More about Neural Networks

PHYS591000 2022.03.30

Outline

- A few more details about how NN work:
  - Back propagation
- More about Regularization:
  - Dropout
  - Early Stopping

Warming up

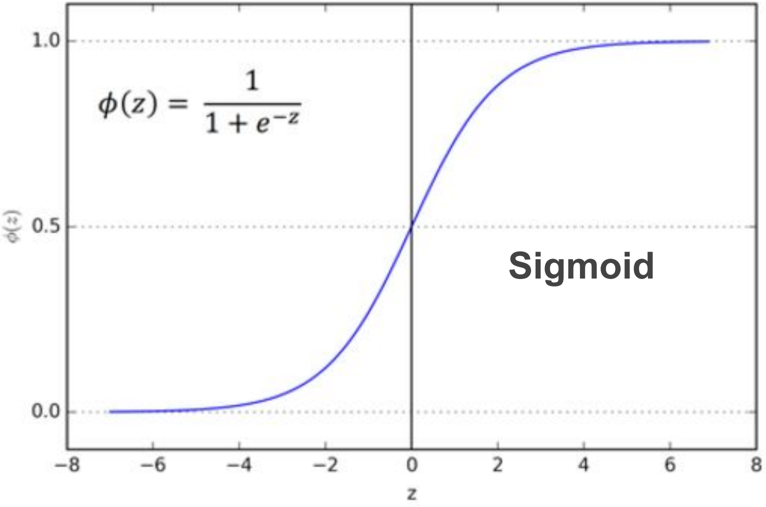
- As usual, take 3 mins to introduce yourself to your teammate for this week!
  – “What do you remember about neural networks from last week?”
  – “We’re halfway through! Any plans for Spring break?”

Review: Activation Function

- Recall that output of each neuron is obtained by feeding an weighted input into an activation function such as **ReLU** or **sigmoid**

$$z = \sum_i w_i x_i + b,$$

$$\text{output} = \sigma(z) = \frac{1}{1 + \exp(-z)}$$



Review: Loss Function

- Recall the goal of training is to find optimal parameters (weights (w_i) and biases (b_j)) which minimize the **loss function** L.

- Typically need to optimize a lot of parameters → Method of Gradient Descent

How to minimize the loss function

- Method of gradient descent: The next step is proportional to the negative of the local gradient

Gradient of Loss (average over the input data) $$\nabla L = \frac{1}{n}\sum_{x}^{n} \nabla L_x$$

$$w_i \rightarrow w_i' = w_i - \eta \frac{\partial L}{\partial w_i}$$

$$b_j \rightarrow b_j' = b_j - \eta \frac{\partial L}{\partial b_j}$$

η: learning rate

a tunable hyperparameter

Courtesy of Prof. Kai-Feng Chen (NTU)

Optimizer for minimizing loss function

- When the input data size is large it will take a lot of time calculating the gradients, and make the NN too slow. There are several **optimizer** to speed up the learning process.

- Most optimizers are based on stochastic gradient descent (SGD), which calculates the gradients using subsets of input data (‘batches’).

Backpropagation

- So it all boils down to calculating the gradient the loss function with respect to many, many parameters.

- In general this means we have to do this numerical calculations many times, and thus make the NN very slow….

- However, the gradients can be calculated in an effective way called **back propagation**.

Backpropagation

- Backpropagation sounds fancy but it's just the chain rule:

$$\frac{\partial L}{\partial w_i} = \frac{\partial L}{\partial \sigma(z_l)} \frac{\partial \sigma(z_l)}{\partial w_i} = \frac{\partial L}{\partial \sigma(z_l)} \frac{\partial \sigma(z_l)}{\partial z_l} \frac{\partial z_l}{\partial w_i}$$

$$= \frac{\partial L}{\partial \sigma(z_l)} \sigma'(z_l) \frac{\partial z_l}{\partial w_i} = \frac{\partial L}{\partial z_l} \frac{\partial z_l}{\partial w_i}$$

where z_l is the weighted input in the l-th layer, $\sigma(z_l)$ is the activation function.

Backpropagation

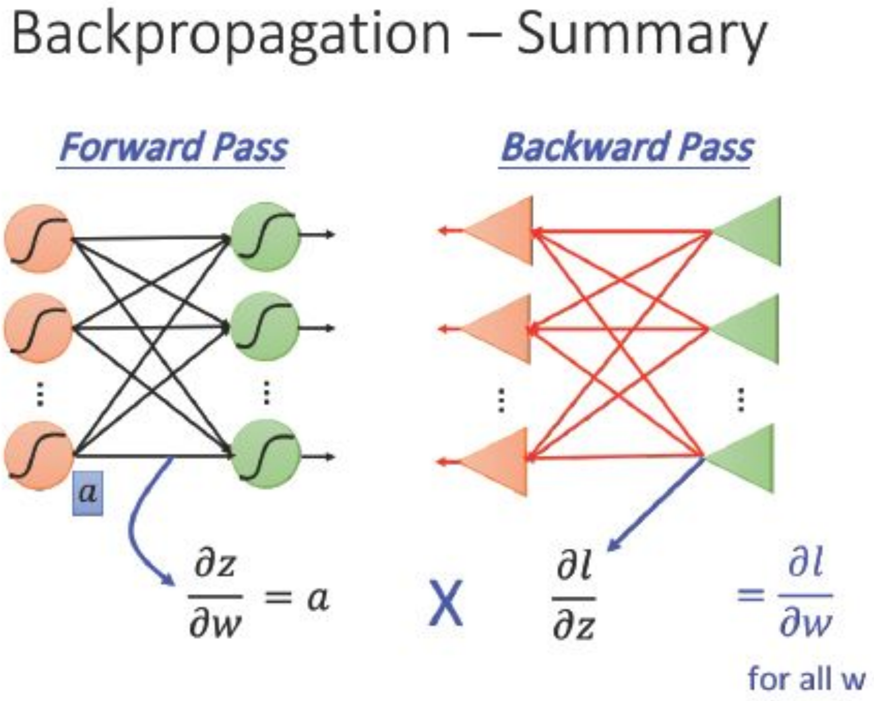
- A few observations:
  - In general it depends on the first derivative of σ(z).
  - $\frac{\partial L}{\partial z_l}$ is *independent* of the weights used for inputs to previous layers (changing weights in this layer won't affect what happened in previous layers). On the other hand, it depends on all weights/gradients applied in next layers.

Backpropagation

- In order to calculate the gradients, we first initialize the weights randomly, and
  - Perform a feedforward calculations to get all $\frac{\partial z_l}{\partial w_i}$
  - Calculate $\frac{\partial L}{\partial z_l}$ from the output (ending) layer, **back propagating** to the second last layer, and to the third last layer,... until we obtained $\frac{\partial L}{\partial z_l}$ for all layers.

Backpropagation

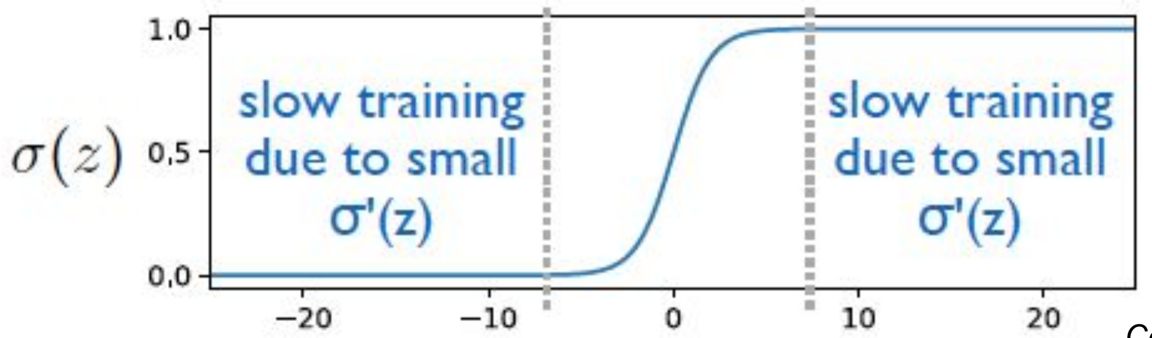
$$\frac{\partial l}{\partial w} = \frac{\partial z}{\partial w}\Big|_{forward\ pass} \cdot \frac{\partial l}{\partial z}\Big|_{backward\ pass}$$



Reference: Slides and lecture video
from Prof. Hung-yi Lee (NTU)

Choice of Loss Function

- This is why we say using mean square error (MSE) as loss function can be slow since one may fall into regions with tiny slope (very small σ'(z)).



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Choice of Loss Function

- And that's why the **cross entropy function** (combined with Softmax output) is another popular choice for loss function:

$$L = -\sum_i t_j \ln(y_j) \quad j\text{: classes}$$

$$y_j = \frac{\exp(z_j)}{\sum_k \exp(z_k)} \quad k\text{: classes}$$

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Choice of Loss Function

$$\boxed{\frac{\partial L}{\partial z_i}} = -t_i \frac{1}{y_i}\frac{\partial y_i}{\partial z_i} - \sum_{j \neq i} t_j \frac{1}{y_j}\frac{\partial y_j}{\partial z_i}$$

$$= -t_i(1-y_i) + \sum_{j \neq i} t_j y_i = -t_i + t_i y_i + \sum_{j \neq i} t_j y_i$$

$$= -t_i + y_i \left(t_i + \sum_{j \neq i} t_j \right) = \boxed{y_i - t_i}$$

t_j = target value for class j
by definition $\Sigma t_j = 1$

It ends up with the same results as before and no dependency on $\sigma'(z)$!

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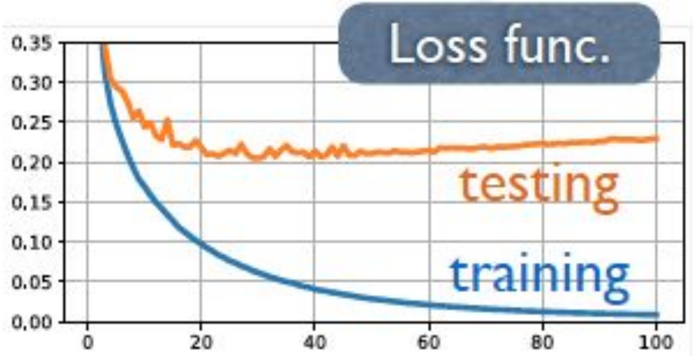
Regularization

- Last week we introduced L1/L2 regularization: Add extra term $\lambda\Sigma i|\mathbf{Wi}|$ (L1) or $\lambda\Sigma i\mathbf{Wi}^2$ (L2) to the loss function

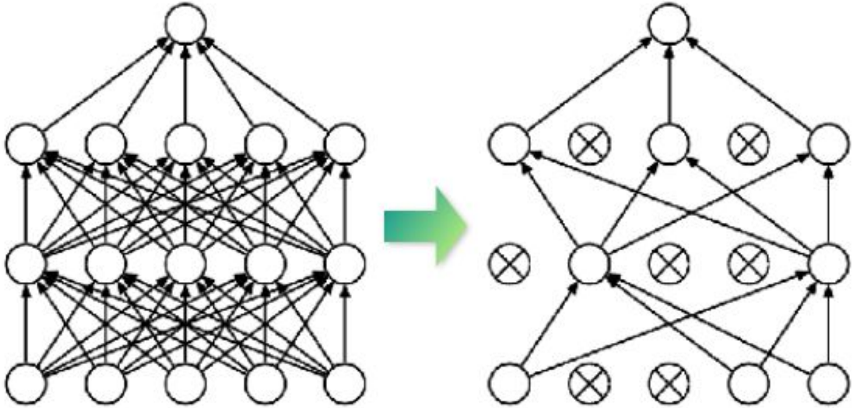
- This week we will work with two other methods: Dropout and Early Stopping.



Number of epochs

Dropout

- Dropout method means to randomly disconnect some of the inputs of a specific layer/neurons at each training cycle, and thus less sensitive to noises and be more general.



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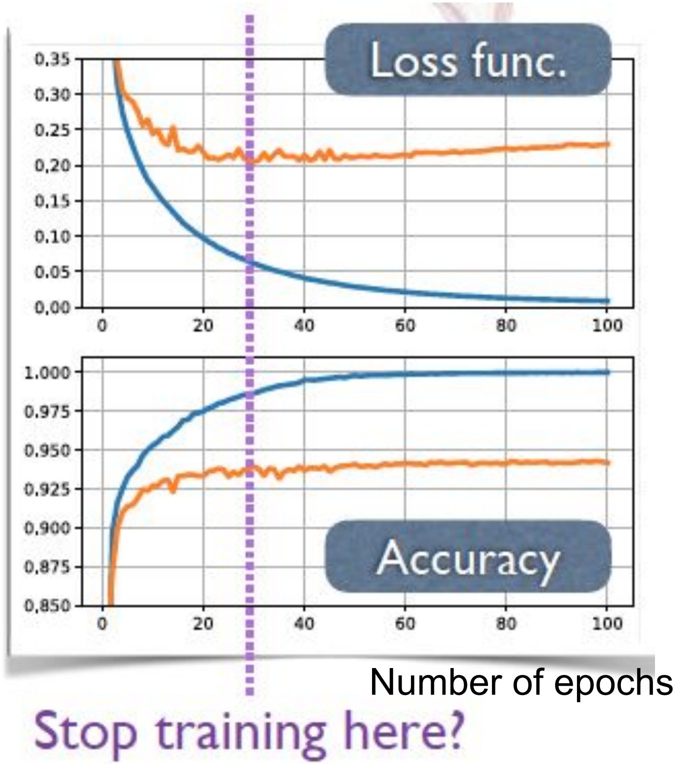
Early Stopping

- Stop training when the model stops improving after certain number of consecutive iterations on a **validation** sample (independent from the train *and* the test data).



Lab for this week

- No in-class exercise this week.

- For the Lab this week, we continue with the same W/Z v.s. QCD jet dataset, and we'll play with

  - Dropout and Early Stopping

  - *KerasTuner* for hyperparameter optimization

Backup