DL_LAB1

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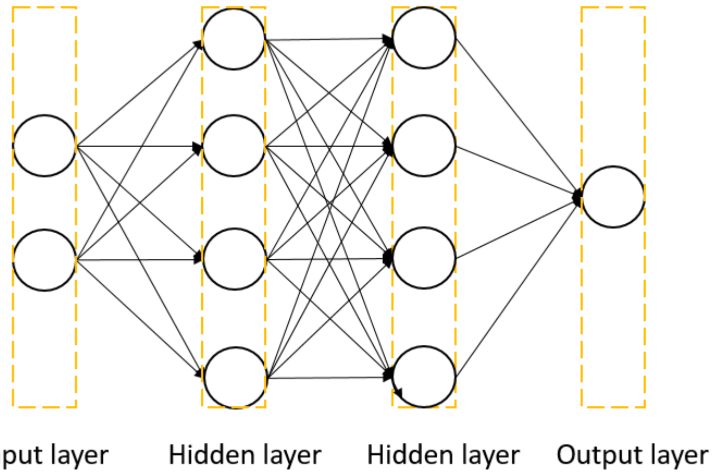
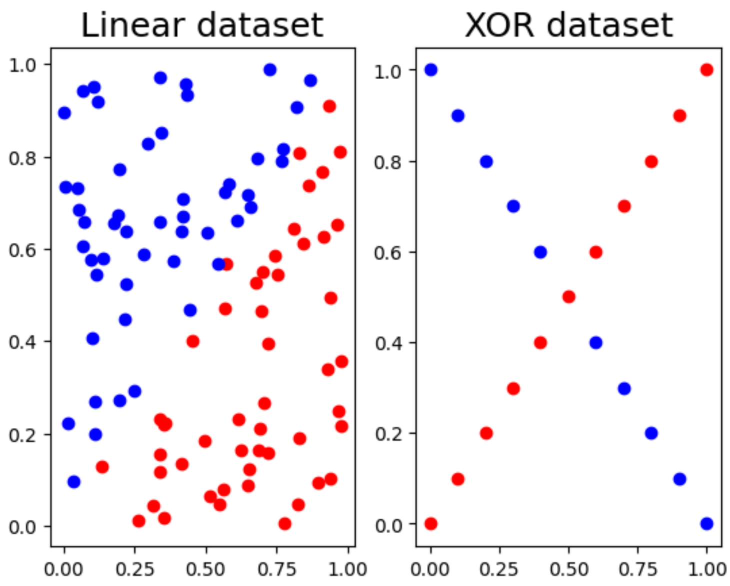
1. Introduction

在這個 Lab 中，需要實作一個具有 2 層 Hidden Layer 的 Multilayer Perceptron(MLP) ，並實現其 forward, back propagation，以及嘗試不同的 activation function 與 optimizer。



MLP

在建立完成 MLP 後，需要利用給定的 Linear Data 以及 XOR Data 進行訓練，並嘗試不同的訓練設定，以了解各項參數對於模型的影響。



Dataset

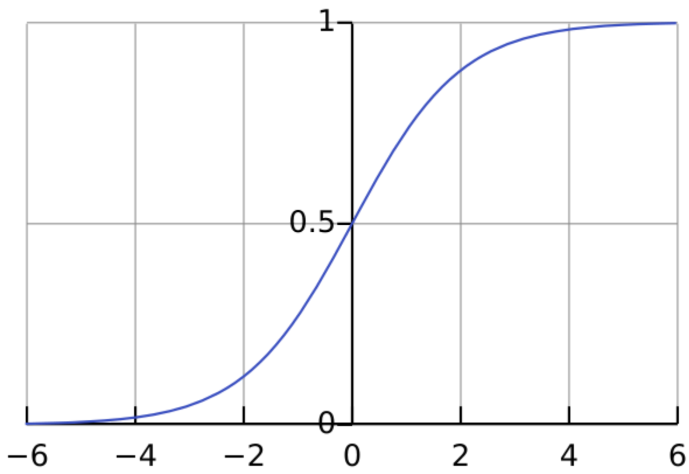
2. Experiment setups

A. Sigmoid functions

使用 Sigmoid 函數作為 Activation Function，其函數如下：

$$\sigma(x) = \frac{1}{1+e^{-x}}$$

由於 Sigmoid 函數輸出的範圍在 $[0, 1]$ 之間，因此可以很適合用來作為 Binary Classification 的 Activation Function。



Sigmoid

在訓練過程中，需要對 Activation Function 進行微分，而 Sigmoid 函數的微分如下：

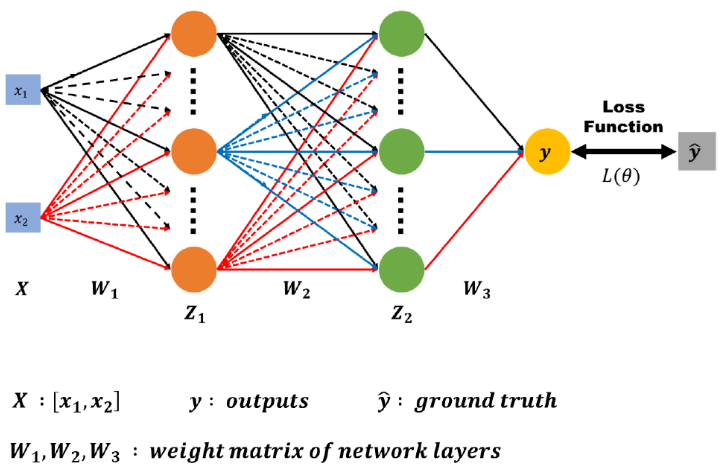
$$\sigma'(x) = \sigma(x) \cdot (1 - \sigma(x))$$

在實作時，我定義了一個 `Sigmoid` class，並在其中定義了 `forward` 與 `backward` 函數，分別用來計算 Sigmoid 函數的正向與反向傳播，其他 Activation Function 也是類似的實作方式。

```
class Sigmoid(Layer):
    def __init__(self):
        super().__init__()
        self.out = None

    def __str__(self) -> str:
        return "Sigmoid"

    def forward(self, x: np.ndarray) -> np.ndarray:
        out = 1.0 / (1.0 + np.exp(-x))
        self.out = out
        return out

    def backward(self, dout: np.ndarray) -> np.ndarray:
        dx = dout * (1.0 - self.out) * self.out
        return dx
```

B. Neural network

使用一個具有多層 Hidden Layer 的 Multilayer Perceptron(MLP) 作為模型，其架構如下：



Model

初始化時，需要指定每一層的輸入維度、輸出維度，以及 Activation Function 和 Optimizer，並且可以指定是否使用 Bias (Linear Layer 或 Affine Layer)。

在初始化參數時，使用了 `np.random.randn` 來初始化權重 W，並且使用 `np.zeros` 來初始化 Bias b，並將這些參數保存在 `params` 中。同時，也使用 `OrderedDict` 來保存每一層的 Layer 使用的 Transformation 和 Activation Function，以便在 Forward 和 Backward 過程中能夠按照順序進行計算。

```
class MLP(Model):
    def __init__(self, input_size: int, hidden_size: List[int
                 lr: float=0.01, optimizer: Optimizer=SGD, la
        super().__init__()
        self.input_size = input_size
        self.hidden_size = hidden_size
        self.output_size = output_size

        self.lr = lr
        self.optimizer = optimizer(lr)
        self.layer = layer
        self.activation = activation

        self.params = {}
        for i, (x, y) in enumerate(pairwise([input_size] + hi
            self.params['W'+str(i)] = np.random.randn(x, y)
            self.params['b'+str(i)] = np.zeros(y)

        self.layers = OrderedDict()
        for i in range(1, len(hidden_size) + 2):
            self.layers[f'Layer{i}'] = self.layer(self.params
            self.layers[f'Activation{i}'] = activation()
```

在本次 Lab 中，我使用了 2 層具有 10 個 Hidden Unit 的 Hidden Layer，並且使用 Sigmoid 函數作為 Activation Function、使用 SGD 作為 Optimizer。

```
model = MLP(input_size=2, hidden_size=[10, 10], output_size=1
            lr=0.01, optimizer=SGD, activation=Sigmoid)
```

C. Backpropagation

在 Forward 過程中，需要將輸入 x 進行 Linear Transformation ，但由於這裡加上了 Bias，因此應為 Affine Transformation。將 Transformation 後的輸出進行 Activation Function 的計算，得到輸出 y。

單一層 Affine Layer 的 Forward 過程如下，圖片中的形狀大小為 3 的部分在本次 Lab 中為 10：

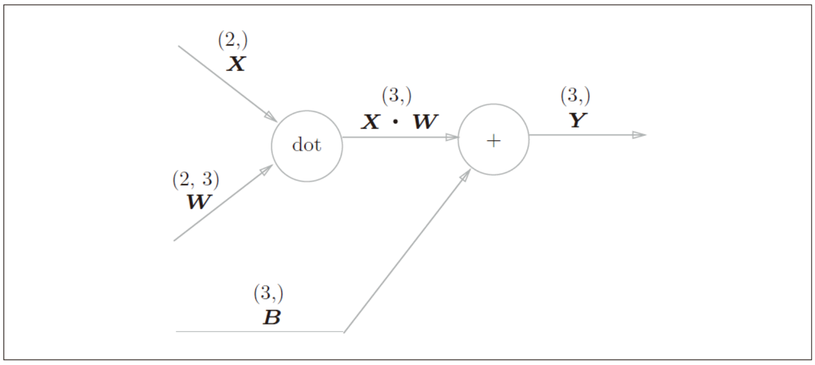


图5-24 Affine层的计算图（注意变量是矩阵，各个变量的上方标记了该变量的形状）

Affine Layer

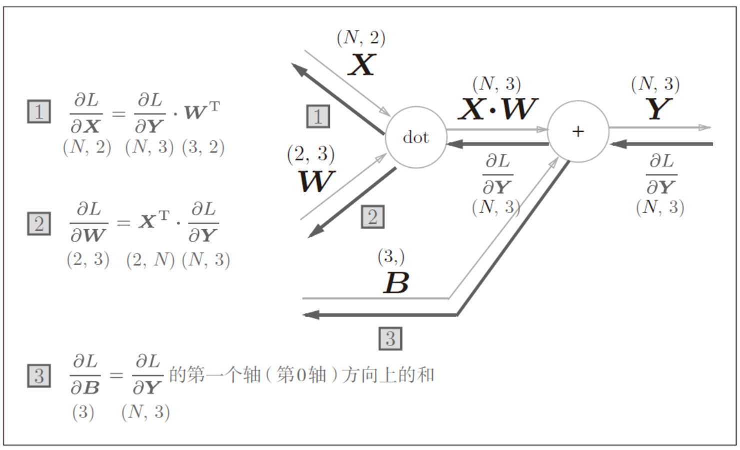
因此整個 Network 的 Forward 過程如下：

$$
\begin{aligned}
z_1 &= \sigma(xW_1 + b_1) \\
z_2 &= \sigma(z_1W_2 + b_2) \\
y &= \sigma(z_2W_3 + b_3)
\end{aligned}
$$

根據模型的輸出 y 和真實的標籤 $\hat{y}$ 之間的差距，可以計算出 Loss Function L，這裡使用了 Mean Squared Error(MSE) 作為 Loss Function。

$$
L = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2
$$

在計算完 loss function 後，需要使用 Backpropagation 來更新模型的權重，因此需要使用 Chain Rule 來計算 $\frac{\partial L}{\partial W_1}$、$\frac{\partial L}{\partial W_2}$、$\frac{\partial L}{\partial W_3}$ 以及 $\frac{\partial L}{\partial b_1}$、$\frac{\partial L}{\partial b_2}$、$\frac{\partial L}{\partial b_3}$。



Affine Layer 的 Backpropagation 計算

程式碼實現如下，其中 $dout$ 為 $\frac{\partial L}{\partial y}$，$dx$ 為 $\frac{\partial L}{\partial x}$，$dW$ 為 $\frac{\partial L}{\partial W}$，$db$ 為 $\frac{\partial L}{\partial b}$。

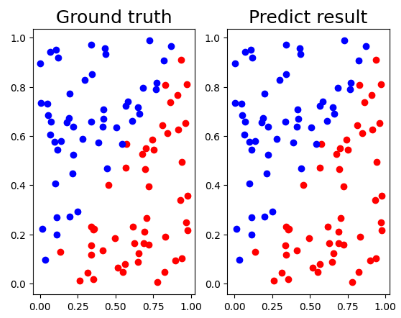
```python
class Affine(Layer):
    def forward(self, x: np.ndarray) -> np.ndarray:
        self.x = x
        out = np.dot(x, self.W) + self.b
        return out

    def backward(self, dout: np.ndarray) -> np.ndarray:
        dx = np.dot(dout, self.W.T)
        self.dW = np.dot(self.x.T, dout)
        self.db = np.sum(dout, axis=0)
        return dx
```

注意到不管是在 `Affine` Layer 還是在 `Sigmoid` Layer 中，都需要保存一些中間過程的變數，以便在 Backward 過程中使用。將這些變數保存在 attribute 中，這樣在 Backward 過程中就可以直接呼叫 `backward` 函數，而不需要再傳入前一層的梯度以外的參數。

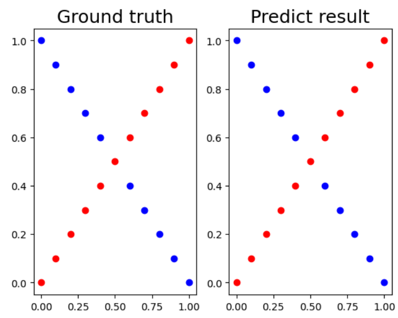
```python
    def forward(self, x):
        for layer in self.layers.values():
            x = layer.forward(x)
        self.pred_y = x
        return x

    def backward(self, y):
        dout = y
        for layer in reversed(self.layers.values()):
            dout = layer.backward(dout)
        return dout
```

3. Results of your testing

A. Screenshot and comparison figure



Linear Dataset



XOR Dataset

B. Show the accuracy of your prediction

Linear Data

loss:

```
epoch  1000 loss : 0.07849912063132942
epoch  2000 loss : 0.04520821461964975
epoch  3000 loss : 0.03313976789135106
epoch  4000 loss : 0.026940282327582377
epoch  5000 loss : 0.0231676558935124
epoch  6000 loss : 0.020597469744500184
epoch  7000 loss : 0.018696248300644046
epoch  8000 loss : 0.0172013349710097
epoch  9000 loss : 0.01597140118800952
epoch 10000 loss : 0.014924860070591127
epoch 11000 loss : 0.014011814589522444
epoch 12000 loss : 0.013200238163389779
epoch 13000 loss : 0.01246870731690159
epoch 14000 loss : 0.011802361939324704
epoch 15000 loss : 0.011190551366477411
epoch 16000 loss : 0.010625407146434231
epoch 17000 loss : 0.010100948298129709
epoch 18000 loss : 0.009612504451975824
epoch 19000 loss : 0.009156335033611893
epoch 20000 loss : 0.008729372736693393
```

prediction:

```
Iter: 0 |    Ground truth: [1] |     Predict: [1]
Iter: 1 |    Ground truth: [0] |     Predict: [0]
Iter: 2 |    Ground truth: [0] |     Predict: [0]
Iter: 3 |    Ground truth: [0] |     Predict: [0]
Iter: 4 |    Ground truth: [1] |     Predict: [1]
Iter: 5 |    Ground truth: [0] |     Predict: [0]
Iter: 6 |    Ground truth: [0] |     Predict: [0]
Iter: 7 |    Ground truth: [1] |     Predict: [1]
Iter: 8 |    Ground truth: [0] |     Predict: [0]
Iter: 9 |    Ground truth: [1] |     Predict: [1]
Iter: 10 |   Ground truth: [1] |     Predict: [1]
Iter: 11 |   Ground truth: [0] |     Predict: [0]
Iter: 12 |   Ground truth: [0] |     Predict: [0]
Iter: 13 |   Ground truth: [0] |     Predict: [0]
Iter: 14 |   Ground truth: [1] |     Predict: [1]
Iter: 15 |   Ground truth: [1] |     Predict: [1]
Iter: 16 |   Ground truth: [1] |     Predict: [1]
Iter: 17 |   Ground truth: [1] |     Predict: [1]
Iter: 18 |   Ground truth: [1] |     Predict: [1]
Iter: 19 |   Ground truth: [0] |     Predict: [0]
Iter: 20 |   Ground truth: [1] |     Predict: [1]
Iter: 21 |   Ground truth: [1] |     Predict: [1]
Iter: 22 |   Ground truth: [0] |     Predict: [0]
Iter: 23 |   Ground truth: [1] |     Predict: [1]
Iter: 24 |   Ground truth: [0] |     Predict: [0]
Iter: 25 |   Ground truth: [0] |     Predict: [0]
Iter: 26 |   Ground truth: [0] |     Predict: [0]
Iter: 27 |   Ground truth: [0] |     Predict: [0]
Iter: 28 |   Ground truth: [1] |     Predict: [1]
Iter: 29 |   Ground truth: [0] |     Predict: [0]
Iter: 30 |   Ground truth: [1] |     Predict: [1]
Iter: 31 |   Ground truth: [1] |     Predict: [1]
Iter: 32 |   Ground truth: [0] |     Predict: [0]
Iter: 33 |   Ground truth: [1] |     Predict: [1]
Iter: 34 |   Ground truth: [1] |     Predict: [1]
Iter: 35 |   Ground truth: [1] |     Predict: [1]
Iter: 36 |   Ground truth: [0] |     Predict: [0]
Iter: 37 |   Ground truth: [0] |     Predict: [0]
Iter: 38 |   Ground truth: [1] |     Predict: [1]
Iter: 39 |   Ground truth: [1] |     Predict: [1]
Iter: 40 |   Ground truth: [1] |     Predict: [1]
Iter: 41 |   Ground truth: [0] |     Predict: [0]
Iter: 42 |   Ground truth: [1] |     Predict: [1]
Iter: 43 |   Ground truth: [0] |     Predict: [0]
Iter: 44 |   Ground truth: [1] |     Predict: [1]
Iter: 45 |   Ground truth: [0] |     Predict: [0]
Iter: 46 |   Ground truth: [0] |     Predict: [0]
Iter: 47 |   Ground truth: [0] |     Predict: [0]
Iter: 48 |   Ground truth: [0] |     Predict: [0]
```

```
Iter: 49 |   Ground truth: [0] |      Predict: [0]
Iter: 50 |   Ground truth: [1] |      Predict: [1]
Iter: 51 |   Ground truth: [0] |      Predict: [0]
Iter: 52 |   Ground truth: [1] |      Predict: [1]
Iter: 53 |   Ground truth: [1] |      Predict: [1]
Iter: 54 |   Ground truth: [0] |      Predict: [0]
Iter: 55 |   Ground truth: [1] |      Predict: [1]
Iter: 56 |   Ground truth: [1] |      Predict: [1]
Iter: 57 |   Ground truth: [1] |      Predict: [1]
Iter: 58 |   Ground truth: [0] |      Predict: [0]
Iter: 59 |   Ground truth: [1] |      Predict: [1]
Iter: 60 |   Ground truth: [1] |      Predict: [1]
Iter: 61 |   Ground truth: [1] |      Predict: [1]
Iter: 62 |   Ground truth: [1] |      Predict: [1]
Iter: 63 |   Ground truth: [1] |      Predict: [1]
Iter: 64 |   Ground truth: [0] |      Predict: [0]
Iter: 65 |   Ground truth: [0] |      Predict: [0]
Iter: 66 |   Ground truth: [0] |      Predict: [0]
Iter: 67 |   Ground truth: [1] |      Predict: [1]
Iter: 68 |   Ground truth: [1] |      Predict: [1]
Iter: 69 |   Ground truth: [1] |      Predict: [1]
Iter: 70 |   Ground truth: [1] |      Predict: [1]
Iter: 71 |   Ground truth: [0] |      Predict: [0]
Iter: 72 |   Ground truth: [1] |      Predict: [1]
Iter: 73 |   Ground truth: [1] |      Predict: [1]
Iter: 74 |   Ground truth: [0] |      Predict: [0]
Iter: 75 |   Ground truth: [0] |      Predict: [0]
Iter: 76 |   Ground truth: [0] |      Predict: [0]
Iter: 77 |   Ground truth: [0] |      Predict: [0]
Iter: 78 |   Ground truth: [1] |      Predict: [1]
Iter: 79 |   Ground truth: [0] |      Predict: [0]
Iter: 80 |   Ground truth: [0] |      Predict: [0]
Iter: 81 |   Ground truth: [0] |      Predict: [0]
Iter: 82 |   Ground truth: [1] |      Predict: [1]
Iter: 83 |   Ground truth: [0] |      Predict: [0]
Iter: 84 |   Ground truth: [0] |      Predict: [0]
Iter: 85 |   Ground truth: [1] |      Predict: [1]
Iter: 86 |   Ground truth: [1] |      Predict: [1]
Iter: 87 |   Ground truth: [1] |      Predict: [1]
Iter: 88 |   Ground truth: [1] |      Predict: [1]
Iter: 89 |   Ground truth: [1] |      Predict: [1]
Iter: 90 |   Ground truth: [0] |      Predict: [0]
Iter: 91 |   Ground truth: [0] |      Predict: [0]
Iter: 92 |   Ground truth: [0] |      Predict: [0]
Iter: 93 |   Ground truth: [1] |      Predict: [1]
Iter: 94 |   Ground truth: [0] |      Predict: [0]
Iter: 95 |   Ground truth: [1] |      Predict: [1]
Iter: 96 |   Ground truth: [0] |      Predict: [0]
Iter: 97 |   Ground truth: [0] |      Predict: [0]
```

```
Iter: 98 |   Ground truth: [0] |     Predict: [0]
Iter: 99 |   Ground truth: [0] |     Predict: [0]
loss=0.00873 accuracy=100.00%
```

XOR Data

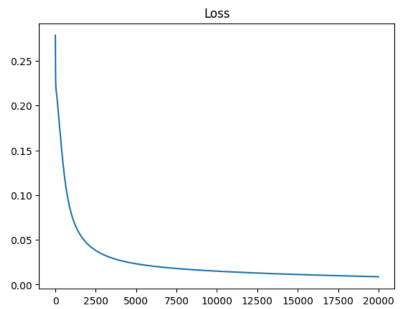
loss:

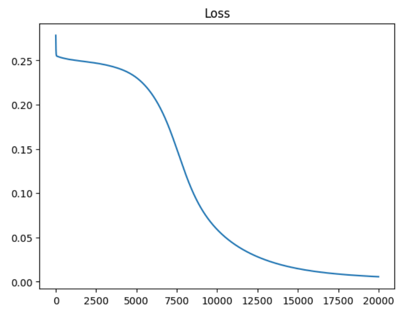
```
epoch  1000 loss : 0.2507043488190884
epoch  2000 loss : 0.24827133390907646
epoch  3000 loss : 0.24530348812303807
epoch  4000 loss : 0.2402814733403033
epoch  5000 loss : 0.23052597643483982
epoch  6000 loss : 0.21082976053330493
epoch  7000 loss : 0.1749271050808638
epoch  8000 loss : 0.12385950082031297
epoch  9000 loss : 0.0832229156422266
epoch 10000 loss : 0.05890902645016745
epoch 11000 loss : 0.04323208060886581
epoch 12000 loss : 0.03235669038687363
epoch 13000 loss : 0.024545998062900892
epoch 14000 loss : 0.01887006239216881
epoch 15000 loss : 0.014738278931597995
epoch 16000 loss : 0.011720456712043657
epoch 17000 loss : 0.009496796793265413
epoch 18000 loss : 0.007836141129906608
epoch 19000 loss : 0.0065758111998092195
epoch 20000 loss : 0.005602855922810573
```

prediction:

```
Iter: 0 |     Ground truth: [0] |      Predict: [0]
Iter: 1 |     Ground truth: [1] |      Predict: [1]
Iter: 2 |     Ground truth: [0] |      Predict: [0]
Iter: 3 |     Ground truth: [1] |      Predict: [1]
Iter: 4 |     Ground truth: [0] |      Predict: [0]
Iter: 5 |     Ground truth: [1] |      Predict: [1]
Iter: 6 |     Ground truth: [0] |      Predict: [0]
Iter: 7 |     Ground truth: [1] |      Predict: [1]
Iter: 8 |     Ground truth: [0] |      Predict: [0]
Iter: 9 |     Ground truth: [1] |      Predict: [1]
Iter: 10 |    Ground truth: [0] |      Predict: [0]
Iter: 11 |    Ground truth: [0] |      Predict: [0]
Iter: 12 |    Ground truth: [1] |      Predict: [1]
Iter: 13 |    Ground truth: [0] |      Predict: [0]
Iter: 14 |    Ground truth: [1] |      Predict: [1]
Iter: 15 |    Ground truth: [0] |      Predict: [0]
Iter: 16 |    Ground truth: [1] |      Predict: [1]
Iter: 17 |    Ground truth: [0] |      Predict: [0]
Iter: 18 |    Ground truth: [1] |      Predict: [1]
Iter: 19 |    Ground truth: [0] |      Predict: [0]
Iter: 20 |    Ground truth: [1] |      Predict: [1]
loss=0.00560 accuracy=100.00%
```

C. Learning curve (loss, epoch curve)





Linear Dataset	XOR Dataset

D. Anything you want to present

- 在 Backpropagation 過程中，若使用 $(y - \hat{y})$ 作為 Loss Function 的梯度，則在使用 Sigmoid 函數作為 Activation Function 時，會訓練的比較快，但在不使用 Activation Function 時，則無法訓練成功。若取 $\frac{2\times(y-\hat{y})}{n}$ 作為 Loss Function 的梯度，則在大部分的情況下，都可以訓練成功，但在以 Sigmoid 函數作為 Activation Function 時，需要相對較多的 Epochs。

4. Discussion

A. Try different learning rates

Parameters:

- hidden layer size = [10, 10]
- optimizer = SGD
- activation function = Sigmoid

lr	epochs	Linear	XOR
1	10000	100%	100%
0.5	10000	100%	100%
0.1	10000	100%	95.24%
0.1	20000	100%	100%
0.05	10000	98%	71.43%
0.05	50000	100%	100%
0.01	20000	98%	52.38%
0.01	50000	98%	71.43%

可以觀察到，在 Learning Rate 大時，模型的收斂速度較快，在 Learning Rate 小時，需要更多的 Epochs。此外，在 Learning Rate 過小時，也有可能會無法到達最佳解的位置。

B. Try different numbers of hidden units

hiddens	epochs	Linear	XOR
[20, 20]	20000	100%	100%
[5, 5]	20000	100%	85.71%
[5, 5]	50000	100%	100%
[2, 2]	20000	100%	71.43%
[2, 2]	50000	100%	100%

可以觀察到，當 Hidden Layer 太小時，模型無法很好的學習到 XOR Data 的特徵，但在增加 Epochs 後，仍然可以達到 100% 的準確率。

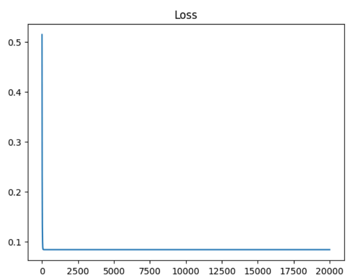
C. Try without activation functions

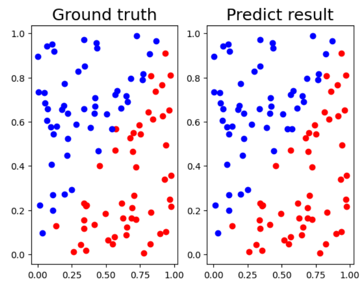
移除 Activation Function 後，部分的程式碼如下：

```
self.params = {}
for i, (x, y) in enumerate(pairwise([input_size] + hidden_siz
    self.params['W'+str(i)] = np.random.randn(x, y)
    self.params['b'+str(i)] = np.zeros(y)

self.layers = OrderedDict()
for i in range(1, len(hidden_size) + 2):
    self.layers[f'Layer{i}'] = self.layer(self.params[f'W{i}'
```

Parameters:

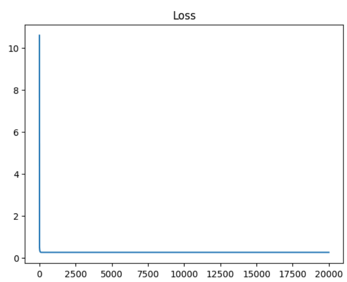
- hidden layer size = [5, 5]
- learning rate = 0.01
- optimizer = SGD
- activation function = Sigmoid
- epochs = 20000

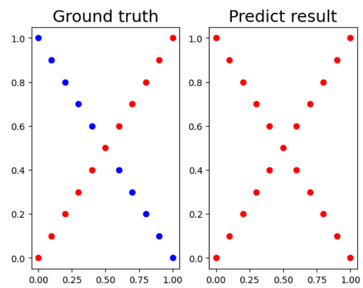




Loss of Linear dataset

Result of Linear dataset (99.00%)





Loss of XOR dataset

Result of XOR dataset (52.38%)

若不使用 Activation Function，則不管使用多少層 Hidden Layer，都仍然只是一個線性模型，無法學習到 XOR Data 的特徵。

5. Extra

A. Implement different optimizers

除了使用 SGD 作為 Optimizer 外，我也實作了 AdaGrad，部分的程式碼如下：

```
class AdaGrad(Optimizer):
    def __init__(self, lr: float=0.01):
        self.lr = lr
        self.eps = 1e-7
        self.h = None

    def update(self, params: Dict[str, np.ndarray], grads: Di
        if self.h is None:
            self.h = {}
            for key, val in params.items():
                self.h[key] = np.zeros_like(val)

        for key in params.keys():
            self.h[key] += grads[key] ** 2
            params[key] -= self.lr * grads[key] / (np.sqrt(se
        return params
```

Parameters:

- hidden layer size = [10, 10]
- activation function = Sigmoid

optimizer	lr	epochs	Linear	XOR
AdaGrad	0.1	10000	100%	100%
SGD	0.1	10000	100%	95.24%
AdaGrad	0.01	10000	99%	100%
SGD	0.01	20000	98%	52.38%

可以觀察到，AdaGrad 需要的 Epochs 較少，且在 XOR Data 上的表現也較好。

B. Implement different activation functions

ReLU

```python
class ReLU(Layer):
    def forward(self, x: np.ndarray) -> np.ndarray:
        self.mask = (x <= 0)
        out = x.copy()
        out[self.mask] = 0
        return out

    def backward(self, dout: np.ndarray) -> np.ndarray:
        dout[self.mask] = 0 # set non-positive elements to 0
        dx = dout
        return dx
```

Parameters:

- hidden layer size = [10, 10]
- learning rate = 0.01
- optimizer = SGD
- activation function = ReLU
- epochs = 10000

Results:

- Linear dataset: 100%
- XOR dataset: 100%

Tanh

```python
class Tanh(Layer):
    def forward(self, x: np.ndarray) -> np.ndarray:
        out = np.tanh(x)
        self.out = out
        return out

    def backward(self, dout: np.ndarray) -> np.ndarray:
        dx = dout * (1 - self.out ** 2)
        return dx
```

Parameters:

- hidden layer size = [10, 10]
- learning rate = 0.01
- optimizer = SGD
- activation function = ReLU
- epochs = 10000

Results:

- Linear dataset: 98%
- XOR dataset: 100%