Deep learning

5.5. Parameter initialization

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Consider the gradient estimation for a standard MLP, as seen in 3.6. “Back-propagation”:

**Forward pass**
\[
x^{(l)} = x, \quad \forall l = 1, \ldots, L, \quad \left\{ \begin{array}{l}
s^{(l)} = w^{(l)} x^{(l-1)} + b^{(l)} \\
x^{(l)} = \sigma(s^{(l)})
\end{array} \right.
\]

**Backward pass**
\[
\begin{align*}
\frac{\partial l}{\partial x^{(L)}} & \quad \text{from the definition of } \ell \\
\text{if } l < L, & \quad \left[ \frac{\partial \ell}{\partial x^{(l)}} \right] = \left( w^{(l+1)} \right)^T \left[ \frac{\partial \ell}{\partial s^{(l+1)}} \right] \\
\left[ \frac{\partial \ell}{\partial w^{(l)}} \right] & = \left[ \frac{\partial \ell}{\partial s^{(l)}} \right] \left( x^{(l-1)} \right)^T \\
\left[ \frac{\partial \ell}{\partial b^{(l)}} \right] & = \left[ \frac{\partial \ell}{\partial s^{(l)}} \right].
\end{align*}
\]
We have
\[
\frac{\partial \ell}{\partial x^{(l)}} = (w^{(l+1)})^T \left( \sigma'(s^{(l)}) \odot \left( \frac{\partial \ell}{\partial x^{(l+1)}} \right) \right).
\]
so the gradient “vanishes” exponentially with the depth if the \(w\)s are ill-conditioned or the activations are in the saturating domain of \(\sigma\).

(Glorot and Bengio, 2010)

Notes

In the process of back-propagation, the norm of the gradient can explode or vanish for two reasons:

- It gets multiplied again and again by the weights \(w^{(l+1)}\). If the weight matrix is ill-conditioned, the gradient may vanish or explode exponentially, and

- It gets multiplied by the derivative of the non-linearity: in the flat regime of a tanh for instance, the gradient of \(\sigma\) is close to zero.

The plot taken from Glorot and Bengio (2010) shows the distribution of the gradient in different layers.

- In layer 5 (next to the output of the network, cyan curve), the gradient is spread out, and the distribution of the norm of the gradient takes large values.

- The more we go back in the initial layers, the norm of the gradient becomes smaller and smaller: here, this is the vanishing gradient effect.

What follows aims at carefully selecting \(w^{(l)}\) at initialization to avoid this effect and not to pay an exponential price during the backward pass.
Weight initialization
The design of the weight initialization aims at controlling

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

so that weights evolve at the same rate across layers during training, and no layer reaches a saturation behavior before others.
We will use that, if $A$ and $B$ are independent

$$V(AB) = V(A) V(B) + V(A) E(B)^2 + V(B) E(A)^2.$$  

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

**Notes**

By using the fact that $V(X) = E(X^2) - E(X)^2$, 

$$V(AB) = E(A^2B^2) - E(AB)^2$$

$$= E(A^2) E(B^2) - E(AB)^2$$

$$= (V(A) + E(A)^2) (V(B) + E(B)^2) - E(A)^2 E(B)^2$$

$$= V(A) V(B) + V(A) E(B)^2 + V(B) E(A)^2$$

In particular, when both $A$ and $B$ are centered, we have $V(AB) = V(A) V(B)$
In a standard layer

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

where \( N_l \) is the number of units in layer \( l \), and \( \sigma \) is the activation function.

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

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

From which, if both the \( w^{(l)} \)s and \( x^{(l-1)} \)s are centered, and biases set to zero:

\[
\mathbb{V} \left( x_j^{(l)} \right) \simeq \mathbb{V} \left( \sum_{j=1}^{N_{l-1}} w_{i,j}^{(l)} x_j^{(l-1)} \right) \\
= \sum_{j=1}^{N_{l-1}} \mathbb{V} \left( w_{i,j}^{(l)} \right) \mathbb{V} \left( x_j^{(l-1)} \right)
\]

and the \( x^{(l)} \)s are centered.
So if the $w_{i,j}$ are sampled i.i.d in each layer, and all the activations have same variance, then

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

$$= N_{l-1} V(w^{(l)}) V(x^{(l-1)}) .$$

So we have for the variance of the activations:

$$V(x^{(l)}) \simeq V(x^{(0)}) \prod_{q=1}^{l} N_{q-1} V(w^{(q)}) ,$$

which leads to a first type of initialization to ensure

$$V(w^{(l)}) = \frac{1}{N_{l-1}} .$$
The standard PyTorch weight initialization for a linear layer

\[ f : \mathbb{R}^N \rightarrow \mathbb{R}^M \]

is

\[ w_{i,j} \sim \mathcal{U} \left[ -\frac{1}{\sqrt{N}}, \frac{1}{\sqrt{N}} \right] \]

hence

\[ \mathbb{V}(w) = \frac{1}{3N}. \]

```python
>>> f = nn.Linear(5, 100000)
>>> f.weight.mean()
tensor(0.0007, grad_fn=<MeanBackward0>)
>>> f.weight.var()
tensor(0.0667, grad_fn=<VarBackward0>)
>>> torch.empty(1000000).uniform_(-1/math.sqrt(5), 1/math.sqrt(5)).var()
tensor(0.0667)
>>> 1./15.
0.06666666666666667
```

**Notes**

This first type of initialization compensates the increase of the variance due to the number of input units by dividing the weights by the square root of the number.
We can look at the variance of the gradient w.r.t. the activations. Since

\[
\frac{\partial \ell}{\partial x_i^{(l)}} \simeq \sum_{h=1}^{N_{l+1}} \frac{\partial \ell}{\partial x_h^{(l+1)}} w_{h,i}^{(l+1)}
\]

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 w.r.t. the activations:

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

Notes

The analysis is the same as for the forward pass, but now what matters is the number of units in the next layer.
Since
\[ x_i^{(l)} \simeq \sum_{j=1}^{N_{l-1}} w_{i,j}^{(l)} x_j^{(l-1)} + b_i^{(l)} \]
we have
\[ \frac{\partial \ell}{\partial w_{i,j}^{(l)}} \simeq \frac{\partial \ell}{\partial x_i^{(l-1)}} x_j^{(l-1)} \]
and we get the variance of the gradient w.r.t. the weights
\[
V \left( \frac{\partial \ell}{\partial w^{(l)}} \right) \simeq V \left( \frac{\partial \ell}{\partial x^{(l)}} \right) V \left( x^{(l-1)} \right)
= V \left( \frac{\partial \ell}{\partial x^{(L)}} \right) \left( \prod_{q=l+1}^{L} N_q V \left( w^{(q)} \right) \right) V \left( x^{(0)} \right) \left( \prod_{q=1}^{L} N_{q-1} V \left( w^{(q)} \right) \right)
= \frac{N_0}{N_l} \left( \prod_{q=1}^{L} N_q V \left( w^{(q)} \right) \right) V \left( x^{(0)} \right) V \left( \frac{\partial \ell}{\partial x^{(L)}} \right).
\]

Notes

Since

- the [variance of the] activations in layer $l$ is proportional to the product of the [variance of the] weights of the layers before,
- the [variance of the] gradient is proportional to the product of the [variance of the] weights in the layers after, and
- the [variance of the] derivative of the loss w.r.t. the weights is the product of the two,

we have this interesting result that the [variance of the] derivative of the loss w.r.t. the weights at layer $l$ does not depend exponentially on the layer (it only depend on $N_l$ alone).
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
\[ \frac{\partial \ell}{\partial b_i^{(l)}} \simeq \frac{\partial \ell}{\partial x_i^{(l)}} \]
so we get the variance of the gradient w.r.t. the biases
\[ \mathbb{V}\left( \frac{\partial \ell}{\partial b_i^{(l)}} \right) \simeq \mathbb{V}\left( \frac{\partial \ell}{\partial x_i^{(l)}} \right) . \]
So the variance of the gradient w.r.t. the weights is the same in all layers.

To control the variance of activations, we need

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

and to control the variance of the gradient w.r.t. activations, and through it the variance of the gradient w.r.t. the biases

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

From which we get as a compromise the “Xavier initialization”

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

(Glorot and Bengio, 2010)

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**Notes**

To summarize, the constrains to initialize the weights are the following:

- In the forward pass, the number of input dimensions matters to control the variance of the activations,
- In the backward pass, the number of output dimensions matters to control the variance of the gradient w.r.t. the biases.

Since we cannot have both together, we average the two.
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)
4.2.2 Gradient Propagation Study

To empirically validate the above theoretical ideas, we have plotted some normalized histograms of activation values, as well as activation values normalized histograms with hyperbolic tangent activation, with standard (top) vs normalized (bottom) initialization. Top: 0-peak increases for layer 1, whereas with the standard initialization, this ratio is 5, whereas with the normalized initialization, this ratio is 8.

The results displayed (Figures 6, 7 and 8) are from experiments on one hundred thousand Shapeset examples and obtained with the other datasets. As first noted by Bradley (2009), we observe (Figure 7) that the variance of the weight gradients is roughly constant across layers, as shown on Figure 8. However, this variance does not remain constant during training (here for a tanh network). Indeed, as can be seen by comparing the evolution of activations with the tanh networks with normalized initialization, the variance of the back-propagated gradients becomes smaller (standard initialization), the variance of the weights gradients is roughly increasing back-propagated gradients (bottom of Figure 7).

Using our normalized initialization we do not see such decrease anymore independent of the activation values and the linearity hypothesis is also violated. This trend is reversed very quickly during learning. The advantages of the normalized initialization, since having smaller variance, they diverge from each other (with larger gradients in the lower layers) as training progresses, especially with tanh networks with normalized initialization. However, this trend is reversed very quickly during learning. The variance of the back-propagated gradients becomes smaller (standard initialization). Note that this might be one of the reasons why these observations on the back-propagated gradients of very different magnitudes at different layers is explained by our theoretical analysis above (eq. 14). In particular, we cannot use simple variance calculations anymore.

The final consideration that we care for is the success of training with different strategies, and this is best illustrated with error curves showing the evolution of test error as training progresses and asymptotes. Figure 11 shows such curves with online training on ImageNet. As a baseline, we optimized RBF SVM model (Glorot and Bengio, 2010)

Notes

The second graph shows that with a proper initialization, the distribution of the norm of the gradient is very similar across layers.
The weights can also be scaled to account for the activation functions.

Remember that if $A$ and $B$ are independent, we have

$$V(AB) = V(A)V(B) + V(A)E(B)^2 + V(B)E(A)^2$$

hence

$$V(AB) = V(A)\left(V(B) + E(B)^2\right) + V(B)E(A)^2$$

$$= V(A)E(B^2) + V(B)E(A)^2.$$
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 \( E \left( w^{(l)} \right) = 0, s^{(l-1)} \) is symmetric, and \( \sigma \) is ReLU, we have
\[
V \left( s_i^{(l)} \right) = N_{l-1} V \left( w^{(l)} \sigma \left( s^{(l-1)} \right) \right) \\
= N_{l-1} V \left( w^{(l)} \right) E \left( \sigma \left( s^{(l-1)} \right)^2 \right) \\
= N_{l-1} V \left( w^{(l)} \right) \frac{1}{2} E \left( \left( s^{(l-1)} \right)^2 \right) \\
= \frac{1}{2} N_{l-1} V \left( w^{(l)} \right) V \left( s^{(l-1)} \right). 
\]

Notes

\[ \ldots \xrightarrow{\sigma} x^{(l-1)} \xrightarrow{w^{(l)}, b^{(l)}} s^{(l)} \xrightarrow{\sigma} x^{(l)} \xrightarrow{w^{(l+1)}, b^{(l+1)}} s^{(l+1)} \xrightarrow{\sigma} \ldots \]

In the derivation above, since \( w^{(l)} \) and \( s^{(l-1)} \) are independent, we have
\[ V \left( w^{(l)} \sigma \left( s^{(l-1)} \right) \right) = V \left( w^{(l)} \right) V \left( \sigma \left( s^{(l-1)} \right) \right) \]

With the result of the previous slide applied to \( A = w^{(l)} \) and \( B = \sigma \left( s^{(l-1)} \right) \), we have
\[
V \left( w^{(l)} \sigma \left( s^{(l-1)} \right) \right) = V \left( w^{(l)} \right) E \left( \sigma \left( s^{(l-1)} \right)^2 \right) + V \left( \sigma \left( s^{(l-1)} \right) \right) E \left( w^{(l)} \right)^2 \\
= V \left( w^{(l)} \right) E \left( \sigma \left( s^{(l-1)} \right)^2 \right) 
\]

And finally, under the assumption that \( s^{(l-1)} \) and \( -s^{(l-1)} \) are identically distributed, we have
\[ E \left( \sigma \left( s^{(l-1)} \right)^2 \right) = \frac{1}{2} E \left( \left( s^{(l-1)} \right)^2 \right). \]
For the backward

\[ V \left( \frac{\partial \ell}{\partial x_i^{(l)}} \right) = \sum_{h=1}^{N_{l+1}} V(\sigma' \left( s_h^{(l+1)} \right)) \frac{\partial \ell}{\partial x_h^{(l+1)}} w_{h,i}^{(l+1)} \]

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

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

\[ = \frac{1}{2} \sum_{h=1}^{N_{l+1}} \frac{\partial \ell}{\partial x_h^{(l+1)}} \frac{\partial \ell}{\partial x_h^{(l+1)}} w_{h,i}^{(l+1)} \]
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)

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

In `torch/nn/init.py`

```python
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.

\[ \mathbb{V}(x^{(0)}) = 1. \]

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

```python
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

```python
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.
References
