Week 3

Deep Learning / MLP

#8 History of DL / MLP Basic

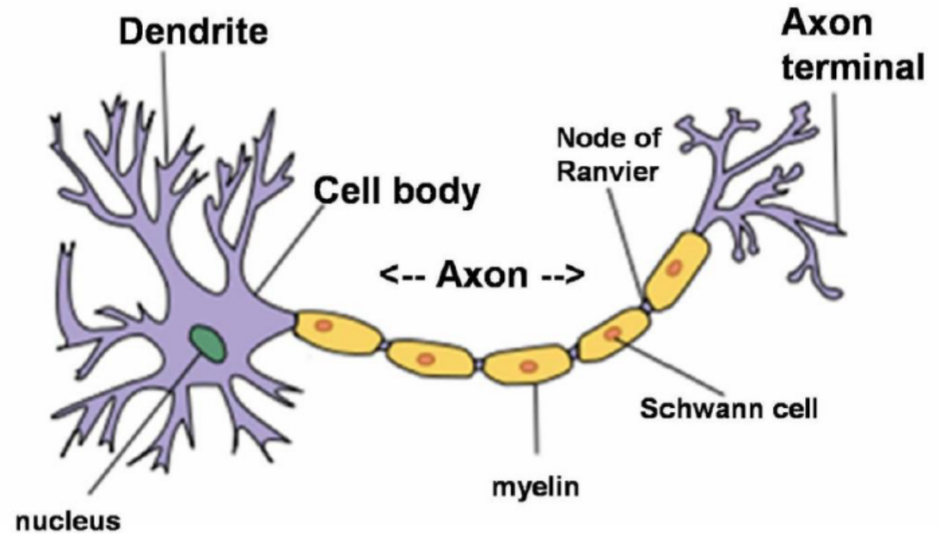
#9 MLP Regression with Pytorch / Assignment 1

#10 Assignment 1 Review

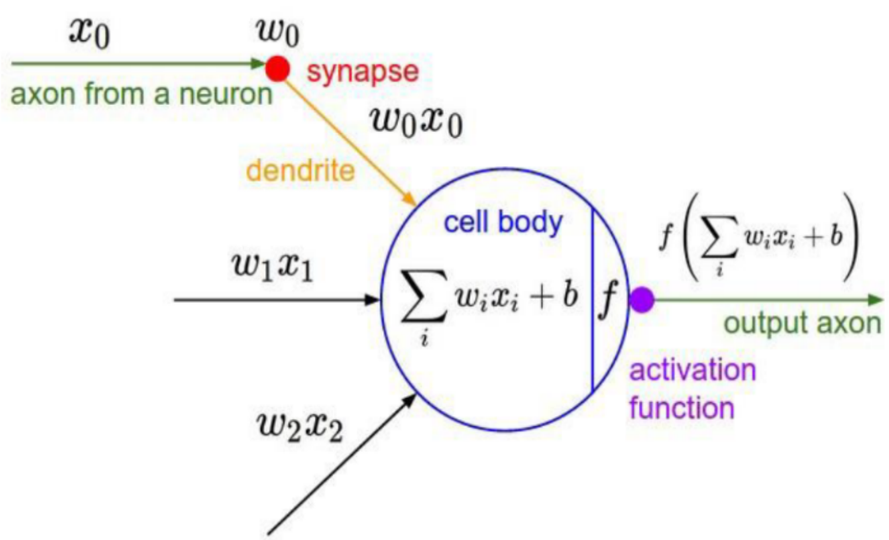
#11 How to parameterize DL code

2021.7.28 (3주차) 조수연

- Structure of Neuron

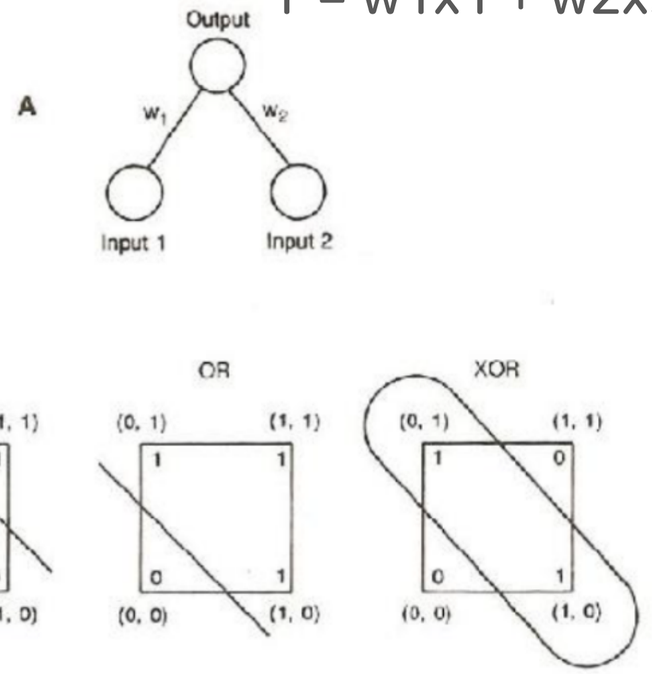


- Modeling Neuron (1957)

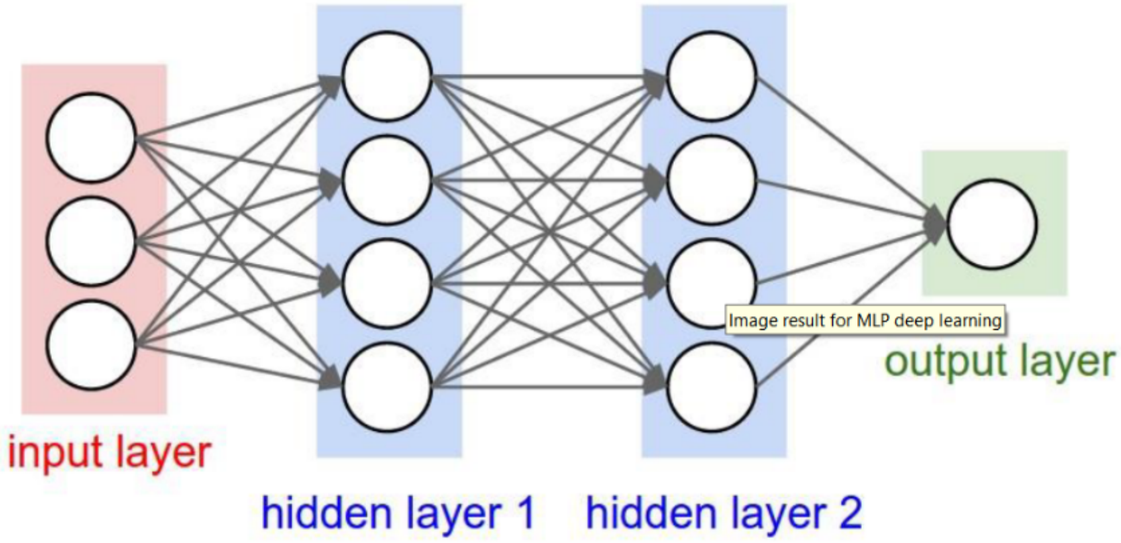


- And / Or Problem

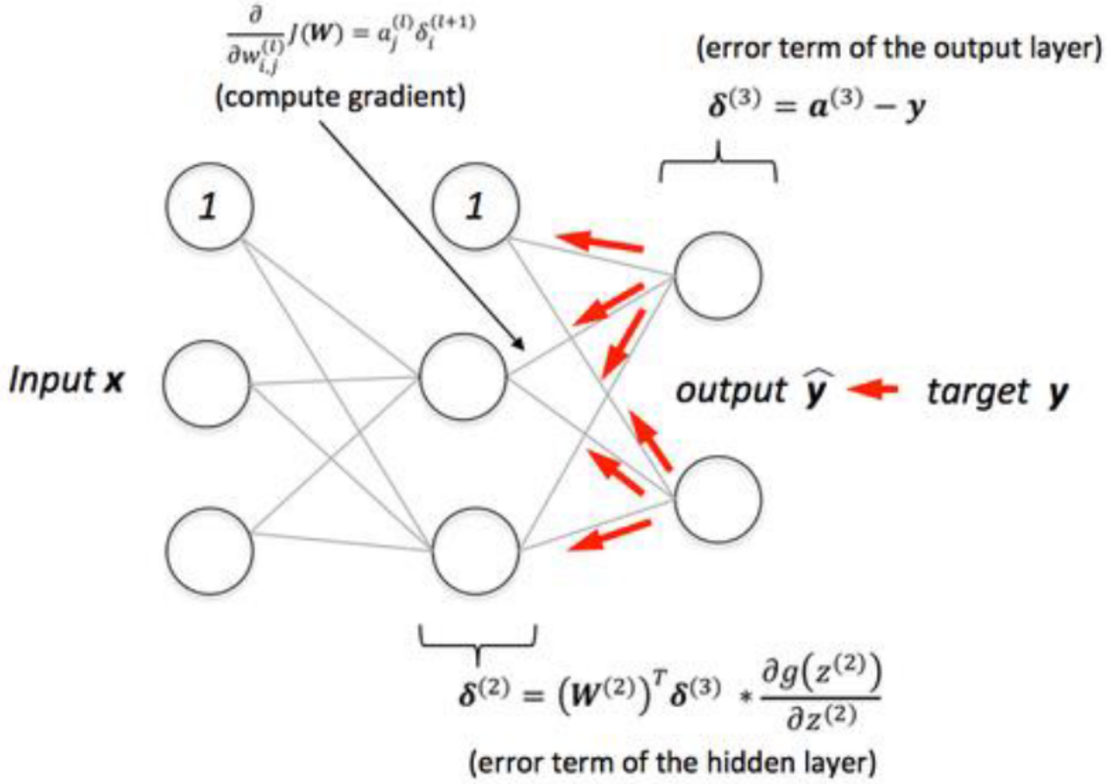
$$Y = w1x1 + w2x2 + b$$



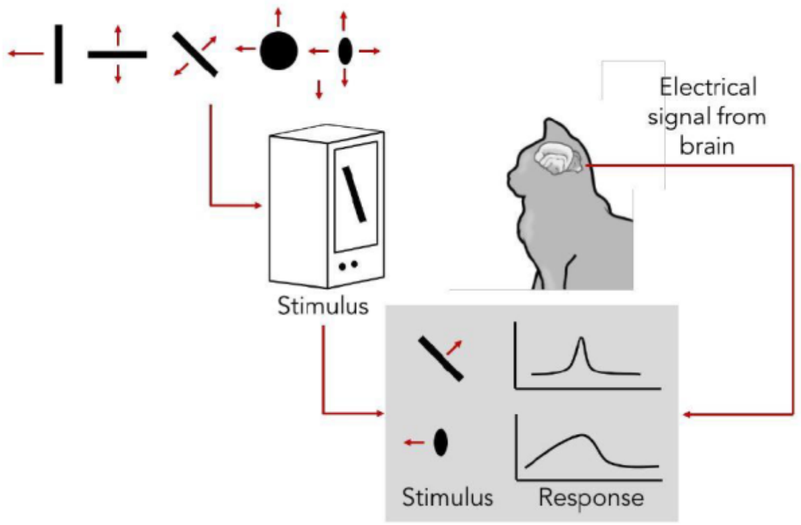
- Multilayer Perceptron (1969)

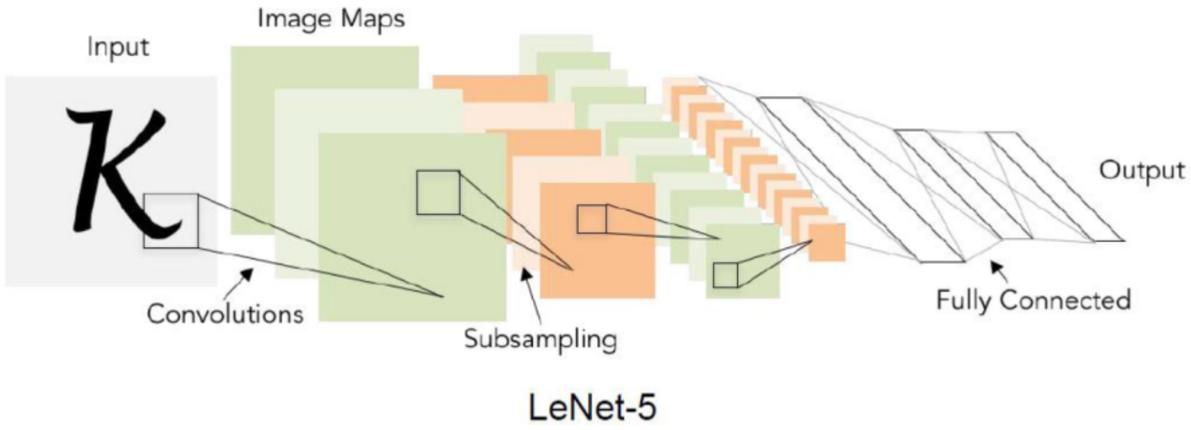


- **Backpropagation** (1986)



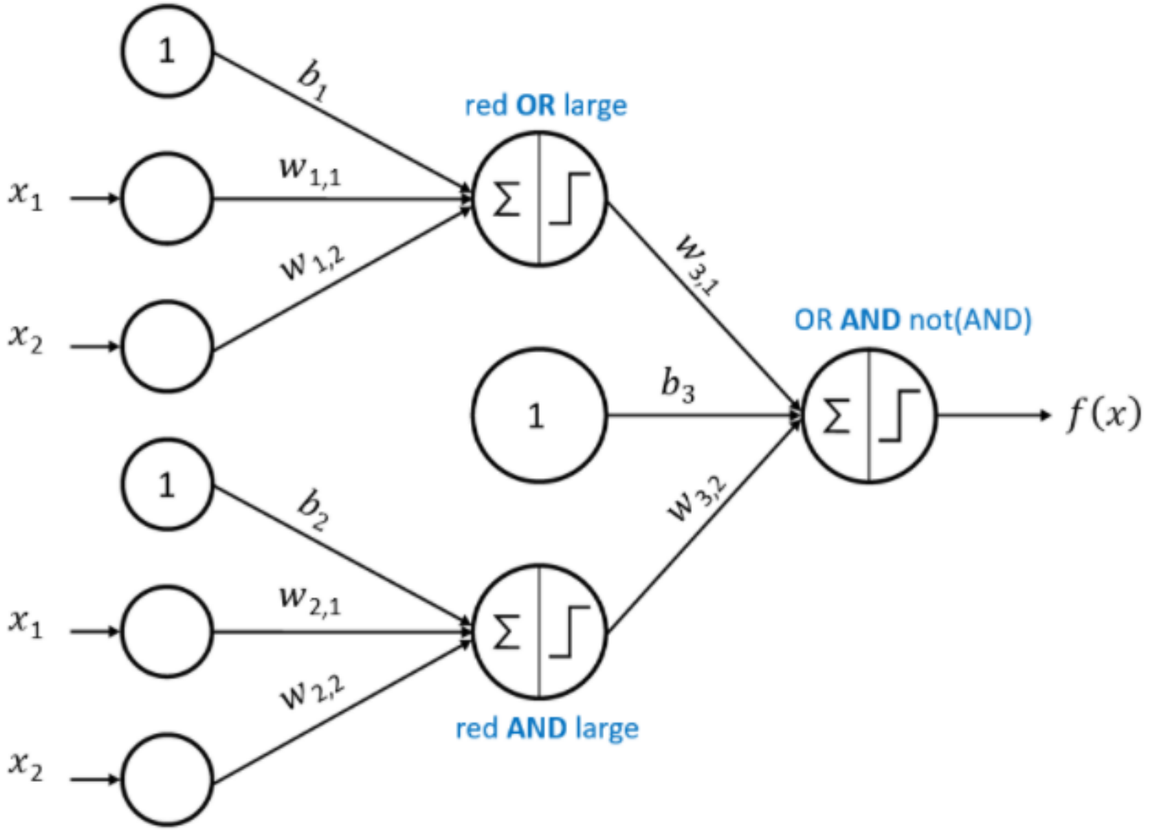
- Convolutional Neural Networks (2012)





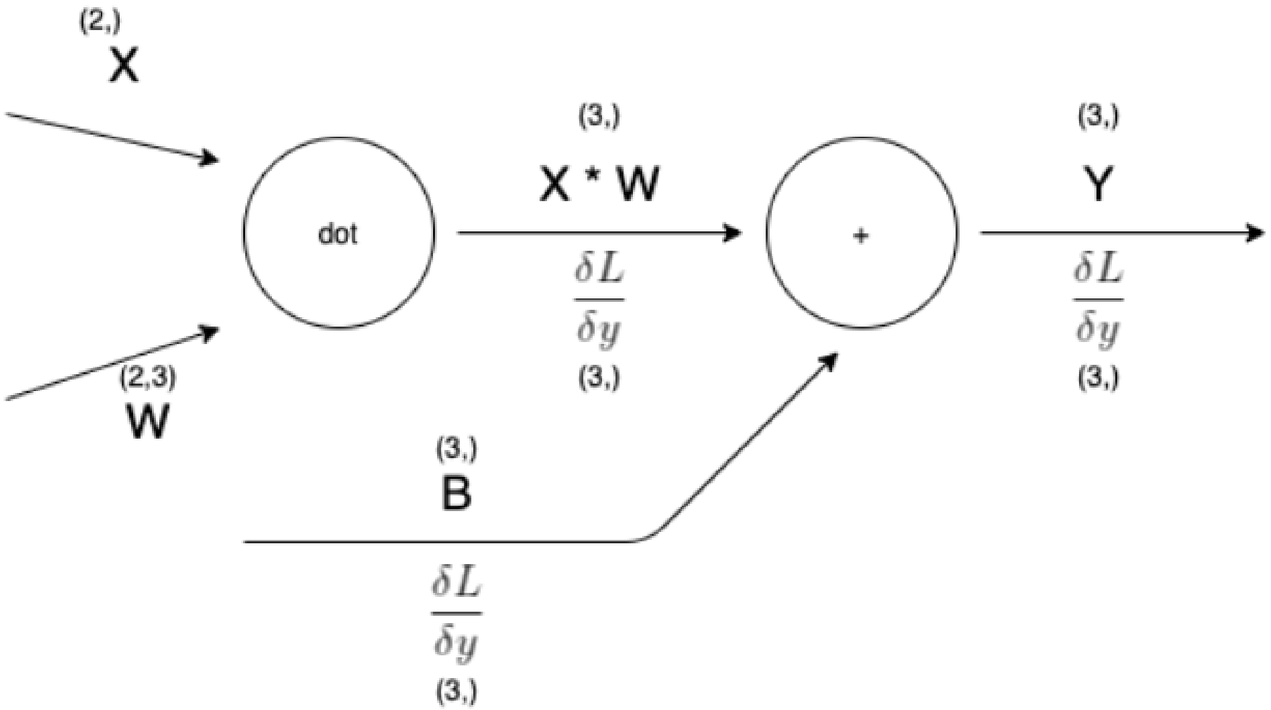
MLP

- Sloving XOR problem



MLP

- Backpropagation with Chain Rule



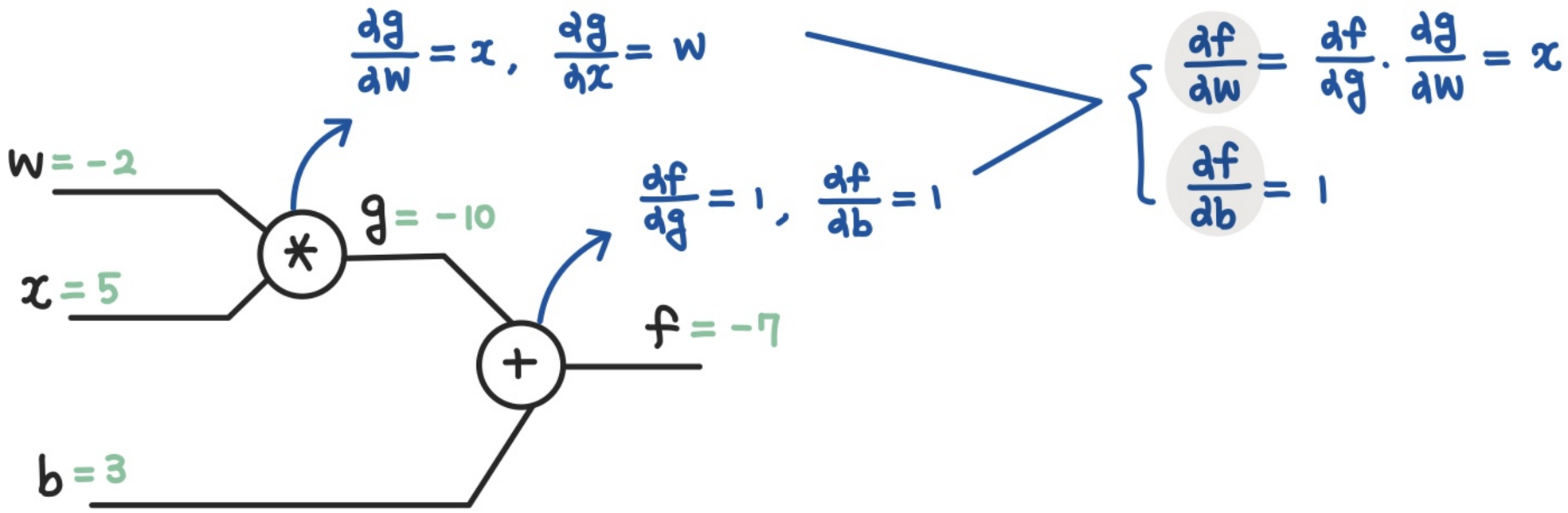
Training 하는 과정

1) Feed forward

2) Backpropagation

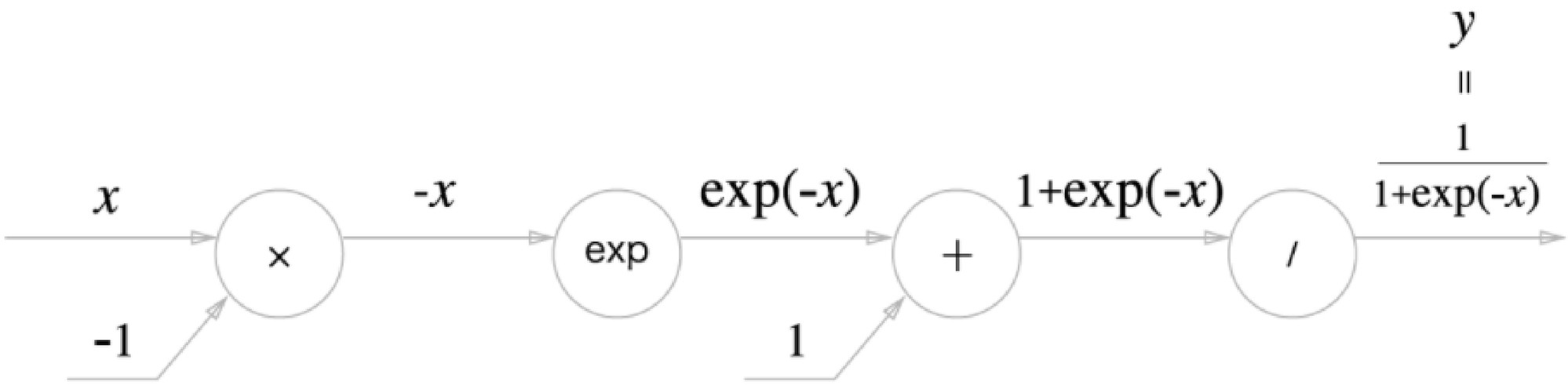
MLP

- 하나의 뉴런 식 : f = g + b = wx + b



MLP

- Sigmoid Function : $y = \frac{1}{1 + \exp(-x)}$



MLP

Linear Model

$$H = XW + b \ \ (W \in \mathcal{R}^{2\times1}, b \in \mathcal{R}^{1}, H \in \mathcal{R}^{N\times1})$$

MLP Model

$$Let\ relu(X) = max(X, 0)$$

$$h = relu(XW_1 + b_1) \ \ (W_1 \in \mathcal{R}^{2\times200}, b_1 \in \mathcal{R}^{200}, h \in \mathcal{R}^{N\times200})$$

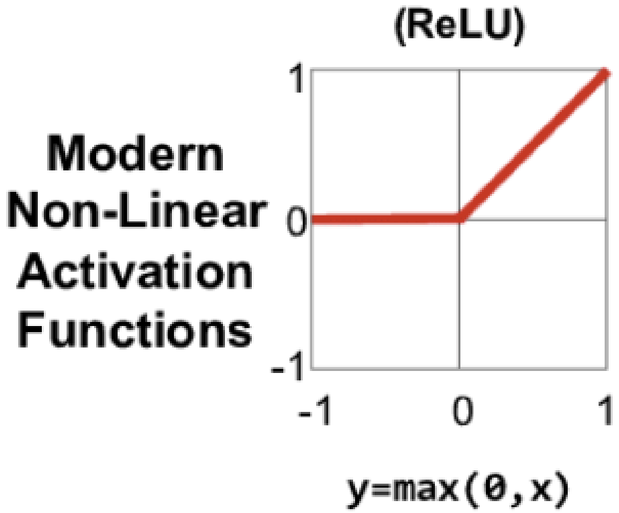
$$H = hW_2 + b_2 \ \ (W_2 \in \mathcal{R}^{200\times1}, b_2 \in \mathcal{R}^{1}, H \in \mathcal{R}^{N\times1})$$

MLP

MLP Regression with Pytorch

```
import torch
import torch.nn as nn
```

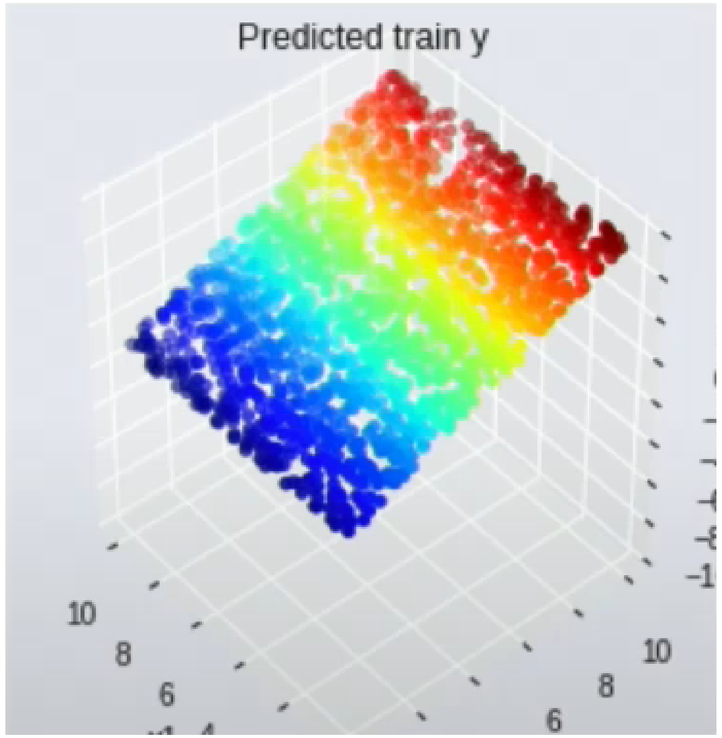
```
class MLPModel(nn.Module):
    def __init__(self):
        super(MLPModel, self).__init__()
        self.linear1 = nn.Linear(in_features=2, out_features=200)
        self.linear2 = nn.Linear(in_features=200, out_features=1)
        self.relu = nn.ReLU()

    def forward(self, x):
    # 인스턴스(샘플) x가 인풋으로 들어왔을 때 모델이 예측하는 y값을 리턴합니다.
        x = self.linear1(x)
        x = self.relu(x)
        x = self.linear2(x)
        return x
```



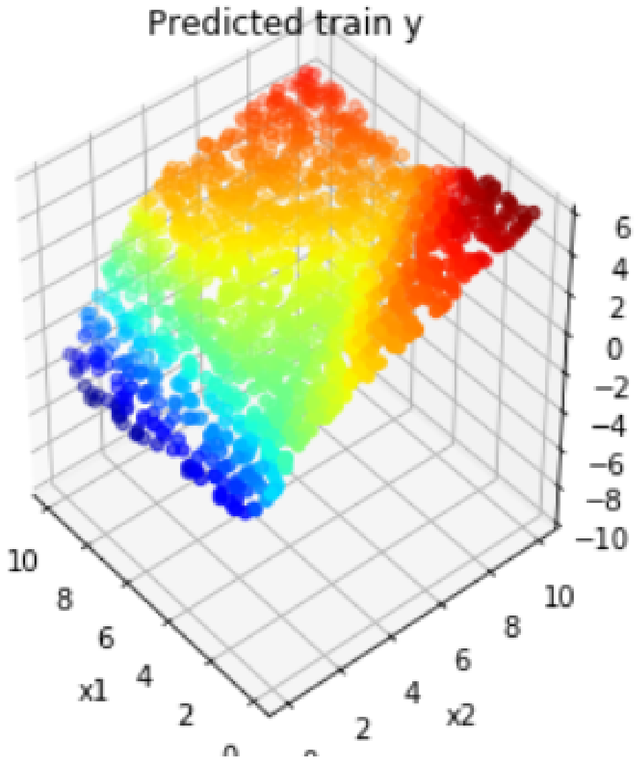
MLP

MLP Regression with Pytorch

- Linear model

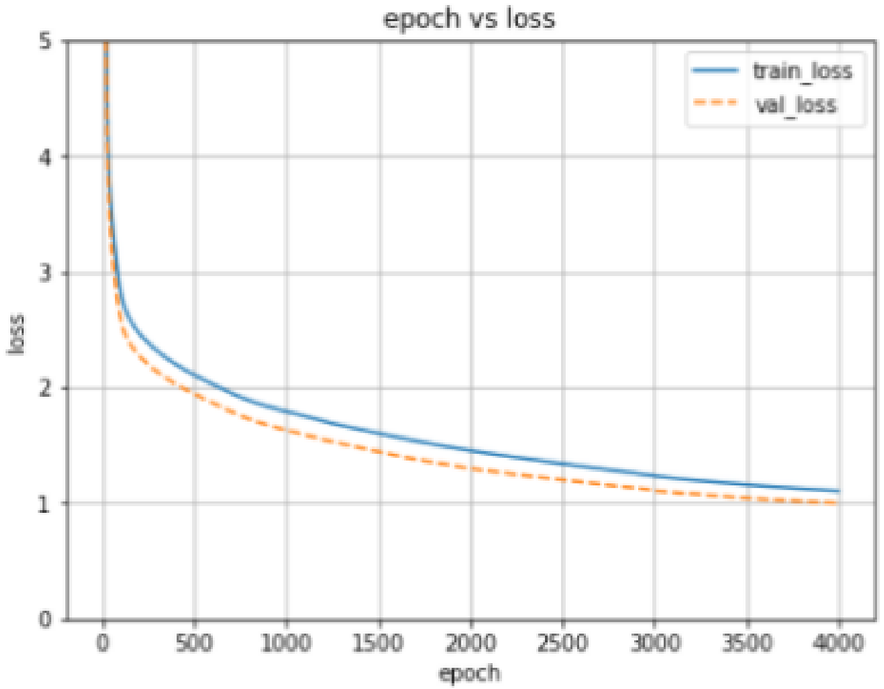


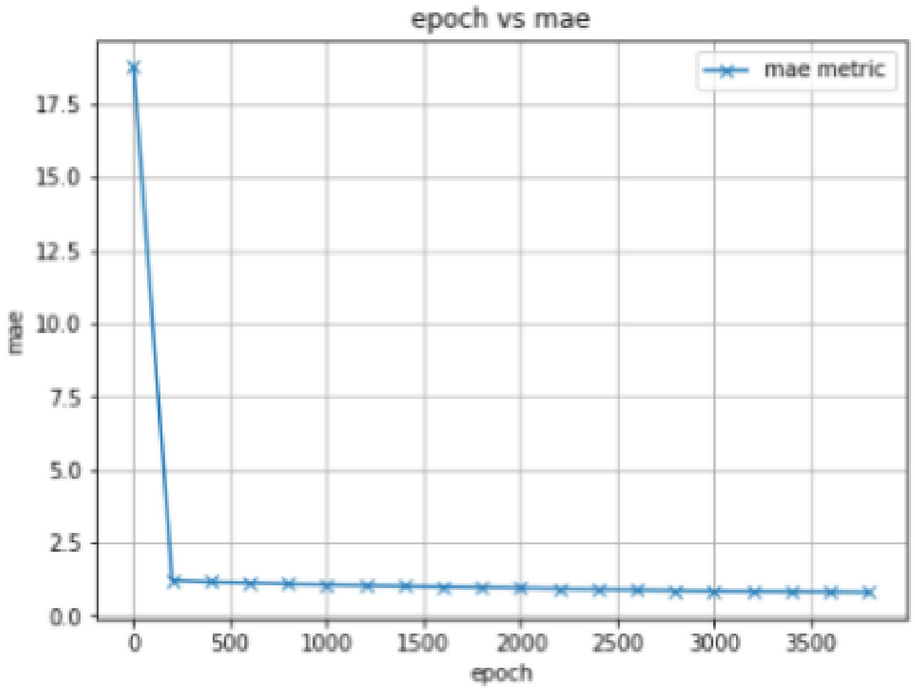
- MLP model



MLP

MLP Regression with Pytorch





Parametrize

How to Parametrize Entire Code

- What is Parametrization?
- Why Parametrization?
- Which parameter? Hyperparameter!

Parametrize

How to Parametrize Entire Code

- Hyperparameter

```
seed = 123
np.random.seed(seed)
torch.manual_seed(seed)
args = parser.parse_args("")

##### SIZE #####
args.vocab_size = 41
args.in_dim = 59
args.out_dim = 256
args.molvec_dim = 512

##### MODEL #####
args.num_layers = 6
args.use_attn = True
args.n_attn_heads = 8
args.use_bn = True
args.sc_type = 'sc'
args.emb_train = True
args.train_logp = True
args.train_mr = True
args.train_tpsa = True
```

Determine Model

```
##### HYPERPARAMETERS #####
args.optim = 'ADAM'
args.lr = 0.001
args.l2_coef = 0.001
args.dp_rate = 0.1

##### EXP #####
args.epoch = 100
args.batch_size = 512
args.test_batch_size = 512
args.save_every = 100
args.validate_every = 100
args.log_every = 20

##### DEVICE #####
args.device = 'cuda' if torch.cuda.is_available() else 'cpu'

##### LOGGING #####
args.log_path = 'runs'
args.model_name = 'exp_test3'
```

Optimizer Related

Training/Evaluation Process Related

Device

Saving Exp Result

Thank you