Lecture G1. Functional Approximation 1

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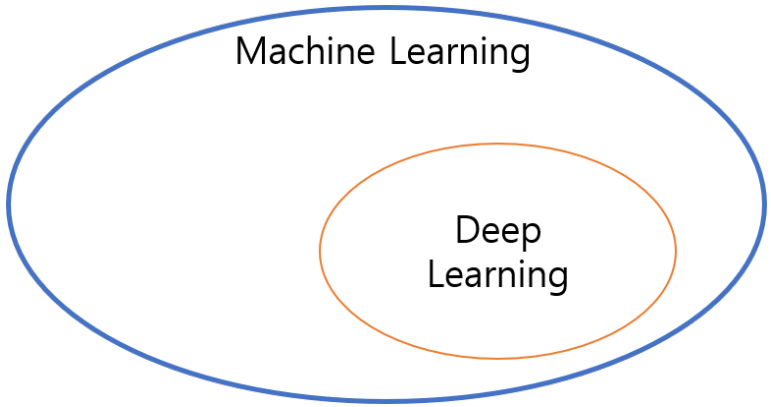
I. Introduction & Motivation

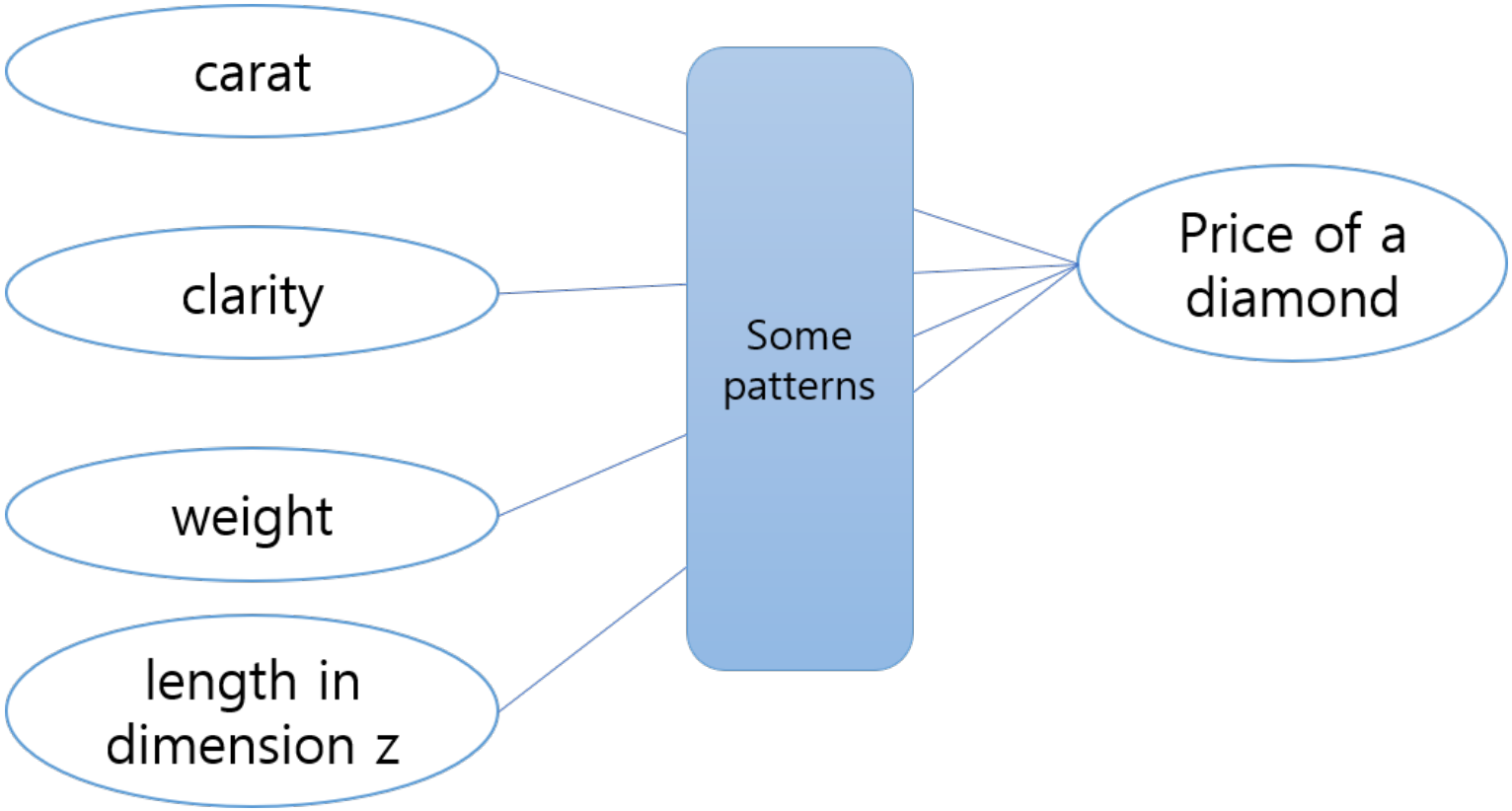
About

- Machine Learning (ML)
  - 'ML is a field of computer science that gives computers the ability to learn without explicitly programmed.' - Wikipedia
  - 'Mathematics is to find patterns.' – R. Feynman
  - My take is, ML is to let the machine to find mathematical patterns
    1. without explicitly programmed
    2. but within the boundary of possible patterns programmed by the researcher.
- Deep Learning (DL)
  - 'DL is part of a broader family of ML Methods.' - Wikipedia
  - DL uses a cascade of multiple layers of nonlinear processing units, i.e. 'deep' neural networks.

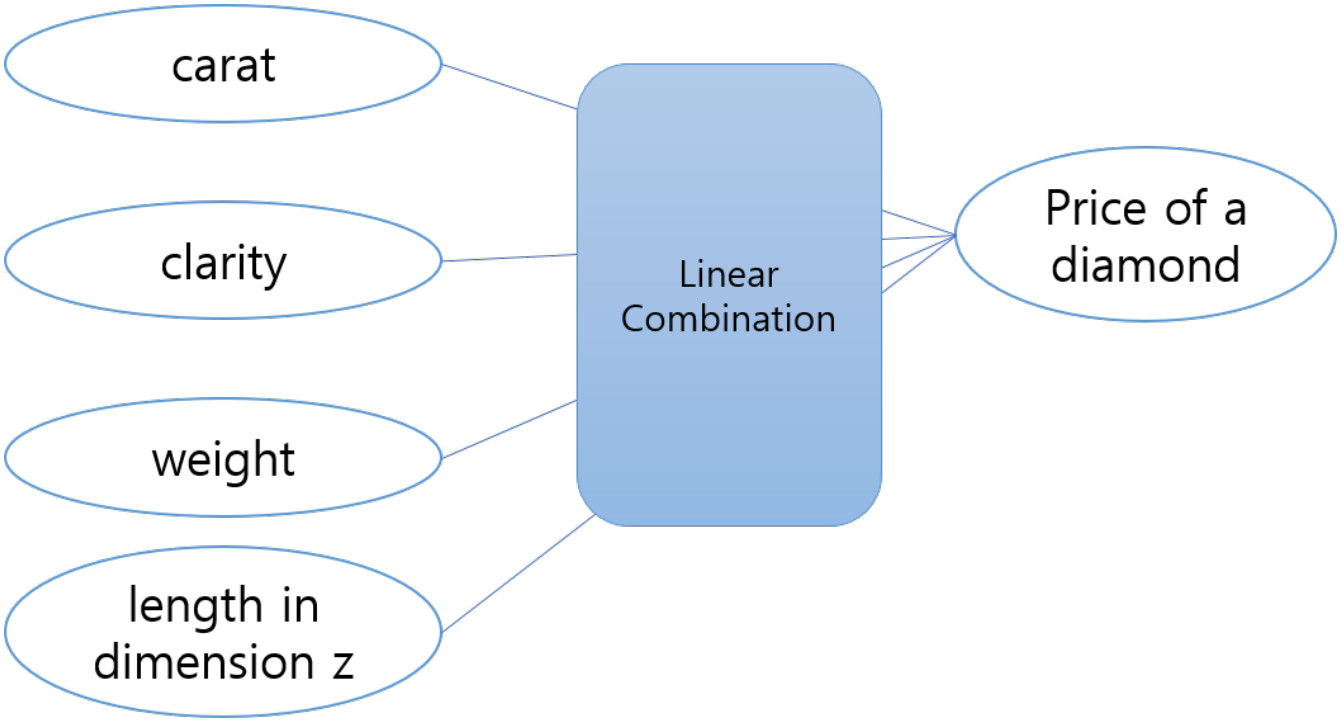


Illustration

"Mathematics is to find patterns." – R. Feynman



Linear regression

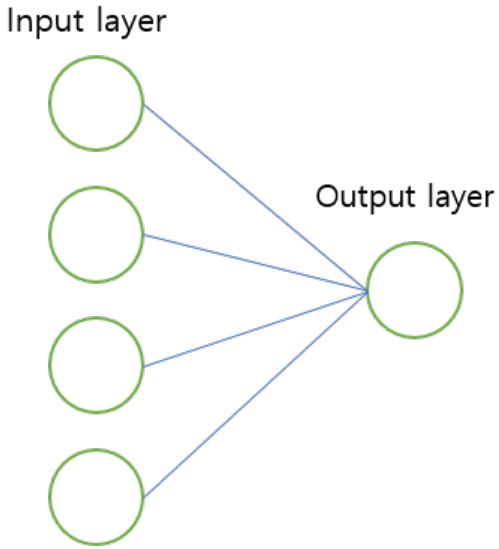


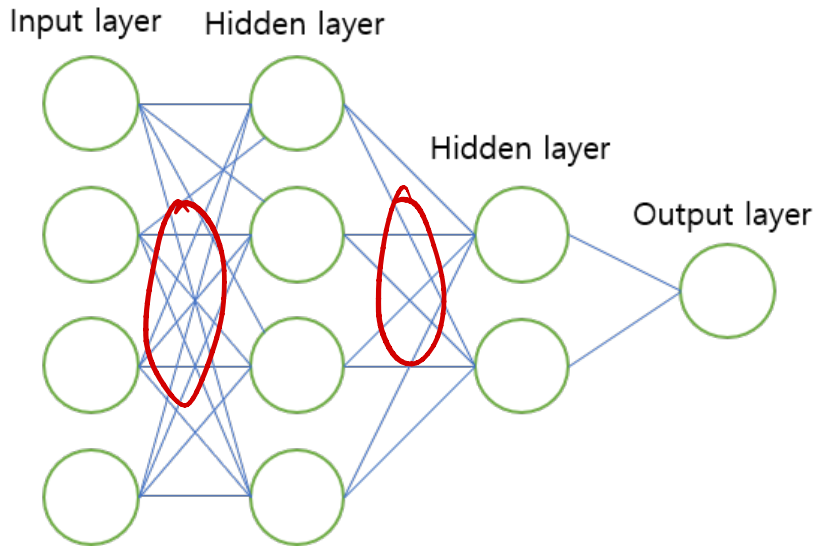
- $Price = \alpha + \beta_{carat} Carat + \beta_{clarity} Clarity + \beta_{weight} Weight + \beta_{len\_z} Len\_z$
- Assumption
  1. Linearity (proportional output change given input change)
  2. Independence (no interaction among input variables)

Sufficiency of linear regression?

- What if the assumptions are not sufficient to find the pattern?
  1. Nonlinearity
     - Price is indeed known to be proportional to square of carat.
     - After the certain level of clarity, it no longer matters.
  2. Interaction
     - Clarity matters more when carat is bigger.
     - Weight is negatively correlated to clarity.
     - Weight is positively correlated to carat.

Linear regression vs Deep neural network





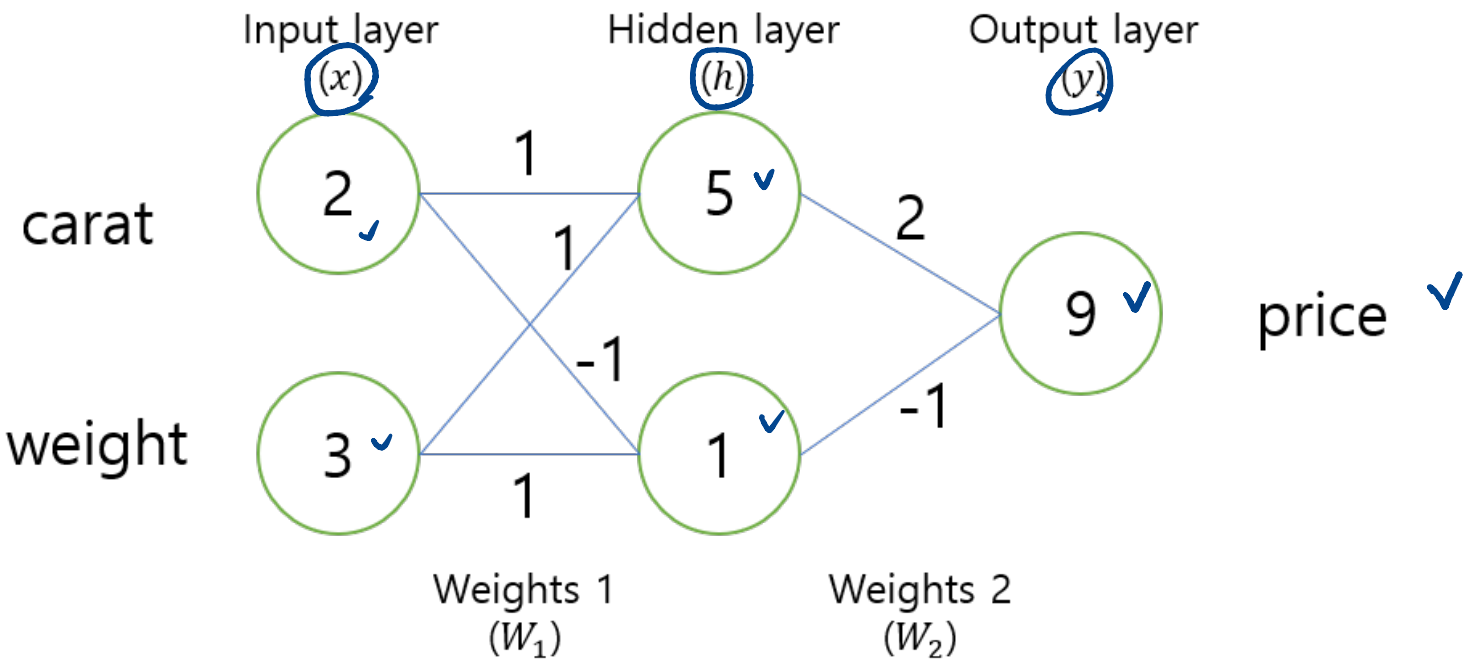
Linear Reg.	Deep Learning
Linear	Nonlinear
Independence	Allows dependence
Intuitive	Less intuitive

II. Mechanism of deep learning

Mechanism anatomy

1. Forward propagation - *the backbone of the network*
2. Activation function - *the essential elements for non-linearity*
3. Loss function - *the performance criteria of your estimate*
4. Gradient descent - *feedback for improvement*
5. Back propagation - *how feedback is propagated*

1. Forward propagation - *the backbone of the network*



- $\mathrm{h} = W_1 \mathrm{x}$
- $\mathrm{y} = W_2 \mathrm{h}$
- The forward propagation process can be summarized as as follows:

$$\mathrm{x} \xrightarrow{\times W_1} \mathrm{h} \xrightarrow{\times W_2} \mathrm{y}$$

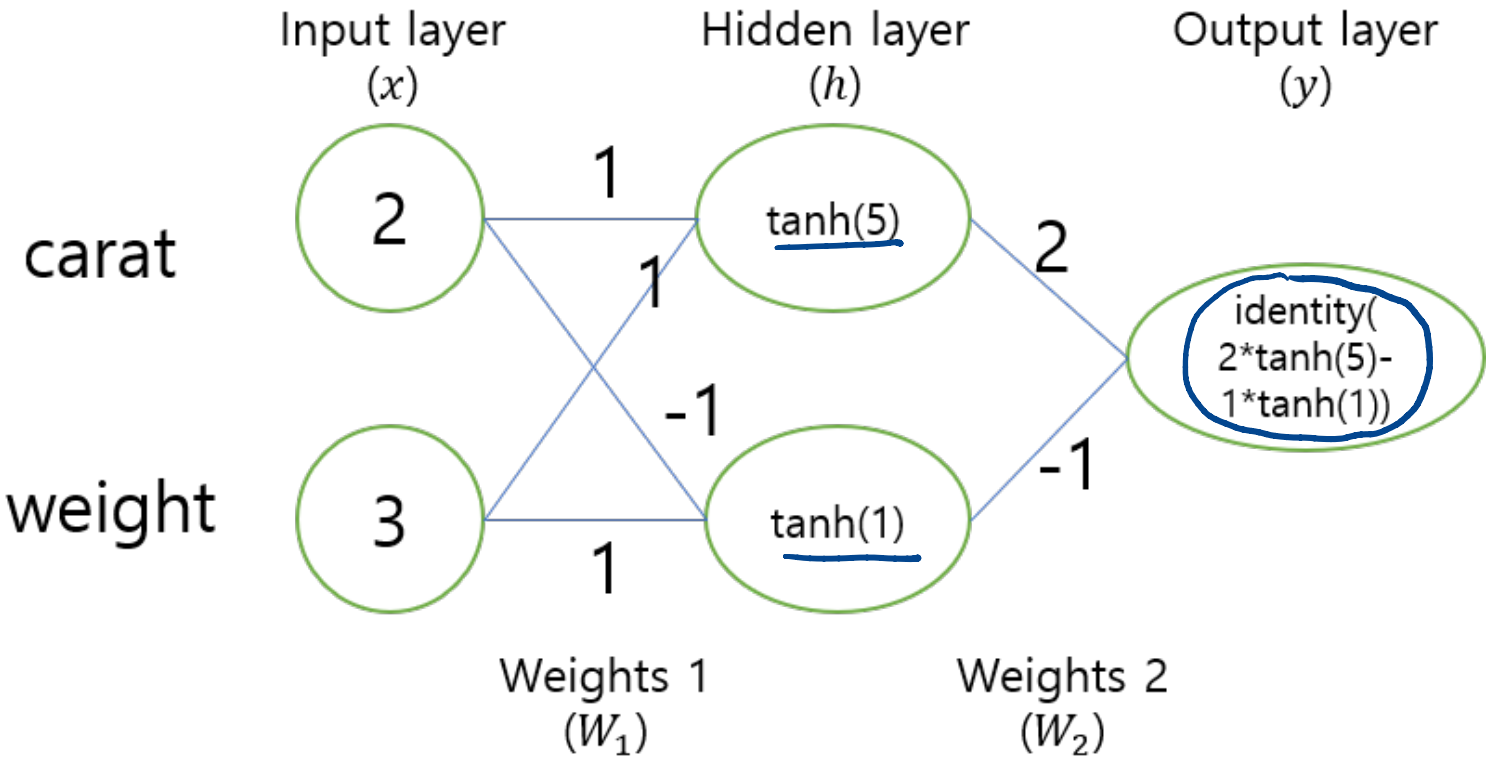
2. Activation function - *the essential elements for non-linearity*

- The previous page's output $9 =$
- Why need activation function?
  - Linear transformation of linear transformation is linear. We need some nonlinearity ~~for~~ to prevent trivial forward propagation.
  - Output layer needs to be structured for desirable output. For example, we may want it to be in range of $(-\infty, \infty)$, $[0, \infty)$, $[0, 1]$, or so on.
- Activation function is a nonlinear function applied to hidden layers or an output layer.

- For hidden layers
  1. ReLU
     - $(-\infty, \infty) \rightarrow [0, \infty)$
     - $f(x) = x^+ = max(x, 0)$
     - Known to be most effective
  2. tanh
     - $(-\infty, \infty) \rightarrow (-1, 1)$
     - $f(x) = tanh(x)$

- For output layer
  3. sigmoid
     - $(-\infty, \infty) \rightarrow (0, 1]$
     - $f(x) = \frac{1}{1+e^{-x}}$
     - Maps to probability space
  4. softmax
     - $(-\infty, \infty)^n \rightarrow (0, 1]^n$
     - $f(x_k) = \frac{exp(x_k)}{\sum_{i=1}^{n} exp(x_i)}$
     - Used for classification problems
  5. linear (identity)
     - $(-\infty, \infty) \rightarrow (-\infty, \infty)$
     - $f(x) = x$
     - Used for regression problems

- The previous forward propagation should be modified, for example, as below:

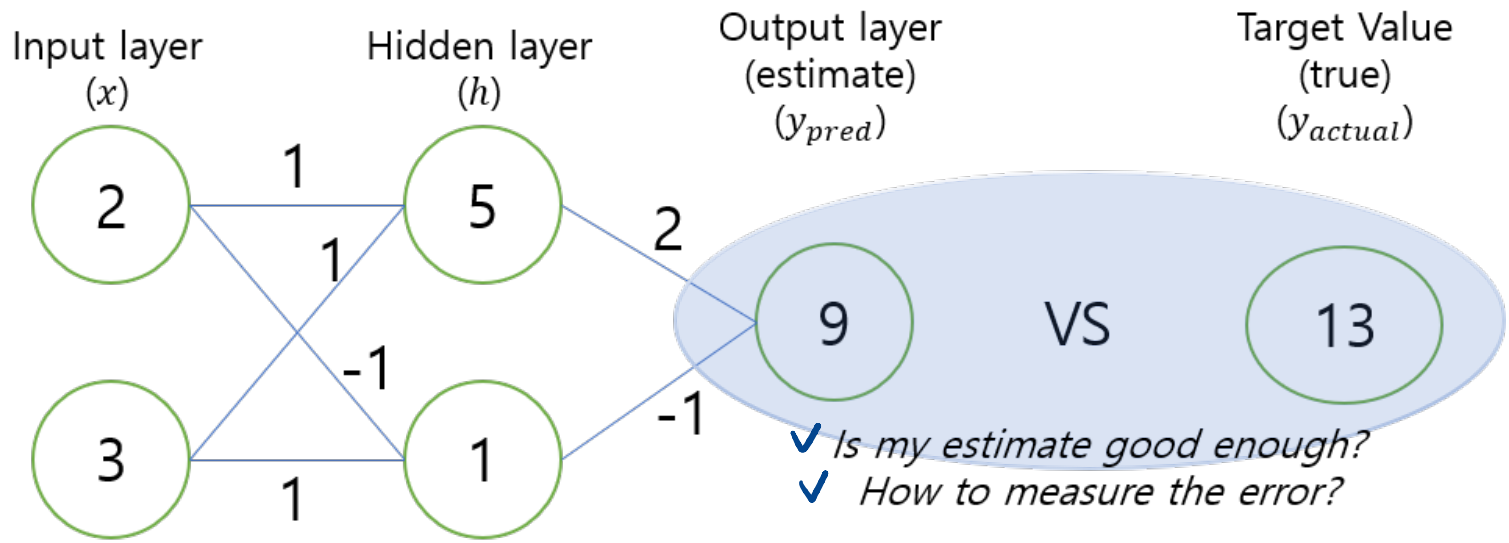


- $\mathrm{h} = tanh(W_1 \mathrm{x})$
- $\mathrm{y} = identity(W_2 \mathrm{h})$
- The forward propagation process should be revised as follows:

$$\mathrm{x} \xrightarrow{\times W_1 \text{ then apply an act. fn.}} \mathrm{h} \xrightarrow{\times W_2 \text{ then apply an act. fn.}} \mathrm{y}$$

3. Loss function - *the performance evaluation of your estimates*

- Assuming, for simplicity of our discussion, that activation functions are all identity (linear) functions.

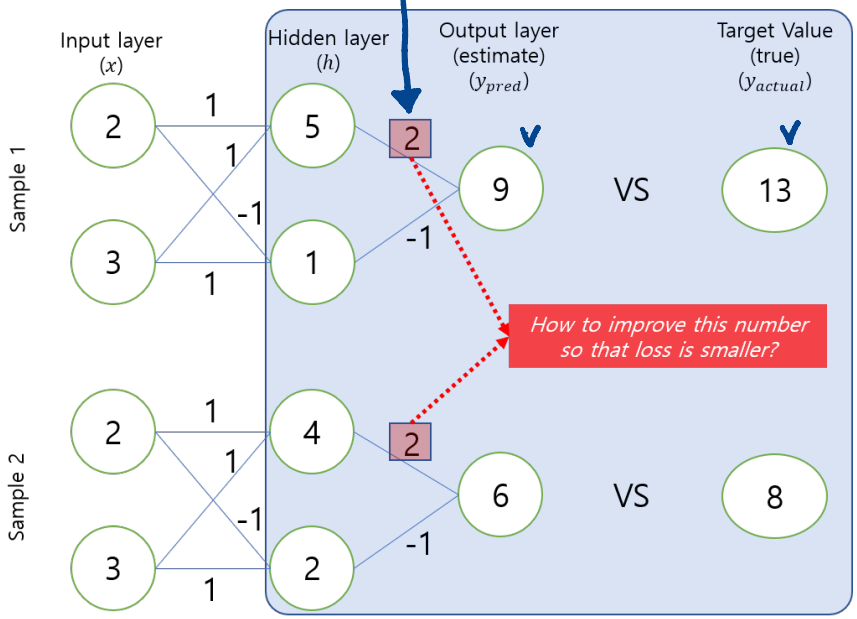


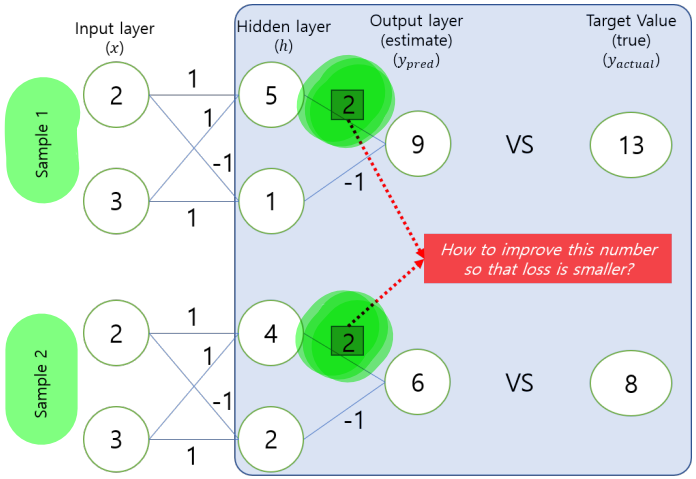
	Estimate $\hat{y}$	True value (target) y	Error $\hat{y}-y$	Squared error (SE) $(\hat{y}-y)^2$
Sample 1	10	20	-10	100
Sample 2	8	3	5	25
Sample 3	6	1	5	25

- Loss function measures aggregated error.
- MAD (Mean Average Deviation)
  - $loss = \frac{|-10|+|5|+|5|}{3}$
  - Though intuitive, not widely used because not differentiable.
- MSE (Mean Squared Error)
  - $loss = \frac{100+25+25}{3}$
  - Most common for parametric target value.
  - Penalizes large errors severely.
- Cross Entrophy
  - Loss: $E = \sum_k t_k log(y_k)$, where t_k is k-th target and y_k is an k-th estimate.
  - Commonly used for classification problem.

4. Gradient descent - *feedback for improvement*

- After measuring loss function, the weights must be improved so that loss becomes smaller.
- Let us confine our attention to W_2, currently $[2\ 1]$, a weight vector for the hidden layer (h). Let us confine further to its first element, currently $W_2(1) = 2$.
- How can we find better value for $W_2(1)$?





h_1	W_2	$\hat{y}$	y	Error	SE	MSE (L)
$\begin{bmatrix}5\\1\end{bmatrix}, \begin{bmatrix}4\\2\end{bmatrix}$	$[0\ \ -1]$	$-1, 2$	$13,\ 8$	$-14, -10$	$(-14)^2, (-10)^2$	148
	$[1\ \ -1]$	$4, 2$		$-9, -6$	$(-9)^2, (-6)^2$	58.5
	$[2\ \ -1]$	$9, 6$		$-4, -2$	$(-4)^2, (-2)^2$	10
	$[3\ \ -1]$	$14, 10$		$1, 2$	$1^2, 2^2$	2.5
	$[4\ \ -1]$	$19, 14$		$6, 6$	$6^2, 6^2$	36

- The current weight $W_2(1)$ should be increased so that L is decreased. The sign of $\frac{\partial L}{\partial W_2(1)}$ is negative. In other words, if $W_2(1)$ is increased, L is decreased.
- This tells us that, the weight is updated in the following way, where α is often called 'learning rate' .

$$W_2^{new}(1) \leftarrow W_2^{old}(1) - \alpha \cdot \frac{\partial L}{\partial W_2(1)}$$

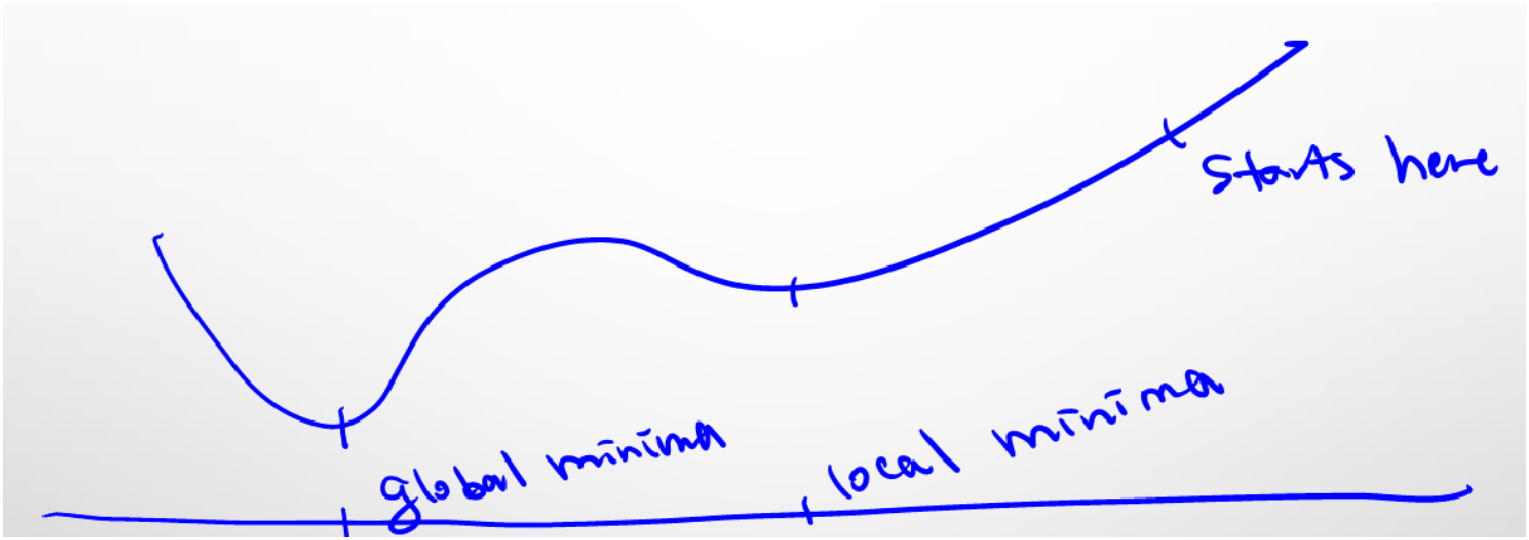
- This updating is to occur simultaneously for all weights.
- If written in a general sense,

$$\mathrm{w} \leftarrow \mathrm{w} - \alpha \cdot \nabla_{\mathrm{w}} L,$$

where $\nabla_{\mathrm{w}} L = (\frac{\partial L}{\partial \mathrm{w}_1}, \frac{\partial L}{\partial \mathrm{w}_2}, \cdots, \frac{\partial L}{\partial \mathrm{w}_n})$ is first-order derivatives of L with respect to all elements of w. $\nabla_{\mathrm{w}} L$ is geometrically slope. ∇ reads 'nabla' .

- This tells us that both loss function and activation functions must be differentiable. They need to be 1) monotone, 2) continuous, and 3) differentiable.

- Optimizer
  - This process of gradient descent is to optimize the weight of neural network. And the algorithm concerning finding learning rate or step size is called ‘optimizer’.
  - Widely used optimizer includes Adam, RMSprop, SGD, and so on.
- Weight initialization
  - It is not always guaranteed to find global optimum given a poor choice of initial weight.
  - Thus, the initial weights must be randomized within a wide range to sufficiently cover the possible optimum.



- Batch and Epoch
  - Conducting differentiation involves numerically cost operation, so it is desirable to collect some number of sample and then to do weight updating.
  - The size of this subset of the data for an update once is called **batch**.
  - One time to go through the whole dataset once is called **epoch**.

5. Back propagation - *how feedback is propagated*

- The weight updating, of course, does not only take place on the last hidden layer, but all weights in front.
- The information is propagated based on 'Chain rule of calculus.'

Summary of deep learning mechanism

1. Forward propagation
   - Choose the number of layer
   - Choose the number of nodes in each layer
2. Activation function
   - Choose the activation function for hidden layers
   - Choose the activation function for the last layer based on the characteristics of target output.
3. Loss function
   - Choose the loss function based on the characteristics of target output
4. Gradient Descent
   - Choose the size of batch
   - Choose the the number of epochs
   - Choose the optimizer
   - (Choose default learning rate)
   - (Choose initial weights)
5. Back propagation

Implementation

- The above mechanism describes supervised learning, because we assume the possesion of correct target values.
- The input data needs to be scaled between [-1,1] range, so that weights effectively cover the variation of data.
- The design factors of neural network summarized in the previous page are called hyperparameter.
- To find hyperparameter, split train-validataion-test sets appropriately.

"Exceptional people, I have found, either start out being optimistic or learn to be optimistic because they realize that they can't get what they want in life without being optimistic.
- B. Rotella in How Champions Think: In Sports and in Life"