5. Weight Initialization

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Today's Goal

- In this time, we will focus on the various initializing methods.
- And we will look at the characteristics of each method through a formula and a picture.

Importance of initialization

- We obtain the appropriate W (often called the parameter matrix) from training a model in MLP, CNN, RNN, etc.
- Because of the large number of parameters, we can't set all of them individually.
- So many people start thinking about various methods how to simply initialize the parameters.

Importance of initialization

- If all of the initial values are 0, there is no learning of the parameters.
- Plus, if the same initial value is used, the correct improvement is not made because the input values are learned by the same ratio.
- Also, even if all of the initial values follow the proper distribution, you
 may not get the desired result as shown in the figures below.

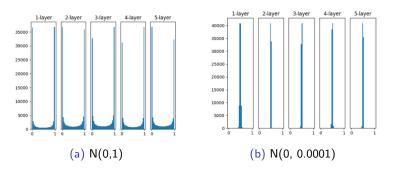


Figure 1: Initial Values Following Normal Distribution

Importance of initialization

- The result of Figure 1 is the distribution of $Y = \sigma(XW + b)$. after each hidden layer.
- Each notation follows:
 - 1 Y is an output.
 - \circ $\sigma(\cdot)$ is a sigmoid function.
 - X is an input.
 - W is a parameter matrix which is initialized.
 - **5** b is a bias term which is initialized with 0.
- Since the intercept term is an added value, it can be initialized to 0.
- The (a) of Figure 1 has eventually gradient vanishing because of being distributed many 0 and 1 values.
- The (b) of Figure 1 does not happen gradient vanishing, but loses the advantage of using nodes a lot.

- Restricted Boltzmann Machine(RBM)[3] is a generative stochastic artificial neural network proposed by Professor Hinton in 2006.
- It is mainly used to determine the initial value and works like unsupervised learning.
- As it is complicated, RBM is not used well these days.

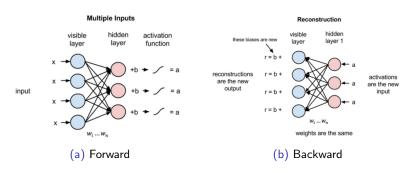


Figure 2: RBM

- "Restricted" means no connection between nodes in each layer.
- Also, calculate W by training until the difference between the input and the result of Figure 2 (a) and (b) is small.
- And last, if you stack multiple RBM, you get Deep Boltzmann Machine(DBM).
- On a lighter note, Deep Belief Network(DBN) is made with the initial values of DBM.

• The DBM can be seen in the figure below.

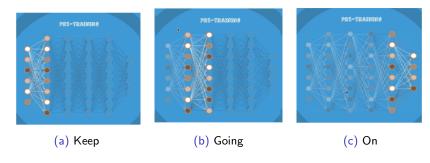


Figure 3: DBM

- ullet Finally, you can use the W, parameter matrix, obtained in this way as the initial value for the training model.
- This initial values assignment is also called 'Fine Tuning'.

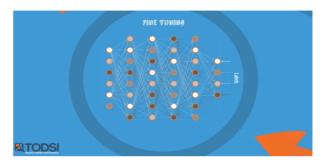


Figure 4: Fine Tuning

2. Simple Uniform Initialization

 Very simply, you can give the initial values to follow the uniform distribution.

$$W$$
's elements $\sim U(-0.5, 0.5)$

- Absolutely, it is not used nowadays.
- Note that W is a parameter matrix.

3. LeCun Initialization

- Also known as the founder of the LeNet and the father of CNN, Yann LeCun suggests giving the following initial values:
- LeCun method[5] have not be used well recently since ReLU came out.
 - LeCun Normal Initialization

$$W$$
's elements $\sim N(0, \sigma^2)$, $\sigma = \sqrt{\frac{1}{n_{in}}}$

LeCun Uniform Initialization

$$W$$
's elements $\sim U(-a,a)$, $a=\sqrt{\frac{3}{n_{in}}}$

• Note that n_{in} is the number of previous layer nodes.

3. LeCun Initialization

Pf)

- Let n=number of input nodes , x=input, Y=output, w=weight. (w, x, Y : R.V. & independent each other)
- And, let's not consider the activation function. Then,

$$Y = w_1x_1 + w_2x_2 + \cdots + w_nx_n$$

Thus, variance of Y is:

$$Var[Y] = Var\left[\sum_{i=1}^{n} w_i x_i\right]$$

$$= n \left[E[x_i]^2 Var[w_i] + E[w_i]^2 Var[x_i] + Var[w_i] Var[x_i]\right]$$

3. LeCun Initialization

Pf)

• Let the mean of x and w be 0. Then,

$$Var[Y] = nVar[w_i]Var[x_i]$$

- Therefore, in order to maintain the variance of x and Y, the variance of w_i must be $\frac{1}{n}$.
- In the end, the appropriate initialization values for normal and uniform distributions are set.
- And activation function can be considered as the variance approximation of the function using the delta method.
 - $> Var[f(X)] \simeq (f'(E[X]))^2 Var(X)$

4. Xavier(Glorot) Initialization

- It is the initialization method that Xavier Glorot first proposed in 2010[1].
- It is still widely used as an initialization method unless otherwise specified.
 - Xavier Normal Initialization

$$W$$
's elements $\sim N(0,\sigma^2)$, $\sigma = \sqrt{\frac{1}{(n_{in} + n_{out})/2}}$

2 Xavier Uniform Initialization

$$W$$
's elements $\sim U(-a,a)$, $a=\sqrt{\frac{3}{(n_{in}+n_{out})/2}}$

- n_{in} : the number of previous layer nodes.
- n_{out}: the number of next layer nodes.

4. Xavier(Glorot) Initialization

• Xavier(or Glorot) initialization is effective when using tanh or sigmoid as an activation function.

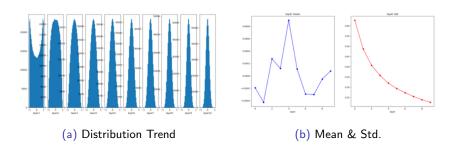


Figure 5: Xavier with Sigmoid

4. Xavier(Glorot) Initialization

- However, it is not effective when using ReLU as an activation function.
- So we use the He initialization, which will be explained in the next slide.

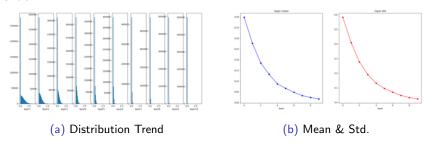


Figure 6: Xavier with ReLU

- It is the initialization method that Kaiming He first proposed in 2015[2].
- He initialization is used a lot in the CNN models with ReLU.
 - He Normal Initialization

$$W$$
's elements $\sim N(0, \sigma^2)$, $\sigma = \sqrt{\frac{2}{n_{in}}}$

4 He Uniform Initialization

$$W$$
's elements $\sim U(-a,a)$, $a=\sqrt{\frac{2\times 3}{n_{in}}}$

- n_{in} : the number of previous layer nodes.
- n_{out}: the number of next layer nodes.

- The difference from Xavier initialization is that the output node is not taken into account and the variance of the initial value is doubled.
- The reason for doubling the variance comes from a simple statistical calculation that takes into account the form of Y = max(0, x).

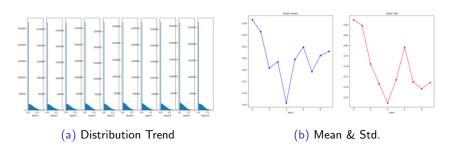


Figure 7: He with ReLU

Showing)

- Let x=output before applying activation function, Y=final output. (Y = max(0, x), i.e. Y = x+ReLU)
- Also, x, Y: R.V. & independent each other.
- And let's look at the relationship between Y's variance and x's variance.
- Thus, variance of Y is:

$$V[Y] = V[X \cdot I(X > 0)]$$

= $V[X] + V[X \cdot I(X \le 0)] - 2Cov[X, X \cdot I(X \le 0)]$
= $V[X] - V[X \cdot I(X \le 0)]$

Showing)

That is,

$$V[X \cdot I(X > 0)] = V[X] - V[X \cdot I(X \le 0)]$$

• Assuming symmetry for x = 0,

$$V[Y] = \frac{1}{2}V[X]$$

• In combination with what we got in slide 13, we multiply the variance of the initial value by 2 to make the output distribution safe.

Interim Summary

• The summary is as follows:

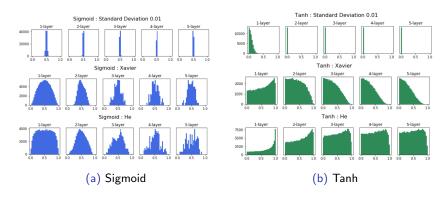


Figure 8: Various Initialization Methods with Sigmoid & Tanh

Interim Summary

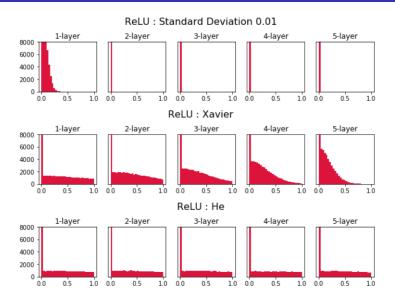


Figure 9: Various Initialization Methods with ReLU

Interim Summary

 Finally, in the end, the initialization is performed in the following distribution.

Activation function	Uniform distribution [-r, r]	Normal distribution
Logistic	$r = \sqrt{\frac{6}{n_{\text{inputs}} + n_{\text{outputs}}}}$	$\sigma = \sqrt{\frac{2}{n_{\rm inputs} + n_{\rm outputs}}}$
Hyperbolic tangent	$r = 4\sqrt{\frac{6}{n_{\rm inputs} + n_{\rm outputs}}}$	$\sigma = 4\sqrt{\frac{2}{n_{\rm inputs} + n_{\rm outputs}}}$
ReLU (and its variants)	$r = \sqrt{2} \cdot \sqrt{\frac{6}{n_{\rm inputs} + n_{\rm outputs}}}$	$\sigma = \sqrt{2} \sqrt{\frac{2}{n_{\rm inputs} + n_{\rm output}}}$

Figure 10: Various Initialization Methods

 To learn more, see 'Aurélien Géron(2017), Hands-On Machine Learning with Scikit-Learn and TensorFlow'.

6. Other Initialization Methods

- The three initialization methods I will introduce are mainly used in RNN.
 - **①** Orthogonal[6]: This is how you initialize using the Singular Value Decomposition(SVD). If $W = U\Lambda V^T$ then W is randomly generated from the standard normal distribution, and U calculated through the SVD is used as the initial value. Especially, it works well on RNN.
 - ② Le et al.[4]: This is the initialization method used with ReLU. By giving W = I and b = 0 to their initial values, they start off ordinarily at first learning.
 - **③** Talathi et al.[7]: This is the initialization method used with ReLU. It is explained specifically in the next slide.

6. Other Initialization Methods

- Talathi et al., hypothesize that an initialization where one eigenvalue is equal to 1 and the rest are less than 1 is better.
- Talathi et al. initialization is as follows:
 - **1** Sample a matrix $\mathbf{A} \in R^{N \times N}$ whose values are drawn from N(0,1) and N is the number of units in the RNN.
 - ② Compute $\mathbf{B} = \frac{1}{N} \mathbf{A} \mathbf{A}^\mathsf{T}$ and let λ_{max} be the largest eigenvalue of the matrix $\mathbf{B} + \mathbf{I}$.
 - **3** Initialize $\mathbf{W} = \frac{1}{\lambda_{max}} \mathbf{B} + \mathbf{I}$.
- Empirically this is better than initializing $\mathbf{W} = \mathbf{I}$.

Conclusion

- Initialization methods are still being studied as a major concern.
- Batch Normalization(BN) has the effect of making the initialization method less important.
- For the initial value distribution, there is no clear usage criteria for normal and uniform distribution.
- ullet Nevertheless, we use nomral initialization rather than uniform, and in the case of CNN, we almost always use a combination of 'He initialization + ReLU'.

Next

- Next time, we'll deal with the followings:
 - Type of loss function.
 - More complex CNN models.
 - About the GAN.
- Of course, Python code learning proceeds at the same time.

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