.01$ i.e when a_i is a small and fixed value [3]. The resultant activation function is of the form $f(y_i) = max(0, y_i) + 0.01 min(0, y_i)$
4. **RReLu**: Randomized Leaky ReLu - the randomized version of leaky ReLu, obtained when a_{ji} is a random number sampled from a uniform distribution $U(l, u)$ i.e $a_{ji} \sim U(l, u);\ l < u \text{ and } l, u \in [0; 1)$. See [2].

Rectifier activation function is simply a threshold at zero hence allowing the network to easily obtain sparse representations. For example, after uniform initialization of the weights, around 50% of hidden units continuous output values are real zeros, and this fraction can easily increase with sparsity-inducing regularization [5].

Take signal $y_i = W_i x + b$, (visualize the signal represented on a bi-dimensional space $y_i \in \mathbb{R}^2$). Applying the rectifier activation function to this signal i.e $f(y_i)$ where f is ReLu results in a scenario where signals existing in regions where $y_i < 0$ are squashed to 0, while those existing in regions where $y_i > 0$ remain unchanged.

The ReLu effect results in *"aggressive data compression"* where information is lost (replaced by real zeros values). A remedy for this would be the PReLu and LReLu

implementations which provides an axle shift that adds a slope a_i to the negative section ensuring from the data some information is retained rather than reduced to zero. Both PReLu and LReLu represented by variations of $f(y_i) = max(0, y_i) + a_i min(0, y_i)$, make use of the factor a_i which serves as the component used to retain some information.

Using ReLu activation function function therefore, only the positive half axis values are obtained hence:

$$E[x_l^2] = \frac{1}{2} Var[y_{l-1}] \tag{6}$$

Putting this in Eqn. (2), we obtain our Eqn. (3) as above:

$$Var[y_l] = n_l Var[w_l] \frac{1}{2} Var[y_{l-1}] \tag{3a}$$

$$= \frac{1}{2} n_l Var[w_l] Var[y_{l-1}] \tag{3b}$$

Note that a proper initialization method should avoid reducing and magnifying the magnitudes of input signals exponentially. For this reason we expect the product in Eqn. (4) to take a proper scalar (e.g., 1). This leads to:

$$\frac{1}{2} n_l Var[w_l] = 1, \quad \forall l \tag{7}$$

From Eqn. (7) above, we can conclude that:

$$Var[w_l] = \frac{2}{n_l} \implies \text{standard deviation (std)} = \sqrt{\frac{2}{n_l}}$$

The initialization according to [1] is a zero-mean Gaussian distribution whose standard deviation (std) is $\sqrt{2/n_l}$. The bias is initialized to zero. The initialization distribution therefore is of the form:

$$W_l \sim \mathcal{N}\left(0, \sqrt{\frac{2}{n_l}}\right) \text{ and } \mathbf{b} = 0.$$

From Eqn. (4), we can observe that for the first layer $(l = 1)$, the variance of weights is given by $n_l Var[w_l] = 1$ because there is no ReLu applied on the input signal. However, the factor of a single layer does not make the overall product exponentially large or small and as such we adopt Eqn. (7) in the first layer for simplicity.

Backward Propagation Case

For back-propagation, the gradient of the conv-layer is computed by:

$$\Delta \mathbf{x}_l = W_l \Delta \mathbf{y}_l. \tag{8}$$

Notation

1. $\Delta \mathbf{x}_l$ is the gradient $\frac{\partial \epsilon}{\partial \mathbf{x}}$
2. $\Delta \mathbf{y}_l$ is the gradient $\frac{\partial \epsilon}{\partial \mathbf{y}}$
3. $\Delta \mathbf{y}_l$ is represented by k by k pixels in d channels and is thus reshaped into $k^2 d$ by 1 vector i.e $\Delta \mathbf{y}_l = k^2 d \times 1$.
4. $\hat{n}$ is given by $k^2 d$ also note that $\hat{n} \neq n$.
5. $\hat{W}$ is a c-by-n matrix where filters are arranged in the back-propagation way. Also $\hat{W}$ and W can be reshaped from each other.
6. $\Delta \mathbf{x}$ is a c-by-1 vector representing the gradient at a pixel of this layer.

Assumptions made here include:

- Assume that w_l and Δy_l are independent of each other then Δx_l has zero mean for all l, when w_l is initialized by a symmetric distribution around zero.
- Assume that $f'(y_l)$ and Δx_{l+1} are independent of each other

In back-propagation we have $\Delta \mathbf{y}_l = f'(y_l)\Delta x_{l+1}$ where f' is the derivative of f. For the ReLu case $f'(y_l)$ is either zero or one with their probabilities being equal i.e $\Pr(0) = \frac{1}{2}$ and $\Pr(1) = \frac{1}{2}$.

Lets build on from some definition here; for a discrete case, the expected value of a discrete random variable, X, is found by multiplying each X-value by its probability and then summing over all values of the random variable. That is, if X is discrete,

$$E[X] = \sum_{\text{all } x} x p(x)$$

The expectation of $f'(y_l)$ then:

$$E[f'(y_l)] = (0)\frac{1}{2} + (1)\frac{1}{2} = \frac{1}{2} \tag{9}$$

With the independence of $f'(y_l)$ and Δx_{l+1}, we can show that: The expectation of $f'(y_l)$ then:

$$E[\Delta y_l] = E[f'(y_l)\Delta x_{l+1}] = E[f'(y_l)]E[\Delta x_{l+1}] \tag{10}$$

Substituting results in Eqn. (9) into Eqn. (10) we obtain:

$$E[\Delta y_l] = \frac{1}{2}E[\Delta x_{l+1}] = 0 \tag{11}$$

In Eqn. (10) Δx_l has zero mean for all l which gives us the result zero. With this we can show that $E[(\Delta y_l)^2] = Var[\Delta y_l]$ using the formula of variance as follows:

$$
\begin{aligned}
Var[\Delta y_l] &= E[(\Delta y_l)^2] - [E[\Delta y_l]]^2 \\
&= E[(\Delta y_l)^2] - 0 \\
&= E[(\Delta y_l)^2]
\end{aligned}
$$

Again with the assumption that Δx_l has zero mean for all l, we show can that the variance of product of two independent variables $f'(y_l)$ and Δx_{l+1} to be

$$
\begin{aligned}
Var[\Delta y_l] &= Var[f'(y_l)\Delta x_{l+1}] \\
&= E[(f'(y_l))^2]E[(\Delta x_{l+1})^2] - [E[f'(y_l)]]^2[E[\Delta x_{l+1}]]^2 \\
&= E[(f'(y_l))^2]E[(\Delta x_{l+1})^2] - 0 \\
&= E[(f'(y_l))^2]E[(\Delta x_{l+1})^2] \qquad (12)
\end{aligned}
$$

From the values of $f'(y_l) \in \{0, 1\}$ we can observe that $1^2 = 1$ and $0^2 = 0$ meaning $f'(y_l) = [f'(y_l)]^2$.

This means that $E[f'(y_l)] = E[(f'(y_l))^2] = \frac{1}{2}$. Using this result in Eqn. (12) we obtain:

$$
\begin{aligned}
Var[\Delta y_l] &= E[(f'(y_l))^2]E[(\Delta x_{l+1})^2] \\
&= \frac{1}{2}E[(\Delta x_{l+1})^2] \qquad (13)
\end{aligned}
$$

Using the formula for variance and yet again the assumption that Δx_l has zero mean for all l, we show can that $Var[\Delta x_{l+1}] = E[(\Delta x_{l+1})^2]$:

$$
\begin{aligned}
Var[\Delta x_{l+1}] &= E[(\Delta x_{l+1})^2] - [E[\Delta x_{l+1}]]^2 \\
&= E[(\Delta x_{l+1})^2] - 0 \\
&= E[(\Delta x_{l+1})^2] \qquad (14)
\end{aligned}
$$

Substituting this result in Eqn. (13) we obtain:

$$
E[(\Delta y_l)^2] = Var[\Delta y_l] = \frac{1}{2}E[(\Delta x_{l+1})^2] \qquad (15)
$$

The variance of Eqn. (8) can be shown to be:

$$
\begin{aligned}
Var[\Delta x_{l+1}] &= \hat{n}Var[w_l]Var[\Delta y_l] \\
&= \frac{1}{2}\hat{n}Var[w_l]Var[\Delta x_{l+1}] \qquad (16)
\end{aligned}
$$

The scalar $1/2$ in both Eqn. (16) and Eqn. (3) is the result of ReLu, though the derivations are different. With L layers put together, we have:

$$
Var[\Delta x_2] = Var[\Delta x_{L+1}] \left(\prod_{l=2}^{L} \frac{1}{2}\hat{n}_l Var[w_l] \right) \qquad (17)
$$

Considering a sufficient condition that the gradient is not exponentially large/small:

$$\frac{1}{2}\hat{n}_l Var[w_l] = 1, \quad \forall l \tag{18}$$

The only difference between Eqn. (18) and Eqn. (7) is that $\hat{n} = k_l^2 d_l$ while $n = k_l^2 c_l = k_l^2 d_{l-1}$. Eqn. (18) results in a zero-mean Gaussian distribution whose standard deviation (std) is $\sqrt{2/\hat{n}_l}$. The initialization distribution therefore is of the form:

$$W_l \sim \mathcal{N}\left(0, \sqrt{\frac{2}{\hat{n}_l}}\right)$$

For the layer $(l = 1)$, we need not compute Δx because it represents the image domain. We adopt Eqn. (18) for the first layer for the same reason as the forward propagation case - the factor of a single layer does not make the overall product exponentially large or small.

It is noted that use of either Eqn. (18) or Eqn. (4) alone is sufficient. For example, if we use Eqn.(18), then in Eqn. (17) the product $\prod_{l=2}^{L} \frac{1}{2}\hat{n}_l Var[w_l] = 1$, and in Eqn. (4) the product $\prod_{l=2}^{L} \frac{1}{2} n_l Var[w_l] = \prod_{l=2}^{L} n_l/\hat{n} = c_2/d_L$, which is not a diminishing number in common network designs. This means that if the initialization properly scales the backward signal, then this is also the case for the forward signal; and vice versa.

For initialization in the PReLu case, it is easy to show that Eqn. (4) becomes:

$$\frac{1}{2}(1 + a^2) n_l Var[w_l] = 1, \tag{19}$$

Where a is the initialized value of the coefficients. If $a = 0$, it becomes the ReLu case; if $a = 1$, it becomes the linear case; same as [2]. Similarly, Eqn. (14) becomes:

$$\frac{1}{2}(1 + a^2) \hat{n}_l Var[w_l] = 1, \tag{20}$$

Applications

The initialization routines derived here, more famously known as **“Kaiming Initialization”** have been successfully applied in various deep learning libraries. Below we shall look at Keras a minimalist, highly modular neural networks library, written in Python and capable of running on top of either TensorFlow or Theano.

The initialization routine here is named “he_” following the name of one of the authors Kaiming He [1]. In the code snippet below, **he_normal** is the implementation of initialization based on Gaussian distribution while **he_uniform** is the equivalent implementation of initialization based on Uniform distribution

```
def get_fans(shape):
    fan_in = shape[0] if len(shape) == 2 else np.prod(shape[
1:])
    fan_out = shape[1] if len(shape) == 2 else shape[0]
return fan_in, fan_out

def he_normal(shape, name=None):
    fan_in, fan_out = get_fans(shape)
    s = np.sqrt(2. / fan_in)
    return normal(shape, s, name=name)

def he_uniform(shape, name=None):
    fan_in, fan_out = get_fans(shape)
    s = np.sqrt(6. / fan_in)
return uniform(shape, s, name=name)
```

References

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