

Week 3

Deep Learning / MLP

#8 History of DL / MLP Basic

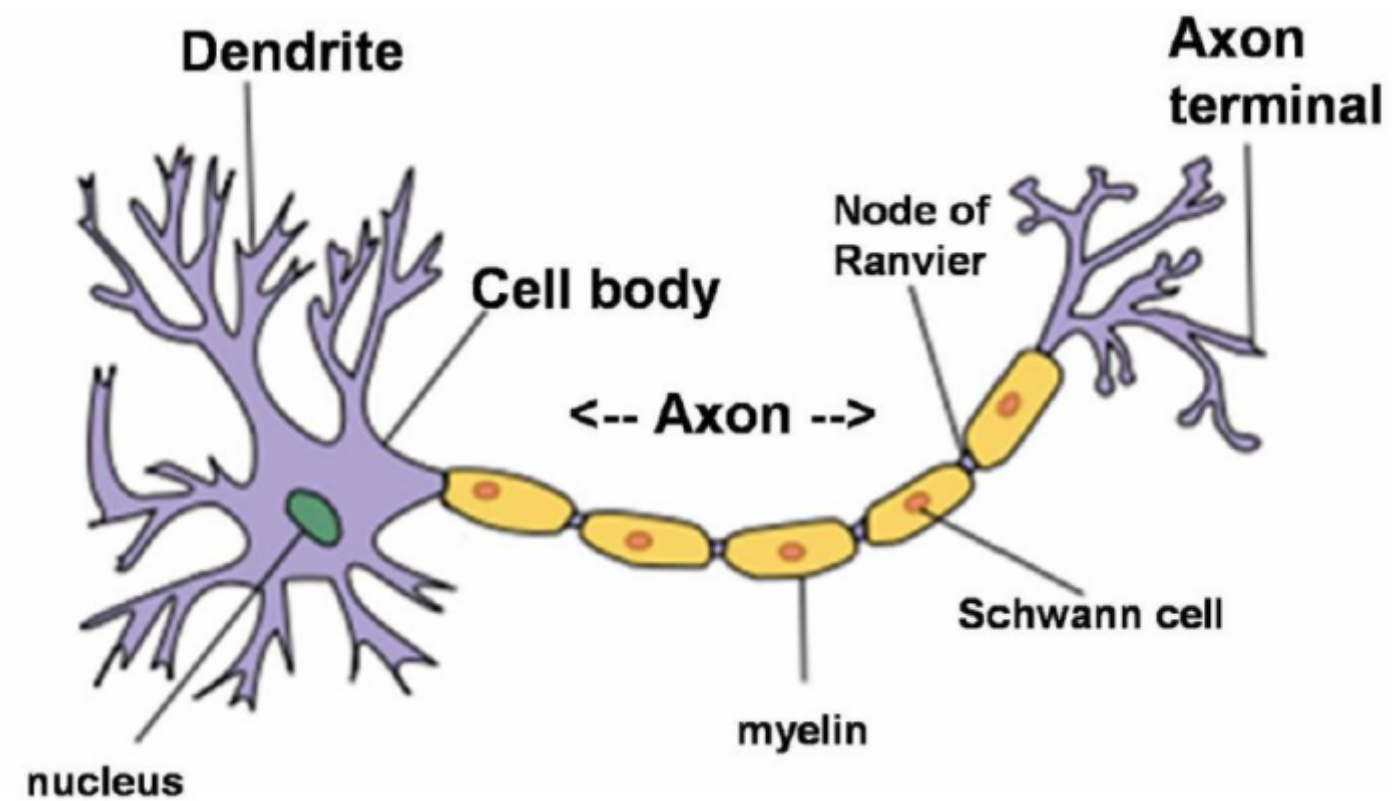
#9 MLP Regression with Pytorch / Assignment 1

#10 Assignment 1 Review

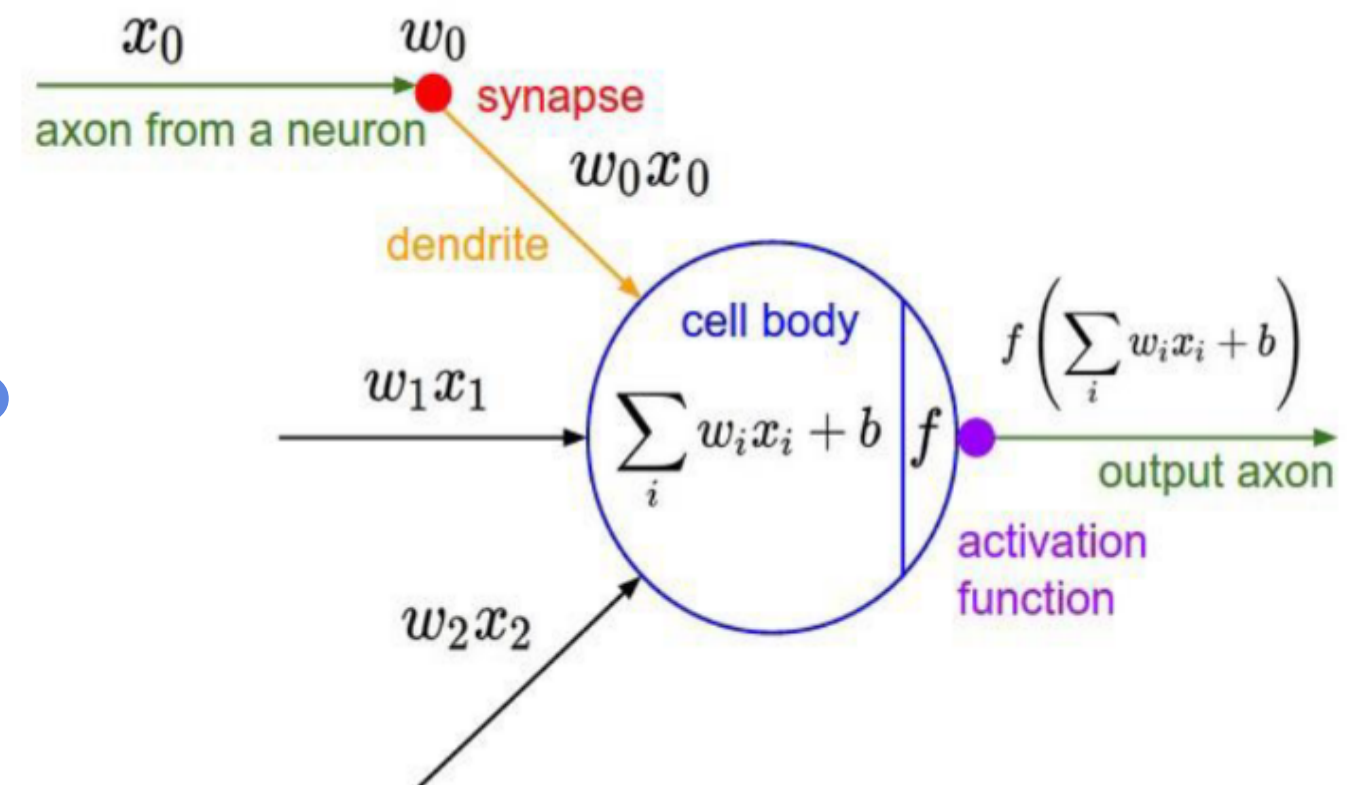
#11 How to parameterize DL code

2021.7.28 (3주차) 조수연

- Structure of Neuron

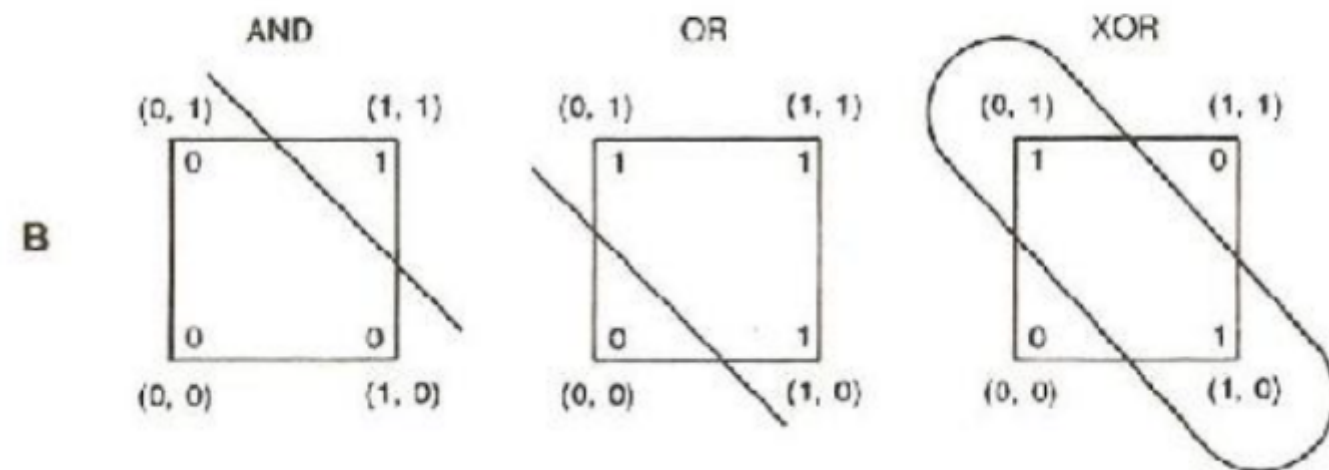
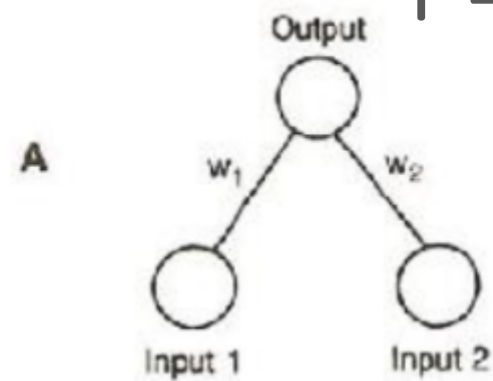


- Modeling Neuron (1957)

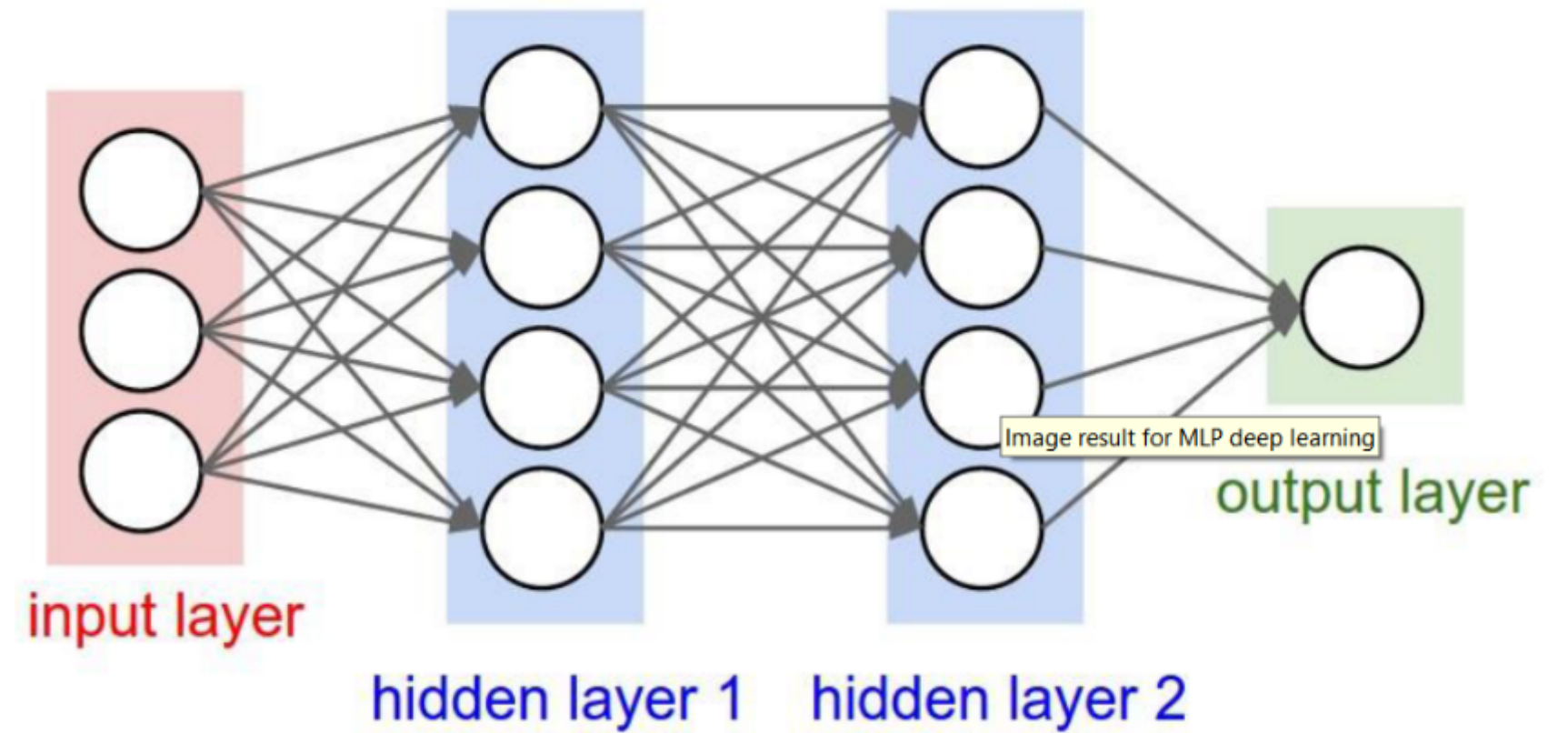


- And / Or Problem

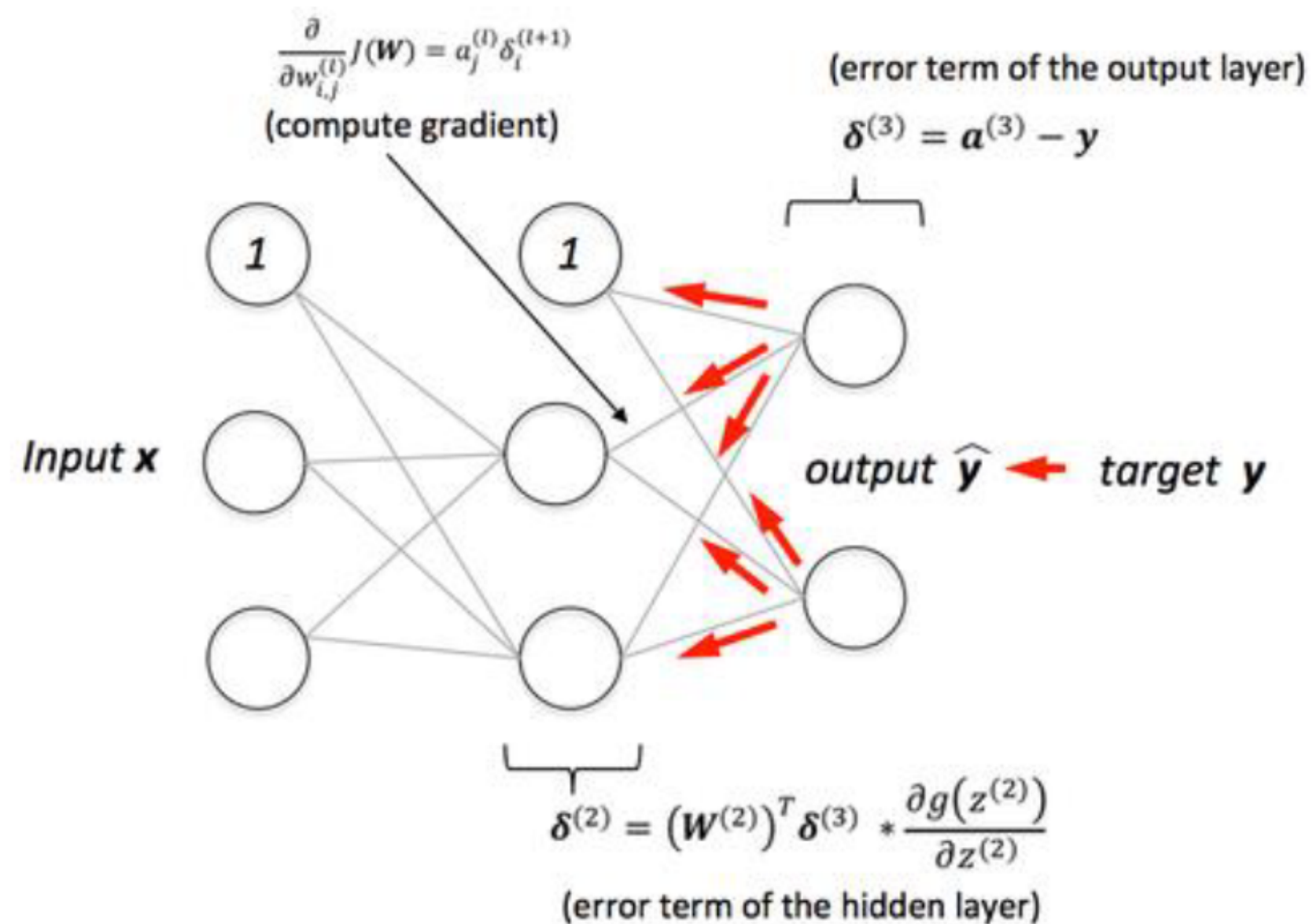
$$Y = w_1x_1 + w_2x_2 + b$$



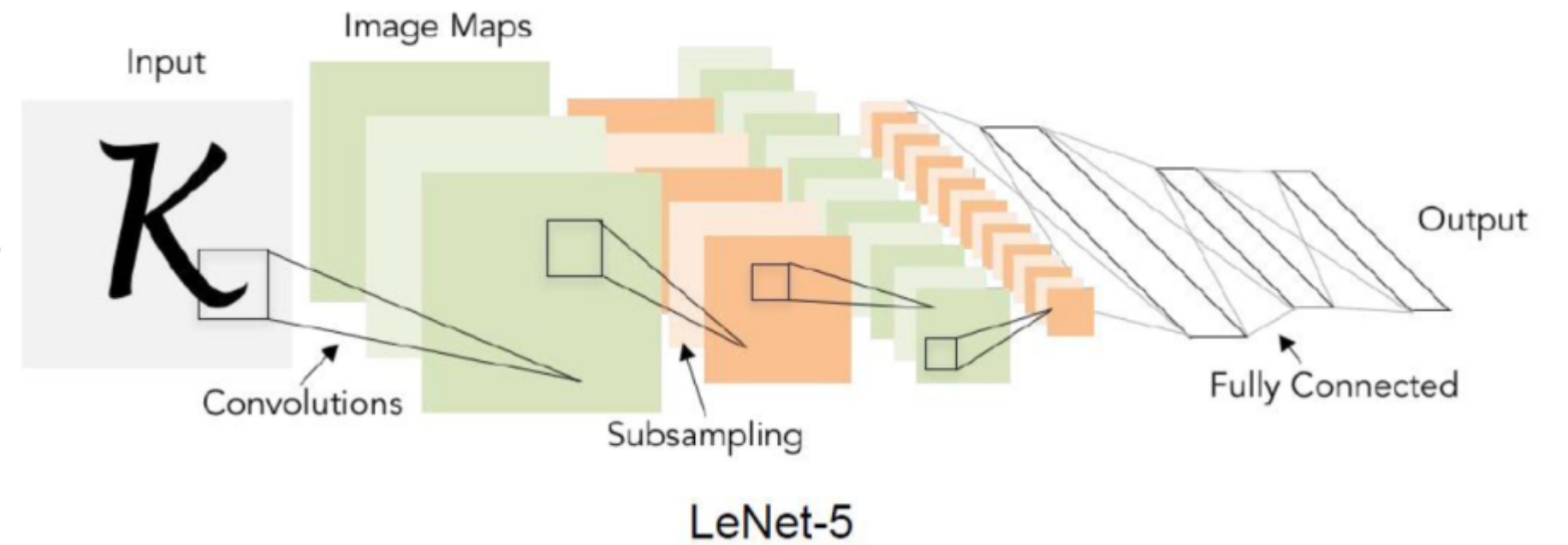
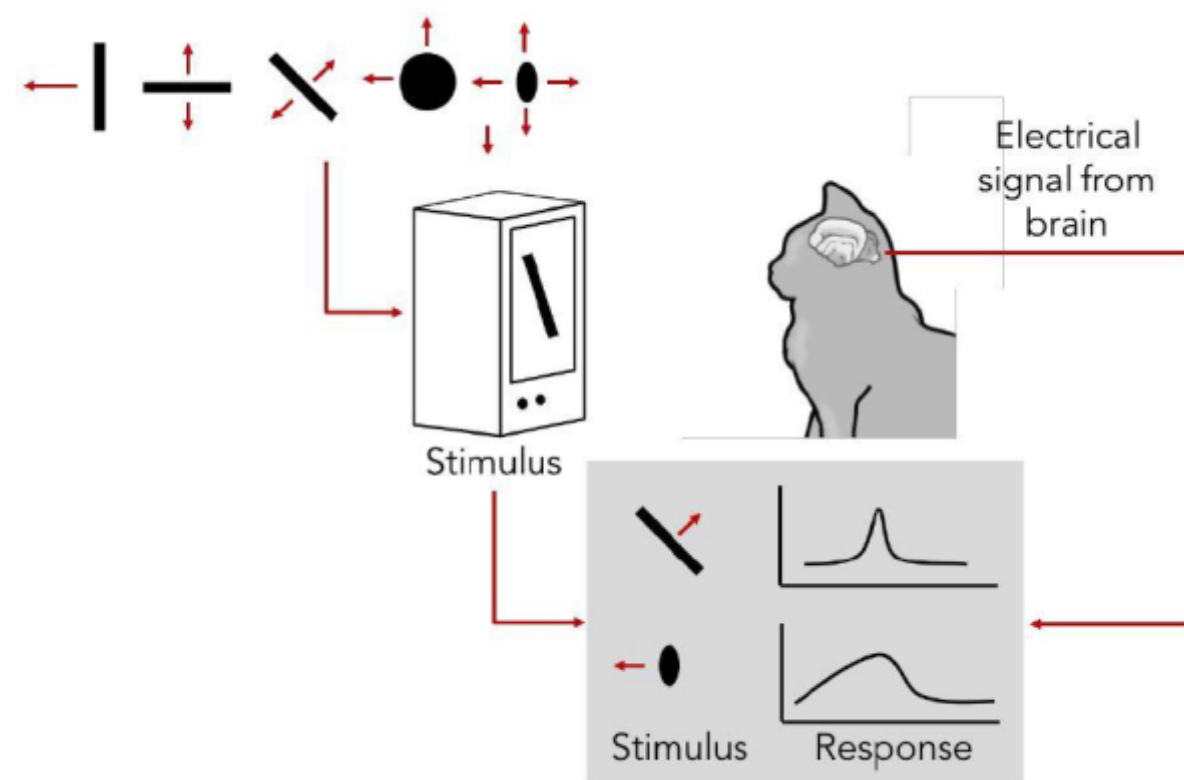
- Multilayer Perception (1969)



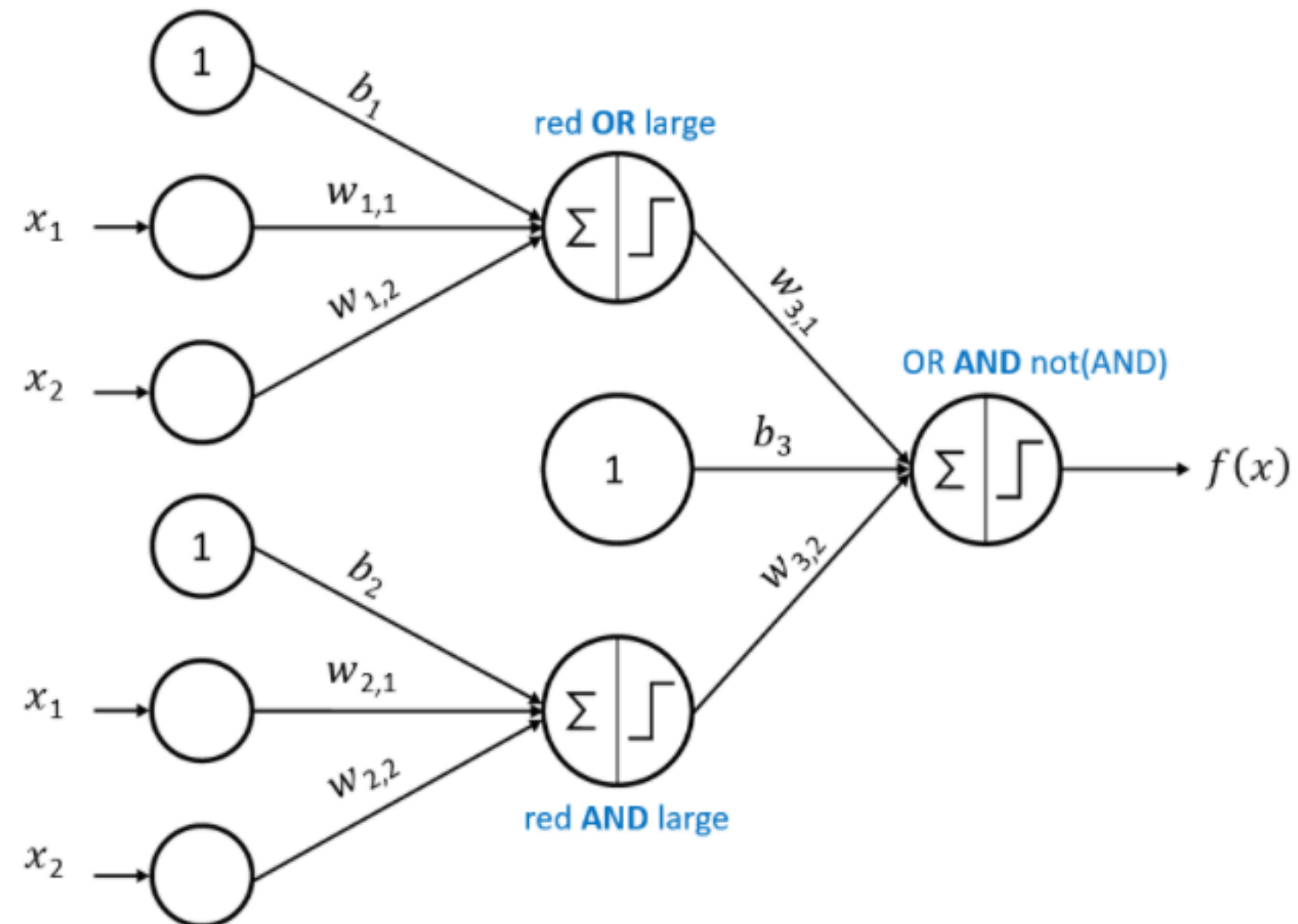
- Backpropagation (1986)



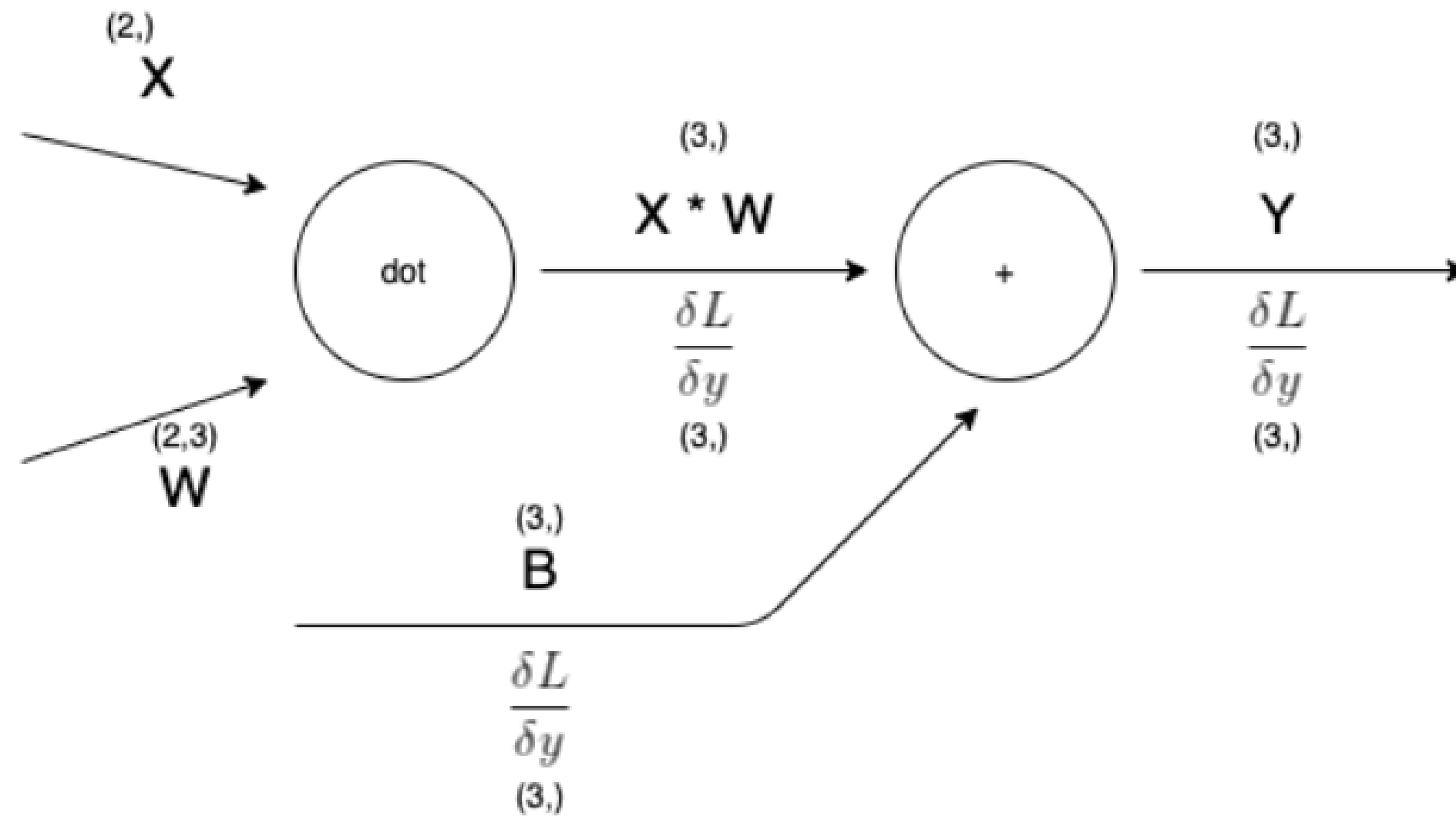
- Convolutional Neural Networks (2012)



- Solving XOR problem

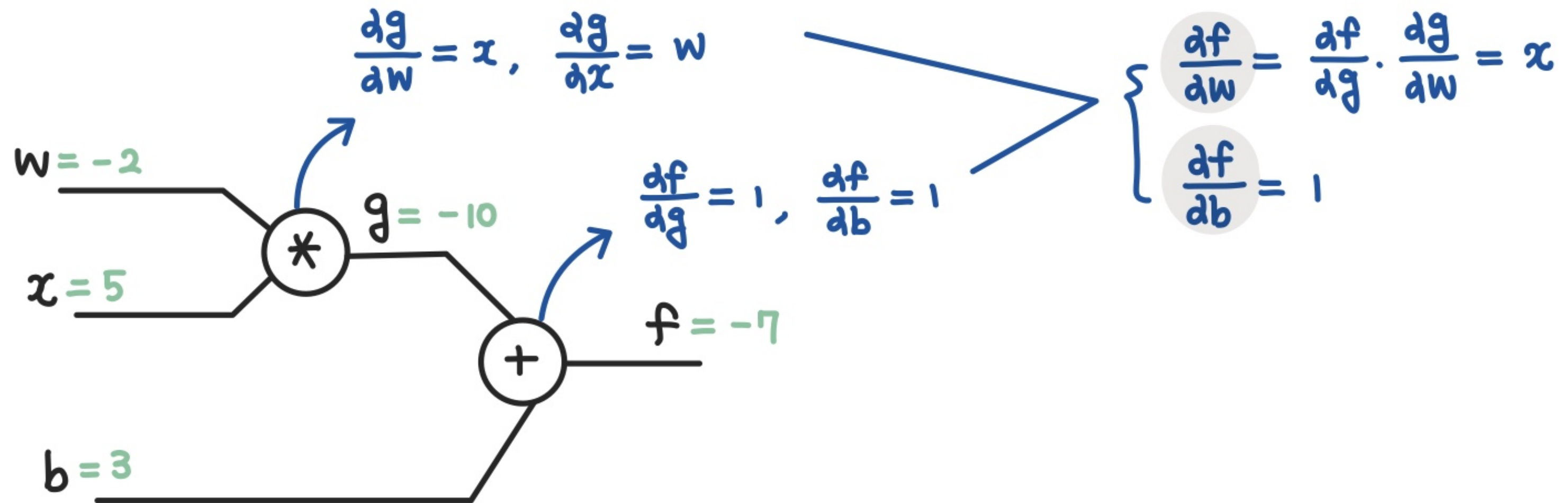


- Backpropagation with Chain Rule

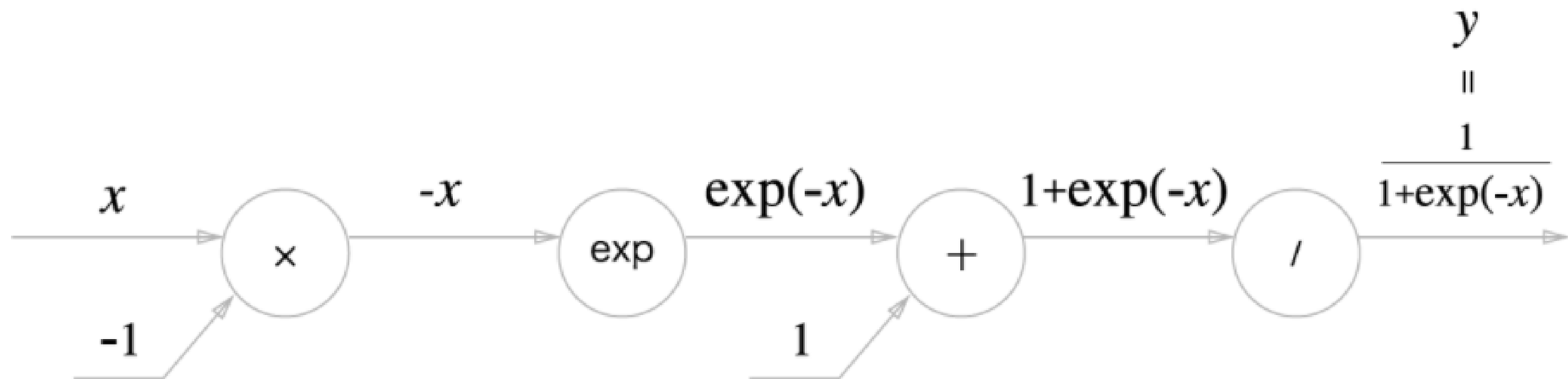


Training 하는 과정
1) Feed forward
2) Backpropagation

- 하나의 뉴런 식 : $f = g + b = wx + b$



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



Linear Model

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

MLP Model

$$\text{Let } \text{relu}(X) = \max(X, 0)$$

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

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

MLP

MLP Regression with Pytorch

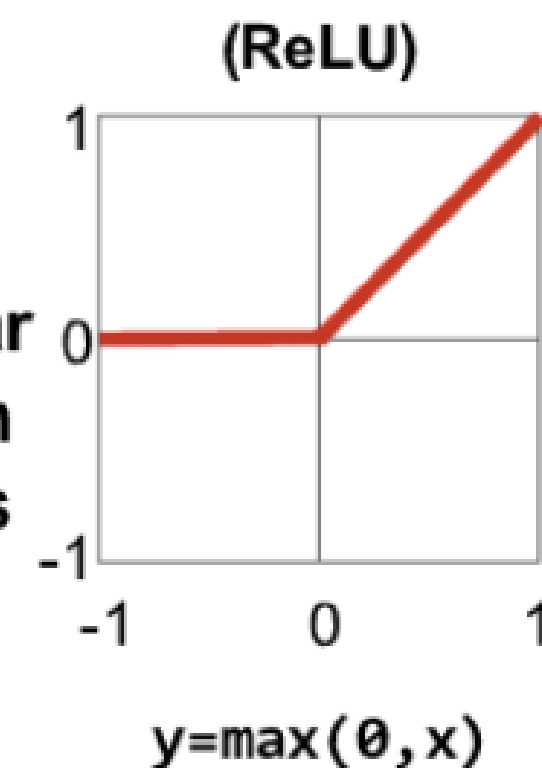


```
import torch
import torch.nn as nn
```

```
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
```

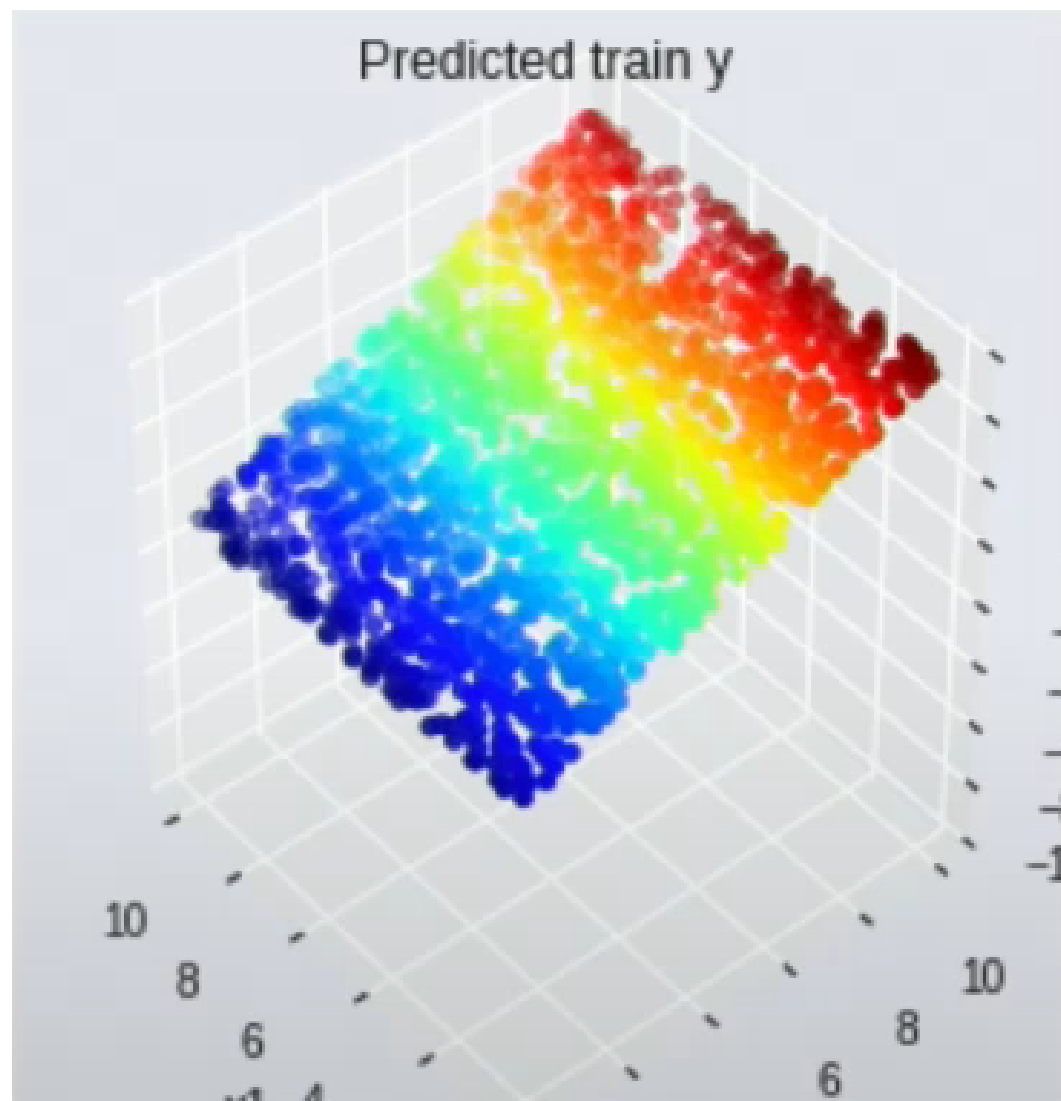
**Modern
Non-Linear
Activation
Functions**



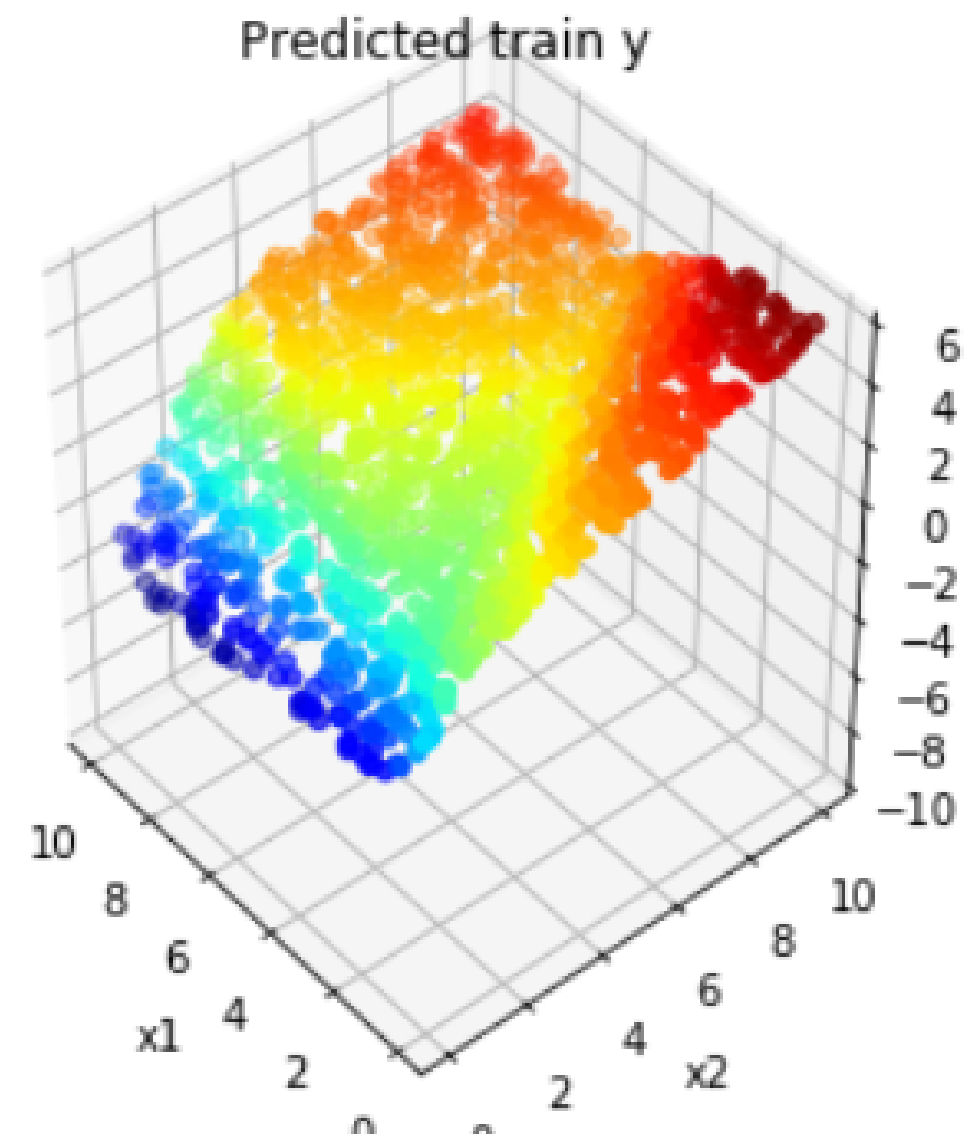
MLP

MLP Regression with Pytorch

- Linear model

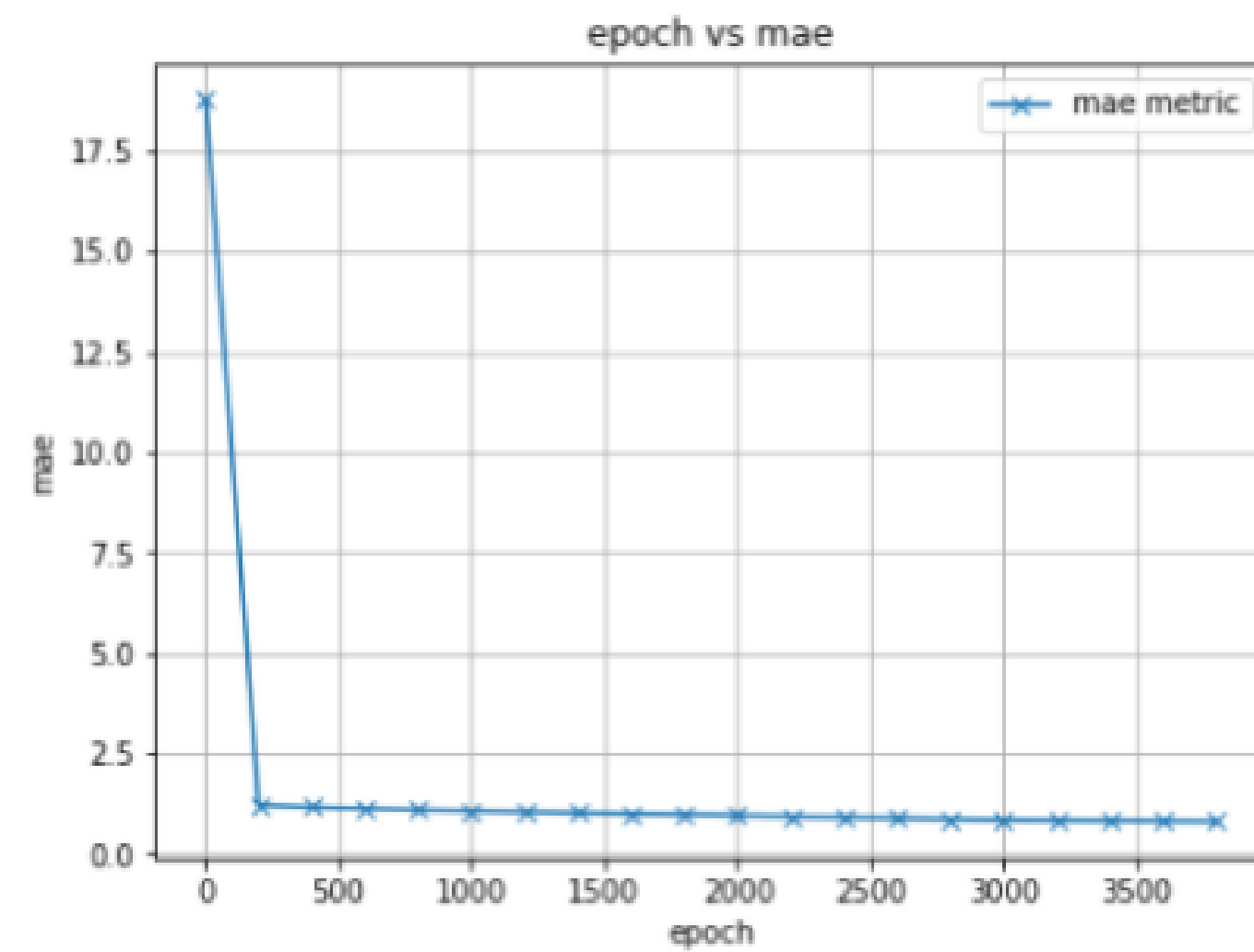
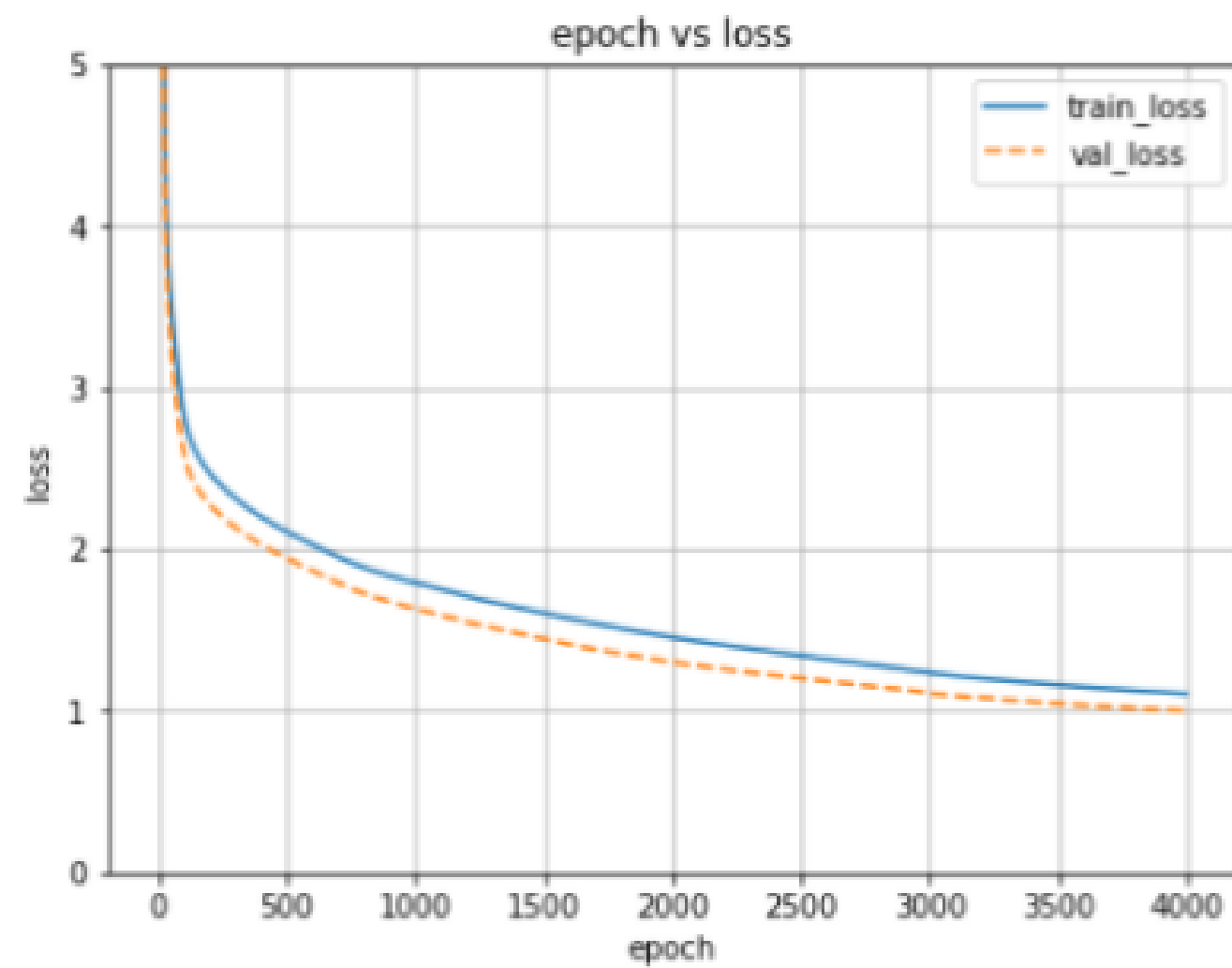


- MLP model



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
```

Optimizer Related

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
```

Training/Evaluation Process Related

DEVICE

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

Device

LOGGING

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

Saving Exp Result

Thank you