

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

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

Backward pass

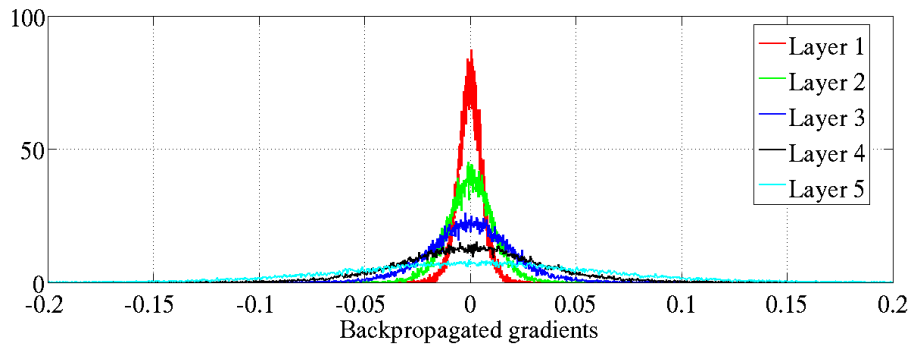
$$\begin{cases} \left[\frac{\partial \ell}{\partial x^{(L)}} \right] \text{ from the definition of } \ell & \left[\frac{\partial \ell}{\partial s^{(l)}} \right] = \left[\frac{\partial \ell}{\partial x^{(l)}} \right] \odot \sigma'(s^{(l)}) \\ \text{if } l < L, \left[\frac{\partial \ell}{\partial x^{(l)}} \right] = (w^{(l+1)})^\top \left[\frac{\partial \ell}{\partial s^{(l+1)}} \right] \end{cases}$$

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

We have

$$\left[\frac{\partial \ell}{\partial \mathbf{x}^{(l)}} \right] = \left(\mathbf{w}^{(l+1)} \right)^\top \left(\sigma'(\mathbf{s}^{(l)}) \odot \left[\frac{\partial \ell}{\partial \mathbf{x}^{(l+1)}} \right] \right).$$

so the gradient “vanishes” exponentially with the depth if the \mathbf{w} s are ill-conditioned or the activations are in the saturating domain of σ .



(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 $\mathbf{w}^{(l+1)}$. 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 σ 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 $\mathbf{w}^{(l)}$ 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

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

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

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

So in particular, if $\mathbb{E}(A) = \mathbb{E}(B) = 0$, then $\mathbb{V}(AB) = \mathbb{V}(A)\mathbb{V}(B)$.

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 $\mathbb{V}(X) = \mathbb{E}(X^2) - \mathbb{E}(X)^2$,

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

In particular, when both A and B are centered, we have $\mathbb{V}(AB) = \mathbb{V}(A) \mathbb{V}(B)$

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

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

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

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

and the $x^{(l)}$ s are centered.

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

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

So we have for the variance of the activations:

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

which leads to a first type of initialization to ensure

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

We can look at the variance of the activations when going through a series of linear layers of various size with a normal weight initialization.

```
s = [ 5, 50, 100, 25, 5 ]
x = torch.randn(1000, s[0])
for n in s[1:]:
    w = torch.randn(x.size(1), n)
    x = x @ w
    print(x.mean(), x.var())
```

prints

```
tensor(0.0045) tensor(5.0118)
tensor(0.0305) tensor(268.1688)
tensor(-0.3304) tensor(22855.8164)
tensor(2.4529) tensor(588037.5625)
```

And the same if we scale the weights in $\frac{1}{\sqrt{N_l-1}}$.

```
s = [ 5, 50, 100, 25, 5 ]
x = torch.randn(1000, s[0])
for n in s[1:]:
    w = torch.randn(x.size(1), n) / math.sqrt(x.size(1))
    x = x @ w
    print(x.mean(), x.var())
```

prints

```
tensor(0.0113) tensor(1.0412)
tensor(3.4459e-05) tensor(1.0622)
tensor(0.0123) tensor(1.1627)
tensor(0.0095) tensor(1.2369)
```

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

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

```
>>> 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:

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

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

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

and we get the variance of the gradient w.r.t. the weights

$$\begin{aligned} \mathbb{V}\left(\frac{\partial \ell}{\partial w^{(l)}}\right) &\simeq \mathbb{V}\left(\frac{\partial \ell}{\partial x^{(l)}}\right) \mathbb{V}\left(x^{(l-1)}\right) \\ &= \mathbb{V}\left(\frac{\partial \ell}{\partial x^{(L)}}\right) \left(\prod_{q=l+1}^L N_q \mathbb{V}\left(w^{(q)}\right)\right) \mathbb{V}\left(x^{(0)}\right) \left(\prod_{q=1}^l N_{q-1} \mathbb{V}\left(w^{(q)}\right)\right) \\ &= \frac{1}{N_l} N_0 \underbrace{\left(\prod_{q=1}^L N_q \mathbb{V}\left(w^{(q)}\right)\right)}_{\text{Does not depend on } l} \mathbb{V}\left(x^{(0)}\right) \mathbb{V}\left(\frac{\partial \ell}{\partial x^{(L)}}\right). \end{aligned}$$

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

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

Finally:

1. there is no exponential behavior to mitigate for the gradients w.r.t. weights,
2. to control the variance of activations (e.g. avoid the saturating part of the non-linearities), we need

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

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

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

The “Xavier initialization” is a compromise

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

(Glorot and Bengio, 2010)

Notes

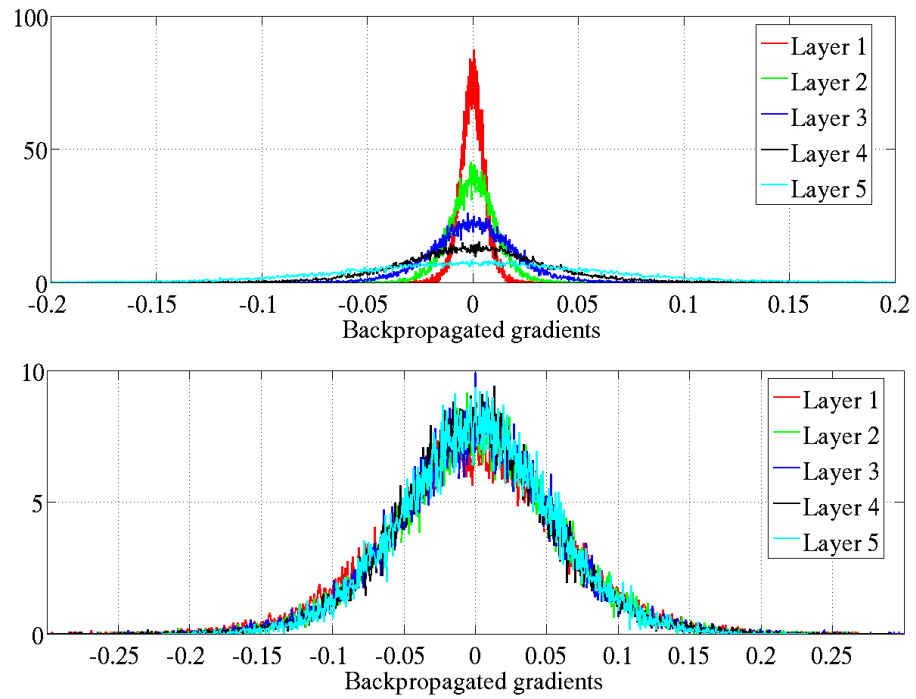
To summarize, the constraints to initialize the weights are the following:

- 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)
```

(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. E.g. ReLU impacts the forward and backward pass as if the weights had half their variances, which motivates multiplying them by $\sqrt{2}$ (He et al., 2015).

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.

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

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.

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.