EE-559 – Deep learning

5.5. Parameter initialization

François Fleuret

https://fleuret.org/ee559/

Wed Aug 29 16:57:37 CEST 2018

idiap RESEARCH INSTITUTE

ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

Vanishing gradient

Consider the gradient estimation for a standard MLP:

Forward pass

$$\forall n,\ x^{(0)} = x, \quad \forall l = 1, \ldots, L, \begin{cases} s^{(l)} = w^{(l)} x^{(l-1)} + b^{(l)} \\ x^{(l)} = \sigma\left(s^{(l)}\right) \end{cases}$$

Consider the gradient estimation for a standard MLP:

Forward pass

$$\forall n,\ x^{(0)} = x, \quad \forall l = 1, \ldots, L, \ \begin{cases} s^{(l)} = w^{(l)} x^{(l-1)} + b^{(l)} \\ x^{(l)} = \sigma\left(s^{(l)}\right) \end{cases}$$

Backward pass

$$\begin{cases} \left[\frac{\partial \ell}{\partial x^{(L)}}\right] = \nabla_1 \ell\left(x^{(L)}\right) \\ \text{if } l < L, \left[\frac{\partial \ell}{\partial x^{(l)}}\right] = \left(w^{(l+1)}\right)^T \left[\frac{\partial \ell}{\partial s^{(l+1)}}\right] \end{cases}$$

$$\left[\frac{\partial \ell}{\partial s^{(l)}}\right] = \left[\frac{\partial \ell}{\partial x^{(l)}}\right] \odot \sigma'\left(s^{(l)}\right)$$

$$\left[\!\left[\frac{\partial \ell}{\partial w^{(l)}}\right]\!\right] = \left[\frac{\partial \ell}{\partial s^{(l)}}\right] \left(x^{(l-1)}\right)^T \qquad \left[\frac{\partial \ell}{\partial b^{(l)}}\right] = \left[\frac{\partial \ell}{\partial s^{(l)}}\right].$$

We have

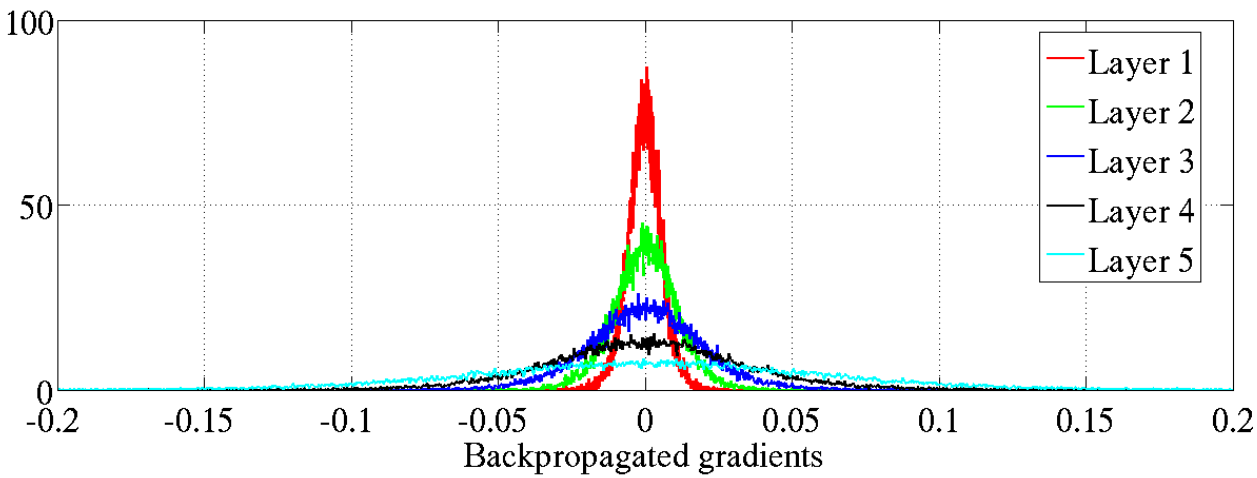
$$\left[\frac{\partial \ell}{\partial x^{(l)}}\right] = \left(w^{(l+1)}\right)^T \left(\sigma'\left(s^{(l)}\right) \odot \left[\frac{\partial \ell}{\partial x^{(l+1)}}\right]\right).$$

so the gradient "vanishes" exponentially with the depth if the ws are ill-conditioned or the activations are in the saturating domain of σ.

We have

$$\left[\frac{\partial \ell}{\partial x^{(l)}}\right] = \left(w^{(l+1)}\right)^T \left(\sigma'\left(s^{(l)}\right) \odot \left[\frac{\partial \ell}{\partial x^{(l+1)}}\right]\right).$$

so the gradient "vanishes" exponentially with the depth if the ws are ill-conditioned or the activations are in the saturating domain of σ.



(Glorot and Bengio, 2010)

Weight initialization

The analysis for the weight initialization relies on controlling

$$\mathbb{V}\left(\frac{\partial \ell}{\partial w_{i,j}^{(l)}}\right) \quad \text{and} \quad \mathbb{V}\left(\frac{\partial \ell}{\partial b_{i}^{(l)}}\right)$$

so that

- the gradient does not vanish, and
- weights evolve at the same rate across layers during training, and no layer reaches a saturation behavior before others.

If two variables X and Y are independent, the variance of their product is given by

We will use that, if A and B are independent

$$\mathbb{V}(AB) = \mathbb{V}(A)\,\mathbb{V}(B) + \mathbb{V}(A)\,\mathbb{E}(B)^2 + \mathbb{V}(B)\,\mathbb{E}(A)^2\,.$$

We will use that, if A and B are independent

$$\mathbb{V}(AB) = \mathbb{V}(A)\,\mathbb{V}(B) + \mathbb{V}(A)\,\mathbb{E}\,(B)^2 + \mathbb{V}(B)\,\mathbb{E}\,(A)^2\,.$$

Notation in the coming slides will drop indexes when variances are identical for all activations or parameters in a layer.

In a standard layer

$$x_i^{(l)} = \sigma\left(\sum_{j=1}^{N_{l-1}} w_{i,j}^{(l)} x_j^{(l-1)} + b_i^{(l)}\right)$$

where N_l is the number of units in layer l, and σ is the activation function.

In a standard layer

$$x_i^{(l)} = \sigma\left(\sum_{j=1}^{N_{l-1}} w_{i,j}^{(l)} x_j^{(l-1)} + b_i^{(l)}\right)$$

where N_l is the number of units in layer l, and σ is the activation function.

Assuming $\sigma'(0) = 1$, and we are in the linear regime

$$x_i^{(l)} \simeq \sum_{j=1}^{N_{l-1}} w_{i,j}^{(l)} x_j^{(l-1)} + b_i^{(l)}.$$

In a standard layer

$$x_i^{(l)} = \sigma\left(\sum_{j=1}^{N_{l-1}} w_{i,j}^{(l)} x_j^{(l-1)} + b_i^{(l)}\right)$$

where N_l is the number of units in layer l, and σ is the activation function.

Assuming $\sigma'(0) = 1$, and we are in the linear regime

linearization of local regime

$$x_i^{(l)} \simeq \sum_{j=1}^{N_{l-1}} w_{i,j}^{(l)} x_j^{(l-1)} + b_i^{(l)}.$$

From which, if both the $w^{(l)}$s and $x^{(l-1)}$s are centered Expectation is ZERO

$$\begin{aligned}\mathbb{V}\left(x_i^{(l)}\right) &\simeq \mathbb{V}\left(\sum_{j=1}^{N_{l-1}} w_{i,j}^{(l)} x_j^{(l-1)}\right) \\ &= \sum_{j=1}^{N_{l-1}} \mathbb{V}\left(w_{i,j}^{(l)}\right) \mathbb{V}\left(x_j^{(l-1)}\right)\end{aligned}$$

and if the $b^{(l)}$ are centered, so are the $x^{(l)}s$.

So if the $w_{i,j}^{(l)}$ are sampled i.i.d in each layer, and the $x_i^{(l)}$ have all the same variance for l fixed

$$\begin{aligned}\mathbb{V}\left(x^{(l)}\right) &\simeq \sum_{j=1}^{N_{l-1}} \mathbb{V}\left(w^{(l)}\right) \mathbb{V}\left(x^{(l-1)}\right) \\ &= N_{l-1} \mathbb{V}\left(w^{(l)}\right) \mathbb{V}\left(x^{(l-1)}\right).\end{aligned}$$

So if the $w_{i,j}^{(l)}$ are sampled i.i.d in each layer, and the $x_i^{(l)}$ have all the same variance for l fixed

$$\begin{aligned}\mathbb{V}\left(x^{(l)}\right) &\simeq \sum_{j=1}^{N_{l-1}} \mathbb{V}\left(w^{(l)}\right) \mathbb{V}\left(x^{(l-1)}\right) \\ &= N_{l-1} \mathbb{V}\left(w^{(l)}\right) \mathbb{V}\left(x^{(l-1)}\right).\end{aligned}$$

So **we have for the variance of the activations:**

$$\mathbb{V}\left(x^{(l)}\right) \simeq \mathbb{V}\left(x^{(0)}\right) \prod_{q=1}^{l} N_{q-1} \mathbb{V}\left(w^{(q)}\right).$$

1) var of the activations --> 1/fan_in

This leads to a first type of initialization

$$\mathbb{V}\left(w^{(l)}\right) = \frac{1}{N_{l-1}}.$$

This leads to a first type of initialization

$$\mathbb{V}\left(w^{(l)}\right) = \frac{1}{N_{l-1}}.$$

In `torch/nn/modules/linear.py`

```
def reset_parameters(self):
    stdv = 1. / math.sqrt(self.weight.size(1))
    self.weight.data.uniform_(-stdv, stdv)
    if self.bias is not None:
        self.bias.data.uniform_(-stdv, stdv)
```

There is a slight mistake here: the standard deviation of $\mathcal{U}[-\delta, \delta] = \sqrt{3}\delta$, hence a $\sqrt{3}$ is missing.

δ/sqrt(3)

We can look at the variance of the gradient wrt the activations. Since

$$\begin{aligned}\frac{\partial \ell}{\partial x_i^{(l)}} &= \sum_{h=1}^{N_{l+1}} \frac{\partial \ell}{\partial x_h^{(l+1)}} \frac{\partial x_h^{(l+1)}}{\partial x_i^{(l)}} \\ &\simeq \sum_{h=1}^{N_{l+1}} \frac{\partial \ell}{\partial x_h^{(l+1)}} w_{h,i}^{(l+1)}\end{aligned}$$

we get

$$\mathbb{V}\left(\frac{\partial \ell}{\partial x^{(l)}}\right) \simeq N_{l+1} \mathbb{V}\left(\frac{\partial \ell}{\partial x^{(l+1)}}\right) \mathbb{V}\left(w^{(l+1)}\right).$$

We can look at the variance of the gradient wrt the activations. Since

$$\begin{aligned}\frac{\partial \ell}{\partial x_i^{(l)}} &= \sum_{h=1}^{N_{l+1}} \frac{\partial \ell}{\partial x_h^{(l+1)}} \frac{\partial x_h^{(l+1)}}{\partial x_i^{(l)}} \\ &\simeq \sum_{h=1}^{N_{l+1}} \frac{\partial \ell}{\partial x_h^{(l+1)}} w_{h,i}^{(l+1)}\end{aligned}$$

we get

$$\mathbb{V}\left(\frac{\partial \ell}{\partial x^{(l)}}\right) \simeq N_{l+1} \mathbb{V}\left(\frac{\partial \ell}{\partial x^{(l+1)}}\right) \mathbb{V}\left(w^{(l+1)}\right).$$

So **we have for the variance of the gradient wrt the activations:**

$$\mathbb{V}\left(\frac{\partial \ell}{\partial x^{(l)}}\right) \simeq \mathbb{V}\left(\frac{\partial \ell}{\partial x^{(L)}}\right) \prod_{q=l+1}^{L} N_q \mathbb{V}\left(w^{(q)}\right).$$

2) var of the grad wrt activations --> 1/fan_out

Since

$$x_i^{(l)} \simeq \sum_{j=1}^{N_{l-1}} w_{i,j}^{(l)} x_j^{(l-1)} + b_i^{(l)}$$

we have

$$\begin{aligned} \frac{\partial \ell}{\partial w_{i,j}^{(l)}} &= \frac{\partial \ell}{\partial x_i^{(l)}} \frac{\partial x_i^{(l)}}{\partial w_{i,j}^{(l)}} \\ &\simeq \frac{\partial \ell}{\partial x_i^{(l)}} x_j^{(l-1)} \end{aligned}$$

Since

$$x_i^{(l)} \simeq \sum_{j=1}^{N_{l-1}} w_{i,j}^{(l)} x_j^{(l-1)} + b_i^{(l)}$$

we have

$$\begin{aligned}\frac{\partial \ell}{\partial w_{i,j}^{(l)}} &= \frac{\partial \ell}{\partial x_i^{(l)}} \frac{\partial x_i^{(l)}}{\partial w_{i,j}^{(l)}} \\ &\simeq \frac{\partial \ell}{\partial x_i^{(l)}} x_j^{(l-1)}\end{aligned}$$

and **we get the variance of the gradient wrt the weights**

$$\begin{aligned}\mathbb{V}\left(\frac{\partial \ell}{\partial w^{(l)}}\right) &\simeq \mathbb{V}\left(\frac{\partial \ell}{\partial x^{(l)}}\right) \mathbb{V}\left(x^{(l-1)}\right) \\ &= \mathbb{V}\left(\frac{\partial \ell}{\partial x^{(L)}}\right) \left(\prod_{q=l+1}^{L} N_q \mathbb{V}\left(w^{(q)}\right)\right) \mathbb{V}\left(x^{(0)}\right) \left(\prod_{q=1}^{l} N_{q-1} \mathbb{V}\left(w^{(q)}\right)\right) \\ &= \frac{N_0}{N_l} \left(\prod_{q=1}^{L} N_q \mathbb{V}\left(w^{(q)}\right)\right) \mathbb{V}\left(x^{(0)}\right) \mathbb{V}\left(\frac{\partial \ell}{\partial x^{(L)}}\right).\end{aligned}$$

3) var of the grad wrt weights --> 1/fan_out

Similarly, since

$$x_i^{(l)} \simeq \sum_{j=1}^{N_{l-1}} w_{i,j}^{(l)} x_j^{(l-1)} + b_i^{(l)}$$

we have

$$\begin{aligned} \frac{\partial \ell}{\partial b_i^{(l)}} &= \frac{\partial \ell}{\partial x_i^{(l)}} \frac{\partial x_i^{(l)}}{\partial b_i^{(l)}} \\ &\simeq \frac{\partial \ell}{\partial x_i^{(l)}} \end{aligned}$$

Similarly, since

$$x_i^{(l)} \simeq \sum_{j=1}^{N_{l-1}} w_{i,j}^{(l)} x_j^{(l-1)} + b_i^{(l)}$$

we have

$$\begin{aligned} \frac{\partial \ell}{\partial b_i^{(l)}} &= \frac{\partial \ell}{\partial x_i^{(l)}} \frac{\partial x_i^{(l)}}{\partial b_i^{(l)}} \\ &\simeq \frac{\partial \ell}{\partial x_i^{(l)}} \end{aligned}$$

so **we get the variance of the gradient wrt the biases**

$$\mathbb{V}\left(\frac{\partial \ell}{\partial b^{(l)}}\right) \simeq \mathbb{V}\left(\frac{\partial \ell}{\partial x^{(l)}}\right).$$

So finally, there is nothing we can do to control the variance of the gradient wrt the weights.

To control the variance of activations, we need

$$\mathbb{V}\left(w^{(l)}\right) = \frac{1}{N_{l-1}},$$

and to control the variance of the gradient wrt activations, and through it the variance of the gradient wrt the biases

$$\mathbb{V}\left(w^{(l)}\right) = \frac{1}{N_l}.$$

So finally, there is nothing we can do to control the variance of the gradient wrt the weights.

To control the variance of activations, we need

$$\mathbb{V}\left(w^{(l)}\right) = \frac{1}{N_{l-1}},$$

and to control the variance of the gradient wrt activations, and through it the variance of the gradient wrt the biases

$$\mathbb{V}\left(w^{(l)}\right) = \frac{1}{N_l}.$$

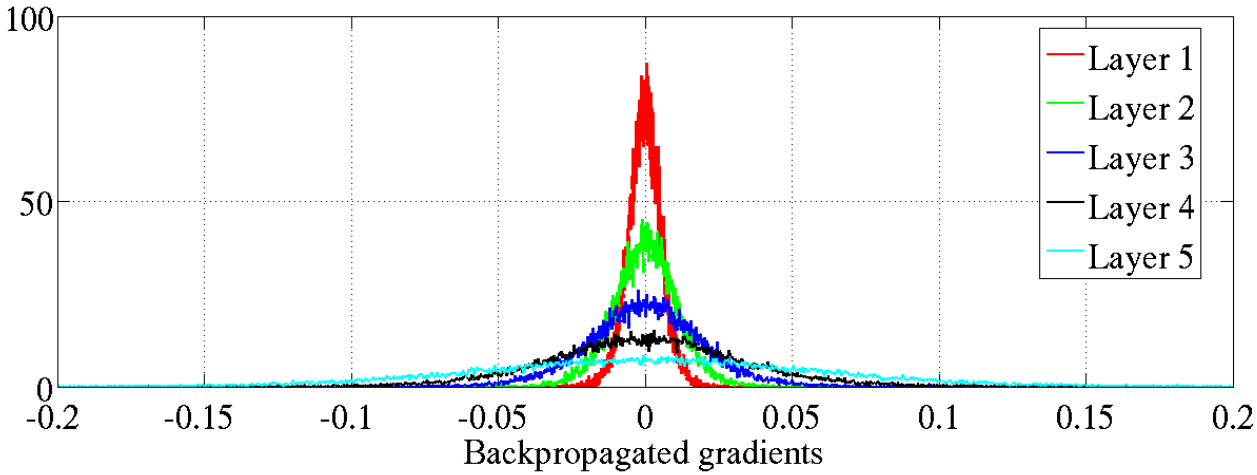
From which we get as a compromise the "Xavier initialization"

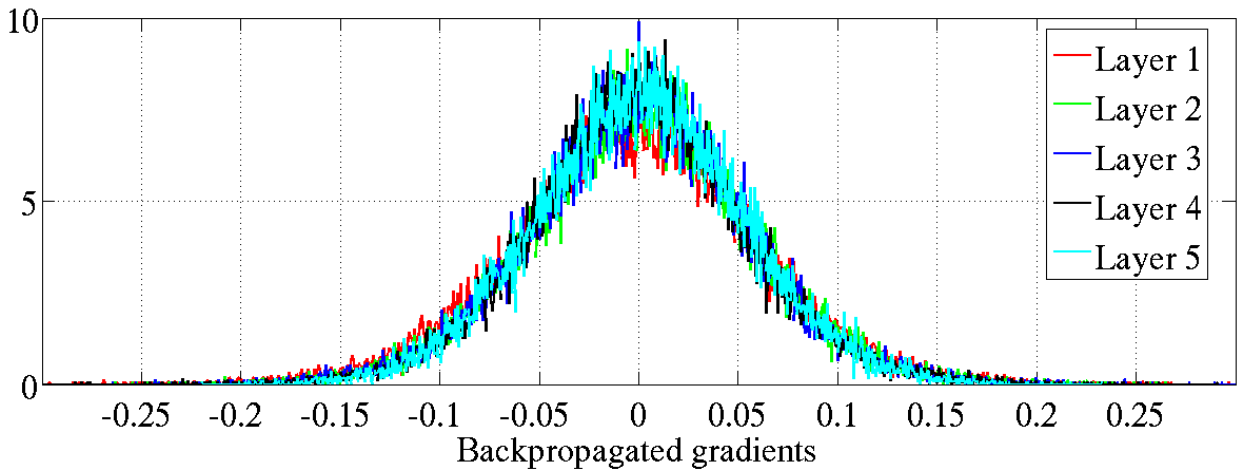
$$\mathbb{V}\left(w^{(l)}\right) = \frac{1}{\frac{N_{l-1}+N_l}{2}} = \frac{2}{N_{l-1}+N_l}.$$

(Glorot and Bengio, 2010)

In `torch/nn/init.py`

```
def xavier_normal_(tensor, gain = 1):
    fan_in, fan_out = _calculate_fan_in_and_fan_out(tensor)
    std = gain * math.sqrt(2.0 / (fan_in + fan_out))
    with torch.no_grad():
        return tensor.normal_(0, std)
```





(Glorot and Bengio, 2010)

The weights can also be scaled to account for the activation functions.

Remember that we have

$$\begin{aligned}\mathbb{V}(AB) &= \mathbb{V}(A)\,\mathbb{V}(B) + \mathbb{V}(A)\,\mathbb{E}(B)^2 + \mathbb{V}(B)\,\mathbb{E}(A)^2 \\ &= \mathbb{V}(A)\,\mathbb{E}\left(B^2\right) + \mathbb{V}(B)\,\mathbb{E}(A)^2\,.\end{aligned}$$

For the forward pass, if

$$s_i^{(l)} = \sum_{j=1}^{N_{l-1}} w_{i,j}^{(l)} \sigma\left(s_j^{(l-1)}\right) + b_i^{(l)}$$
$$x_i^{(l)} = \sigma\left(s_i^{(l)}\right),$$

and $\mathbb{E}\left(w^{(l)}\right) = 0$, $s^{(l-1)}$ is symmetric, and σ is ReLU, we have

$$\begin{aligned}
\mathbb{V}\left(s_i^{(l)}\right) &= N_{l-1}\mathbb{V}\left(w^{(l)}\sigma\left(s^{(l-1)}\right)\right) \\
&= N_{l-1}\mathbb{V}\left(w^{(l)}\right)\mathbb{E}\left(\sigma\left(s^{(l-1)}\right)^2\right) \\
&= N_{l-1}\mathbb{V}\left(w^{(l)}\right)\frac{1}{2}\mathbb{E}\left(\left(s^{(l-1)}\right)^2\right) \\
&= \frac{1}{2}N_{l-1}\mathbb{V}\left(w^{(l)}\right)\mathbb{V}\left(s^{(l-1)}\right).
\end{aligned}$$

1) var of the weighted sum --> 2/fan_in

For the backward

$$\mathbb{V}\left(\frac{\partial \ell}{\partial x_i^{(l)}}\right) = \sum_{h=1}^{N_{l+1}} \mathbb{V}\Big(\underbrace{\sigma'\left(s_h^{(l+1)}\right)}_{0/1} \underbrace{\frac{\partial \ell}{\partial x_h^{(l+1)}} w_{h,i}^{(l+1)}}_{\mathbb{E}(.)=0, \text{ symmetric}} \Big)$$

$$= \sum_{h=1}^{N_{l+1}} \mathbb{E}\left(\sigma'\left(s_h^{(l+1)}\right)\left(\frac{\partial \ell}{\partial x_h^{(l+1)}} w_{h,i}^{(l+1)}\right)^2\right)$$

$$= \sum_{h=1}^{N_{l+1}} \frac{1}{2}\mathbb{E}\left(\left(\frac{\partial \ell}{\partial x_h^{(l+1)}} w_{h,i}^{(l+1)}\right)^2\right)$$

$$= \frac{1}{2}\sum_{h=1}^{N_{l+1}} \mathbb{V}\left(\frac{\partial \ell}{\partial x_h^{(l+1)}}\right)\mathbb{V}\left(w_{h,i}^{(l+1)}\right).$$

2) var of the grad wrt activation --> 2/fan_in

So ReLU impacts the forward and backward pass as if the weights had half their variances, which motivates multiplying them by a corrective gain of $\sqrt{2}$.

(He et al., 2015)

So ReLU impacts the forward and backward pass as if the weights had half their variances, which motivates multiplying them by a corrective gain of $\sqrt{2}$.

Var(w_l) = 2 / (N_l-1)
similar to first type initialization (He et al., 2015)
apart from factor 2

The same type of reasoning can be applied to other activation functions.

In `torch/nn/init.py`

```
def calculate_gain(nonlinearity, param=None):

    linear_fns = ['linear', 'conv1d', 'conv2d', 'conv3d',
                  'conv_transpose1d', 'conv_transpose2d', 'conv_transpose3d']
    if nonlinearity in linear_fns or nonlinearity == 'sigmoid':
        return 1
    elif nonlinearity == 'tanh':
        return 5.0 / 3
    elif nonlinearity == 'relu':
        return math.sqrt(2.0)
    /.../
```

Data normalization

The analysis for the weight initialization relies on keeping the activation variance constant.

For this to be true, not only the variance has to remained unchanged through layers, but it has to be correct for the input too.

$$\mathbb{V}\left(x^{(0)}\right) = 1.$$

The analysis for the weight initialization relies on keeping the activation variance constant.

For this to be true, not only the variance has to remained unchanged through layers, but it has to be correct for the input too.

$$\mathbb{V}\left(x^{(0)}\right) = 1.$$

This can be done in several ways. Under the assumption that all the input components share the same statistics, we can do

```
mu, std = train_input.mean(), train_input.std()
train_input.sub_(mu).div_(std)
test_input.sub_(mu).div_(std)
```

The analysis for the weight initialization relies on keeping the activation variance constant.

For this to be true, not only the variance has to remained unchanged through layers, but it has to be correct for the input too.

$$\mathbb{V}\left(x^{(0)}\right) = 1.$$

This can be done in several ways. Under the assumption that all the input components share the same statistics, we can do

```
mu, std = train_input.mean(), train_input.std()
train_input.sub_(mu).div_(std)
test_input.sub_(mu).div_(std)
```

Thanks to the magic of broadcasting we can normalize component-wise with

```
mu, std = train_input.mean(0), train_input.std(0)
train_input.sub_(mu).div_(std)
test_input.sub_(mu).div_(std)
```

To go one step further, some techniques initialize the weights explicitly so that the empirical moments of the activations are as desired.

As such, they take into account the statistics of the network activation induced by the statistics of the data.

The end

References

X. Glorot and Y. Bengio. Understanding the difficulty of training deep feedforward neural networks. In *International Conference on Artificial Intelligence and Statistics (AISTATS)*, 2010.

K. He, X. Zhang, S. Ren, and J. Sun. Delving deep into rectifiers: Surpassing human-level performance on imagenet classification. *CoRR*, abs/1502.01852, 2015.