Design 1

Run "4.1. Classification with MSE loss.ipynb"

- NN output layer has one node y.
- Use MSE as loss function to train NN.
- After training, if y≤0.5 → class1; if y>0.5 → class2.

In [7]:
```
MyNet = nn.Sequential(
    nn.Linear(2, 50),
    nn.ReLU(),
    nn.Linear(50, 100),
    nn.ReLU(),
    nn.Linear(100, 50),
    nn.ReLU(),
    nn.Linear(50, 1),
)
MyNet.to(device)
loss_func = nn.MSELoss()
optimizer = torch.optim.Ac
.005)
```

X = (x1, x2)

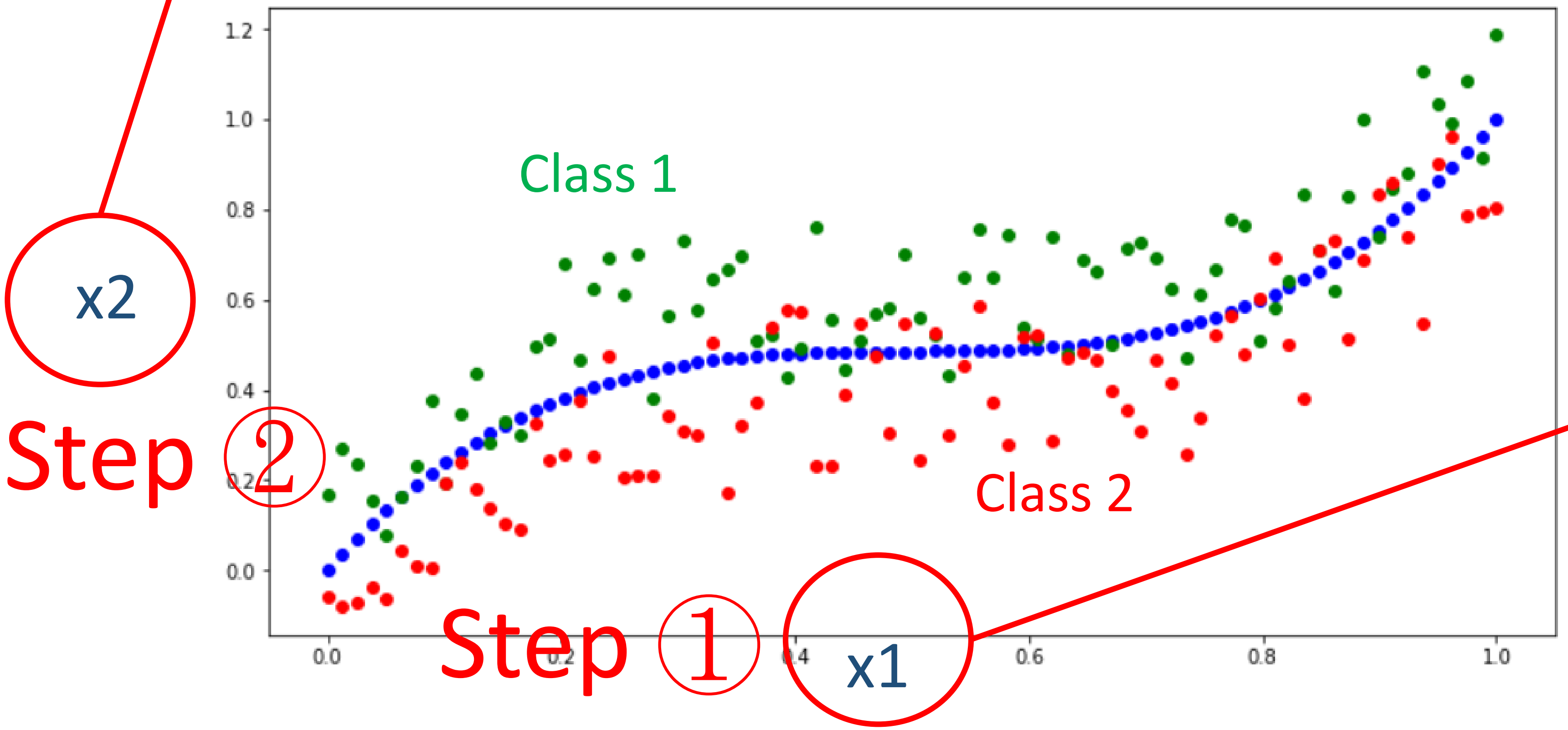
$\hat{y}$ = 0, 1

$y \leq 0.5$ → class 1
$y > 0.5$ → class 2

$$L(w,b) = \sum_{n=1}^{N} (\hat{y}^n - y^n)^2$$

Generate data

In [7]:
```
lstX20 = []
lstX21 = []
for i in range(len(lstX1)):
  lstX20.append(lstY1[i] + random.uniform(-0.1, 0.3))
  lstX21.append(lstY1[i] - random.uniform(-0.1, 0.3))
```




```
x = -10
while(x<10):
  y=3*x*x*x + 2*x*x + 5*x
  lstY1.append(y)
  lstX1.append(x)
  x = x + 0.25
print(len(lstX1), len(lstY1))

#normalized to [0,1]
lstX1= [(float(i)-min(lstX1))/(
lstY1= [(float(i)-min(lstY1))/(
```

Combine list x1, x20, x21 to generate X and Y

X = (x1, x2)
Y = 0, 1

Step ③

In [9]:
```
lstX=[]
lstY=[]
for i in range(len(lstX1)):
   lstX.append([lstX1[i],lstX20[i]])
   lstY.append([0])
   lstX.append([lstX1[i],lstX21[i]])
   lstY.append([1])
numpyX = np.array(lstX)
numpyY = np.array(lstY)
print(numpyX.shape, numpyY.shape)
```

```
(160, 2) (160, 1)
```

Train with mini-batches

```
In [11]: import torch.utils.data as Data
         torch_dataset = Data.TensorDataset(tensorX, tensorY_hat)
```

```
In [12]: loader = Data.DataLoader(
             dataset=torch_dataset,
             batch_size=BATCH_SIZE,
             shuffle=True,
             num_workers=0,    # subprocesses for loading data
         )
```

```
In [13]: # initialize NN weights
         for name, param in MyNet.named_parameters():
           if(param.requires_grad):
             torch.nn.init.normal_(param, mean=0.0, std=0.02)

         lossLst = []
         for epoch in range(1, 500):
           for (batchX, batchY_hat) in loader:
             tensorY = MyNet(batchX)
             loss = loss_func(batchY_hat, tensorY)
             lossLst.append(float(loss))
             optimizer.zero_grad()
             loss.backward()
             optimizer.step()
```

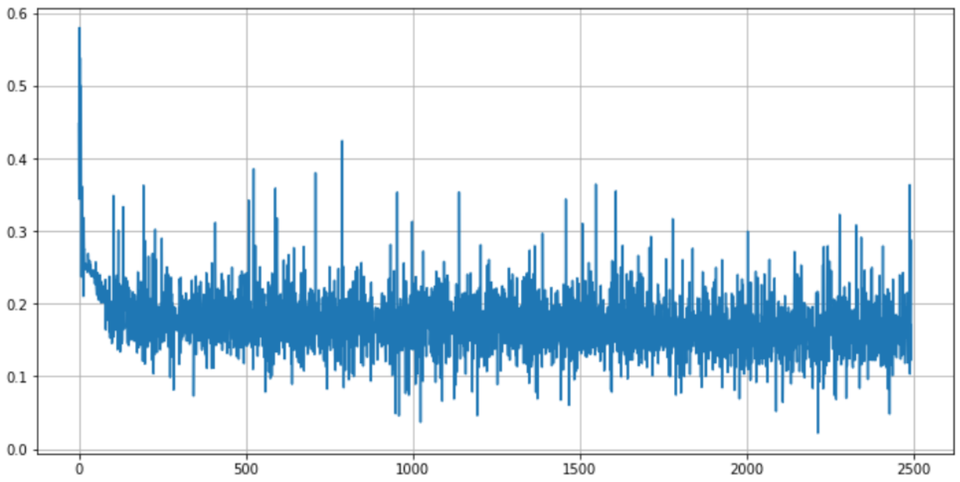
Train with whole data

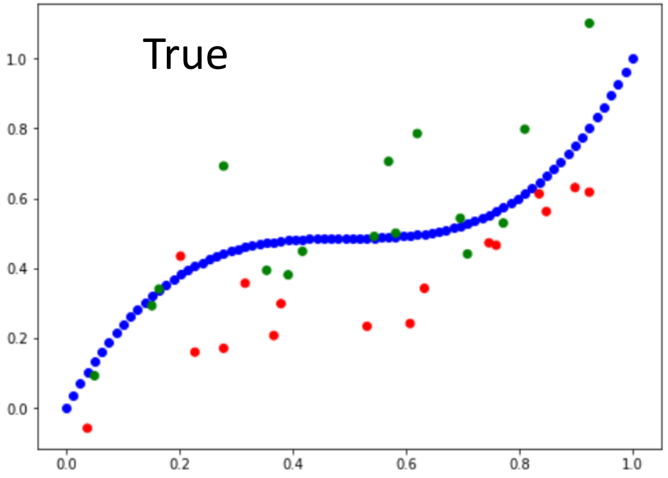
```
lossLst = []
for epoch in range(1, 2000):
    tensorY = MyNet(tensorX)
    loss = loss_func(tensorY_hat, tensorY)
    loss1 = float(loss)
    lossLst.append(float(loss))
    optimizer.zero_grad()
    loss.backward()
    optimizer.step()
```

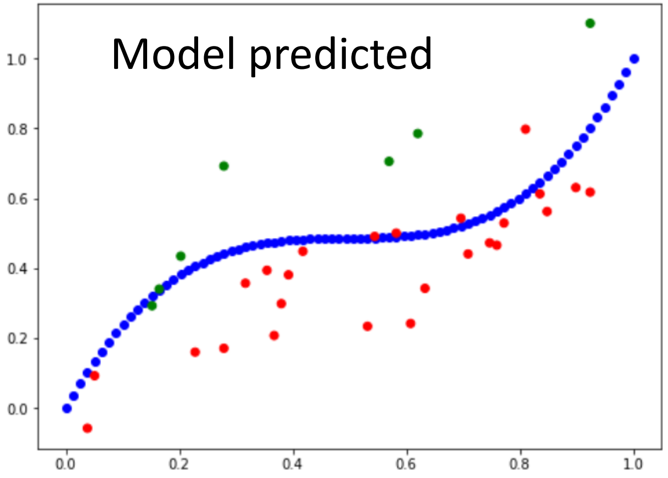
Classification with threshold = 0.5

```
correctNo = 0
for i in range(Y.size):
  if(Y[i][0]<=0.5):
    lstColor.append("green")
    if(testY_hat[i][0]==0):
      correctNo = correctNo + 1
  else:
    lstColor.append("red")
    if(testY_hat[i][0]==1):
      correctNo = correctNo + 1
accuracy = correctNo/Y.size
```

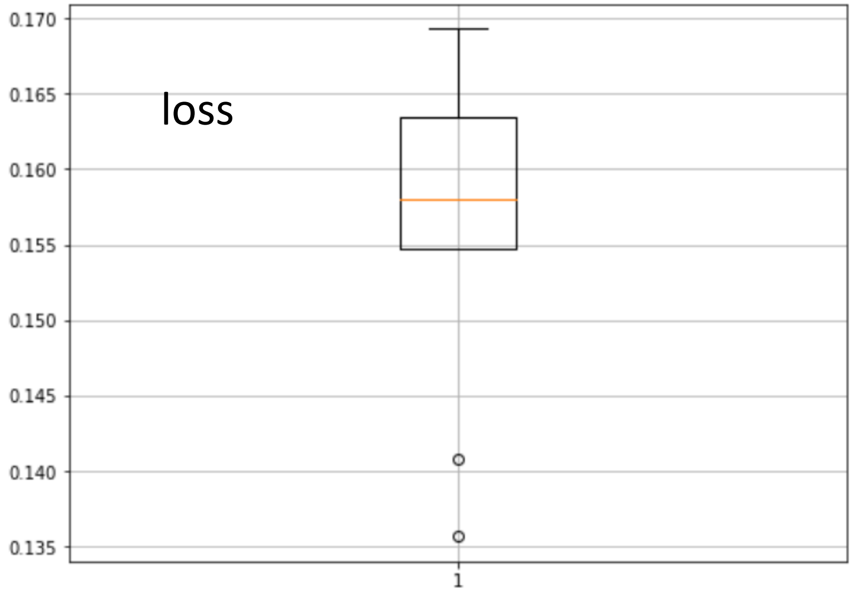
Performance visualization

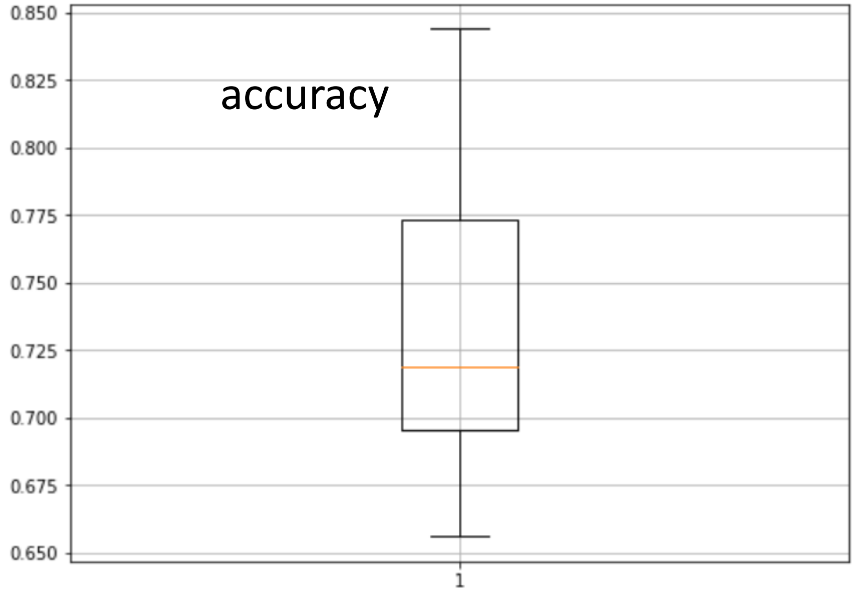






N=10





Design 2

Run " 4.2. Classification with CE loss"

- NN output layer contains two nodes, y_1 and y_2, where $y_1 = P(C_1|x)$, $y_2 = P(C_2|x)$.
- Use cross entropy as loss function to train NN.

In [7]:
```
MyNet = nn.Sequential(
    nn.Linear(2, 50),
    nn.ReLU(),
    nn.Linear(50, 100),
    nn.ReLU(),
    nn.Linear(100, 50),
    nn.ReLU(),
    nn.Linear(50, 2),
)
MyNet.to(device)
loss_func = nn.CrossEntropyLoss()
optimizer = torch.optim.Adam(MyNet.parameters(), lr=0.005)
```

2 classes

Entropy

More information → more uncertain → larger entropy

$$Entropy = -\sum_i p_i log_2(p_i)$$

Excel formula: =LOG(N, 2)
LOG(2, 2)=1
LOG(0.5, 2) = -1

Use Excel to verify

75% × 0.41
+ 25% × 2
= 0.81 bits

https://r23456999.medium.com/%E4%BD%95%E8%AC%82-cross-entropy-%E4%BA%A4%E5%8F%89%E7%86%B5-b6d4cef9189d

Cross entropy

Measures the differences between the true probability p_i and the predicted probability q_i

$$H(p,q) = -\sum_i p_i \ \ ln\ (q_i)$$ Excel formula: =LN(x)

Use Excel to verify

動物	實際機率分佈	預測機率分佈	Entropy
Cat	0%	2%	0% * -log(2%) = 0
Dog	0%	30%	0% * -log(30%) = 0
Fox	0%	45%	0% * -log(45%) = 0
Cow	0%	0%	0% * -log(0%) = 0
Red Panda	100%	25%	100% * -log(25%) = 1.386
Bear	0%	5%	0% * -log(5%) = 0
Dolphin	0%	0%	0% * -log(0%) = 0
總計: cross-entropy = 1.386			

https://r23456999.medium.com/%E4%BD%95%E8%AC%82-cross-entropy-%E4%BA%A4%E5%8F%89%E7%86%B5-b6d4cef9189d

CE vs MSE

Use Excel to compare CE vs MSE

p_i: Red Panda 99.4, others 0.01

q_i : Cat 99.4, others 0.01

$$H(p,q) = -\sum_i p_i \;\; ln\ (q_i)$$

動物	實際機率分佈	預測機率分佈	Entropy
Cat	0%	2%	0% * -log(2%) = 0
Dog	0%	30%	0% * -log(30%) = 0
Fox	0%	45%	0% * -log(45%) = 0
Cow	0%	0%	0% * -log(0%) = 0
Red Panda	100%	25%	100% * -log(25%) = 1.386
Bear	0%	5%	0% * -log(5%) = 0
Dolphin	0%	0%	0% * -log(0%) = 0
總計: cross-entropy = 1.386			

https://r23456999.medium.com/%E4%BD%95%E8%AC%82-cross-entropy-%E4%BA%A4%E5%8F%89%E7%86%B5-b6d4cef9189d

We can use Bayesian's rule to derive $y_i = p(C_i|x)$

$$y_1 = P(C_1|x) = \frac{P(x|C_1)P(C_1)}{P(x|C_1)P(C_1) + P(x|C_2)P(C_2)}$$

Generative Model $P(x) = P(x|C_1)P(C_1) + P(x|C_2)P(C_2)$

Reference: 李弘毅 ML Lecture 4 https://youtu.be/fZAZUYEeIMg

Probabilistic Generative Model

$$f_{\mu^1,\Sigma^1}(x) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma^1|^{1/2}} exp\left\{-\frac{1}{2}(x-\mu^1)^T(\Sigma^1)^{-1}(x-\mu^1)\right\}$$

P(C1)
= 79 / (79 + 61) =0.56

$$\mu^1 = \begin{bmatrix} 75.0 \\ 71.3 \end{bmatrix} \quad \Sigma^1 = \begin{bmatrix} 874 & 327 \\ 327 & 929 \end{bmatrix}$$

Assuming x^n are sampled from a Gaussian distribution, then we can use maximum likelihood to find the best Gaussian distribution behind them.

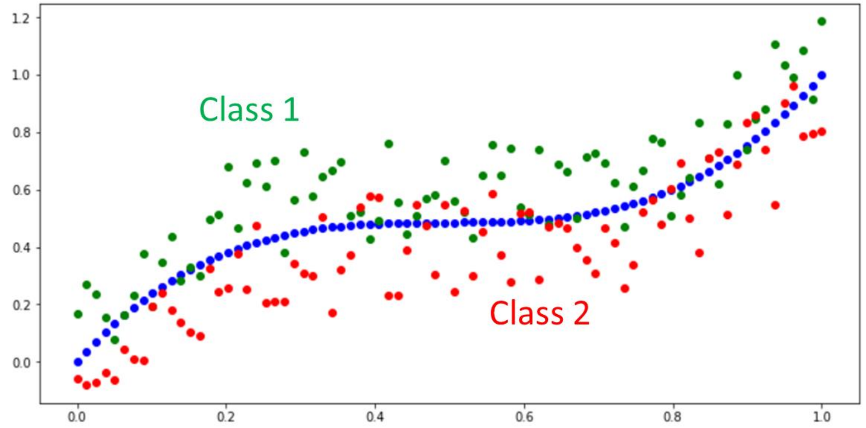
$$P(C_1|x) = \frac{P(x|C_1)P(C_1)}{P(x|C_1)P(C_1) + P(x|C_2)P(C_2)}$$

$$f_{\mu^2,\Sigma^2}(x) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma^2|^{1/2}} exp\left\{-\frac{1}{2}(x-\mu^2)^T(\Sigma^2)^{-1}(x-\mu^2)\right\}$$

P(C2)
= 61 / (79 + 61)
=0.44

$$\mu^2 = \begin{bmatrix} 55.6 \\ 59.8 \end{bmatrix} \quad \Sigma^2 = \begin{bmatrix} 847 & 422 \\ 422 & 685 \end{bmatrix}$$

If $P(C_1|x) > 0.5$



Reference: 李弘毅 ML Lecture 4 https://youtu.be/fZAZUYEeIMg

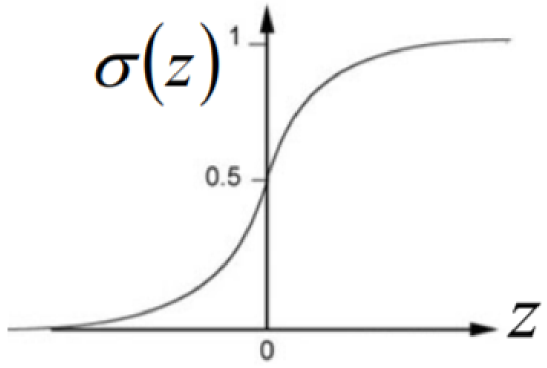
Posterior probability $y_i = p(C_i|x)$ can be represented as a sigmoid function of z

$$\boxed{y_1 = P(C_1|x)} = \frac{P(x|C_1)P(C_1)}{P(x|C_1)P(C_1) + P(x|C_2)P(C_2)}$$

$$= \frac{1}{1 + \frac{P(x|C_2)P(C_2)}{P(x|C_1)P(C_1)}} = \frac{1}{1 + exp(-z)} \boxed{= \sigma(z)}$$

Sigmoid function

$$\boxed{z = ln \frac{P(x|C_1)P(C_1)}{P(x|C_2)P(C_2)}}$$



The posterior probability $y_i = p(C_i|x)$ can be represented as sigmoid function of linear combination of x

$$P(C_1|x) = \sigma(z)$$

Assuming the covariance matrices of the two classes are the same

$$\boxed{\begin{aligned} z = & \cancel{ln\frac{|\Sigma^2|^{1/2}}{|\Sigma^1|^{1/2}}} \cancel{-\frac{1}{2}x^T(\Sigma^1)^{-1}x} + (\mu^1)^T(\Sigma^1)^{-1}x - \frac{1}{2}(\mu^1)^T(\Sigma^1)^{-1}\mu^1 \\ & \cancel{+\frac{1}{2}x^T(\Sigma^2)^{-1}x} - (\mu^2)^T(\Sigma^2)^{-1}x + \frac{1}{2}(\mu^2)^T(\Sigma^2)^{-1}\mu^2 + ln\frac{N_1}{N_2} \end{aligned}}$$

$$\Sigma_1 = \Sigma_2 = \Sigma$$

$$z = \underbrace{(\mu^1 - \mu^2)^T\Sigma^{-1}}_{\boldsymbol{w^T}}x \underbrace{- \frac{1}{2}(\mu^1)^T\Sigma^{-1}\mu^1 + \frac{1}{2}(\mu^2)^T\Sigma^{-1}\mu^2 + ln\frac{N_1}{N_2}}_{\text{b}}$$

$$\boxed{y_1 = P(C_1|x) = \sigma(w \cdot x + b)}$$

How about directly find ***w*** and b?

In generative model, we estimate $N_1, N_2, \mu^1, \mu^2, \Sigma$

Then we have ***w*** and b

Logistic Regression

If we use gradient decent to find optimal w and b for the posterior probability $y_1 = p(C_1|x) = \sigma(w \cdot x + b)$, then the problem becomes logistic regression.

We want to find $P_{w,b}(C_1|x)$

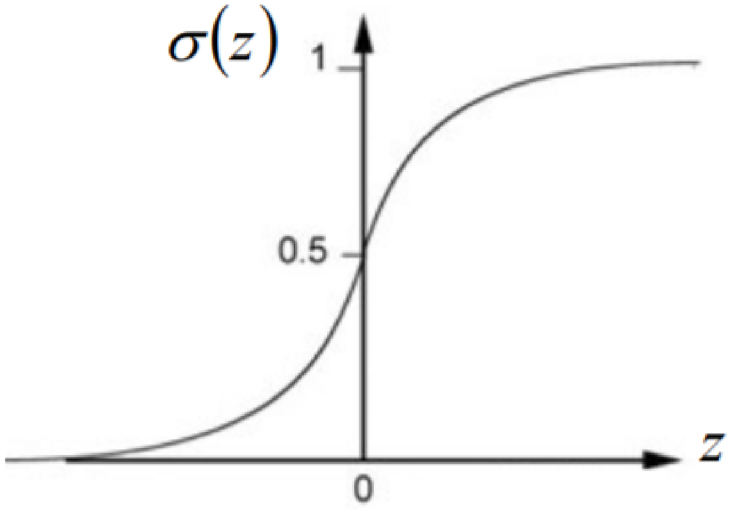
If $P_{w,b}(C_1|x) \geq 0.5$, output C_1

Otherwise, output C_2

$$P_{w,b}(C_1|x) = \sigma(z)$$

$$z = w \cdot x + b$$

$$\sigma(z) = \frac{1}{1 + exp(-z)}$$



Logistic Regression vs Regression

Logistic Regression

$$f_{w,b}(x) = \sigma\left(\sum_i w_i x_i + b\right)$$

Output: between 0 and 1

Linear Regression

$$f_{w,b}(x) = \sum_i w_i x_i + b$$

Output: any value

Reference: 李弘毅 ML Lecture 5 https://youtu.be/hSXFuypLukA

Use maximum likelihood to derive loss function for logistic regression

Assuming the training data is generated from $y_1 = P_{w,b}(C_1|\,x) = \sigma(w \cdot x + b)$, what is the probability of generating the data?

Training Data

x^1	x^2	x^3	……	x^N
C_1	C_1	C_2		C_1

max $$L(w,b) = f_{w,b}(x^1)f_{w,b}(x^2)\left(1 - f_{w,b}(x^3)\right)\cdots f_{w,b}(x^N)$$

min $$-lnL(w,b) = -lnf_{w,b}(x^1) - lnf_{w,b}(x^2) - ln\left(1 - f_{w,b}(x^3)\right)\cdots$$

$\hat{y}^n$: 1 for class 1, 0 for class 2

$$= \sum_n -\underbrace{\left[\hat{y}^n lnf_{w,b}(x^n) + (1-\hat{y}^n)ln\left(1 - f_{w,b}(x^n)\right)\right]}_{\text{Cross entropy between two Bernoulli distribution}}$$

Reference: 李弘毅 ML Lecture 5 https://youtu.be/hSXFuypLukA

Loss function for logistic regression vs regression

Training data: $(x^n, \hat{y}^n)$

$\hat{y}^n$: 1 for class 1, 0 for class 2

$$L(f) = \sum_n C(f(x^n), \hat{y}^n)$$

Training data: $(x^n, \hat{y}^n)$

$\hat{y}^n$: a real number

$$L(f) = \frac{1}{2}\sum_n (f(x^n) - \hat{y}^n)^2$$

Cross entropy:

$$C(f(x^n), \hat{y}^n) = -\left[\hat{y}^n ln f(x^n) + (1 - \hat{y}^n) ln\left(1 - f(x^n)\right)\right]$$

Reference: 李弘毅 ML Lecture 5 https://youtu.be/hSXFuypLukA

Generate training data

In [5]:
```python
lstX=[]
lstY=[]
for i in range(len(lstX1)):
  lstX.append([lstX1[i],lstX20[i]])
  lstY.append(0)
  lstX.append([lstX1[i],lstX21[i]])
  lstY.append(1)
numpyX = np.array(lstX)
numpyY = np.array(lstY)
print(numpyX.shape, numpyY.shape)
```

(160, 2) (160,) Y is a vector

4.2. Classification with CE loss

In [9]:
```python
lstX=[]
lstY=[]
for i in range(len(lstX1)):
  lstX.append([lstX1[i],lstX20[i]])
  lstY.append([0])
  lstX.append([lstX1[i],lstX21[i]])
  lstY.append([1])
numpyX = np.array(lstX)
numpyY = np.array(lstY)
print(numpyX.shape, numpyY.shape)
```

(160, 2) (160, 1) Y is a matrix

4.1. Classification with MSE loss

Calculate cross entropy loss

```
In [12]: for (batchX, batchY_hat) in loader:
             break
         print(batchX.shape, batchY_hat)
```

```
torch.Size([5, 2]) tensor([0, 0, 0, 1, 1], device='cuda:0')
```

Send batchX to NN

```
In [13]: tensorY = MyNet(batchX)
         print(tensorY.shape,"\n", tensorY)
```

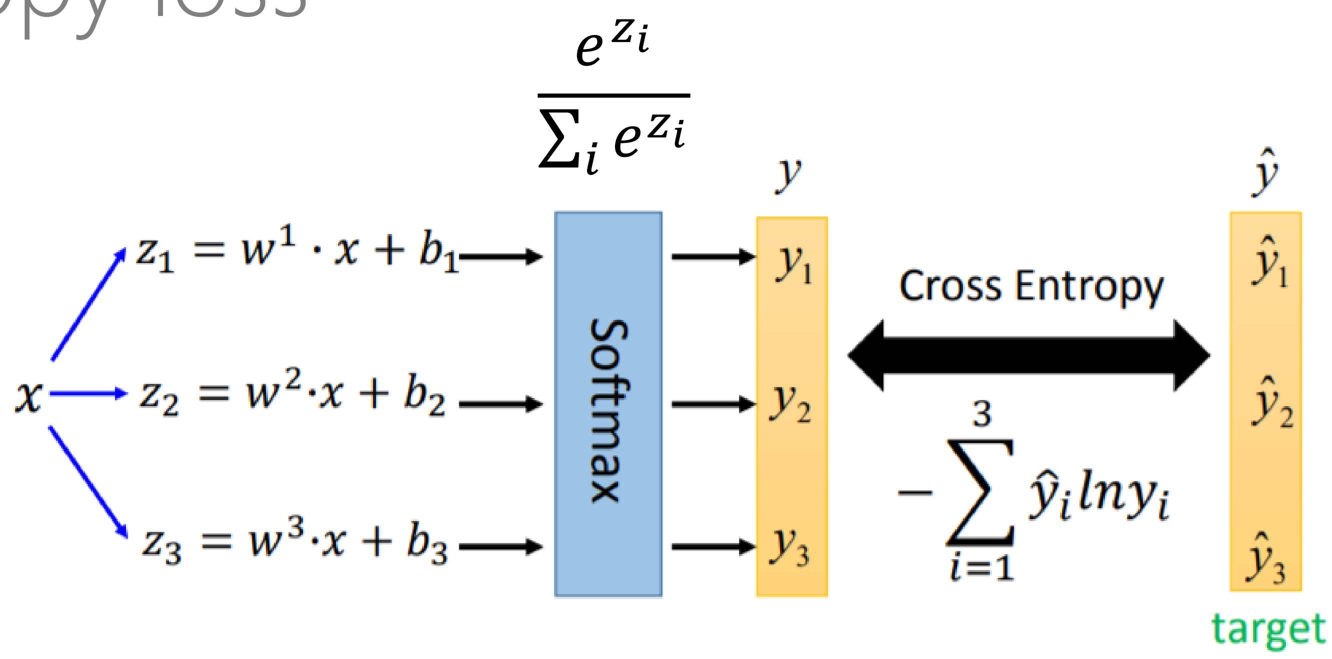
```
torch.Size([5, 2])
 tensor([[-0.0180,  0.0855],
        [-0.0244,  0.0741],
        [-0.0187,  0.0850],
        [-0.0258,  0.0687],
        [-0.0267,  0.0617]], device='cuda:0', grad_fn=<AddmmBackward>)
```

Calculate cross entropy between y and y-hat

```
In [14]: loss = loss_func(tensorY, batchY_hat)
         print(tensorY.shape, batchY_hat.shape, loss)
```

```
torch.Size([5, 2]) torch.Size([5]) tensor(0.7066, device='cuda:0', grad_
```

Cross entropy loss



3-classe example

A	B	C	D	E	F	G	H	I	J	K
z1	z2	y-hat	p1	p2	EXP(z1)	EXP(z2)	F+G	q1	q2	-(P1*LN(Q1)+P2*LN(Q2))
-0.018	0.0855	0	1	0	0.982	1.089	2.071	0.474	0.526	0.74624
-0.0244	0.0741	0	1	0	0.976	1.077	2.053	0.475	0.525	0.74361
-0.0187	0.085	0	1	0	0.981	1.089	2.070	0.474	0.526	0.74634
-0.0258	0.0687	1	0	1	0.975	1.071	2.046	0.476	0.524	0.64701
-0.0267	0.0617	1	0	1	0.974	1.064	2.037	0.478	0.522	0.64992
										0.70662

Calculate accuracy rate

In [12]:
```
for (batchX, batchY_hat) in loader:
    break
print(batchX.shape, batchY_hat)
```

```
torch.Size([5, 2]) tensor([0, 0, 0, 1, 1],
```

In [15]:
```
print(tensorY.shape,"\n", tensorY)
```

```
torch.Size([5, 2])
 tensor([[-0.0180,  0.0855],
        [-0.0244,  0.0741],
        [-0.0187,  0.0850],
        [-0.0258,  0.0687],
        [-0.0267,  0.0617]], device=
```

In [16]:
```
# apply softmax
tensorY = torch.softmax(tensorY, 1)
print(tensorY.shape,"\n", tensorY)
```

```
torch.Size([5, 2])
 tensor([[0.4742, 0.5258],
        [0.4754, 0.5246],
        [0.4741, 0.5259],
        [0.4764, 0.5236],
        [0.4779, 0.5221]], device='cu
```

In [19]:
```
correct = 0
MaxIdxOfEachRow = torch.max(tensorY, 1)[1]
for i in range(batchY_hat.shape[0]):
  print(int(MaxIdxOfEachRow[i]), int(batchY_hat[i]),
  if (int(MaxIdxOfEachRow[i]) == int(batchY_hat[i])
    print("correct")
    correct += 1
  else:
    print("wrong")
print(correct)
accuracy = correct/batchY_hat.shape[0]
print("%.2f" % accuracy)
```

```
1 0==>wrong
1 0==>wrong
1 0==>wrong
1 1==>correct
1 1==>correct
2
0.40
```

Soft max and torch.max

```
In [15]: print(tensorY.shape,"\n", tensorY)

torch.Size([5, 2])
 tensor([[-0.0180,  0.0855],
        [-0.0244,  0.0741],
        [-0.0187,  0.0850],
        [-0.0258,  0.0687],
        [-0.0267,  0.0617]], device='cuda:0', grad_fn=<
```

```
In [16]: # apply softmax
         tensorY = torch.softmax(tensorY, 1)
         print(tensorY.shape,"\n", tensorY)

torch.Size([5, 2])
 tensor([[0.4742, 0.5258],
        [0.4754, 0.5246],
        [0.4741, 0.5259],
        [0.4764, 0.5236],
        [0.4779, 0.5221]], device='cuda:0', grad_fn=<So
```

torch.softmax(tensor, 1)

$$\frac{e^{y_1}}{e^{y_1}+e^{y_2}} \qquad \frac{e^{y_2}}{e^{y_1}+e^{y_2}}$$

0: ↓

1: →

```
In [17]: MaxOfEachRow = torch.max(tensorY, 1)
         print(MaxOfEachRow)

torch.return_types.max(
values=tensor([0.5258, 0.5246, 0.5259, 0.5236, 0.5221],
       grad_fn=<MaxBackward0>),
indices=tensor([1, 1, 1, 1, 1], device='cuda:0'))
```

torch.max(tentor, 1)

Torch.max

```
tensor([[0.4742, 0.5258],
        [0.4754, 0.5246],
        [0.4741, 0.5259],
        [0.4764, 0.5236],
        [0.4779, 0.5221]],
```

torch.max(tentor, 1)[1]

[1]: The 2nd item of torch.max results

In [17]:
```
MaxOfEachRow = torch.max(tensorY, 1)
print(MaxOfEachRow)
```

```
torch.return_types.max(
values=tensor([0.5258, 0.5246, 0.5259, 0.5236, 0.5221], device='c
       grad_fn=<MaxBackward0>),
indices=tensor([1, 1, 1, 1, 1], device='cuda:0'))
```

In [18]:
```
MaxIdxOfEachRow = torch.max(tensorY, 1)[1]
print(MaxIdxOfEachRow)
```

```
tensor([1, 1, 1, 1, 1], device='cuda:0')
```

In [19]:
```
correct = 0
MaxIdxOfEachRow = torch.max(tensorY, 1)[1]
for i in range(batchY_hat.shape[0]):
  print(int(MaxIdxOfEachRow[i]), int(batchY_hat[i]), end="==>")
  if (int(MaxIdxOfEachRow[i]) == int(batchY_hat[i])):
    print("correct")
    correct += 1
  else:
    print("wrong")
print(correct)
accuracy = correct/batchY_hat.shape[0]
print("%.2f" % accuracy)
```

```
1 0==>wrong
1 0==>wrong
1 0==>wrong
1 1==>correct
1 1==>correct
2
0.40
```

Mini-batch training

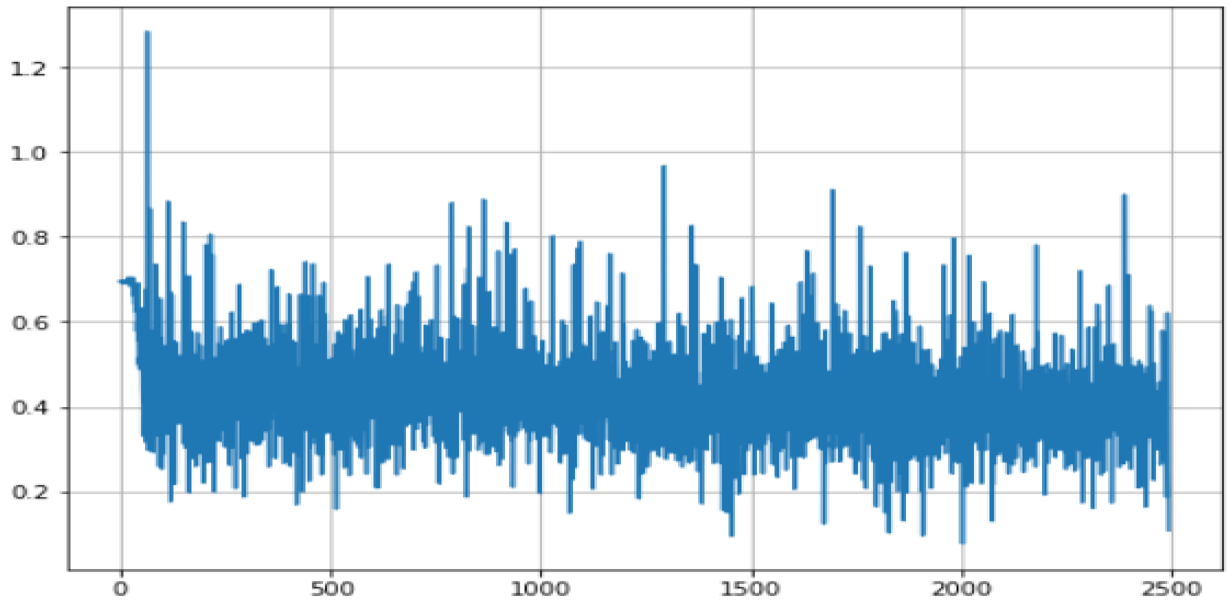
```
for epoch in range(1, 500):
  for (batchX, batchY_hat) in loader:
    tensorY = MyNet(batchX)
    tensorY = torch.softmax(tensorY, 1)
    loss = loss_func(tensorY, batchY_hat)
    lossLst.append(float(loss))
    optimizer.zero_grad()
    loss.backward()
    optimizer.step()

    correct = 0
    MaxIdxOfEachRow = torch.max(tensorY, 1)[1]
    for i in range(batchY_hat.shape[0]):
      if (int(MaxIdxOfEachRow[i]) == int(batchY_hat[i])):
        correct += 1
    accuracy = correct/batchY_hat.shape[0]
    accuracyLst.append(accuracy)
```

4.2. Classification with CE loss

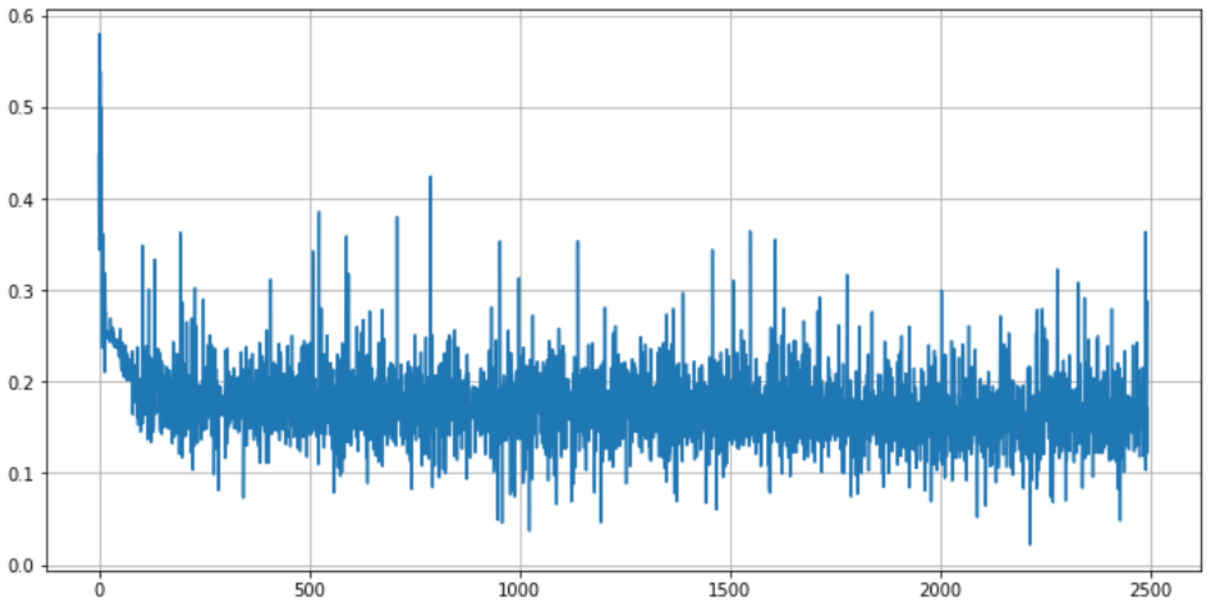
```
for epoch in range(1, 500):
  for (batchX, batchY_hat) in loader:
    tensorY = MyNet(batchX)
    loss = loss_func(batchY_hat, tensorY)
    lossLst.append(float(loss))
    optimizer.zero_grad()
    loss.backward()
    optimizer.step()
```

4.1. Classification with MSE loss

Loss plot



4.2. Classification with CE loss



4.1. Classification with MSE loss

Model performance on test data

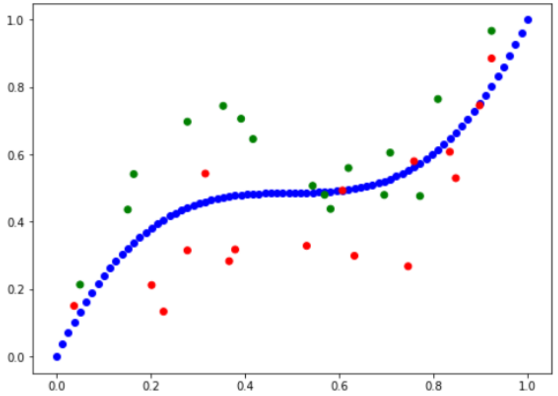
```python
# show model predicted classification
lstColor = []
correctNo = 0
MaxIdxOfEachRow = torch.max(tensorY, 1)[1]
for i in range(tensorY.shape[0]):
  if (int(MaxIdxOfEachRow[i]) == 0):
    lstColor.append("green")
    if(int(testY_hat[i])==0):
      correctNo += 1
  else:
    lstColor.append("red")
    if(testY_hat[i]==1):
      correctNo = correctNo + 1
print(correctNo)
accuracy = correctNo/tensorY.shape[0]
```

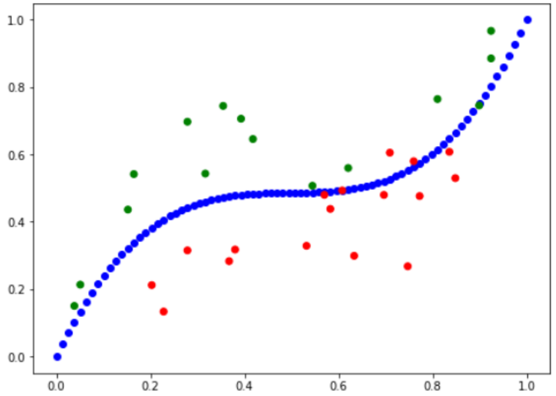
4.2. Classification with CE loss

```python
# show model predicted classification
lstColor = []
correctNo = 0
for i in range(Y.size):
  if(Y[i][0]<=0.5):
    lstColor.append("green")
    if(testY_hat[i][0]==0):
      correctNo = correctNo + 1
  else:
    lstColor.append("red")
    if(testY_hat[i][0]==1):
      correctNo = correctNo + 1
accuracy = correctNo/Y.size
```

4.1. Classification with MSE loss

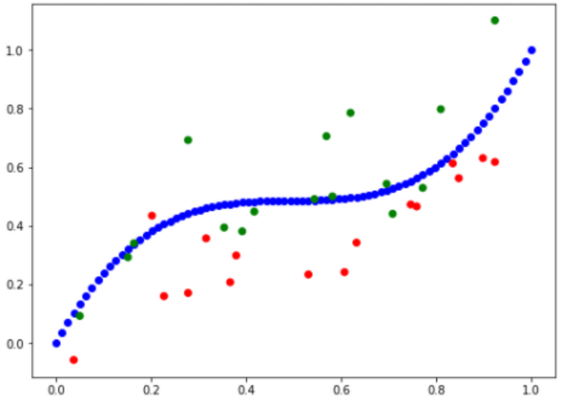
Model performance on test data

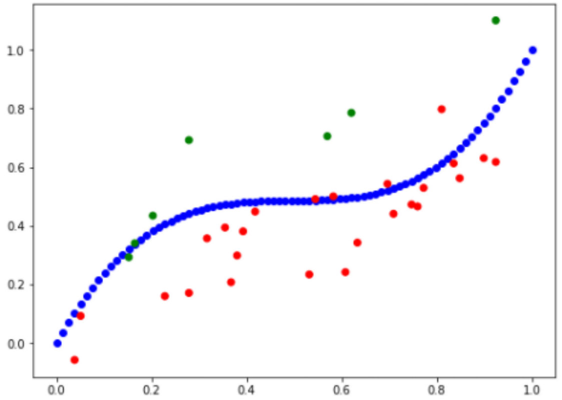





```
correct No.= 23 , accuracy =  0.72
```

4.2. Classification with CE loss

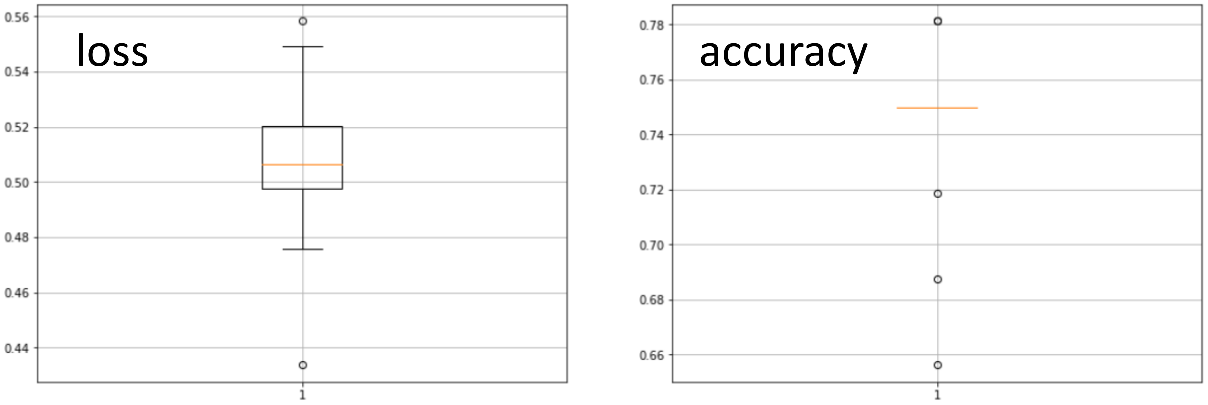




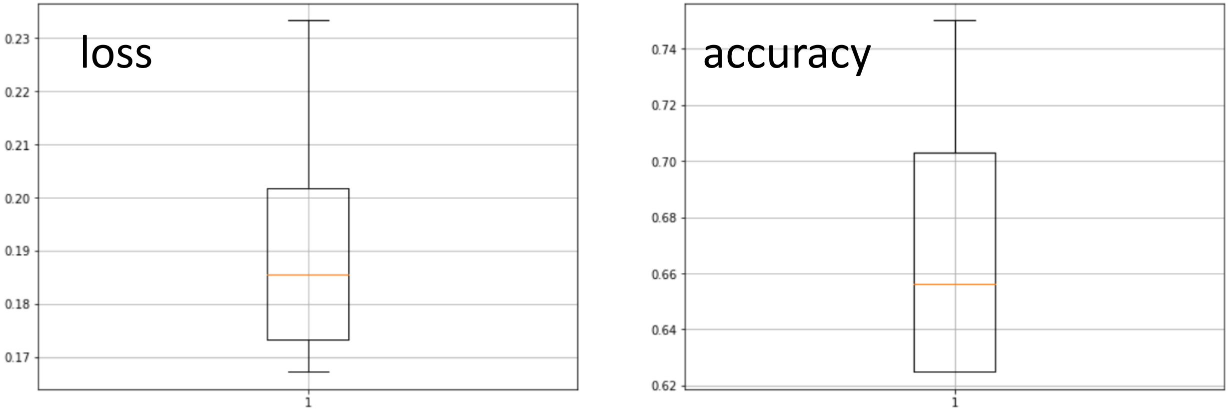

```
correct No.= 21 , accuracy =  0.66
```

4.1. Classification with MSE loss

Variance of model performance on test data

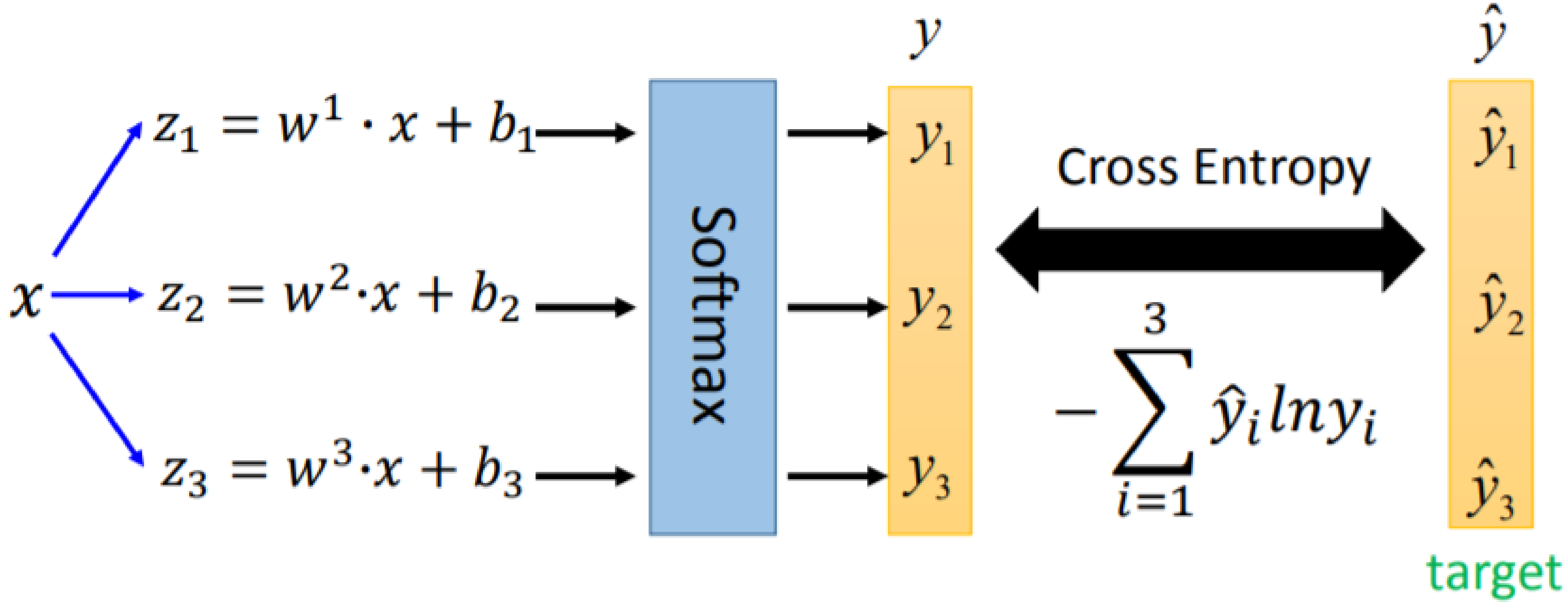


4.2. Classification with CE loss



4.1. Classification with MSE loss

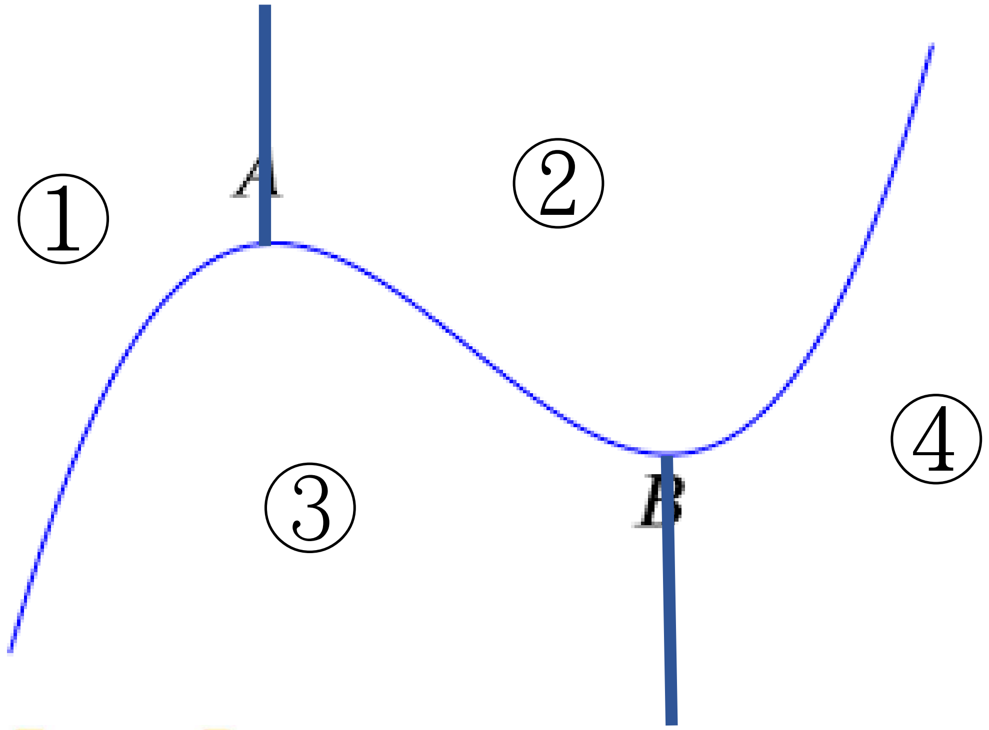
Multi-class classification



Reference: 李弘毅 ML Lecture 5 https://youtu.be/hSXFuypLukA

HW4

- Extend the example to 4 classes. Compare the classification performance (loss plot, scatter plot, box plot) between MSE and CE loss functions.



HW4

Evaluation of Neural Architectures Trained with Square Loss vs Cross-Entropy in Classification Tasks

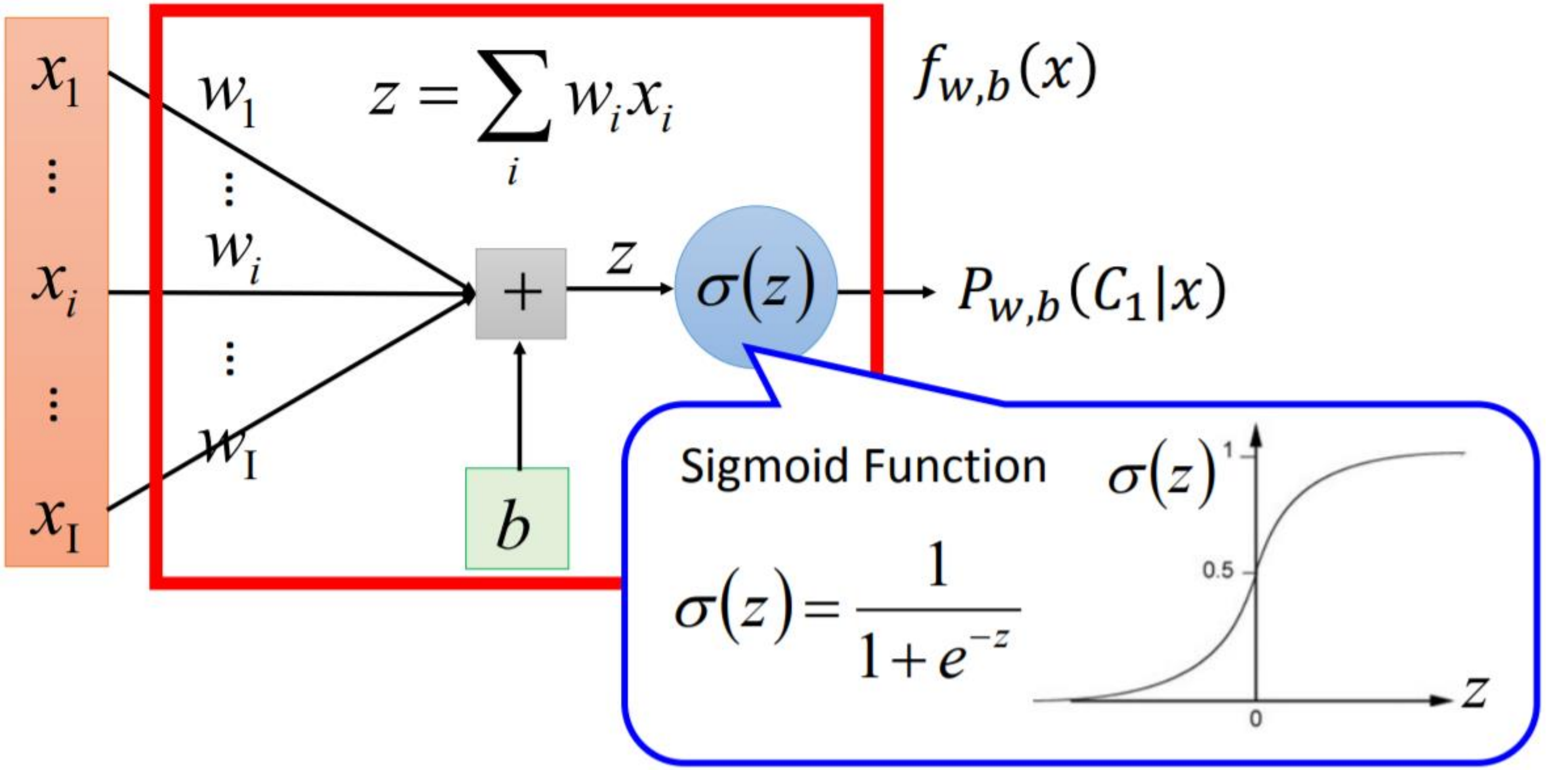
Like Hui, Mikhail Belkin

https://arxiv.org/abs/2006.07322

中文解讀: https://ai-scholar.tech/zh/articles/deep-learning/closs-square

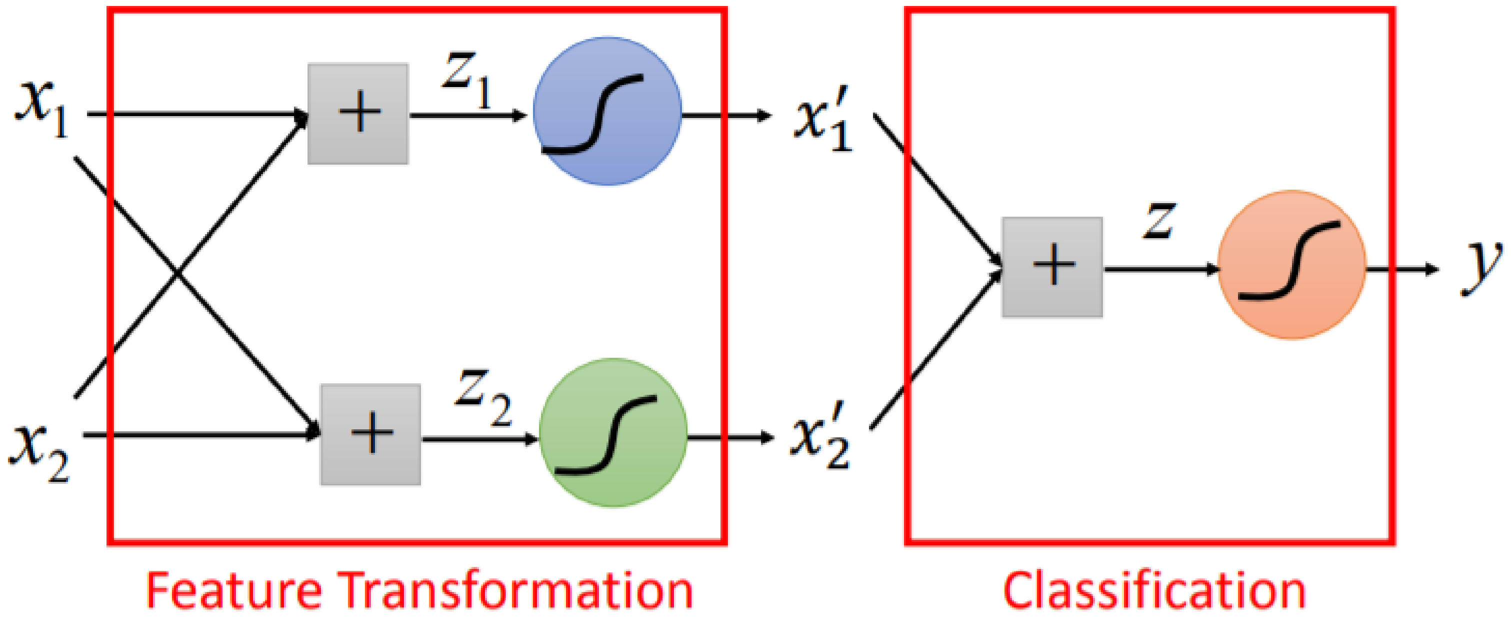
Each neuron in a NN performs logistic regression to classify its inputs

$$P(C_1|\, x) = \sigma(w \cdot x + b) = \sigma\left(\sum_i w_i x_i + b\right)$$



Reference: 李弘毅 ML Lecture 5 https://youtu.be/hSXFuypLukA

A neural network can be seen as cascading logistic regression models



Reference: 李弘毅 ML Lecture 5 https://youtu.be/hSXFuypLukA