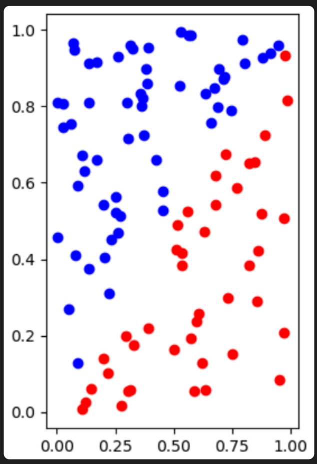
Lab 1 Back-propagation

313551055 柯柏旭

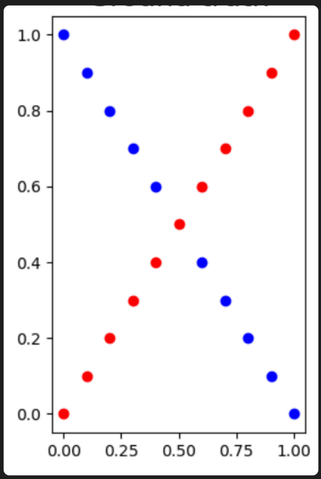
1. Introduction

在本報告中，我們將探討使用反向傳播算法訓練神經網絡的過程與結果。在 section `4.Discussion` 和 `5.Extra` ，我們將利用不同的學習率、激活函數、和優化器等等來訓練，目的是評估這些因素對模型性能的影響。通過詳細的測試和討論，我們將展示這些方法如何影響網絡在處理**Linear數據**和**XOR數據**時的學習和預測能力，以下為Linear數據和XOR數據的呈現方式:

- Linear data



- XOR data



對於 section `2.Experiment setups` 和 `3.Result of testing` 皆由 base code 的 `main.py` 來陳述。

至於 section `4.Discussion` 和 `5.Extra` 則會另外寫成 `diff_` 開頭的 codes。

2. Experiment setups

Hardware overview

```
Model Name: MacBook Pro
Model Identifier: Mac15,6
Model Number: MRX33TA/A
Chip: Apple M3 Pro
Total Number of Cores: 11 (5 performance and 6 efficiency)
Memory: 18 GB
```

Python version

```
Python 3.9.19
```

A. Sigmoid functions

```python
def sigmoid(x):
    return 1.0 / (1.0 + np.exp(-x))

def derivative_sigmoid(x):
    return np.multiply(x, 1.0 - x)
```

(refer to lab1 document)

B. Neural network

```python
def forward_propagation(X, weights):
    Z1 = np.dot(X, weights['W1']) + weights['b1']
    A1 = sigmoid(Z1)
    Z2 = np.dot(A1, weights['W2']) + weights['b2']
    A2 = sigmoid(Z2)
    Z3 = np.dot(A2, weights['W3']) + weights['b3']
    A3 = sigmoid(Z3)
    return Z1, A1, Z2, A2, Z3, A3
```

Each hidden layers is $y = wx + b$ and $sigmoid$ function

C. Backpropagation

```python
def back_propagation(X, y, weights, Z1, A1, Z2, A2, Z3, A3,
learning_rate):
    m = y.shape[0] # number of samples

    # compute gradients
    dZ3 = (A3 - y) * 2
    dW3 = np.dot(A2.T, dZ3) / m
    db3 = np.sum(dZ3, axis=0, keepdims=True) / m # 沿著 row 求和，並保持
維度

    dA2 = np.dot(dZ3, weights['W3'].T)
    dZ2 = dA2 * derivative_sigmoid(A2)
    dW2 = np.dot(A1.T, dZ2) / m
    db2 = np.sum(dZ2, axis=0, keepdims=True) / m

    dA1 = np.dot(dZ2, weights['W2'].T)
    dZ1 = dA1 * derivative_sigmoid(A1)
    dW1 = np.dot(X.T, dZ1) / m
    db1 = np.sum(dZ1, axis=0, keepdims=True) / m

    # update weights
    weights['W3'] -= learning_rate * dW3
    weights['b3'] -= learning_rate * db3
    weights['W2'] -= learning_rate * dW2
    weights['b2'] -= learning_rate * db2
    weights['W1'] -= learning_rate * dW1
    weights['b1'] -= learning_rate * db1
```

拿 $Z3, A3, W3$ 為例，推導如下：

首先定義$dZ3$如下

$dZ3 = \frac{\partial L}{\partial Z3}$ ，$dZ3 = 2 * (A3 - y)$

接著我們需要計算損失函數 (L) 對 權重(W3) 的梯度 ($dW3 = \frac{\partial L}{\partial W3}$)。

由於 ($Z3 = A2 \cdot W3 + b3$)，我們可以將 (L) 對 (W3) 的偏微分寫成：
$\frac{\partial L}{\partial W3} = \frac{\partial L}{\partial Z3} \cdot \frac{\partial Z3}{\partial W3}$

然後運用 chain rule，

首先計算 ($\frac{\partial Z3}{\partial W3}$) ：
$Z3 = A2 \cdot W3 + b3$

$\frac{\partial Z3}{\partial W3} = A2$

将上面的结果代入链式法则：
$\frac{\partial L}{\partial W3} = \frac{\partial L}{\partial Z3} \cdot A2$

由于 ($dZ3 = \frac{\partial L}{\partial Z3}$)，我们可以得到：
$dW3 = dZ3 \cdot A2$

D. Weight Initialization

```
def initialize_weights(input_size, hidden_size1, hidden_size2,
output_size):
    weights = {
        'W1': np.random.randn(input_size, hidden_size1), # shape:
(input_size, hidden_size1)
        'b1': np.zeros((1, hidden_size1)), # shape: (1, hidden_size1)
        'W2': np.random.randn(hidden_size1, hidden_size2),
        'b2': np.zeros((1, hidden_size2)),
        'W3': np.random.randn(hidden_size2, output_size),
        'b3': np.zeros((1, output_size))
    }
    return weights
```

$weights$大多會初始化在[-3, 3]之間

$bias$皆初始化為0

E. Loss function

```
# cost(loss) function: MSE
def compute_loss(y_true, y_pred):
    return np.mean((y_true - y_pred) ** 2)
```

loss (cost) function 為傳統 L2 norm

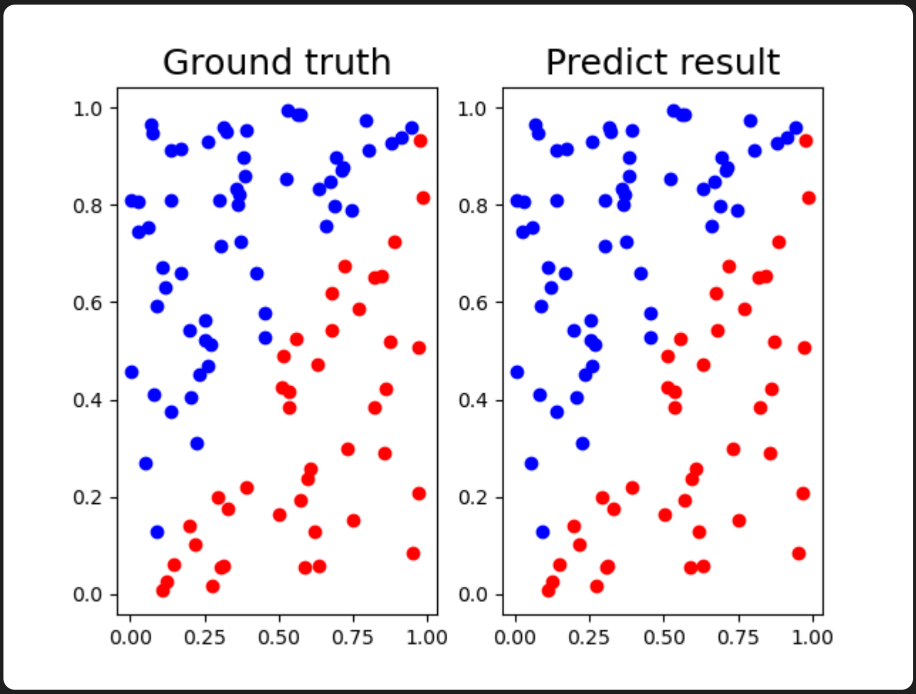
F. Train

```python
def train(X, y, input_size, hidden_size1, hidden_size2, output_size, learning_rate, epochs):
    weights = initialize_weights(input_size, hidden_size1, hidden_size2, output_size)

    for epoch in range(epochs):
        Z1, A1, Z2, A2, Z3, A3 = forward_propagation(X, weights)
        loss = compute_loss(y, A3)
        back_propagation(X, y, weights, Z1, A1, Z2, A2, Z3, A3, learning_rate)

        if epoch % 5000 == 0:
            print(f'Epoch {epoch}, Loss: {loss}')

    return weights
```

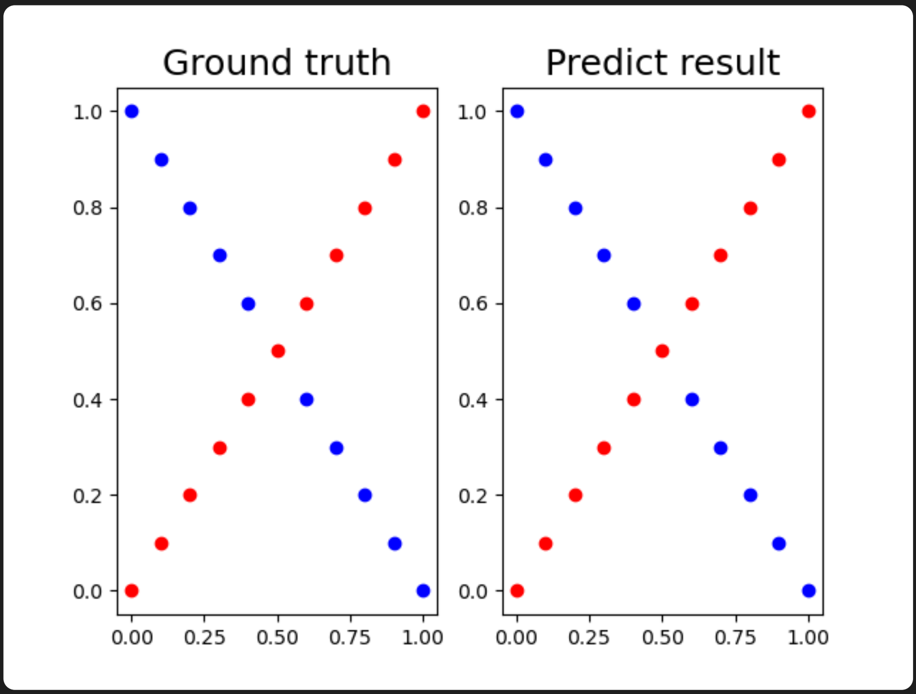
3. Result of testing

A. Screenshot and comparison figure

- Linear data



- XOR data



B. Show the accuracy of your prediction

- Linear data (acc = 100%)

```
Iter1 | Ground truth: 0 | prediction: 0.00000 |
Iter2 | Ground truth: 1 | prediction: 1.00000 |
Iter3 | Ground truth: 0 | prediction: 0.00000 |
Iter4 | Ground truth: 1 | prediction: 1.00000 |
Iter5 | Ground truth: 0 | prediction: 0.00000 |
Iter6 | Ground truth: 0 | prediction: 0.00000 |
Iter7 | Ground truth: 0 | prediction: 0.00000 |
Iter8 | Ground truth: 0 | prediction: 0.00000 |
Iter9 | Ground truth: 1 | prediction: 1.00000 |
Iter10 | Ground truth: 1 | prediction: 1.00000 |
Iter11 | Ground truth: 1 | prediction: 1.00000 |
Iter12 | Ground truth: 1 | prediction: 1.00000 |
Iter13 | Ground truth: 1 | prediction: 1.00000 |
Iter14 | Ground truth: 1 | prediction: 1.00000 |
Iter15 | Ground truth: 1 | prediction: 1.00000 |
Iter16 | Ground truth: 1 | prediction: 1.00000 |
Iter17 | Ground truth: 0 | prediction: 0.00000 |
Iter18 | Ground truth: 1 | prediction: 1.00000 |
Iter19 | Ground truth: 1 | prediction: 1.00000 |
```

```
Iter20 | Ground truth: 1 | prediction: 1.00000 |
Iter21 | Ground truth: 0 | prediction: 0.00000 |
Iter22 | Ground truth: 1 | prediction: 0.98980 |
Iter23 | Ground truth: 1 | prediction: 1.00000 |
Iter24 | Ground truth: 0 | prediction: 0.02334 |
Iter25 | Ground truth: 0 | prediction: 0.00000 |
Iter26 | Ground truth: 0 | prediction: 0.00000 |
Iter27 | Ground truth: 0 | prediction: 0.00000 |
Iter28 | Ground truth: 0 | prediction: 0.00000 |
Iter29 | Ground truth: 1 | prediction: 1.00000 |
Iter30 | Ground truth: 1 | prediction: 1.00000 |
Iter31 | Ground truth: 1 | prediction: 1.00000 |
Iter32 | Ground truth: 0 | prediction: 0.00000 |
Iter33 | Ground truth: 0 | prediction: 0.00002 |
Iter34 | Ground truth: 1 | prediction: 1.00000 |
Iter35 | Ground truth: 0 | prediction: 0.00000 |
Iter36 | Ground truth: 0 | prediction: 0.00000 |
Iter37 | Ground truth: 0 | prediction: 0.00000 |
Iter38 | Ground truth: 0 | prediction: 0.00000 |
Iter39 | Ground truth: 1 | prediction: 0.99978 |
Iter40 | Ground truth: 0 | prediction: 0.00000 |
Iter41 | Ground truth: 1 | prediction: 1.00000 |
Iter42 | Ground truth: 1 | prediction: 1.00000 |
Iter43 | Ground truth: 0 | prediction: 0.00000 |
Iter44 | Ground truth: 0 | prediction: 0.00000 |
Iter45 | Ground truth: 0 | prediction: 0.00000 |
Iter46 | Ground truth: 1 | prediction: 1.00000 |
Iter47 | Ground truth: 0 | prediction: 0.00003 |
Iter48 | Ground truth: 0 | prediction: 0.00000 |
Iter49 | Ground truth: 0 | prediction: 0.00000 |
Iter50 | Ground truth: 0 | prediction: 0.00006 |
Iter51 | Ground truth: 1 | prediction: 1.00000 |
Iter52 | Ground truth: 0 | prediction: 0.00000 |
Iter53 | Ground truth: 0 | prediction: 0.00000 |
Iter54 | Ground truth: 1 | prediction: 1.00000 |
Iter55 | Ground truth: 1 | prediction: 1.00000 |
Iter56 | Ground truth: 1 | prediction: 1.00000 |
```

```
Iter57 | Ground truth: 1 | prediction: 1.00000 |
Iter58 | Ground truth: 1 | prediction: 1.00000 |
Iter59 | Ground truth: 0 | prediction: 0.00000 |
Iter60 | Ground truth: 1 | prediction: 1.00000 |
Iter61 | Ground truth: 0 | prediction: 0.00000 |
Iter62 | Ground truth: 0 | prediction: 0.00000 |
Iter63 | Ground truth: 1 | prediction: 1.00000 |
Iter64 | Ground truth: 0 | prediction: 0.00000 |
Iter65 | Ground truth: 0 | prediction: 0.00000 |
Iter66 | Ground truth: 1 | prediction: 1.00000 |
Iter67 | Ground truth: 0 | prediction: 0.00000 |
Iter68 | Ground truth: 0 | prediction: 0.00000 |
Iter69 | Ground truth: 1 | prediction: 0.99995 |
Iter70 | Ground truth: 1 | prediction: 1.00000 |
Iter71 | Ground truth: 1 | prediction: 1.00000 |
Iter72 | Ground truth: 1 | prediction: 1.00000 |
Iter73 | Ground truth: 0 | prediction: 0.00000 |
Iter74 | Ground truth: 0 | prediction: 0.00000 |
Iter75 | Ground truth: 1 | prediction: 1.00000 |
Iter76 | Ground truth: 1 | prediction: 1.00000 |
Iter77 | Ground truth: 1 | prediction: 1.00000 |
Iter78 | Ground truth: 1 | prediction: 1.00000 |
Iter79 | Ground truth: 0 | prediction: 0.00000 |
Iter80 | Ground truth: 1 | prediction: 1.00000 |
Iter81 | Ground truth: 0 | prediction: 0.00000 |
Iter82 | Ground truth: 1 | prediction: 1.00000 |
Iter83 | Ground truth: 1 | prediction: 0.98803 |
Iter84 | Ground truth: 1 | prediction: 1.00000 |
Iter85 | Ground truth: 0 | prediction: 0.00000 |
Iter86 | Ground truth: 1 | prediction: 1.00000 |
Iter87 | Ground truth: 1 | prediction: 1.00000 |
Iter88 | Ground truth: 1 | prediction: 1.00000 |
Iter89 | Ground truth: 0 | prediction: 0.00000 |
Iter90 | Ground truth: 0 | prediction: 0.00000 |
Iter91 | Ground truth: 1 | prediction: 1.00000 |
Iter92 | Ground truth: 0 | prediction: 0.00000 |
Iter93 | Ground truth: 0 | prediction: 0.00000 |
```

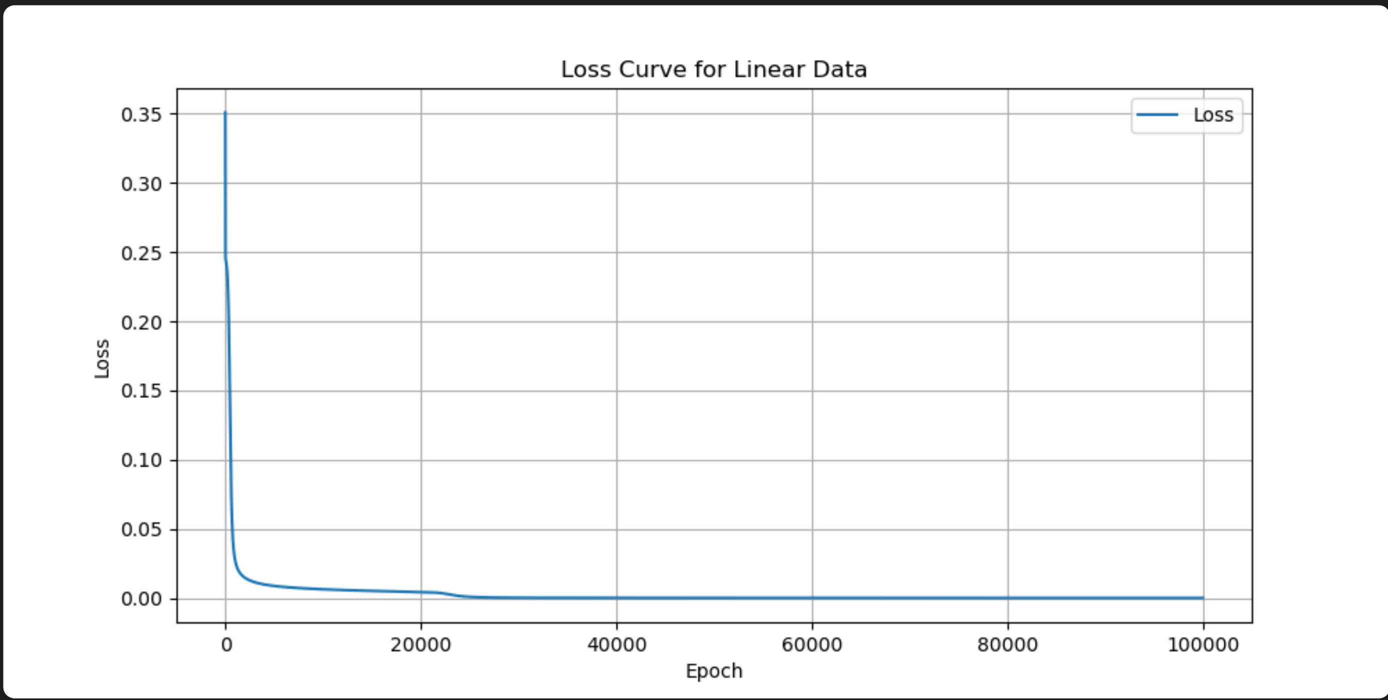
```
Iter94 | Ground truth: 1 | prediction: 1.00000 |
Iter95 | Ground truth: 0 | prediction: 0.00000 |
Iter96 | Ground truth: 1 | prediction: 1.00000 |
Iter97 | Ground truth: 1 | prediction: 1.00000 |
Iter98 | Ground truth: 0 | prediction: 0.00001 |
Iter99 | Ground truth: 1 | prediction: 1.00000 |
Iter100 | Ground truth: 1 | prediction: 1.00000 |
loss=0.0000079244 accuracy=100.00%
```

- XOR data (acc = 100%)

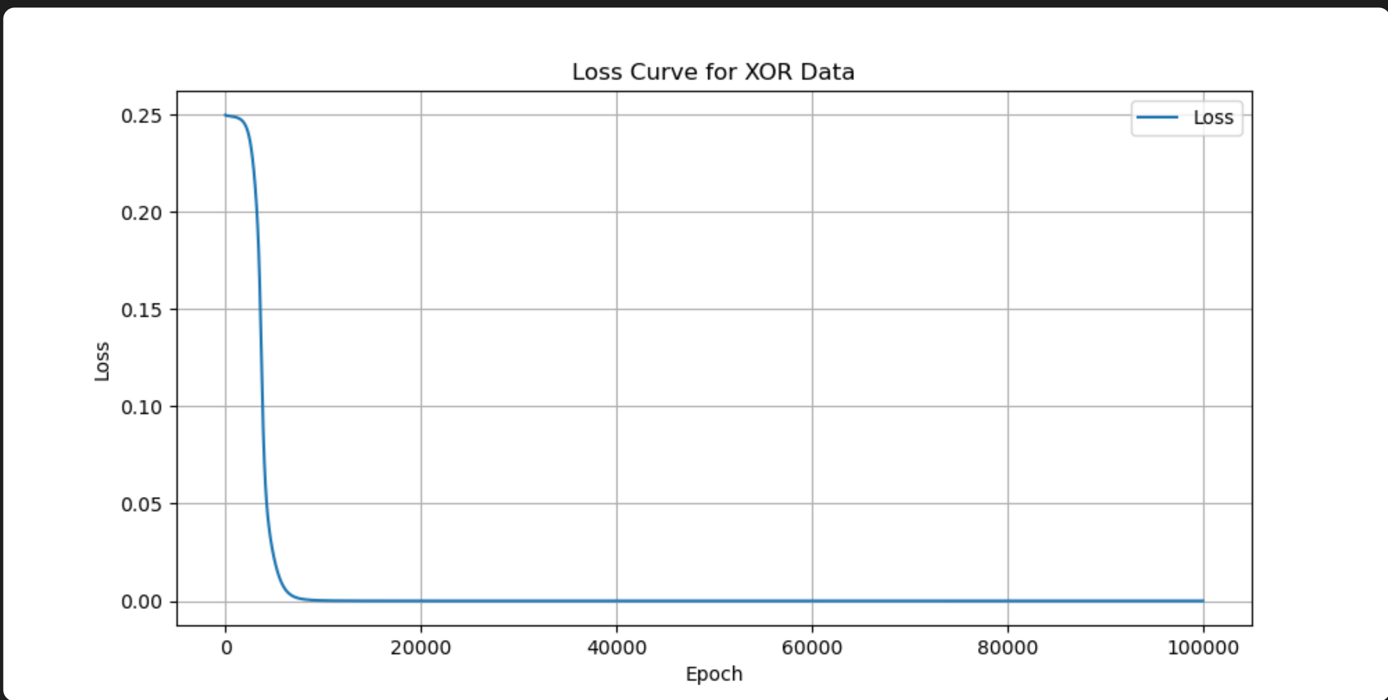
```
Iter1 | Ground truth: 0 | prediction: 0.00021 |
Iter2 | Ground truth: 1 | prediction: 0.99973 |
Iter3 | Ground truth: 0 | prediction: 0.00023 |
Iter4 | Ground truth: 1 | prediction: 0.99973 |
Iter5 | Ground truth: 0 | prediction: 0.00027 |
Iter6 | Ground truth: 1 | prediction: 0.99973 |
Iter7 | Ground truth: 0 | prediction: 0.00031 |
Iter8 | Ground truth: 1 | prediction: 0.99971 |
Iter9 | Ground truth: 0 | prediction: 0.00035 |
Iter10 | Ground truth: 1 | prediction: 0.99902 |
Iter11 | Ground truth: 0 | prediction: 0.00037 |
Iter12 | Ground truth: 0 | prediction: 0.00036 |
Iter13 | Ground truth: 1 | prediction: 0.99909 |
Iter14 | Ground truth: 0 | prediction: 0.00034 |
Iter15 | Ground truth: 1 | prediction: 0.99992 |
Iter16 | Ground truth: 0 | prediction: 0.00031 |
Iter17 | Ground truth: 1 | prediction: 0.99993 |
Iter18 | Ground truth: 0 | prediction: 0.00029 |
Iter19 | Ground truth: 1 | prediction: 0.99993 |
Iter20 | Ground truth: 0 | prediction: 0.00026 |
Iter21 | Ground truth: 1 | prediction: 0.99994 |
loss=0.0000001487 accuracy=100.00%
```

C. Learning curve (loss, epoch curve)

- Linear data



- XOR data

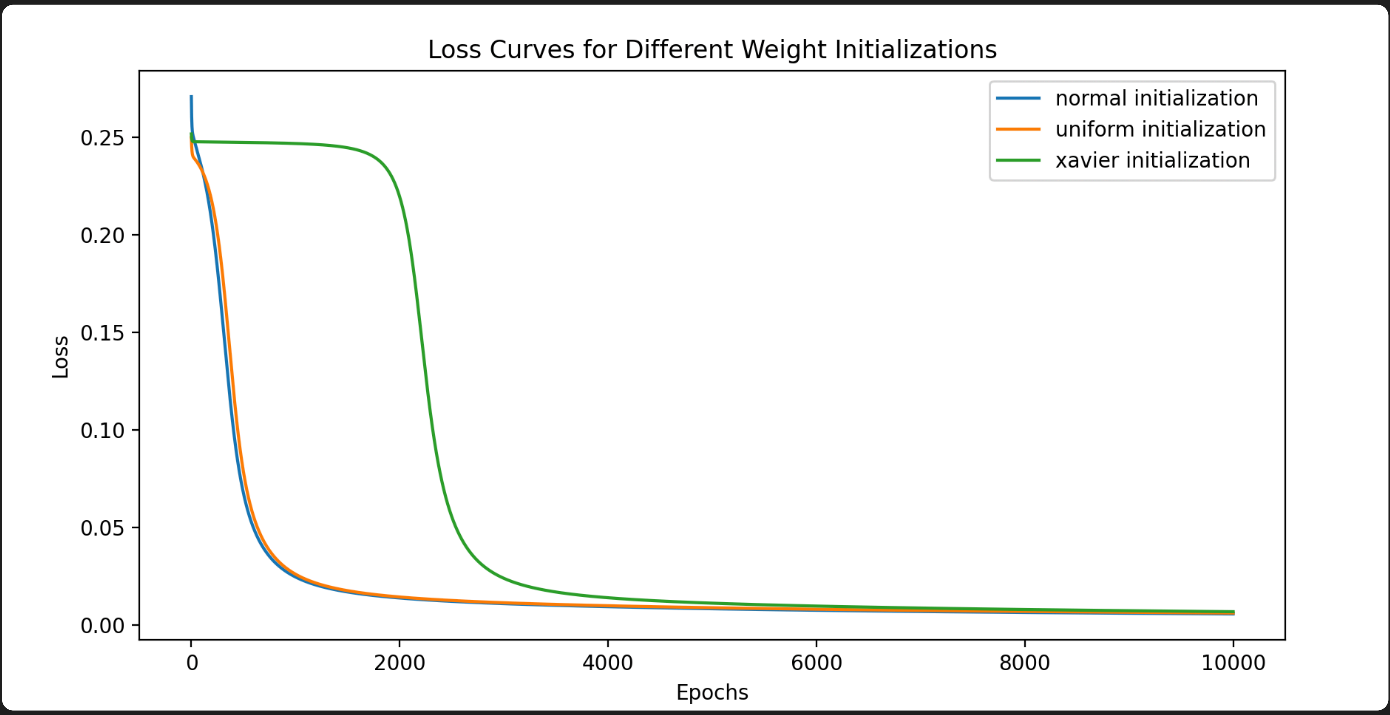


D. Anything you want to present

對於不同的 weight 初始化方法，我做了以下實驗比較:

- Normal (原始的方法)
- Uniform
- Xavier

```
  if method == 'normal':
      weight_initializer = lambda x, y: np.random.randn(x, y)
  elif method == 'uniform':
      weight_initializer = lambda x, y: np.random.uniform(-1.0, 1.0, 
(x, y))
  elif method == 'xavier':
      weight_initializer = lambda x, y: np.random.randn(x, y) * 
np.sqrt(1 / x)
```



對於 weight initialization 的收斂速度比較為

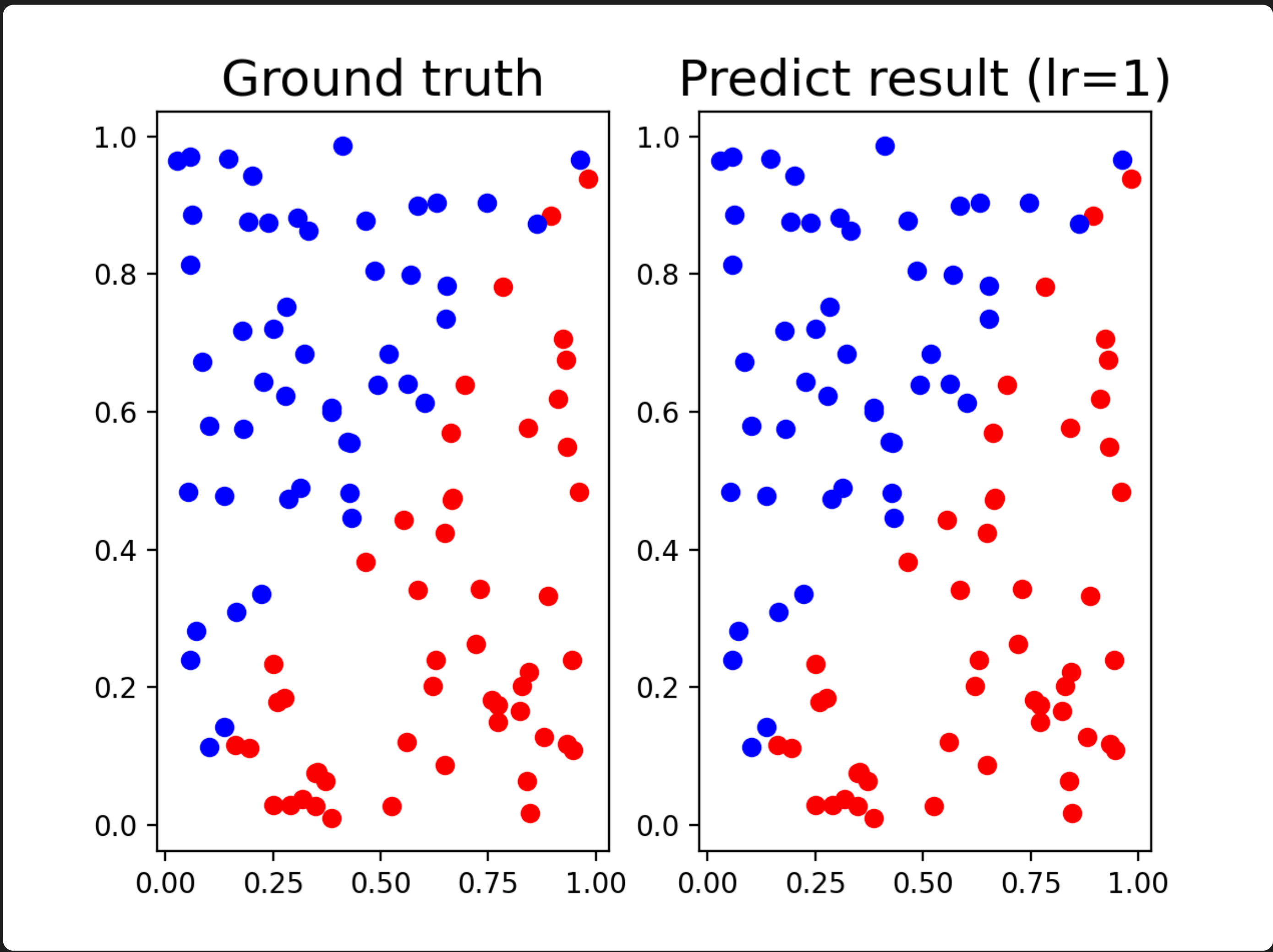
Normal >= Uniform >> Xavier

4. Discussion

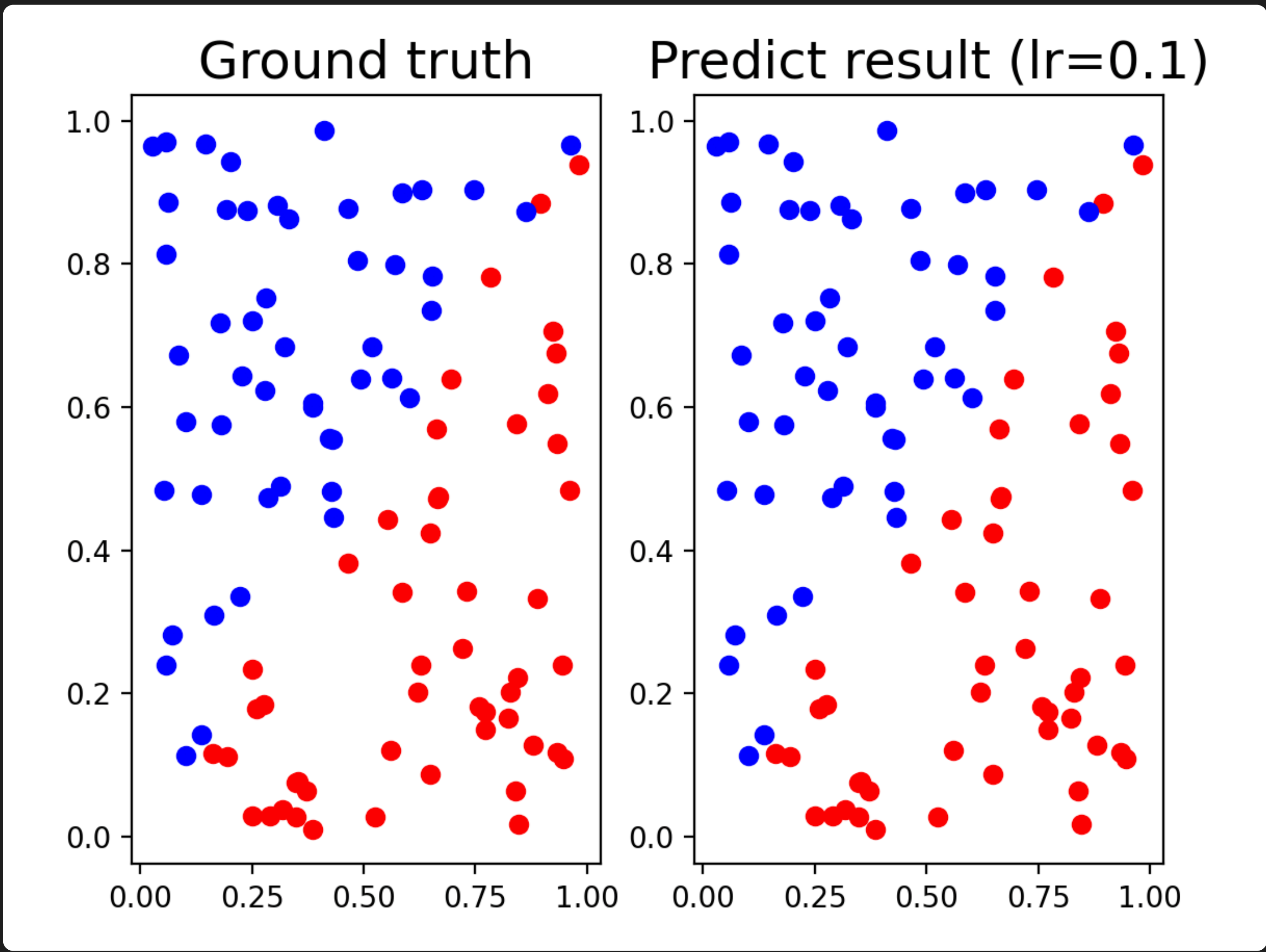
A. Try different learning rates

For linear data

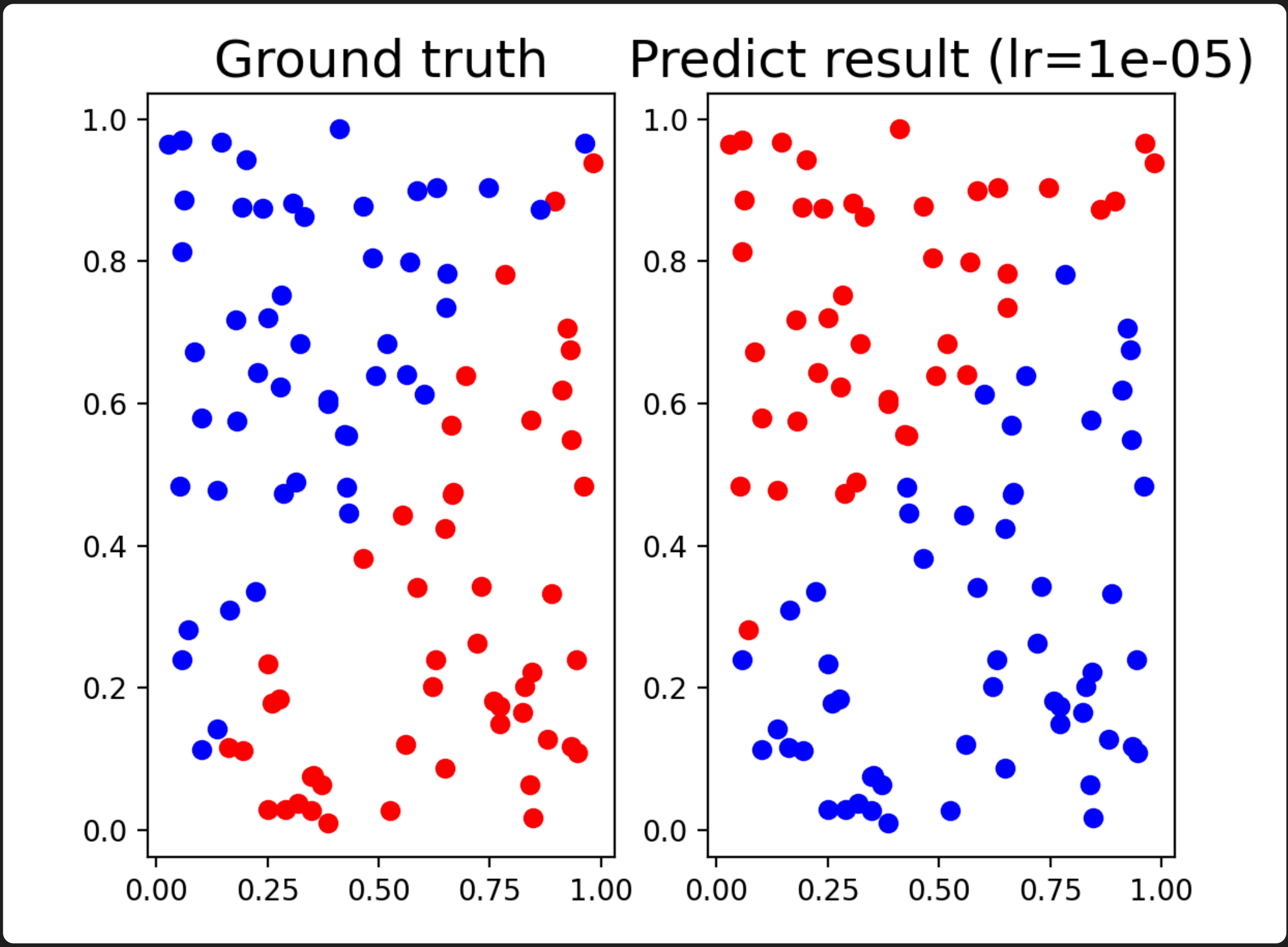
- lr = 1, acc = 100%


Ground truth
Predict result (lr=1)
1.0
0.8
0.6
0.4
0.2
0.0
0.00
0.25
0.50
0.75
1.00

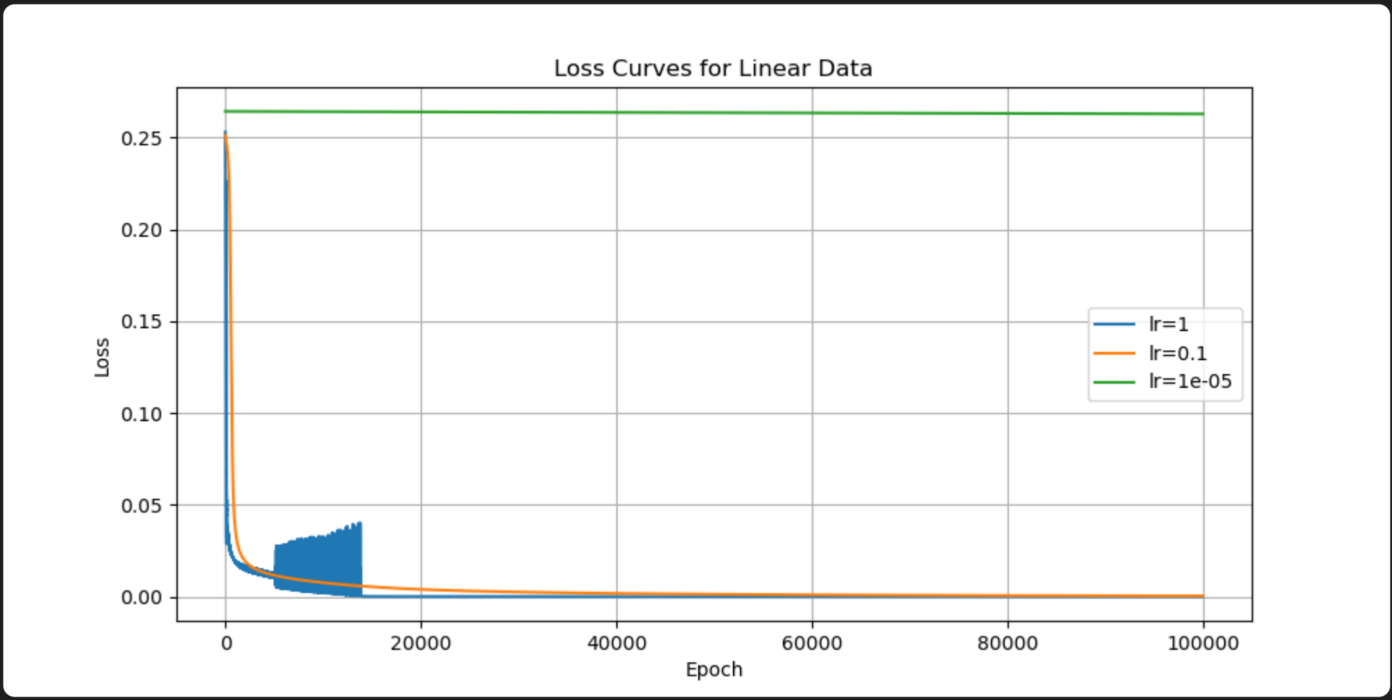
- lr = 0.1, acc = 100%



- lr = 0.0001, acc = 52%

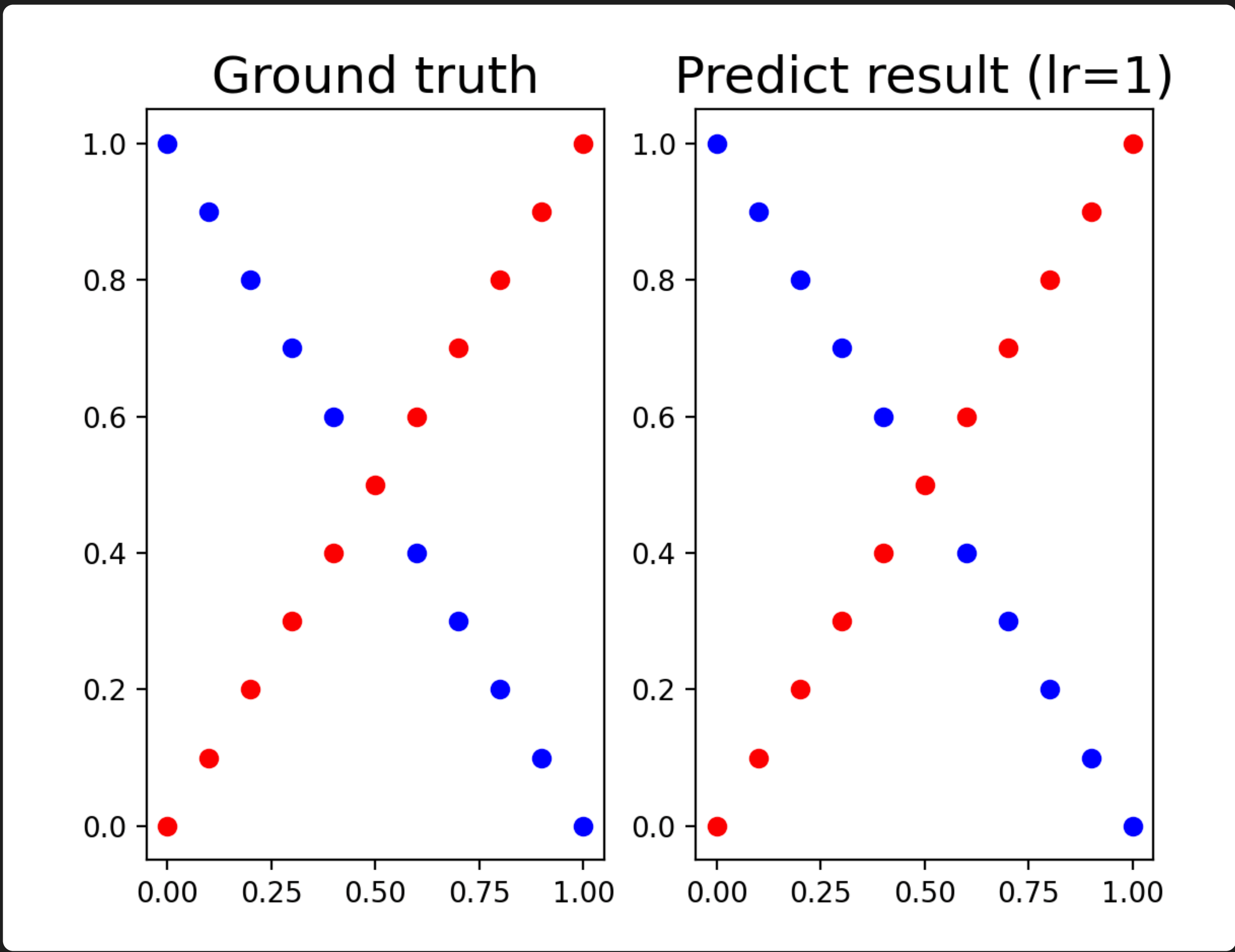


- Comparison figure

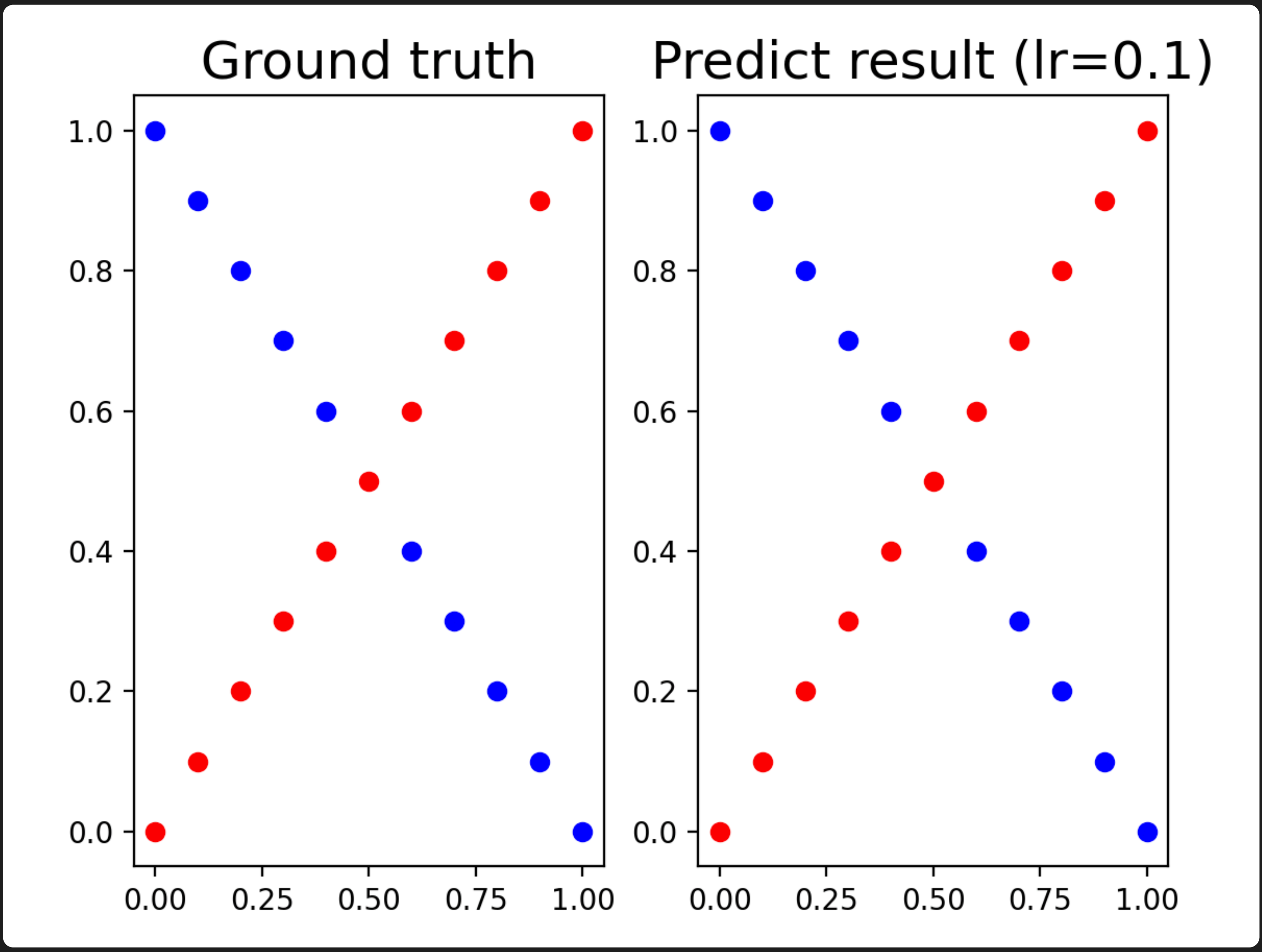


For XOR data

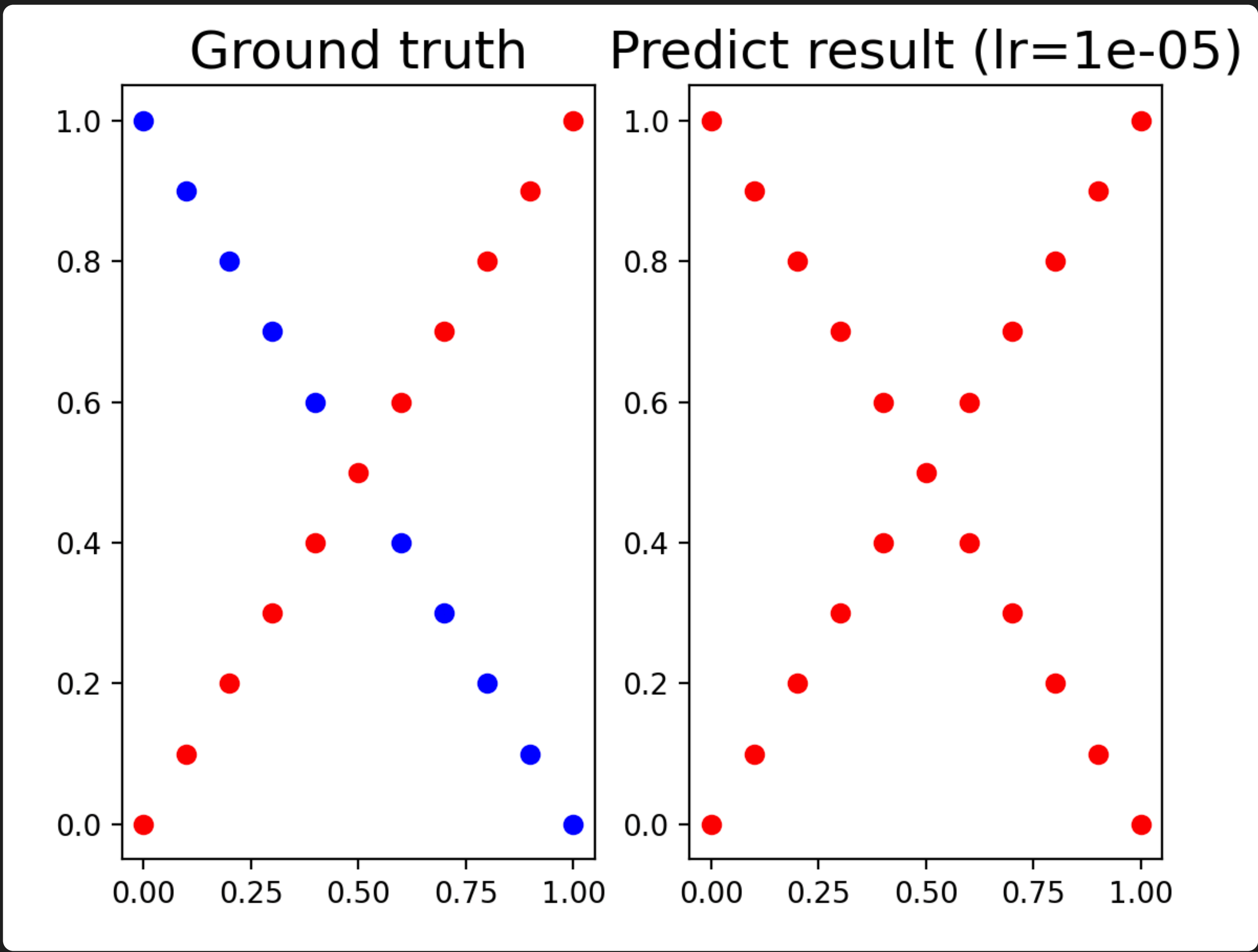
- lr = 1, acc = 100%


Ground truth
Predict result (lr=1)
1.0
0.8
0.6
0.4
0.2
0.0
0.00
0.25
0.50
0.75
1.00

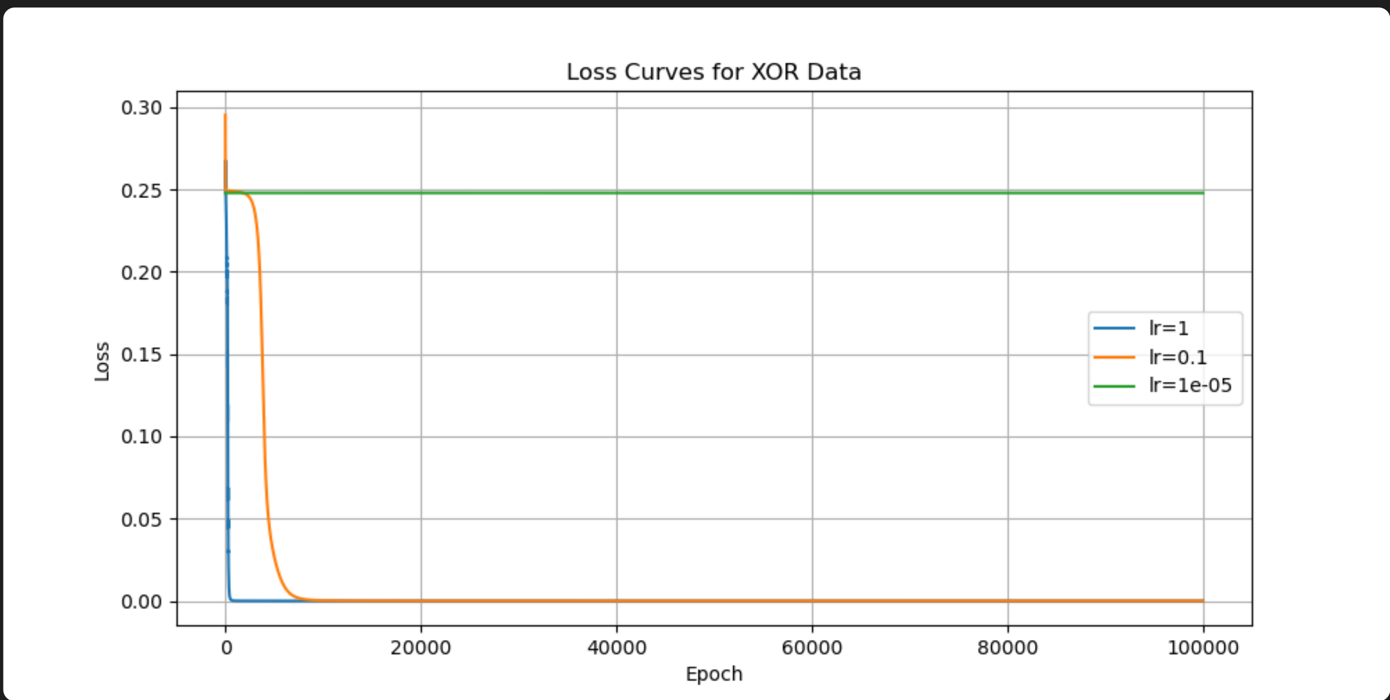
- lr = 0.1, acc = 100%



- lr = 0.0001, acc = 52.38%



- Comparison figure

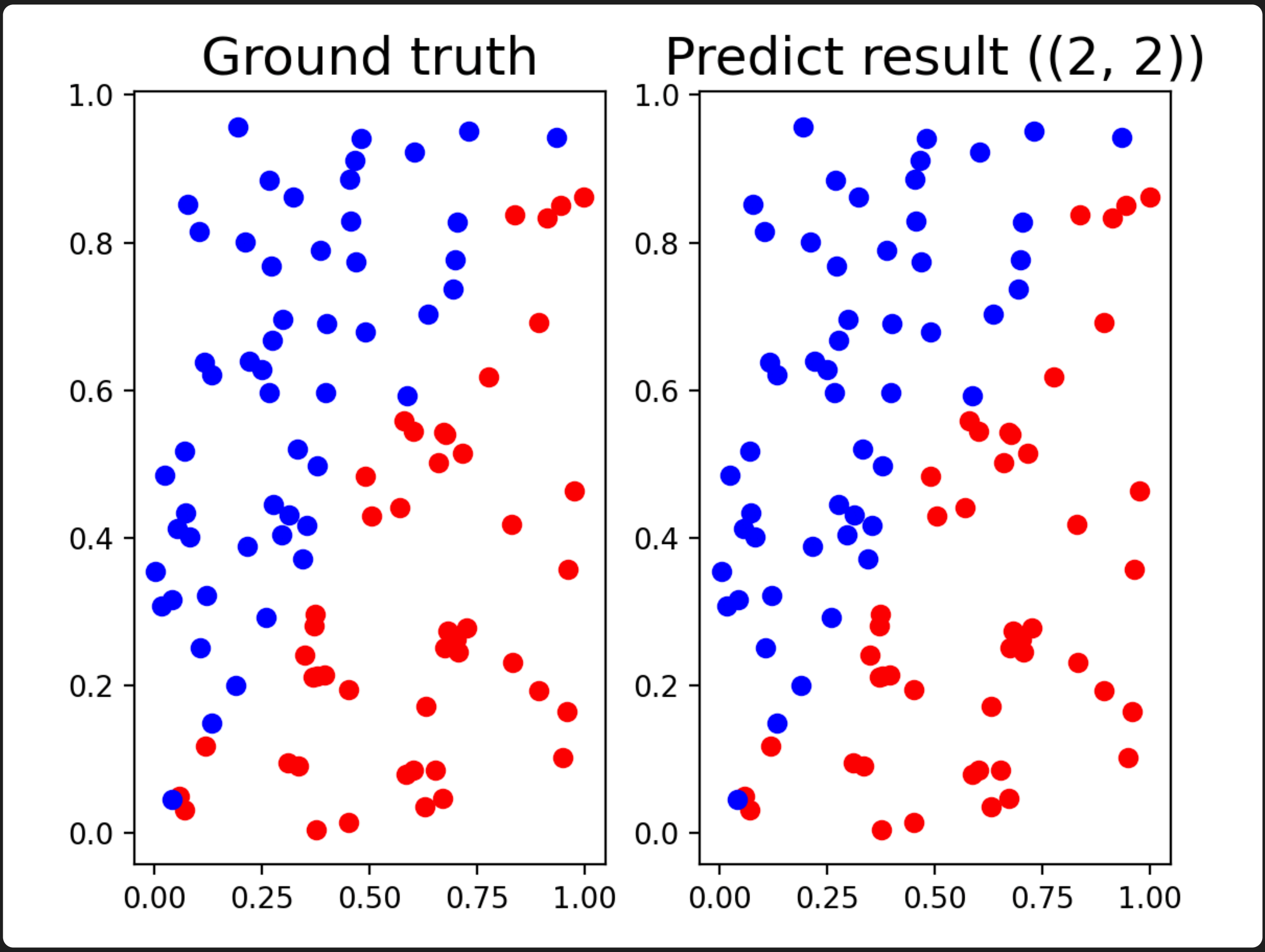


Learning rate 設在 0.00001 太小了，原本以為是 epochs 不夠多無法讓他收斂，但觀察上面的比較圖後，看起來模型早在 10000 epoch 就沒有辦法降低 loss 了。

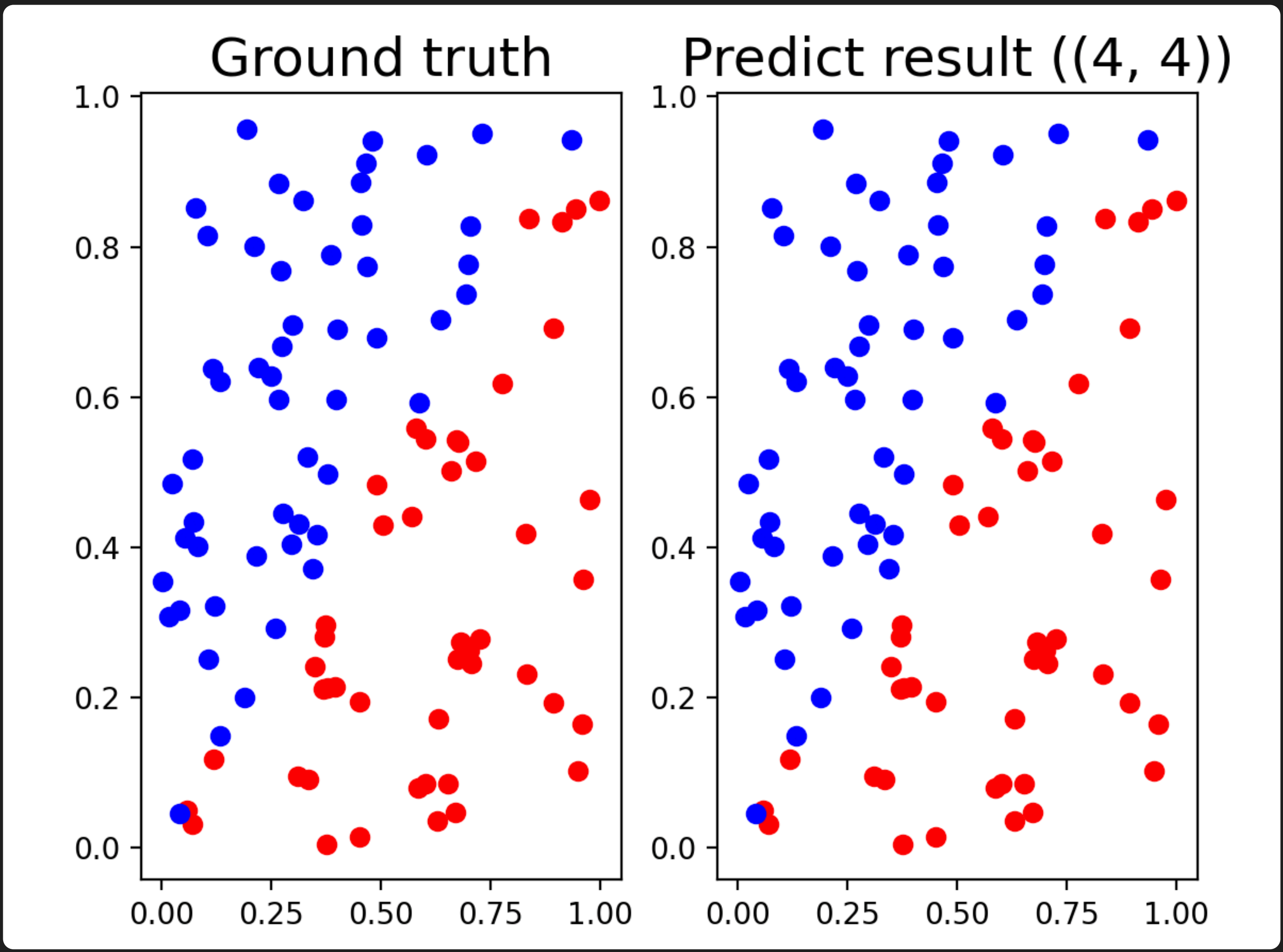
B. Try different numbers of hidden units

For linear data

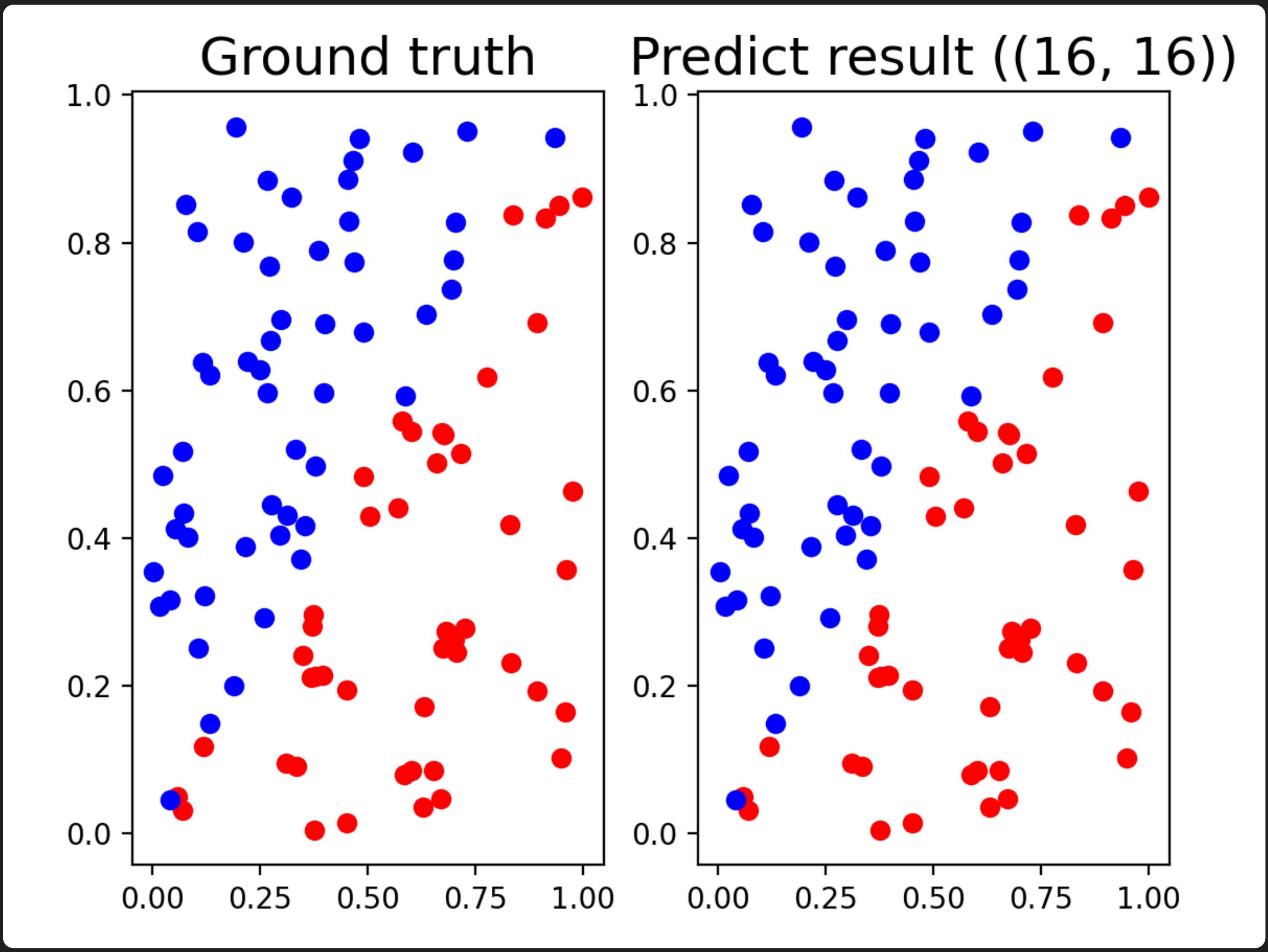
- hidden units = (2, 2) , acc = 100%



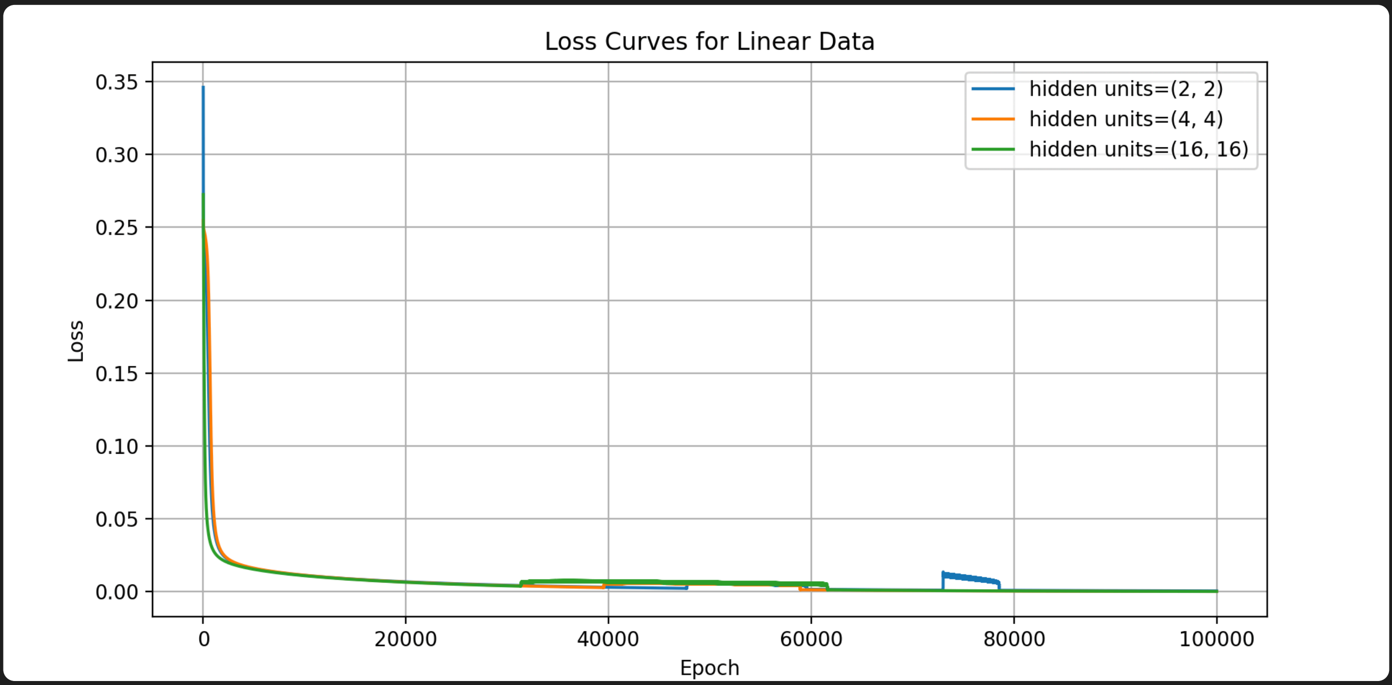
- hidden units = (4, 4) , acc = 100%



- hidden units = (16, 16) , acc = 100%

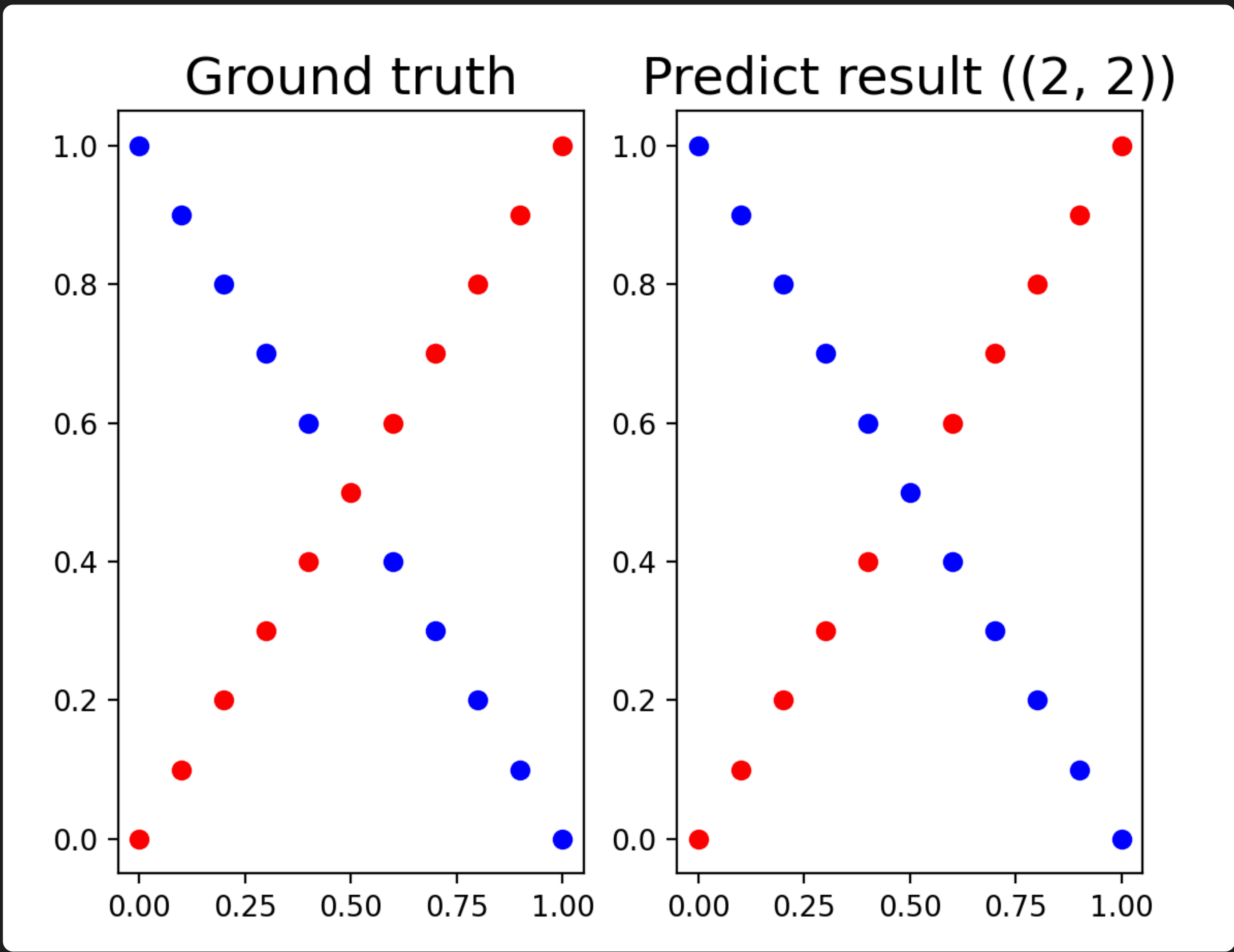


- Comparison figure

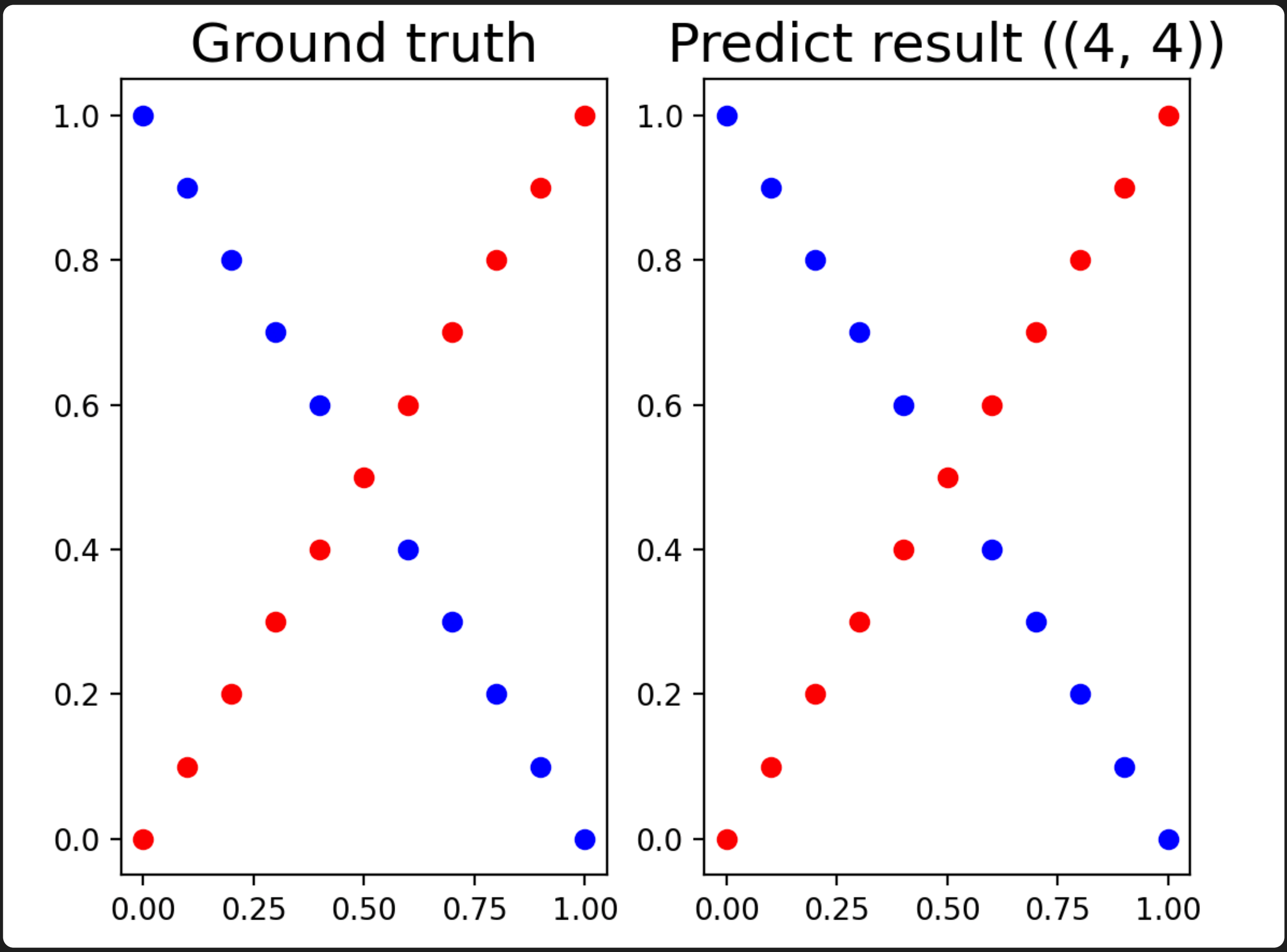


For XOR data

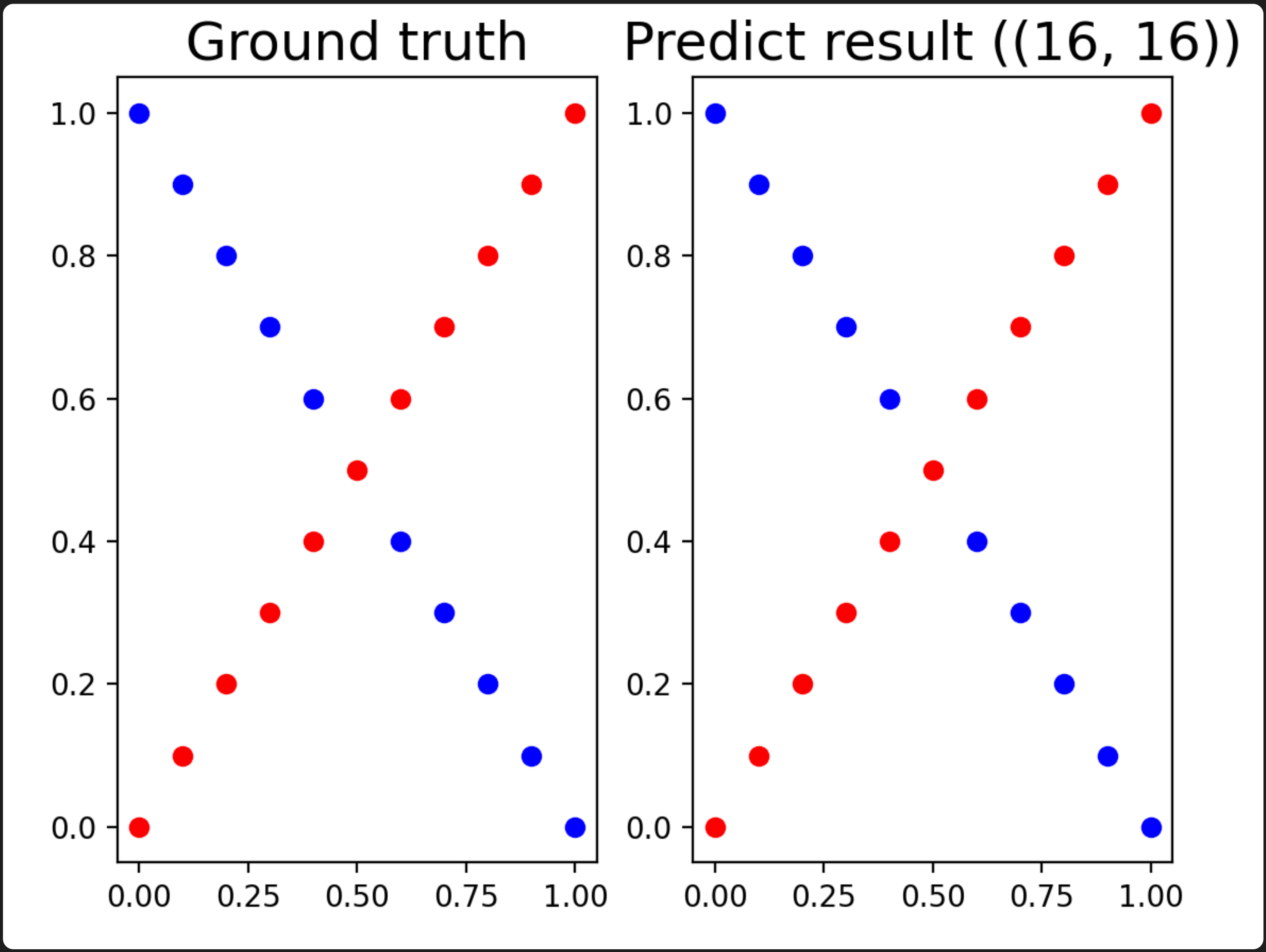
- hidden units = (2, 2), acc = 100%



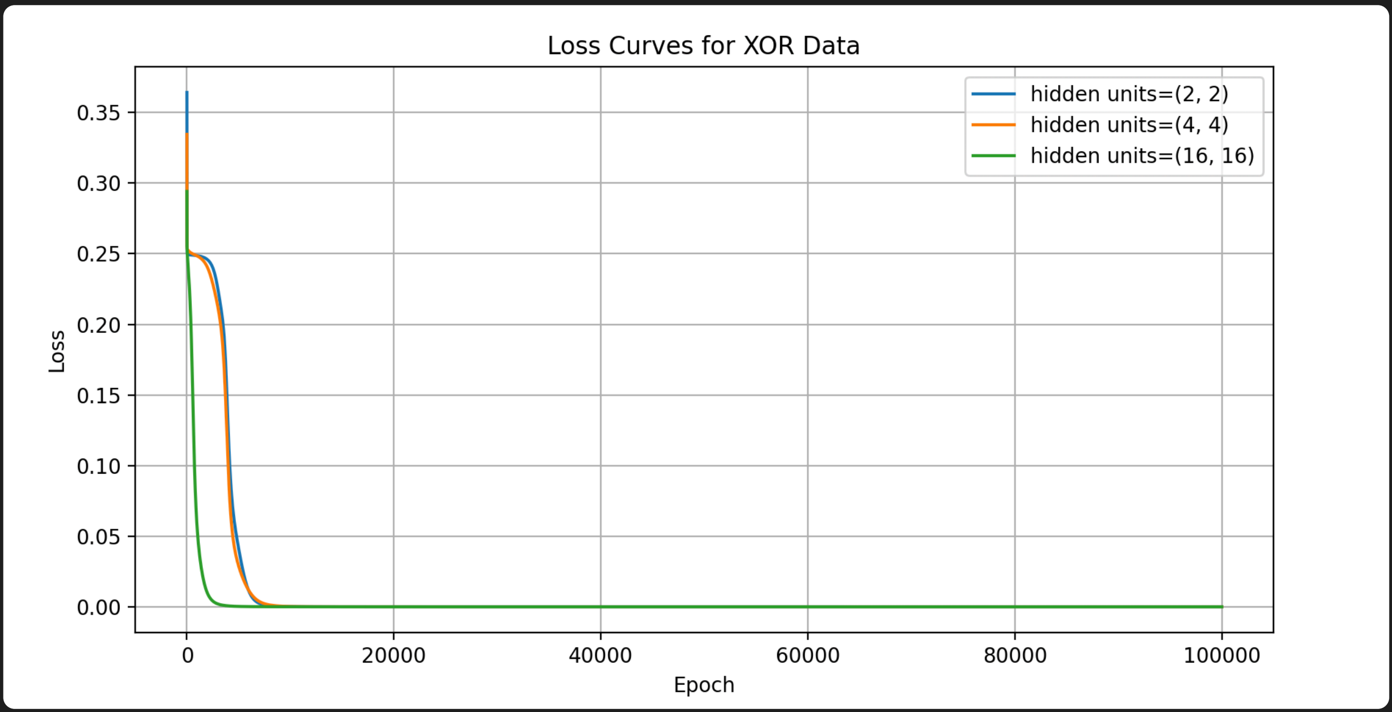
- hidden units = (4, 4), acc = 100%



- hidden units = (16, 16), acc = 100%



- Comparison figure



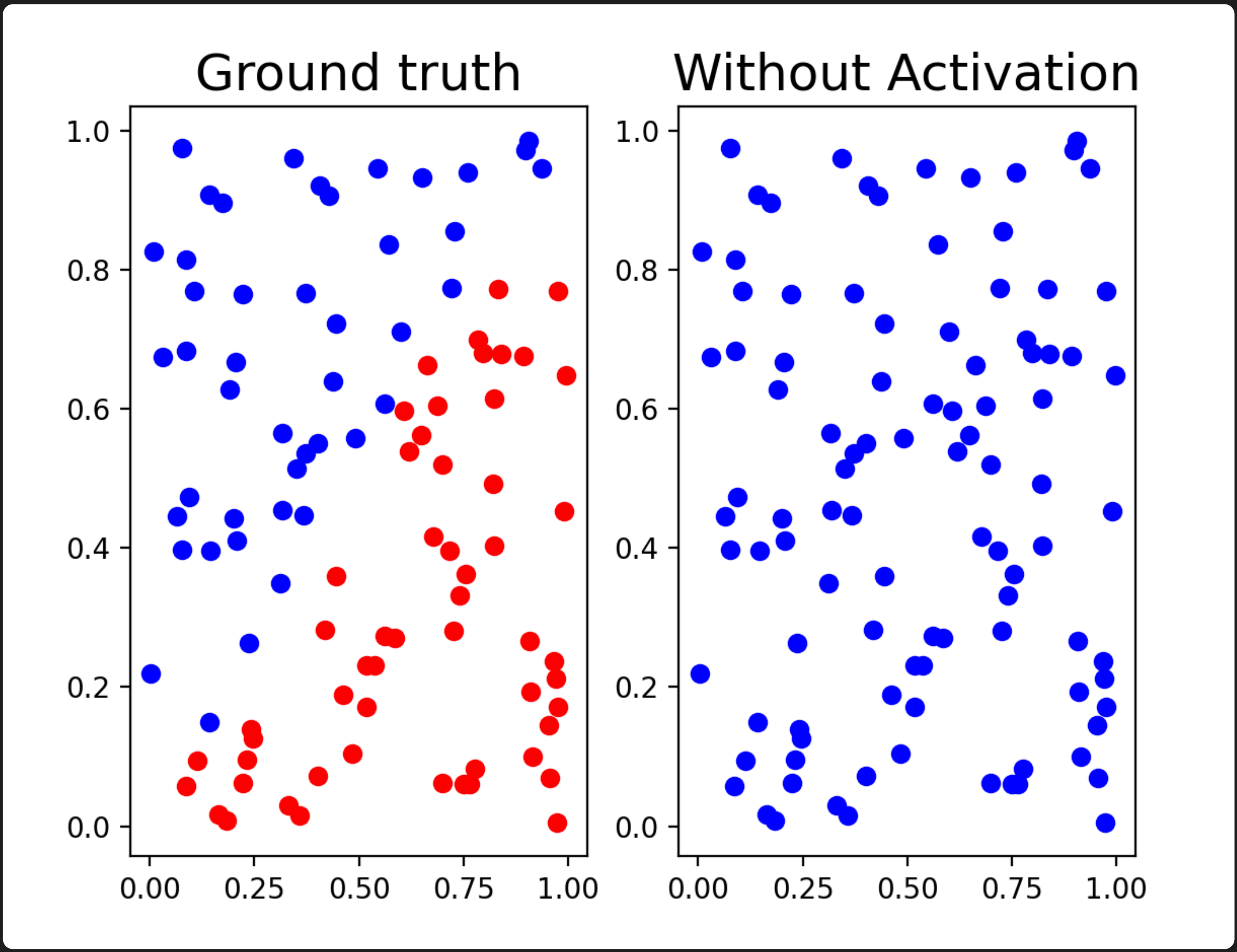
觀察下來，好像 hidden units 設在 (16, 16)，收斂速度會更快一些。

C. Try without activation functions

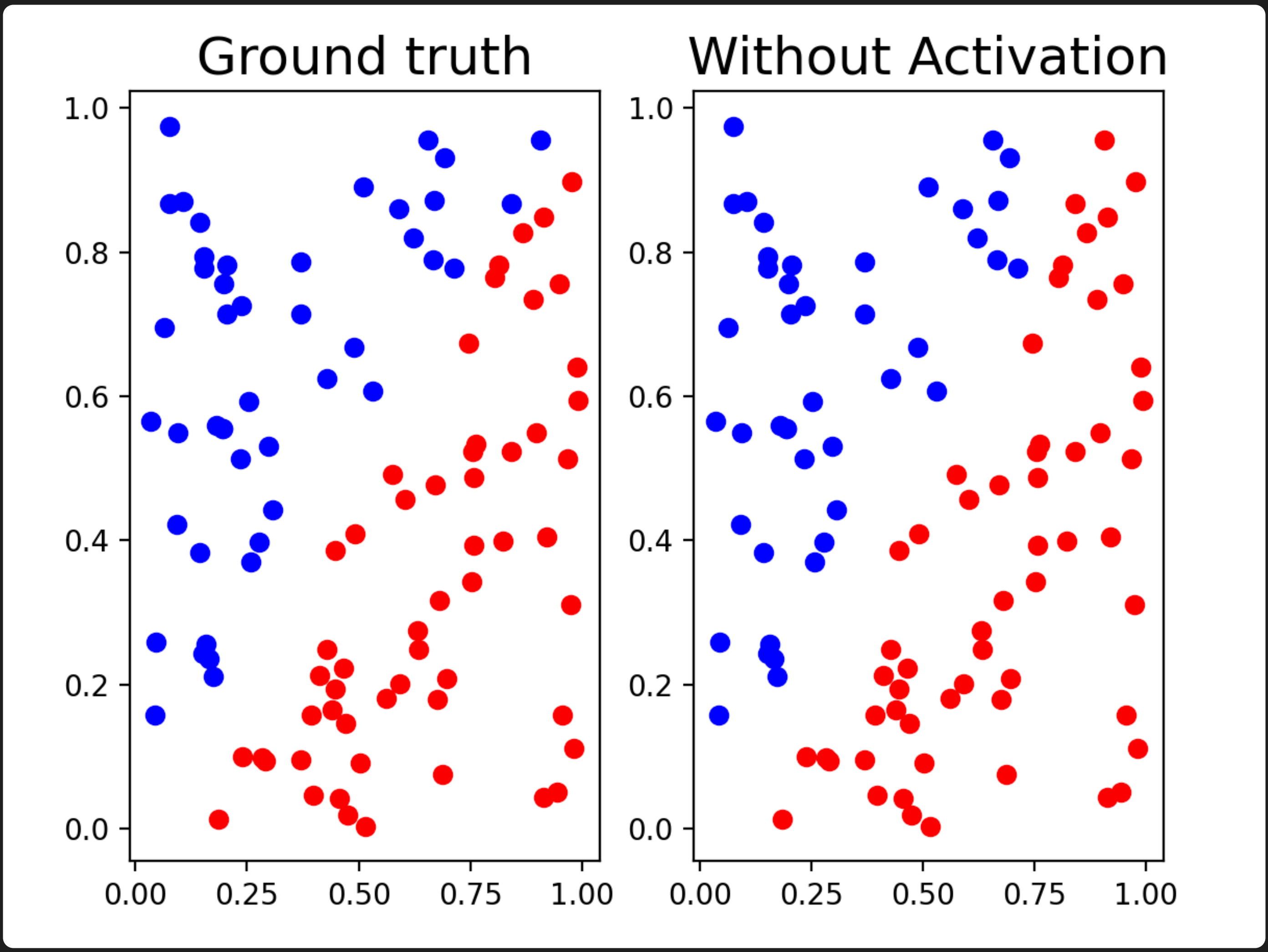
Without activation function (acc 還是能反映大致訓練狀況，但僅參考...)

- Linear data

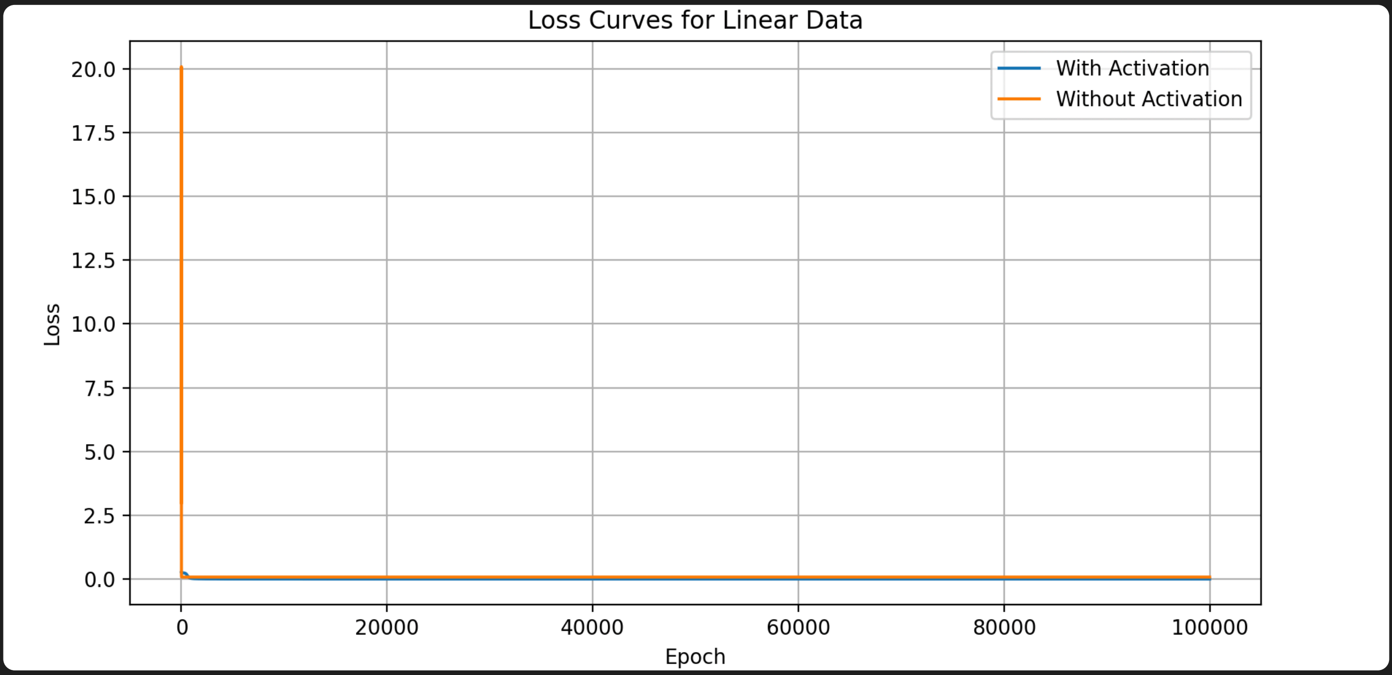
少數情況會完全 train 不起來，acc = 55%



通常是都 train 得起來，acc = 98%，但還是找不到最佳解

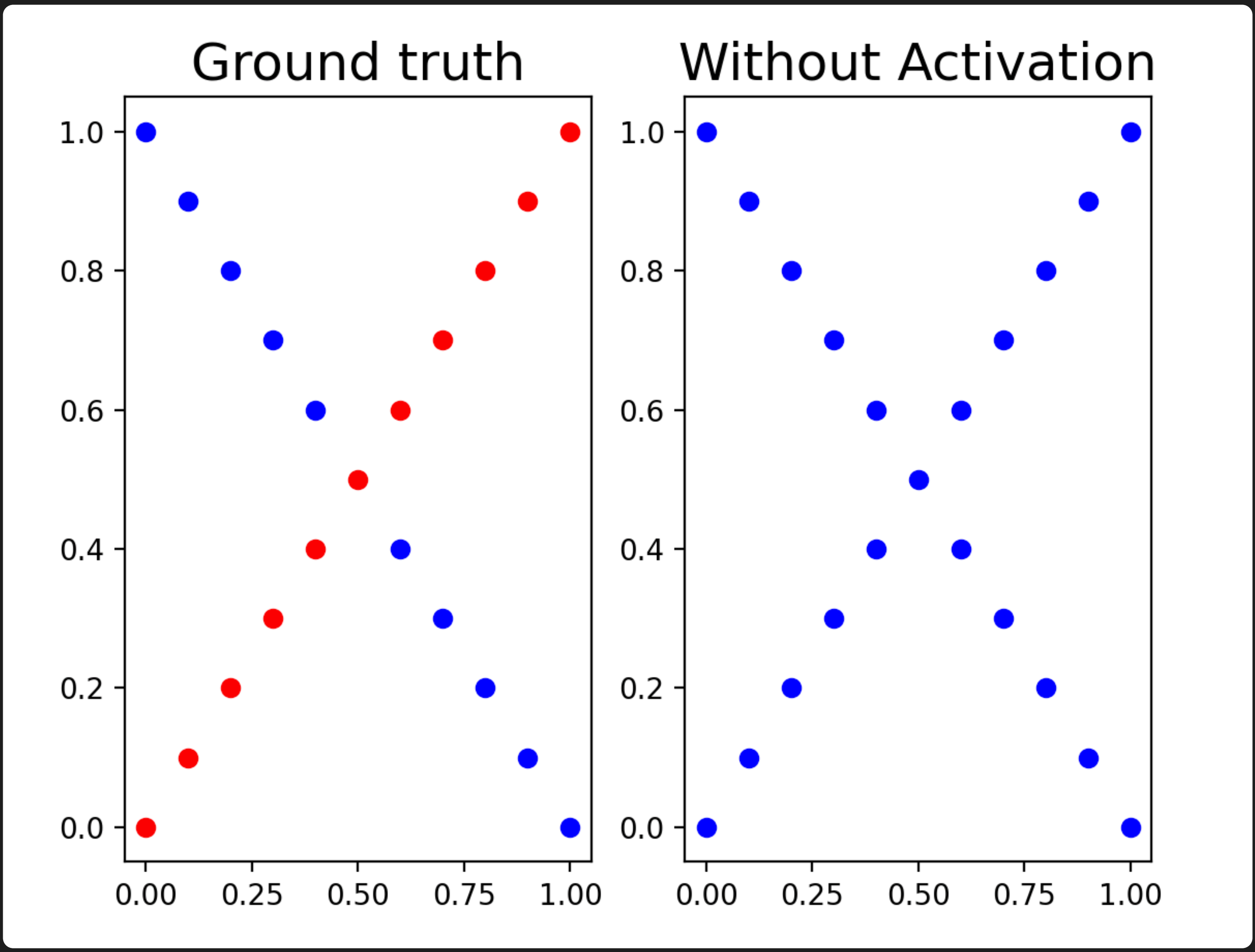


Comparison figure

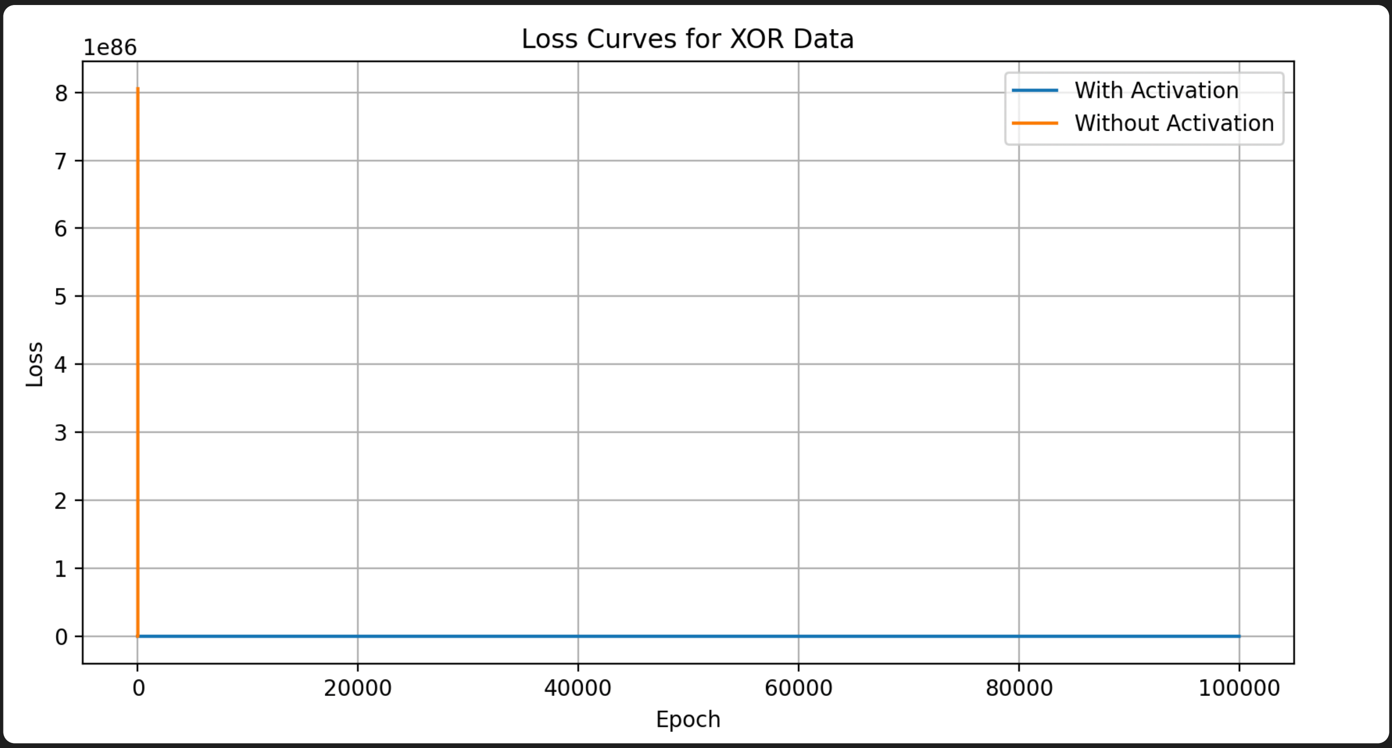


- XOR data

完全無法 train，acc = 52 %



Comparison figure



loss 會直接突破天際...

D. Anything you want to share

嘗試了一下不同的 loss function (MSE -> Cross entropy)

$$L(y, \hat{y}) = -\left(y \log(\hat{y}) + (1 - y) \log(1 - \hat{y})\right)$$

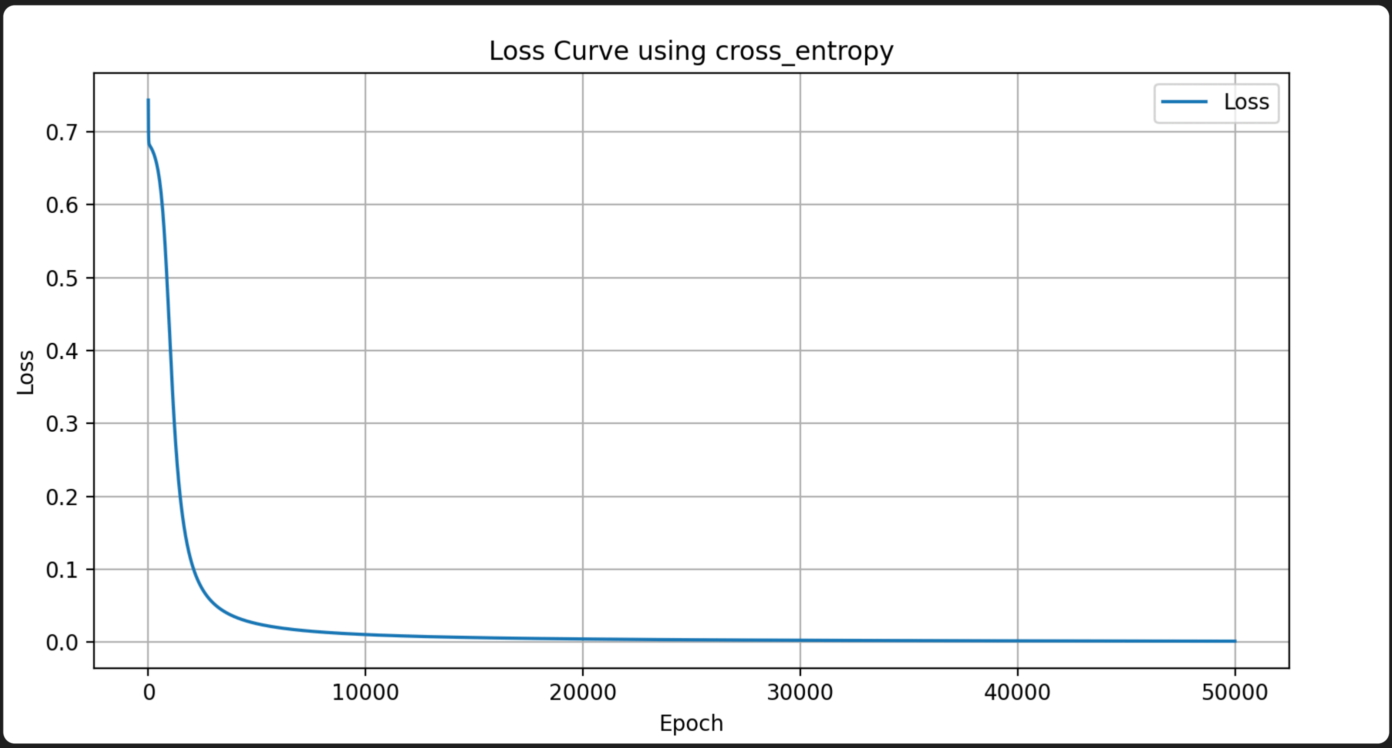
```
def cross_entropy_loss(y_true, y_pred):
    epsilon = 1e-12
    y_pred = np.clip(y_pred, epsilon, 1 - epsilon)
    return -np.mean(y_true * np.log(y_pred) + (1 - y_true) * np.log(1
- y_pred))
```

- Back propgation 的開頭變這樣

```
    if loss_type == 'cross_entropy':
        dA3 = -(y / A3) + (1 - y) / (1 - A3)
        dZ3 = dA3 * derivative_sigmoid(A3)
    else:  # mse
        dZ3 = (A3 - y) * 2 * derivative_sigmoid(A3)
```

依然可以正常收斂

```
Epoch 0, Loss (cross_entropy): 0.7435800152511739
Epoch 5000, Loss (cross_entropy): 0.025269957090769O4
Epoch 10000, Loss (cross_entropy): 0.010364841964053 97
Epoch 15000, Loss (cross_entropy): 0.006214804735750703
Epoch 20000, Loss (cross_entropy): 0.004303550005177803
Epoch 25000, Loss (cross_entropy): 0.003226119856241756
Epoch 30000, Loss (cross_entropy): 0.0025451117385857764
Epoch 35000, Loss (cross_entropy): 0.0020810679549495576
Epoch 40000, Loss (cross_entropy): 0.0017474324652610776
Epoch 45000, Loss (cross_entropy): 0.0014976622444989268
Final accuracy using cross_entropy: 100.00%
```



5. Extra

A. Implement different optimizers

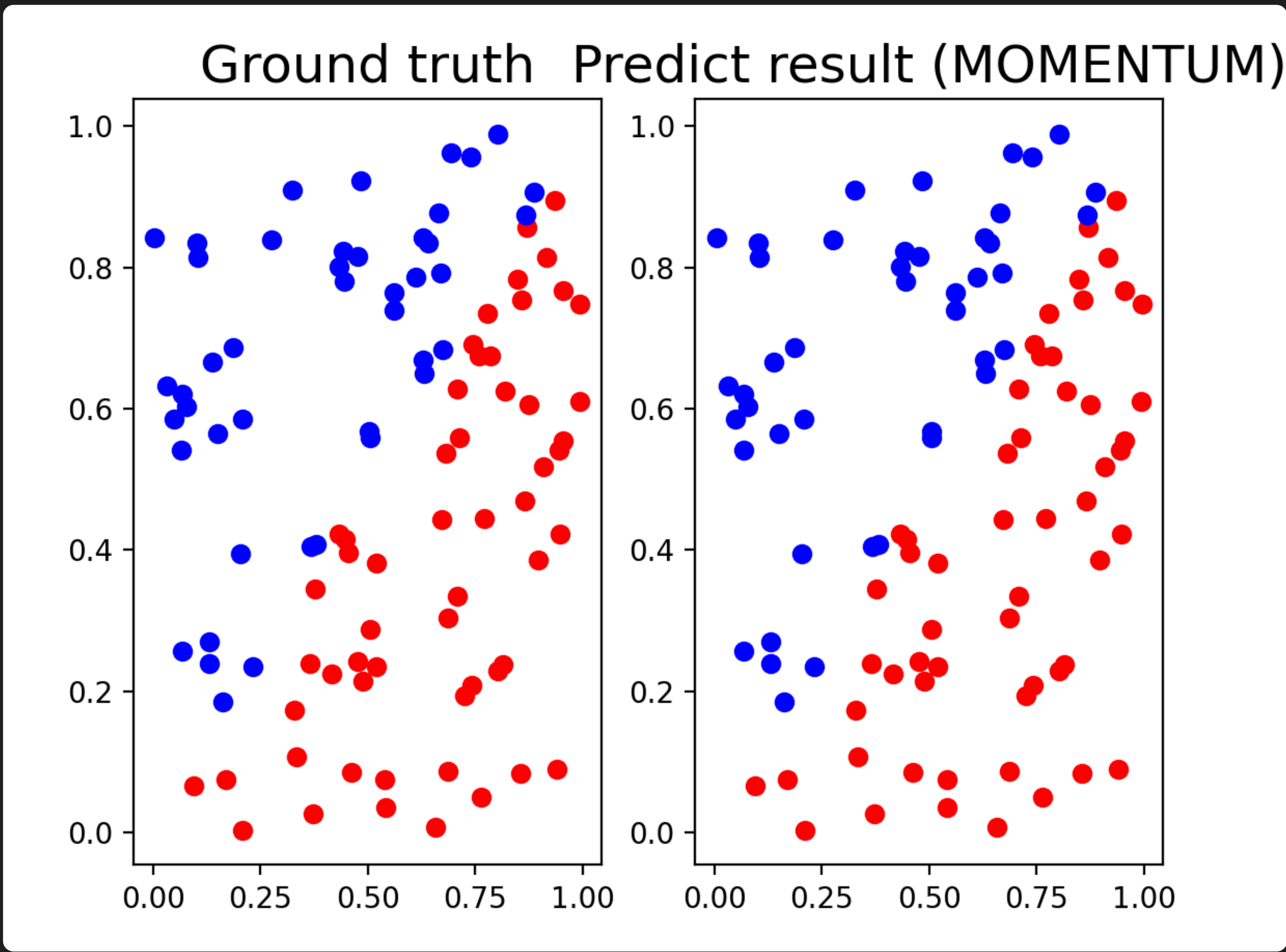
Momentum

```
def momentum_update(weights, grads, velocity, learning_rate, momentum=0.9):
    for key in weights.keys():
        velocity[key] = momentum * velocity[key] - learning_rate * grads[key]
        weights[key] += velocity[key]
    return weights, velocity
```

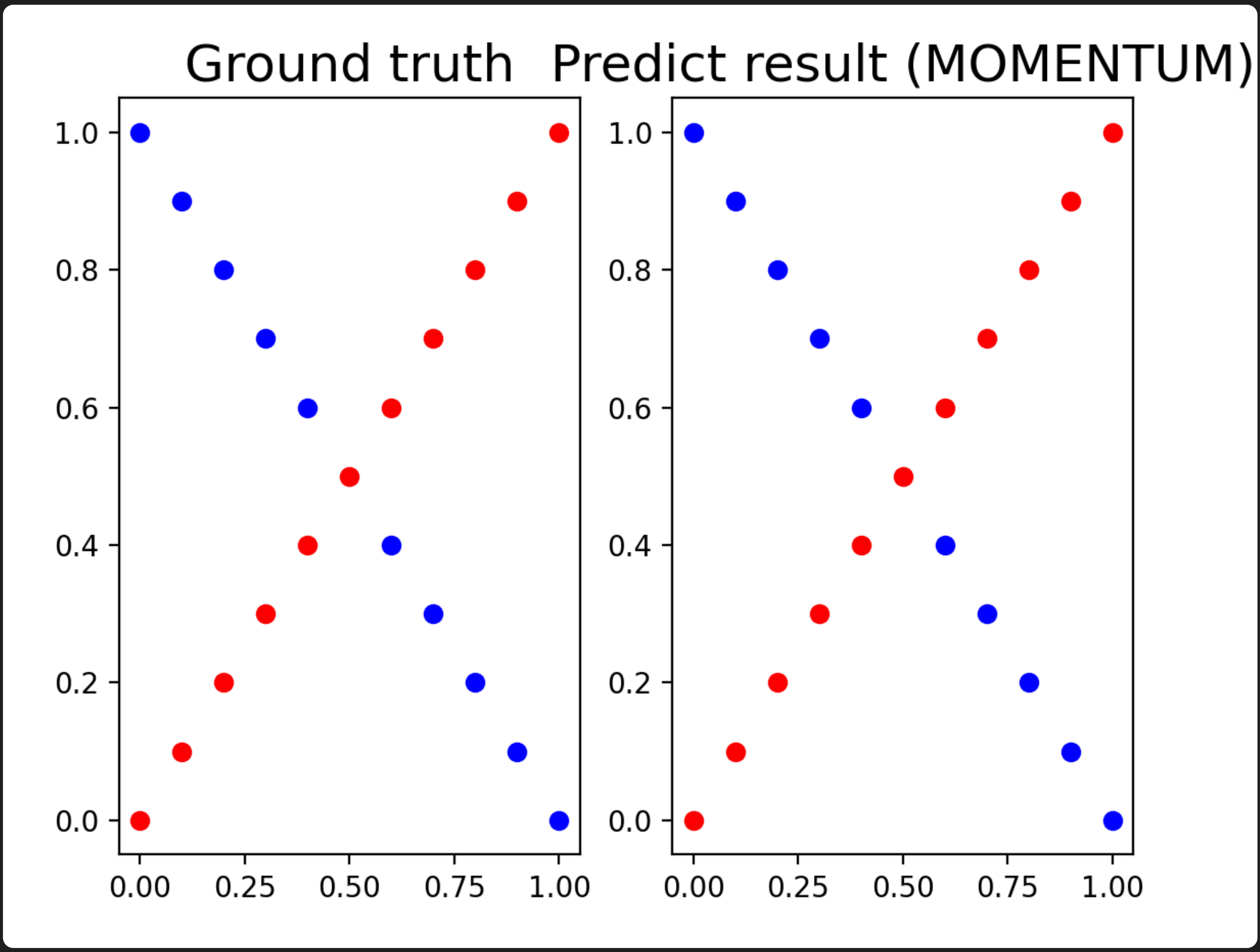
`velocity[key]` 表示上一次更新的速度。

(如果更新方向和上次相反，這次更新速度會變慢，反之則變快。)

- Linear data (acc = 100%)



- XOR data (acc = 100%)



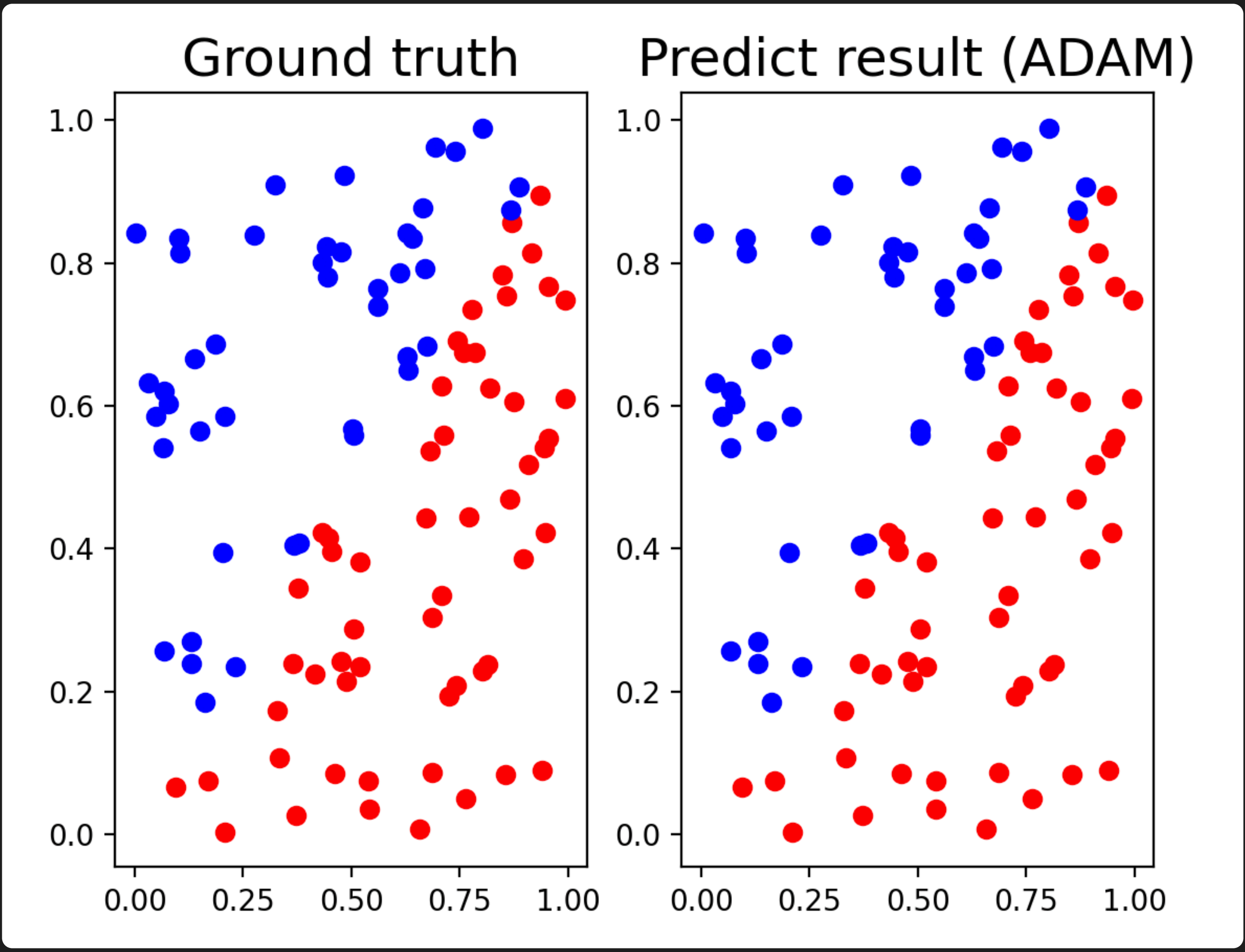
Adam

```
def adam_update(weights, grads, m, v, t, learning_rate, beta1=0.9,
beta2=0.999, epsilon=1e-8):
    m_hat = {}
    v_hat = {}
    for key in weights.keys():
        m[key] = beta1 * m[key] + (1 - beta1) * grads[key]
        v[key] = beta2 * v[key] + (1 - beta2) * np.square(grads[key])
        m_hat[key] = m[key] / (1 - beta1 ** t)
        v_hat[key] = v[key] / (1 - beta2 ** t)
        weights[key] -= learning_rate * m_hat[key] /
(np.sqrt(v_hat[key]) + epsilon)
    return weights, m, v
```

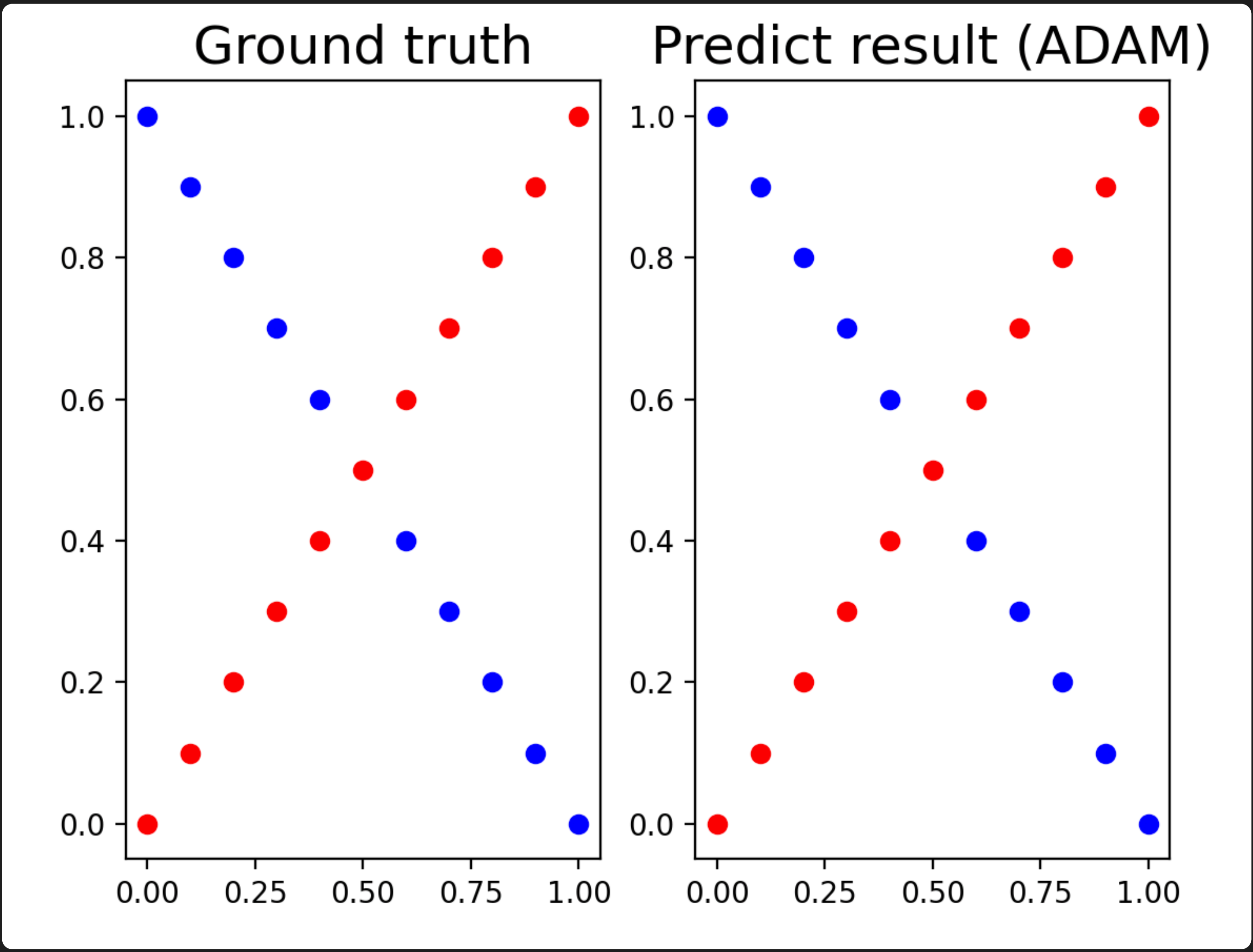
其中：

- weights: 當前的權重參數。
- grads: 當前計算出的梯度。
- m: 一階矩估計（動量）。
- v: 二階矩估計（RMSProp）。
- t: 當前的時間步（迭代次數）。
- learning_rate: 學習率。
- beta1: 一階矩估計的衰減率，通常設為 0.9。
- beta2: 二階矩估計的衰減率，通常設為 0.999。
- epsilon: 防止除零的小數值，通常設為 1e-8。

- Linear data (acc = 100%)

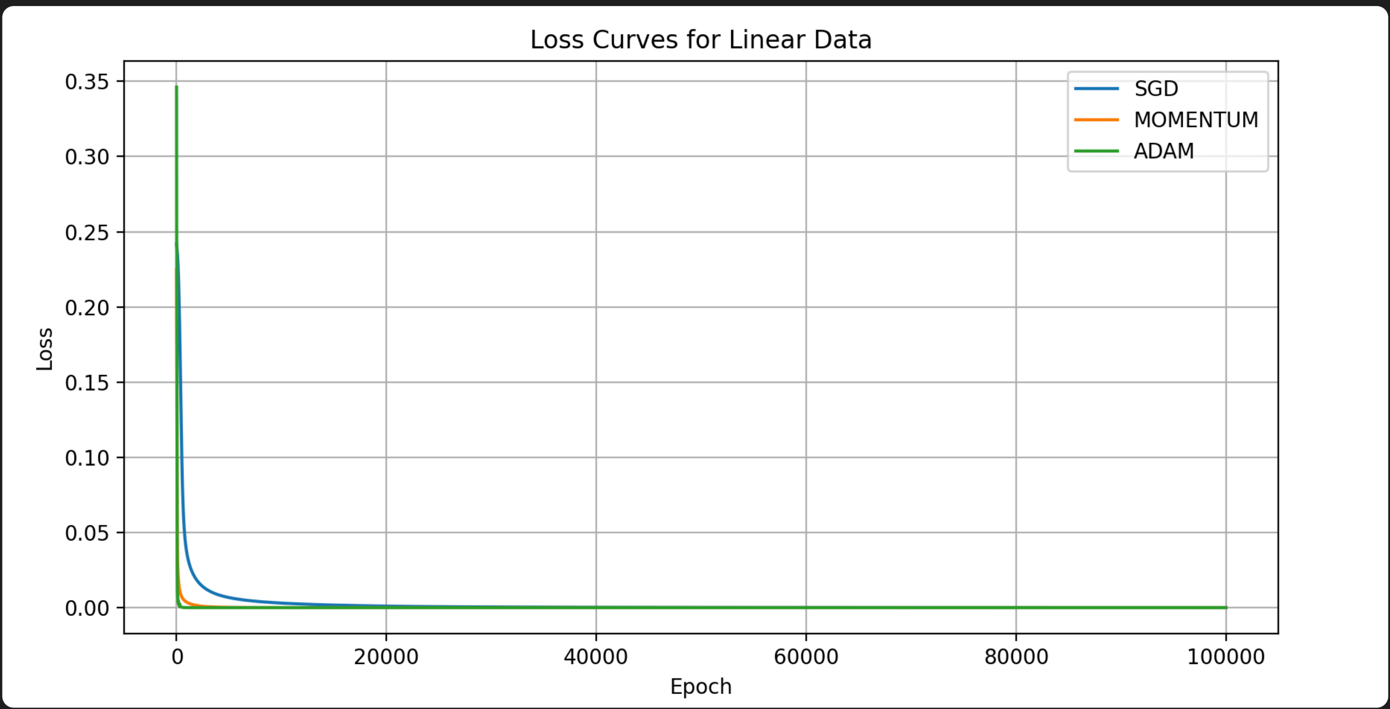


- XOR data (acc = 100%)

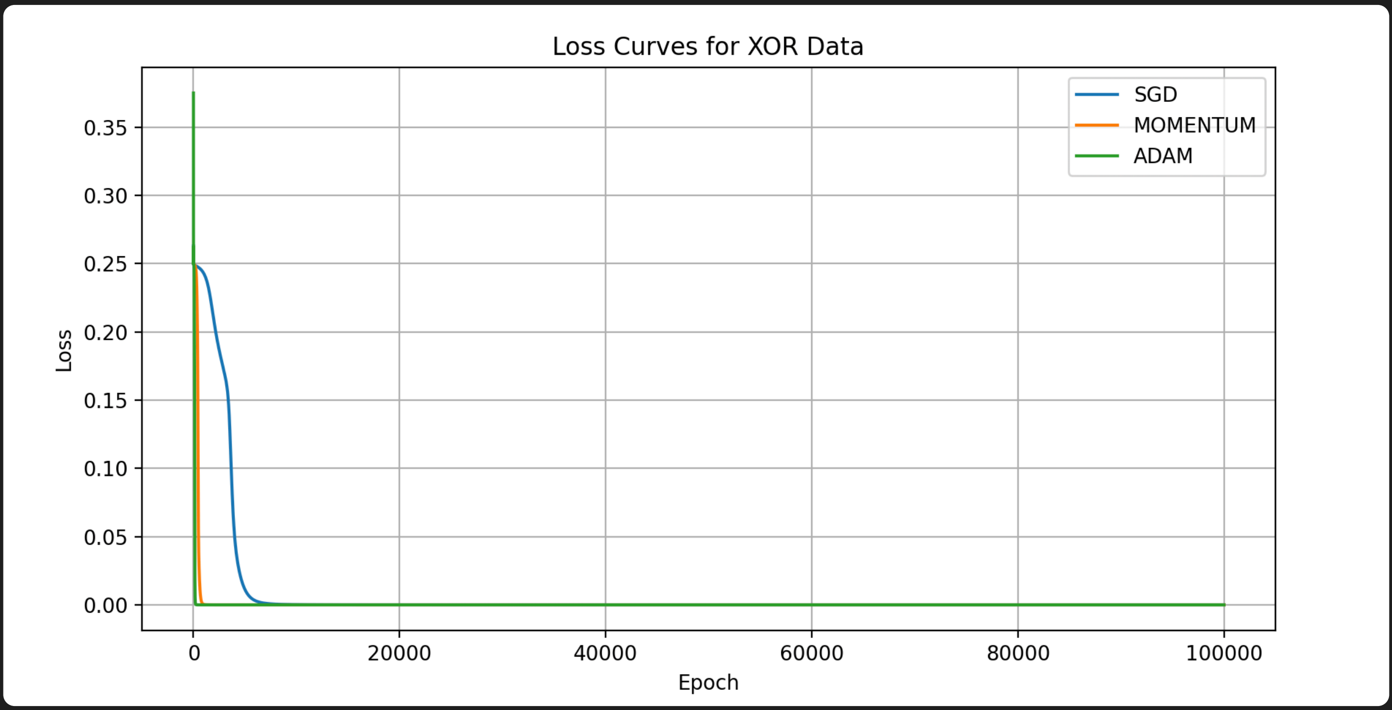


Compare figure

- Linear data



- XOR data



經過觀察可以發現，收斂速度為 `ADAM` > `MOMENTUM` > `SGD`

B. Implement different activation functions.

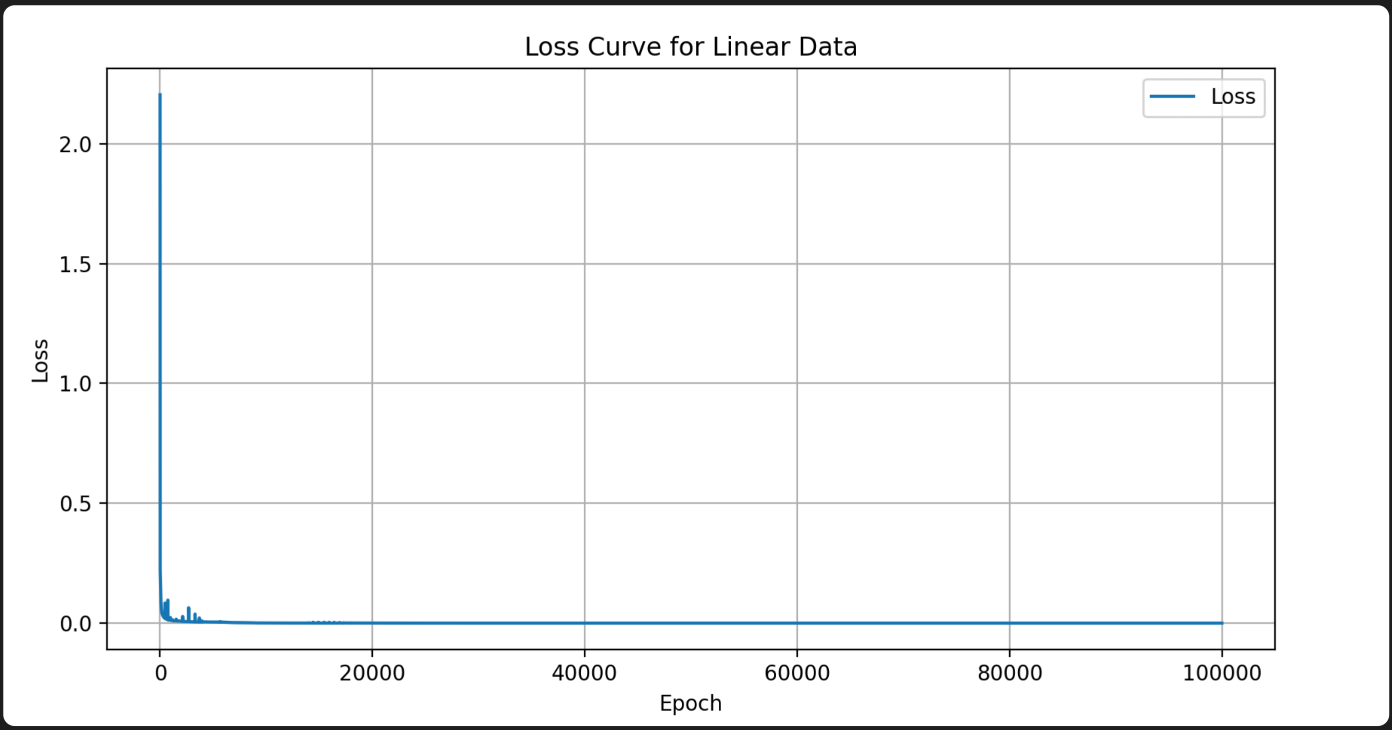
將 `sigmoid` 換成 `relu`

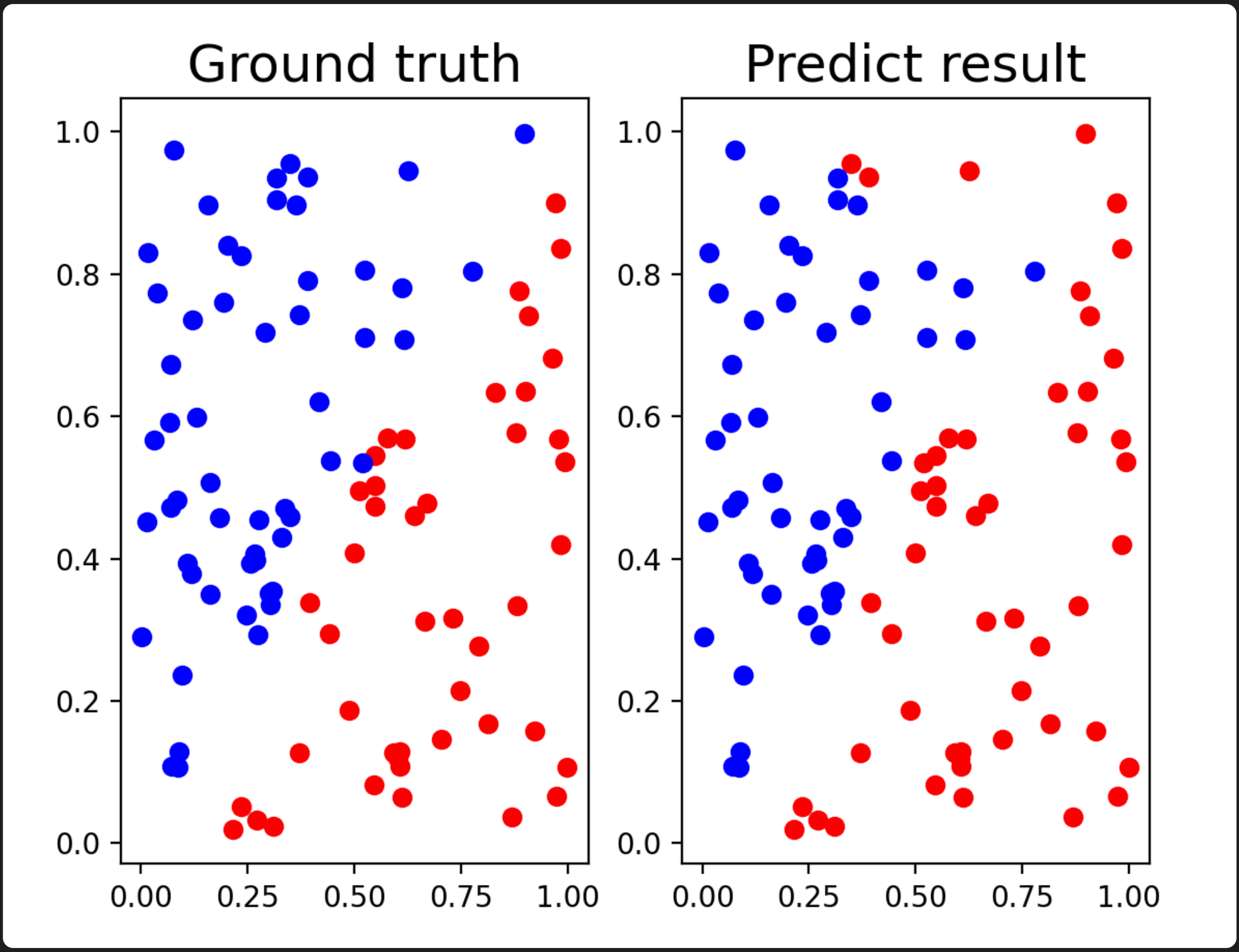
```
def relu(x):
    return np.maximum(0, x)

def derivative_relu(x):
    return np.where(x > 0, 1, 0)
```

因為對於 ReLU，通常輸出值的範圍為 [0, ∞)，這邊的實驗將試著根據訓練數據的輸出值來動態調整閾值，即使用輸出值的中位數作為 threshold，但 acc 還是不能參考...

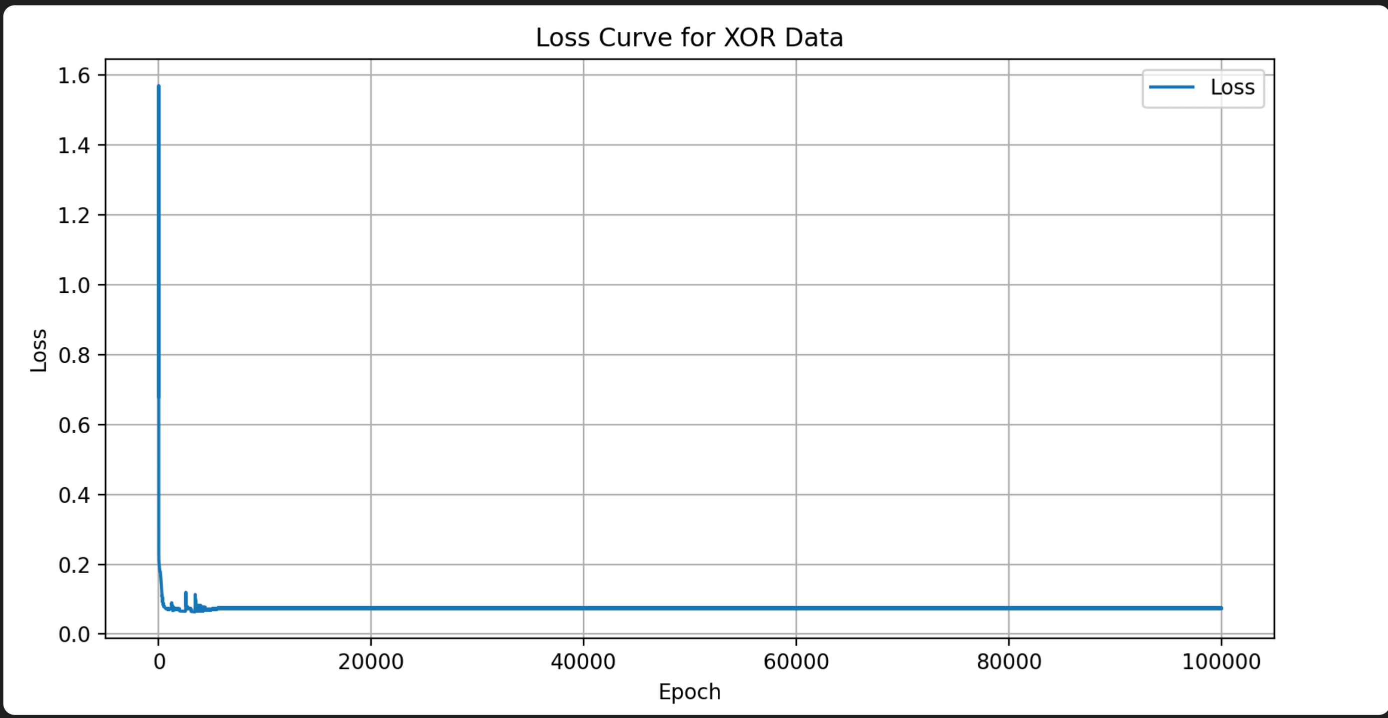
跟 sigmoid 比較起來，好像 relu 的收斂穩定度沒有它來得高。

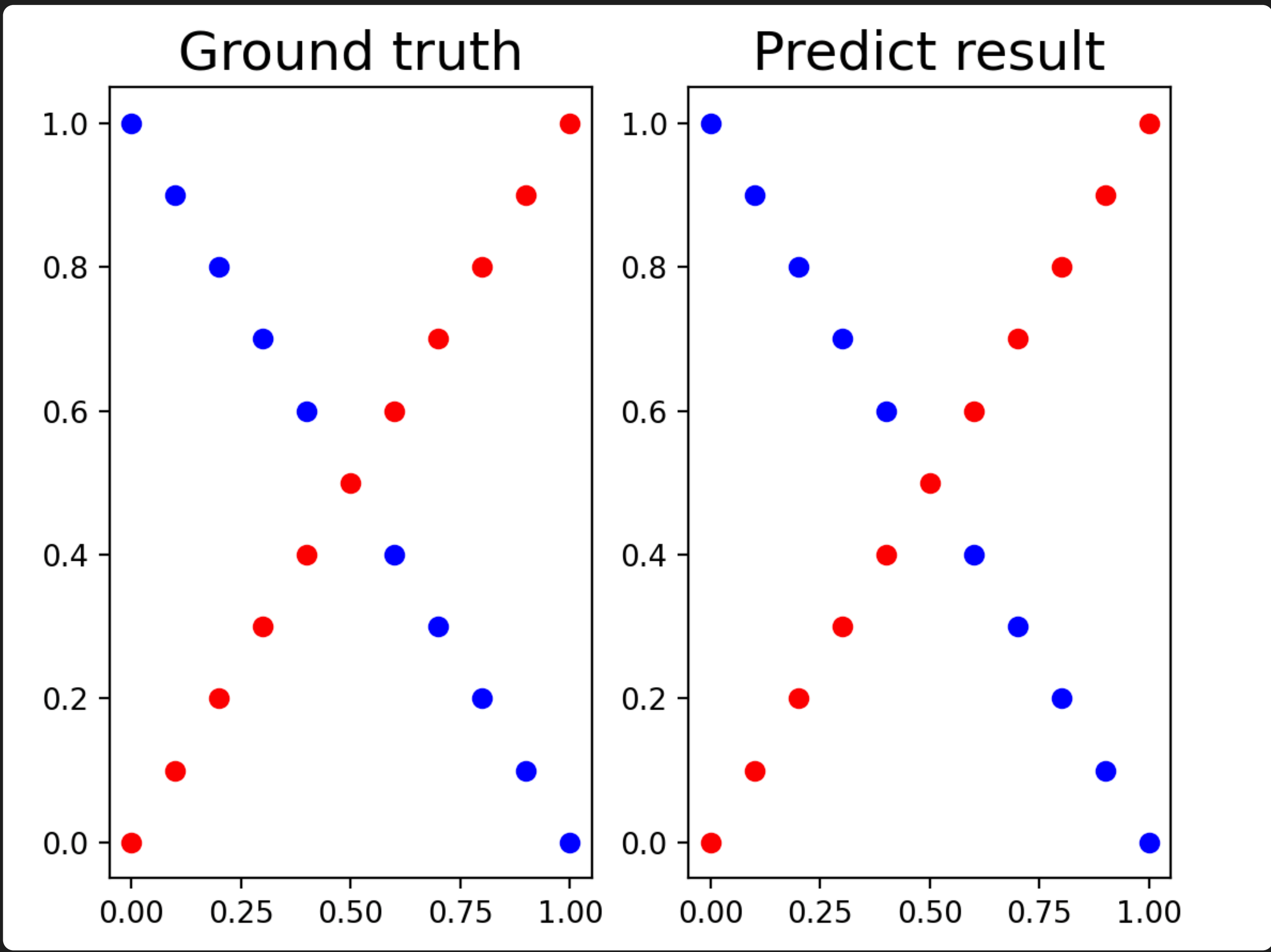
- Linear data (acc = 98%)





- XOR data (acc = 100%)





Reference

- https://hackmd.io/@allen108108/H1l4zqtp4 (Adagrad、RMSprop、Momentum and Adam – 特殊的學習率調整方式)

- https://www.brilliantcode.net/1670/convolutional-neural-networks-4-backpropagation-in-kernels-of-cnns/ (卷積核的Back propagation)
- ChatGPT