# Lecture G1 Functional Approximation 1

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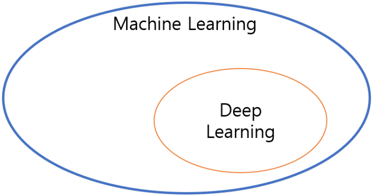
# I. Introduction & Motivation

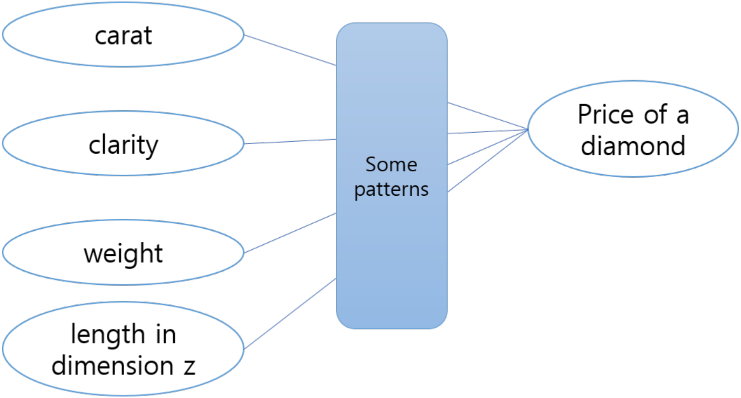
# About

- 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.

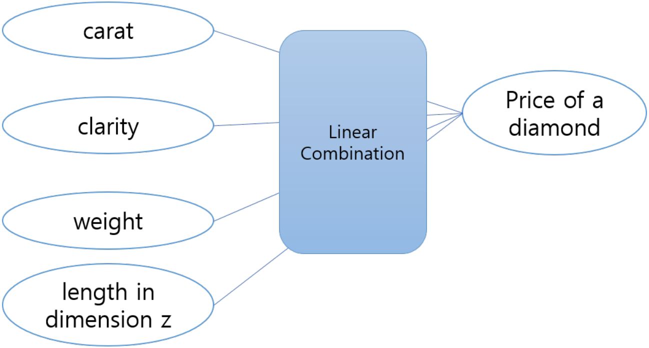


# Illustration

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



# Linear regression

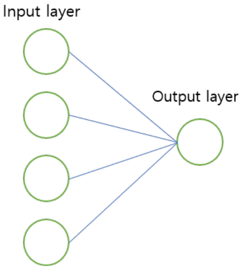


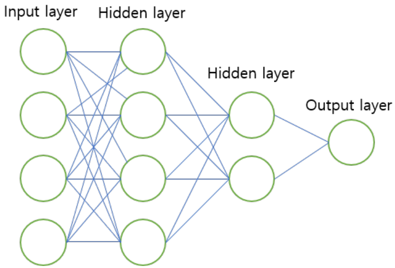

- $Price =$
  $\alpha + \beta_{carat} Carat + \beta_{clarity} Clarity + \beta_{weight} Weight + \beta_{len\_z} Len\_z$
- Assumption
  1. Linearity (proportional output change given input change)
  2. Independence (no interaction among input variables)

# 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



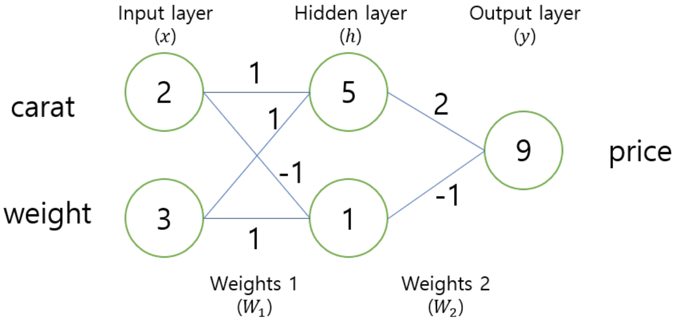

| Linear Reg. | Deep Learning |
|---|---|
| Linear | Nonlinear |
| Independence | Allows dependence |
| Intuitive | Less intuitive |

# 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:

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

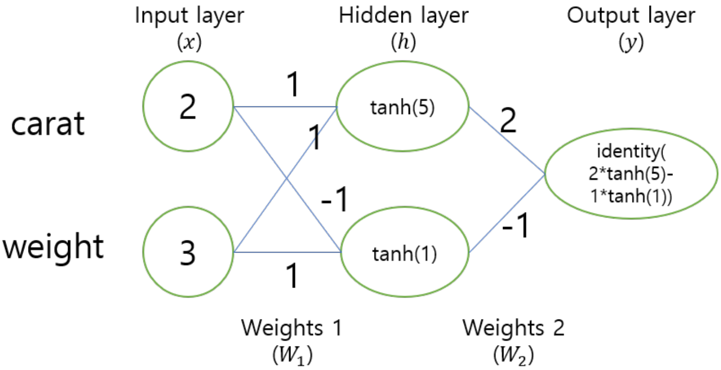
## 2. Activation function - *the essential elements for non-linearity*

- The previous page's output $9 =$
- Why need activation function?
  - Linear transformation of linear transformation is linear. We need some nonlinearity for 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
     - $(-\infty, \infty) \to [0, \infty)$
     - $f(x) = x^+ = max(x, 0)$
     - Known to be most effective
  2. tanh
     - $(-\infty, \infty) \to (-1, 1)$
     - $f(x) = tanh(x)$

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

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

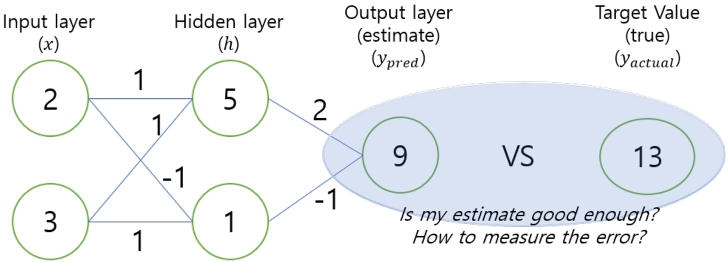



- $\mathrm{h} = tanh(W_1 \mathrm{x})$
- $\mathrm{y} = identity(W_2 \mathrm{h})$
- The forward propagation process should be revised as follows:

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

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

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

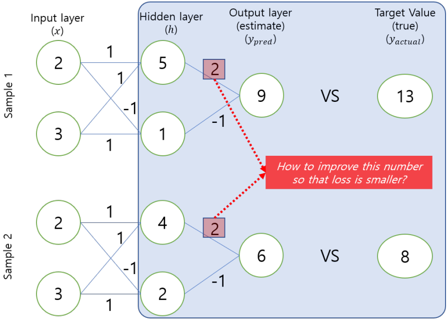


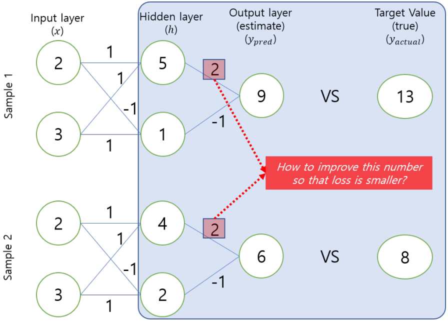
| | Estimate $\hat{y}$ | True value (target) $y$ | Error $\hat{y}-y$ | Squared error (SE) $\hat{y}-y$ |
|---|---|---|---|---|
| Sample 1 | 10 | 20 | -10 | 100 |
| Sample 2 | 8 | 3 | 5 | 25 |
| Sample 3 | 6 | 1 | 5 | 25 |

- 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 Entropy
  - 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 ($L$) |
|---|---|---|---|---|---|---|
| | $[0 \;\; -1]$ | $-1, 2$ | | $-14, -10$ | $(-14)^2, (-10)^2$ | 148 |
| | $[1 \;\; -1]$ | $4, 2$ | | $-9, -6$ | $(-9)^2, (-6)^2$ | 58.5 |
| $\begin{bmatrix}5\\1\end{bmatrix}, \begin{bmatrix}4\\2\end{bmatrix}$ | $[2 \;\; -1]$ | $9, 6$ | $13, \;\; 8$ | $-4, -2$ | $(-4)^2, (-2)^2$ | 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 $\alpha$ is often called 'learning rate'.

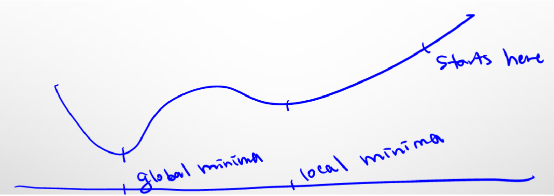
$$W_2^{new}(1) \leftarrow W_2^{old}(1) - \alpha \cdot \frac{\partial L}{\partial W_2(1)}$$

- 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. $\nabla$ 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 beased 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.

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"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"
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