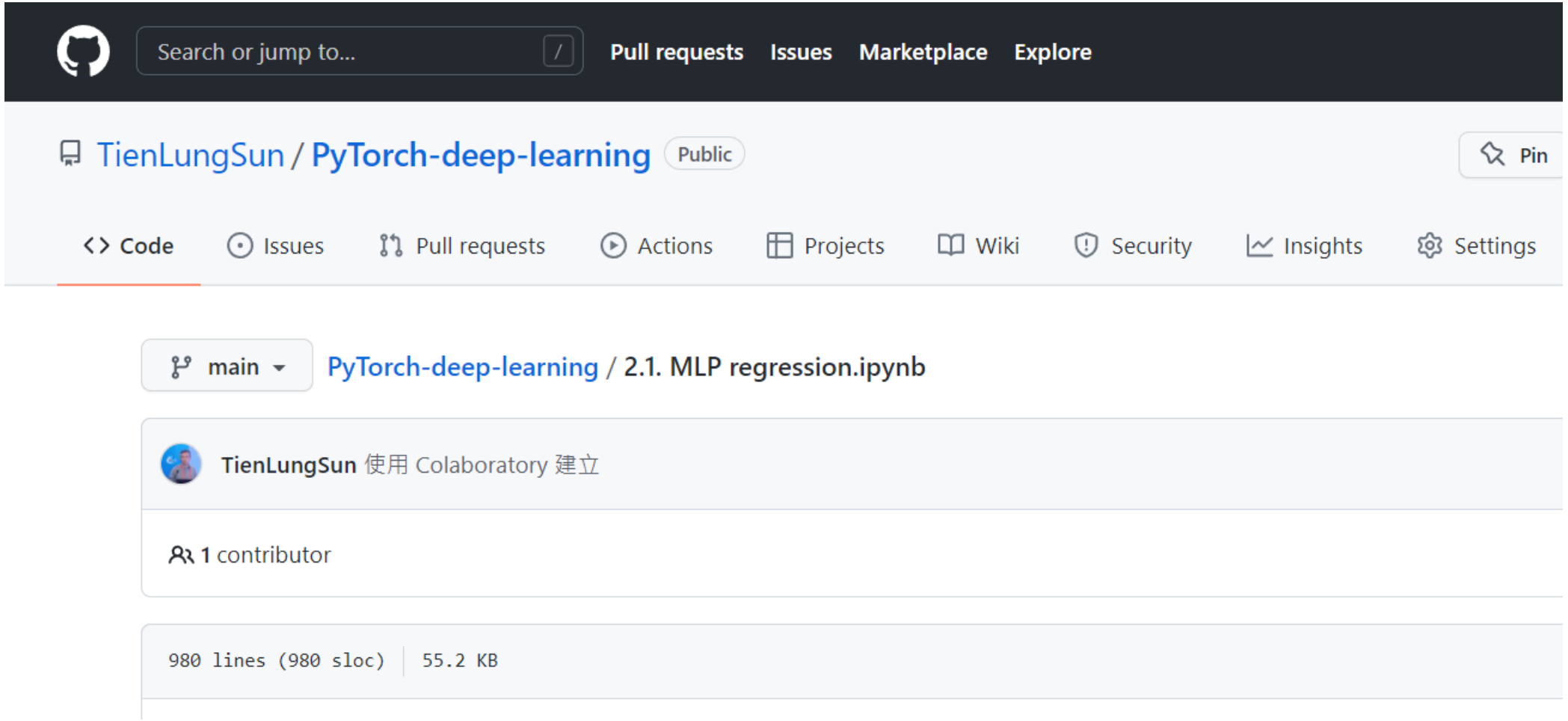
Regression

2.1 MLP regression.ipynb



How machine learns from data?

- Regression
- Classification

$$y = f(x)$$

- Define a function to be learned: $y = f(x)$
- Define a loss function $\mathcal{L}$ to describe the error between $\hat{y} = f(x)$ and y
- Find the optimal parameters of f that minimize $\mathcal{L}$

Statistics vs Machine Learning

Statistics versus machine learning

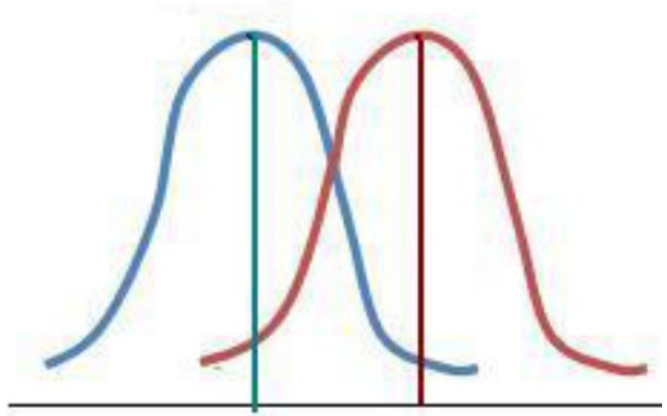
Statistics draws population inferences from a sample, and machine learning finds generalizable predictive patterns.

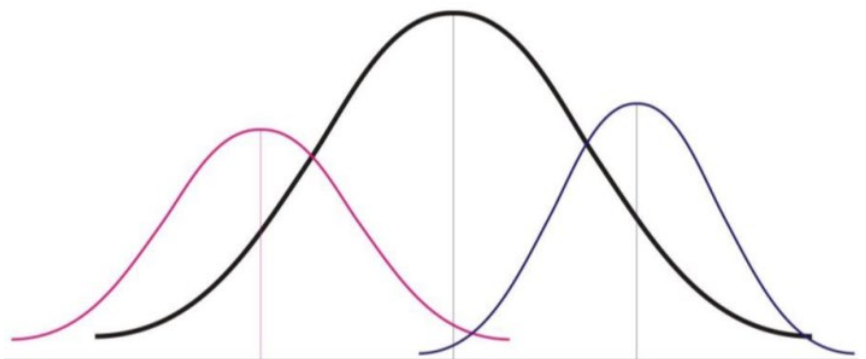
$$y = f(x)$$

Ij, H. (2018). Statistics versus machine learning. *Nat Methods*, *15*(4), 233.

Statistics draw population inferences

動作	range (delta D)
A1	8.20
A1	6.42
A1	8.26
A1	14.55
A1	11.70
A1	11.75
A1	12.72
A1	11.96
A1	6.03
A1	9.20
A1	14.25
A1	13.93
A2	14.17
A2	19.91
A2	9.40
A2	8.48
A2	10.61
A2	13.86
A2	7.15
A2	7.66
A2	6.09
A2	13.18
A2	9.15
A2	13.29





Evaluation of generalizable prediction performance with test data

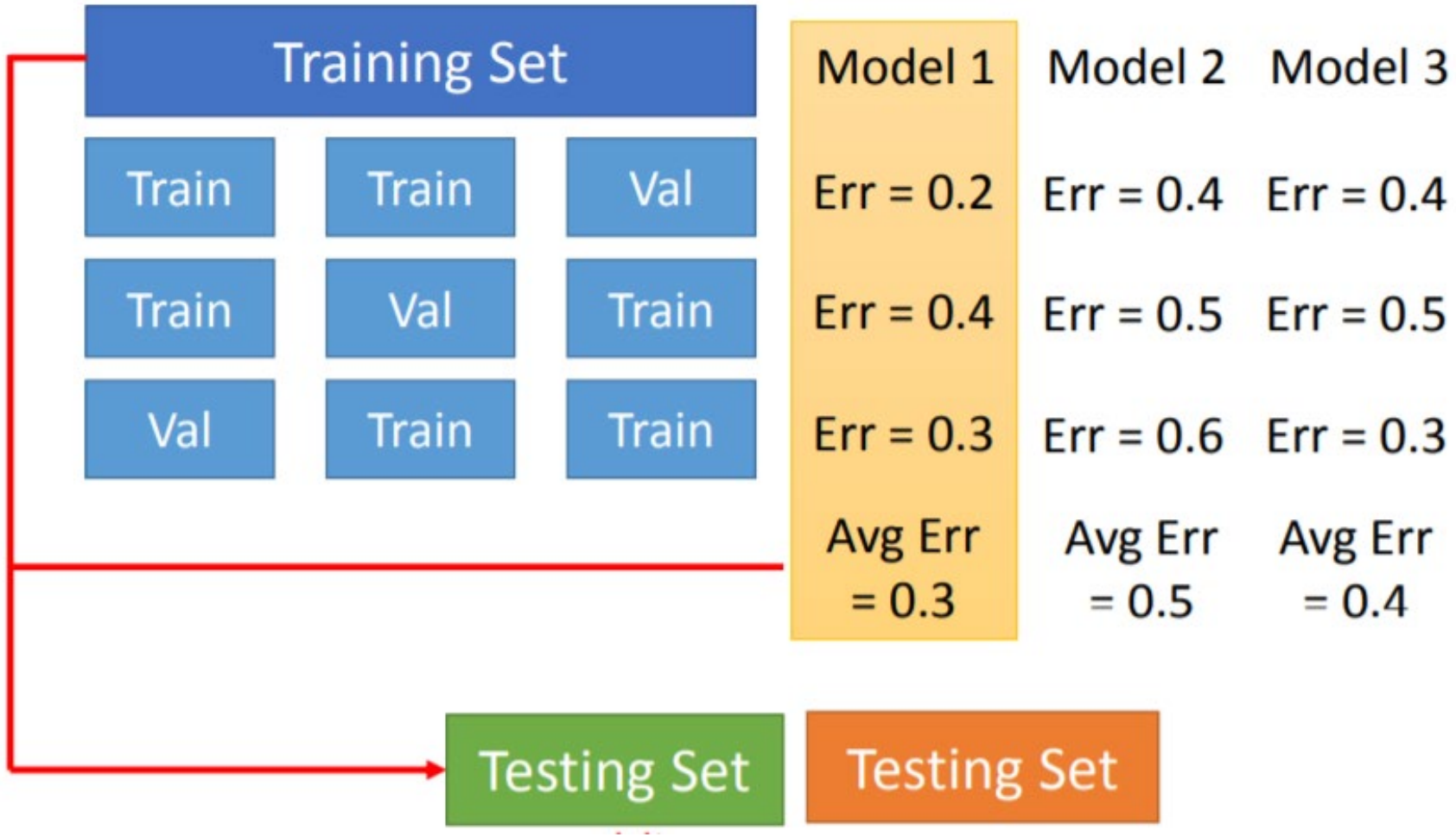
Split input data to train and test data

In [5]:

```
from sklearn.model_selection import train_test_split
trainX, testX, trainY, testY = train_test_split(numpyX, numpyY, test_size=0.20, random_state=0)
print(trainX.shape, testX.shape, trainY.shape, testY.shape)
```

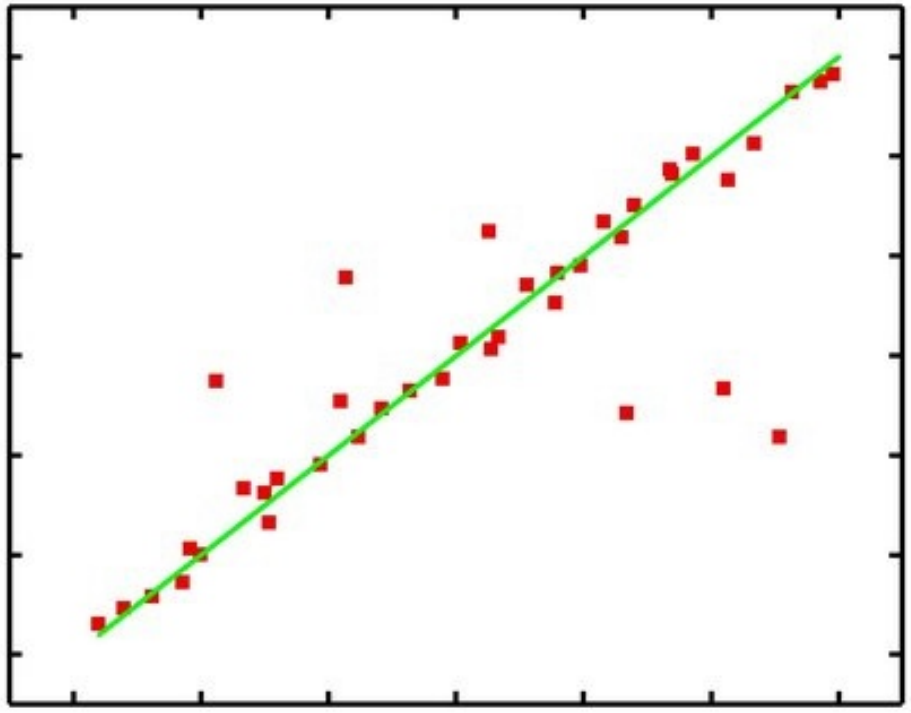
```
(1600, 7) (400, 7) (1600, 1) (400, 1)
```

Cross validation



Reference: 李弘毅 ML Lecture 2 https://youtu.be/D_S6y0Jm6dQ

Statistics vs Machine Learning



(b) Linear Regression

Statistics – R^2 of the variance explained

ML – MSE, MAE of test data which are unseen by the model

Input data

Try 5000, 1000, and 200 data

y	x1	x2	…
0.578			
0.64			
-0.96			
0.23			
…			

$$y = 0.323{x_1}^2 + 0.586x_1x_2 + 0.4x_3 + 0.8972{x_5}^3 + 0.267{x_3}^2x_5x_6 + 0.78{x_7}^2$$

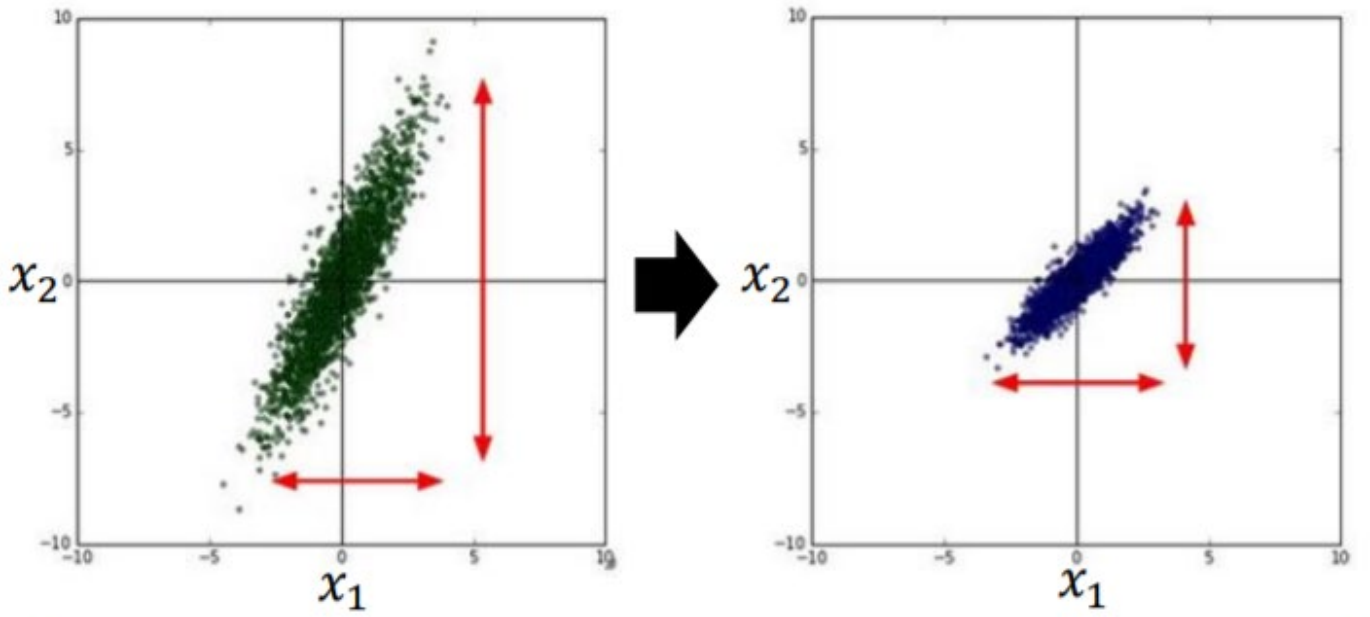
$$x_1 \sim \mathcal{N}(0.5, 0.3)$$

$$x_2 \sim \mathcal{N}(0.8, 0.5)$$

$$\dots$$

Feature scaling

$$y = b + w_1 x_1 + w_2 x_2$$

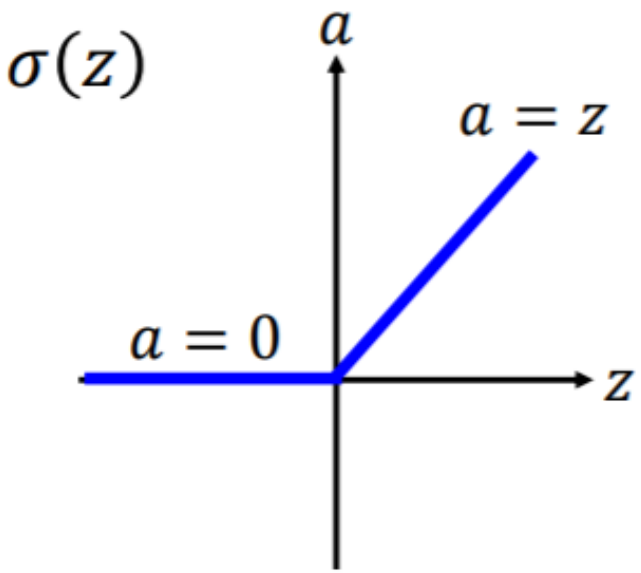


Make different features have the same scaling

Reference: 李弘毅 ML Lecture 3-1 https://youtu.be/yKKNr-QKz2Q

ReLU activation function

- Rectified Linear Unit (ReLU)



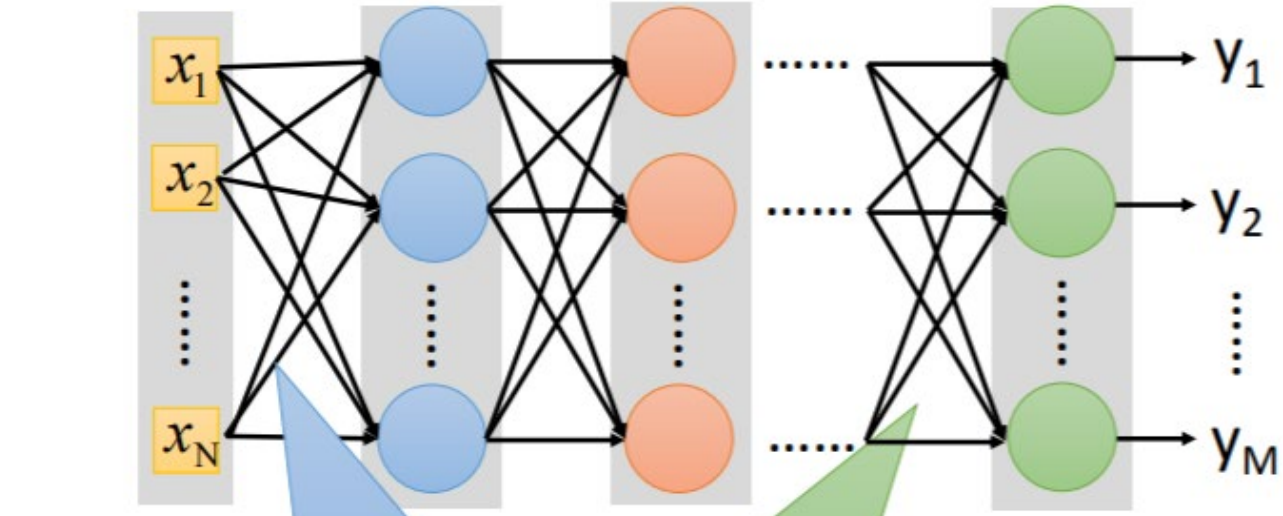
[Xavier Glorot, AISTATS'11]
[Andrew L. Maas, ICML'13]
[Kaiming He, arXiv'15]

Reason:

1. Fast to compute
2. Biological reason
3. Infinite sigmoid with different biases
4. Vanishing gradient problem

Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

Vanishing gradient problem



Smaller gradients

Learn very slow

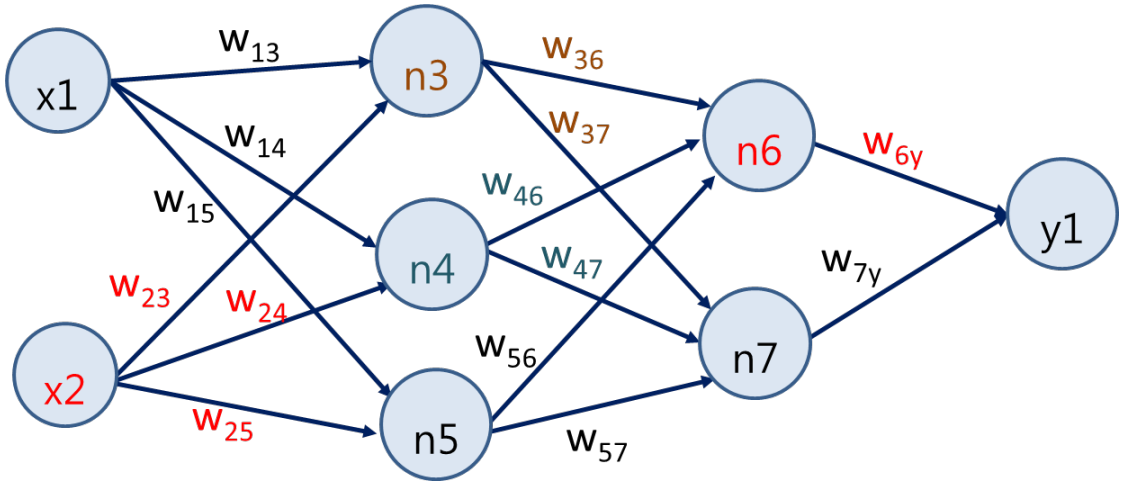
Almost random

Larger gradients

Learn very fast

Already converge

based on random!?

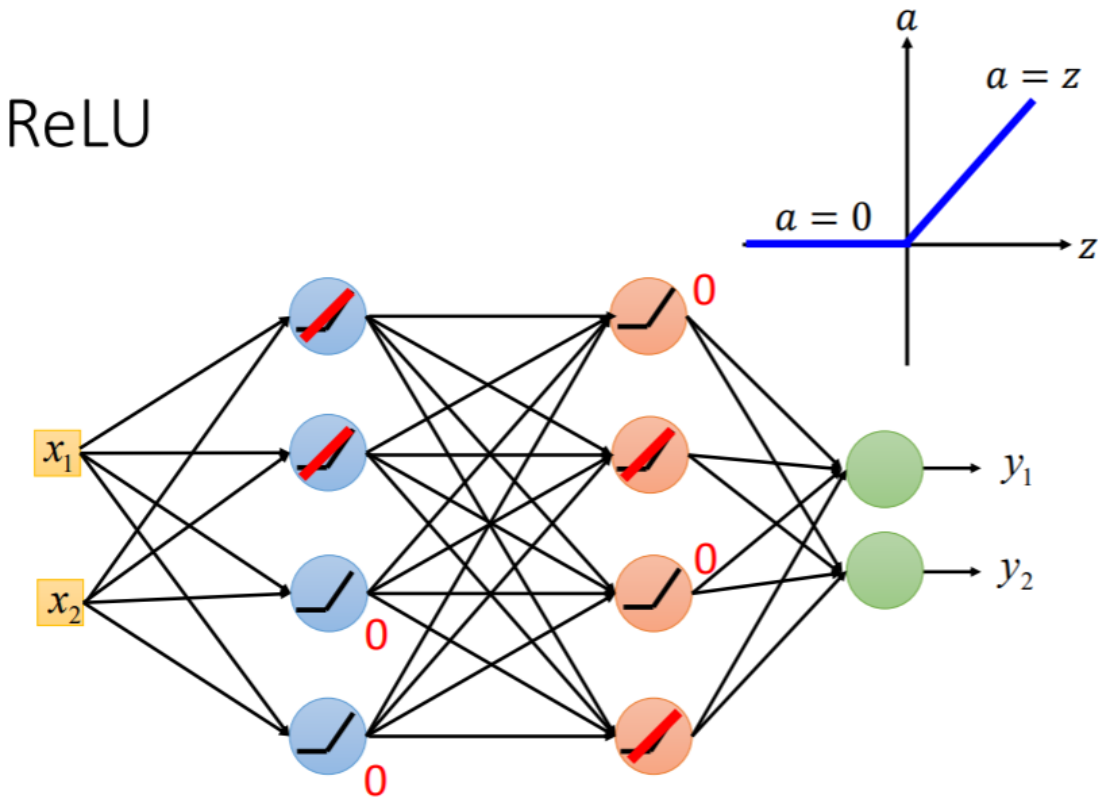


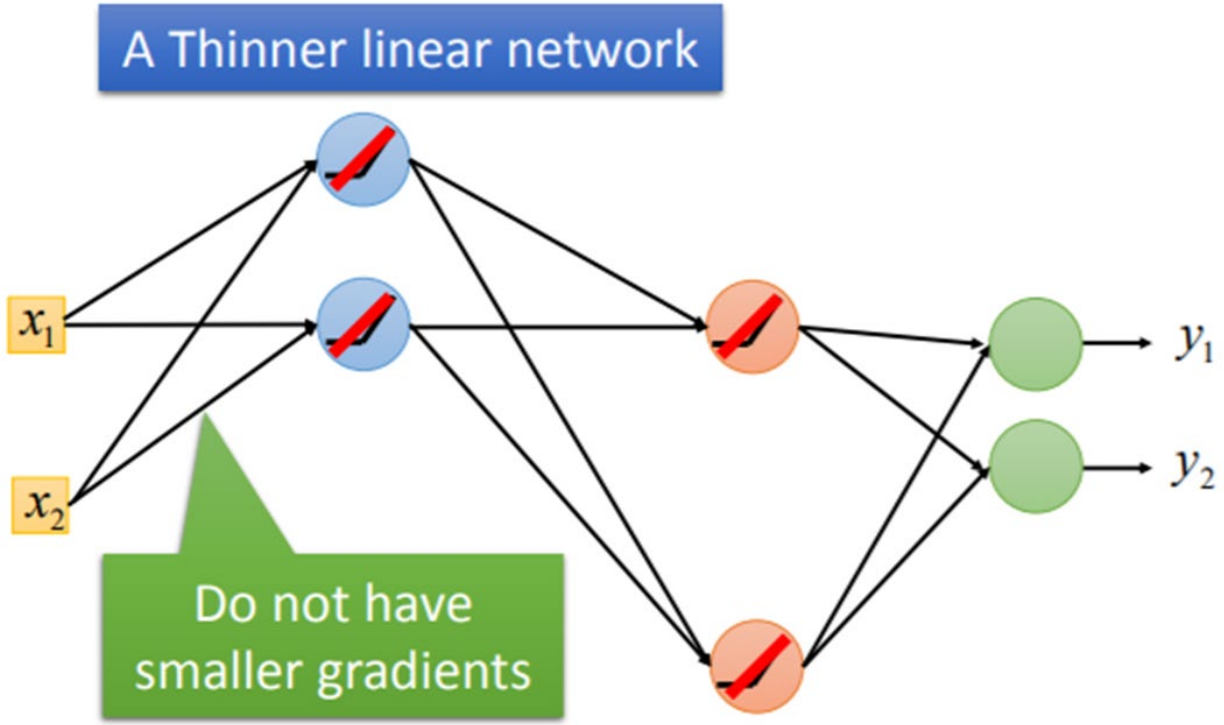
$$\frac{\partial L}{\partial w_{6y}} = \frac{\partial L}{\partial y_1}\frac{\partial y_1}{\partial w_{6y}}$$

$$\frac{\partial L}{\partial w_{57}} = \frac{\partial L}{\partial y_1}\frac{\partial y_1}{\partial n_7}\frac{\partial n_7}{\partial w_{57}}$$

Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

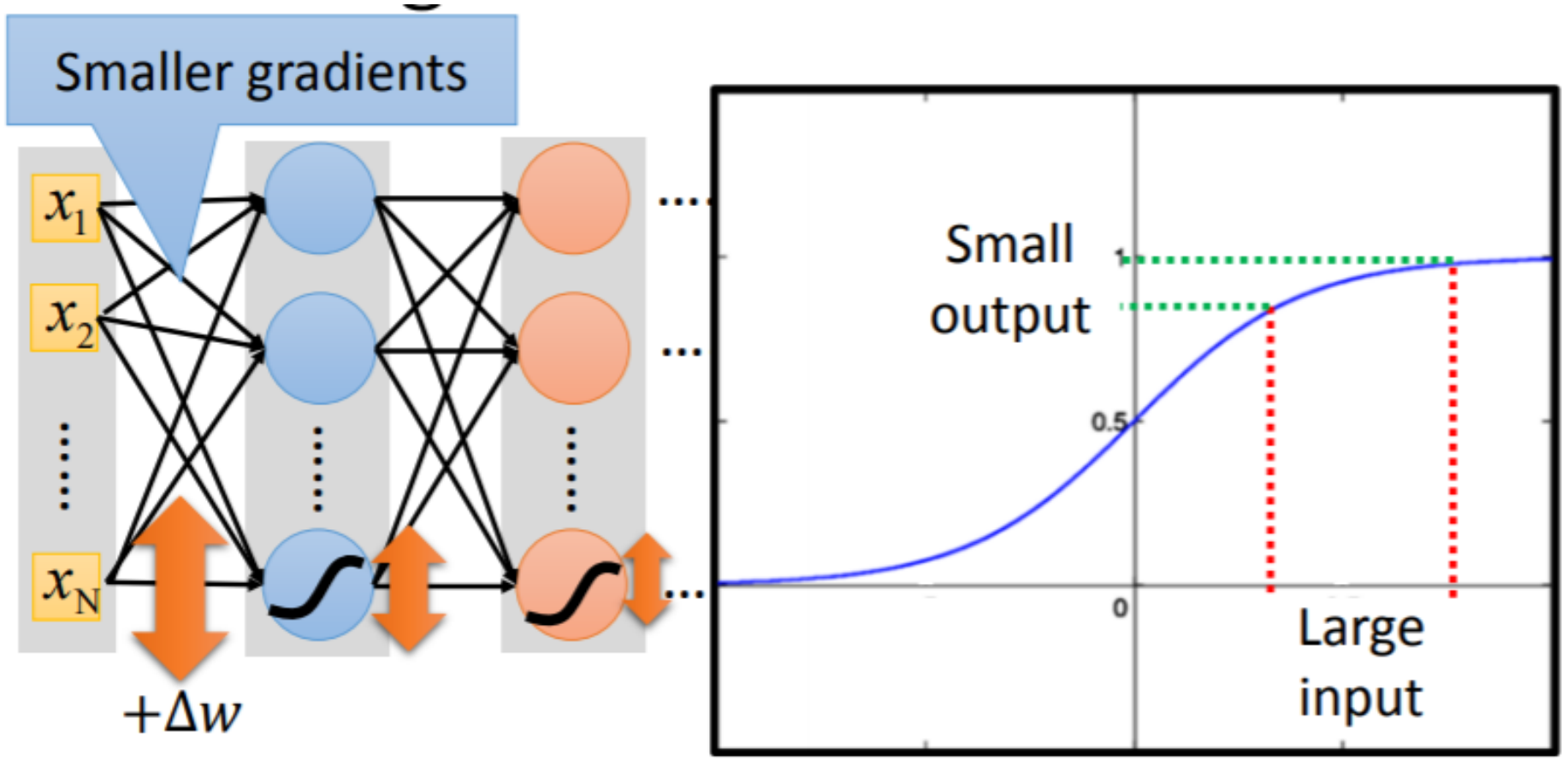
ReLU results in a thinner linear network





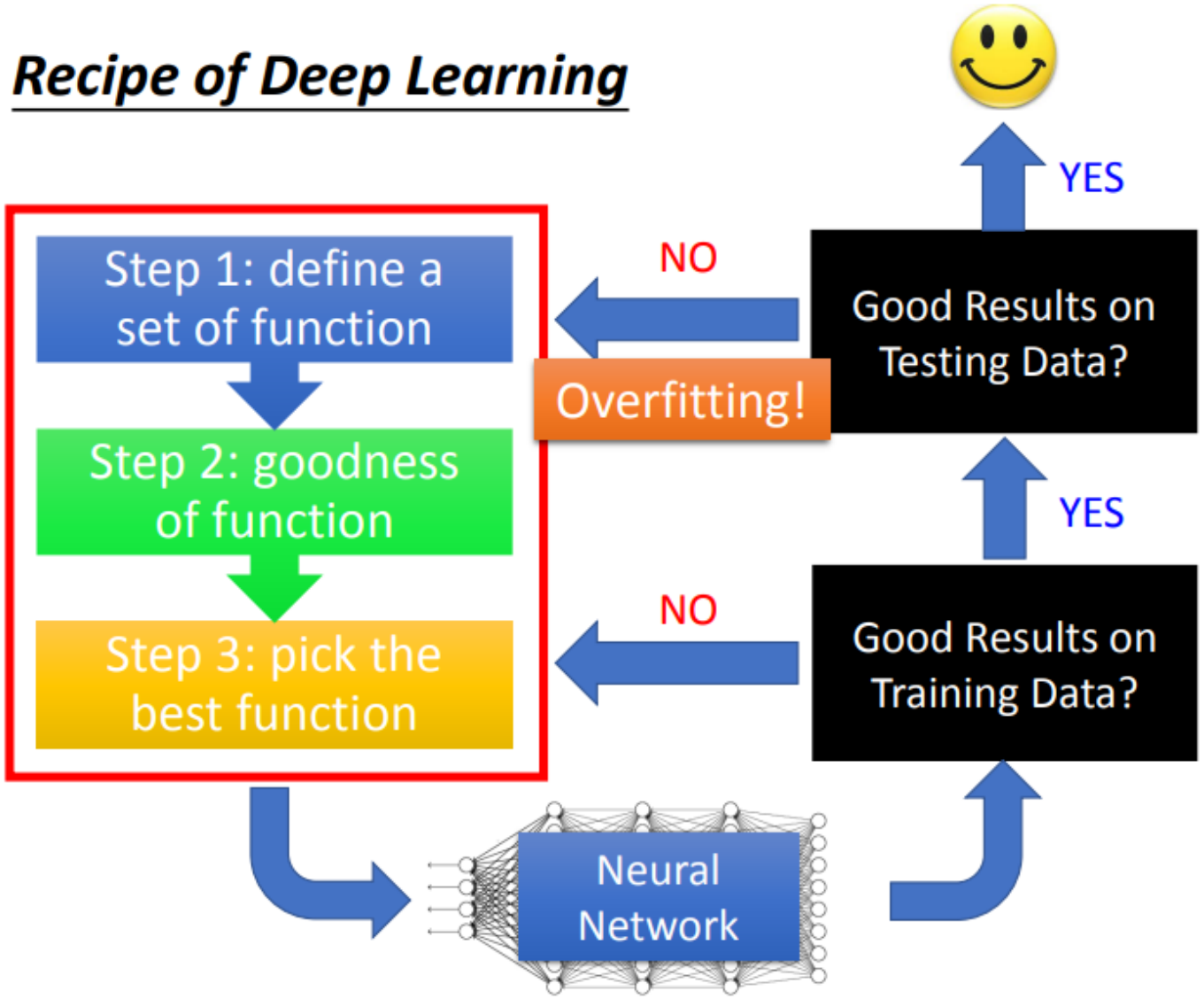
Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

Sigmoid is hard to get the power of deep



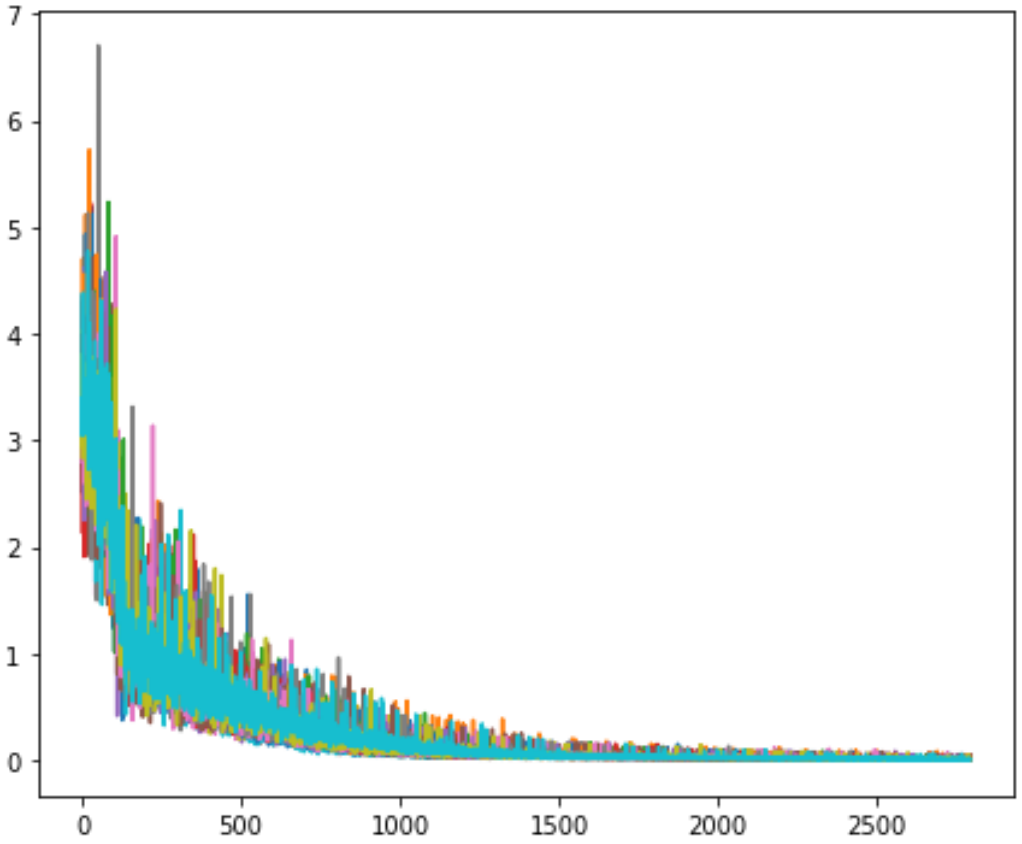
Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

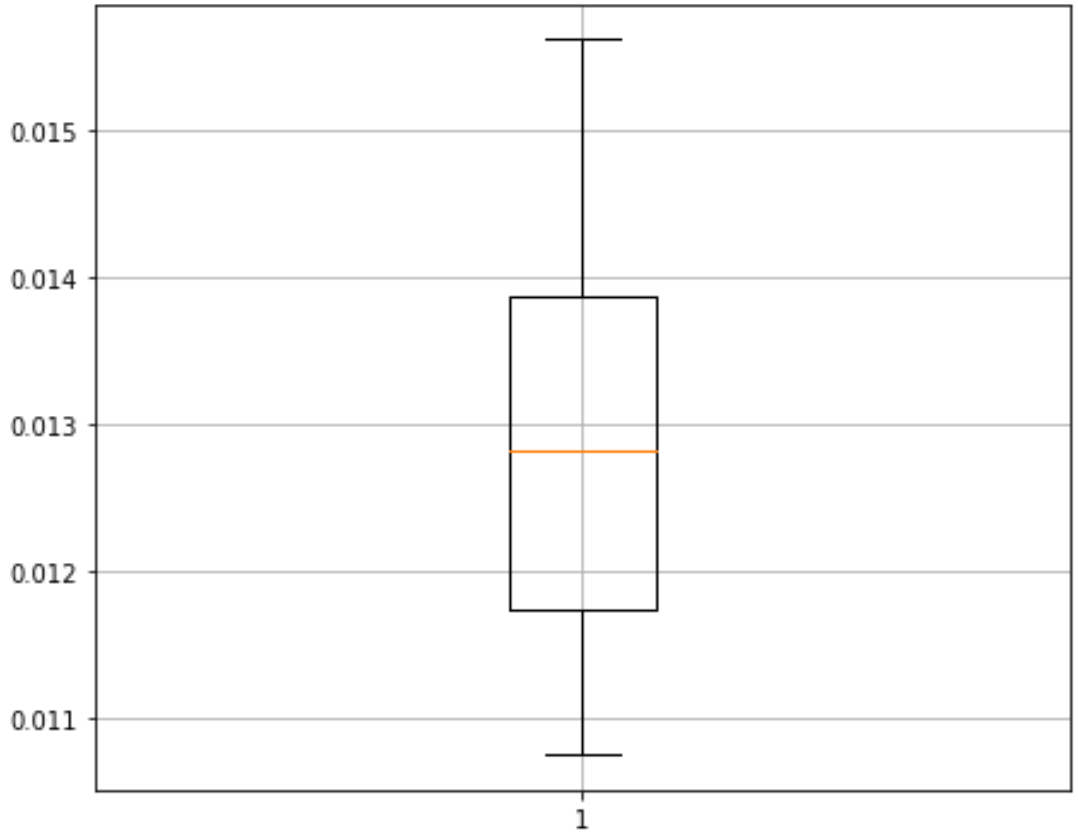
ML finds generalizable predictive patterns



Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

ML finds generalizable predictive patterns



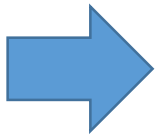


Good results on training data?

Good results on test data?

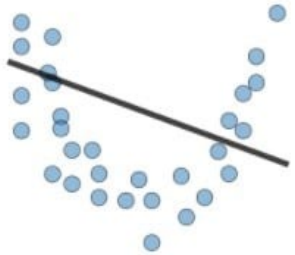
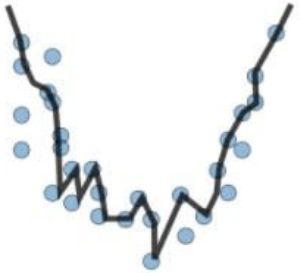
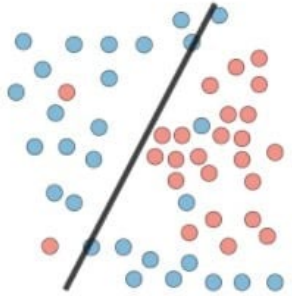
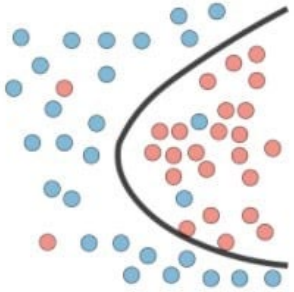
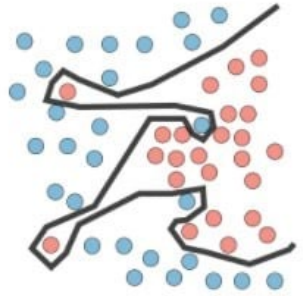
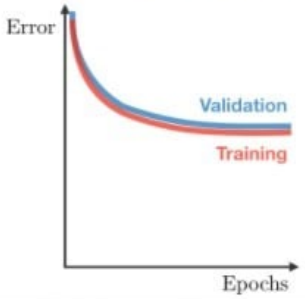
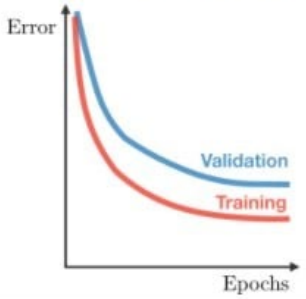
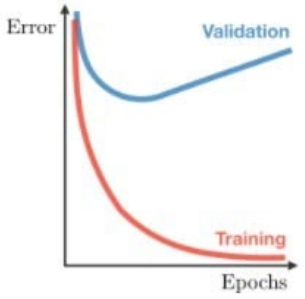
Try different NNs

- 7-56-56-1
- 7-256-256-256-1
- 7-512-512-512-512-1
- 7-1024-1024-1024-1024-1024-1



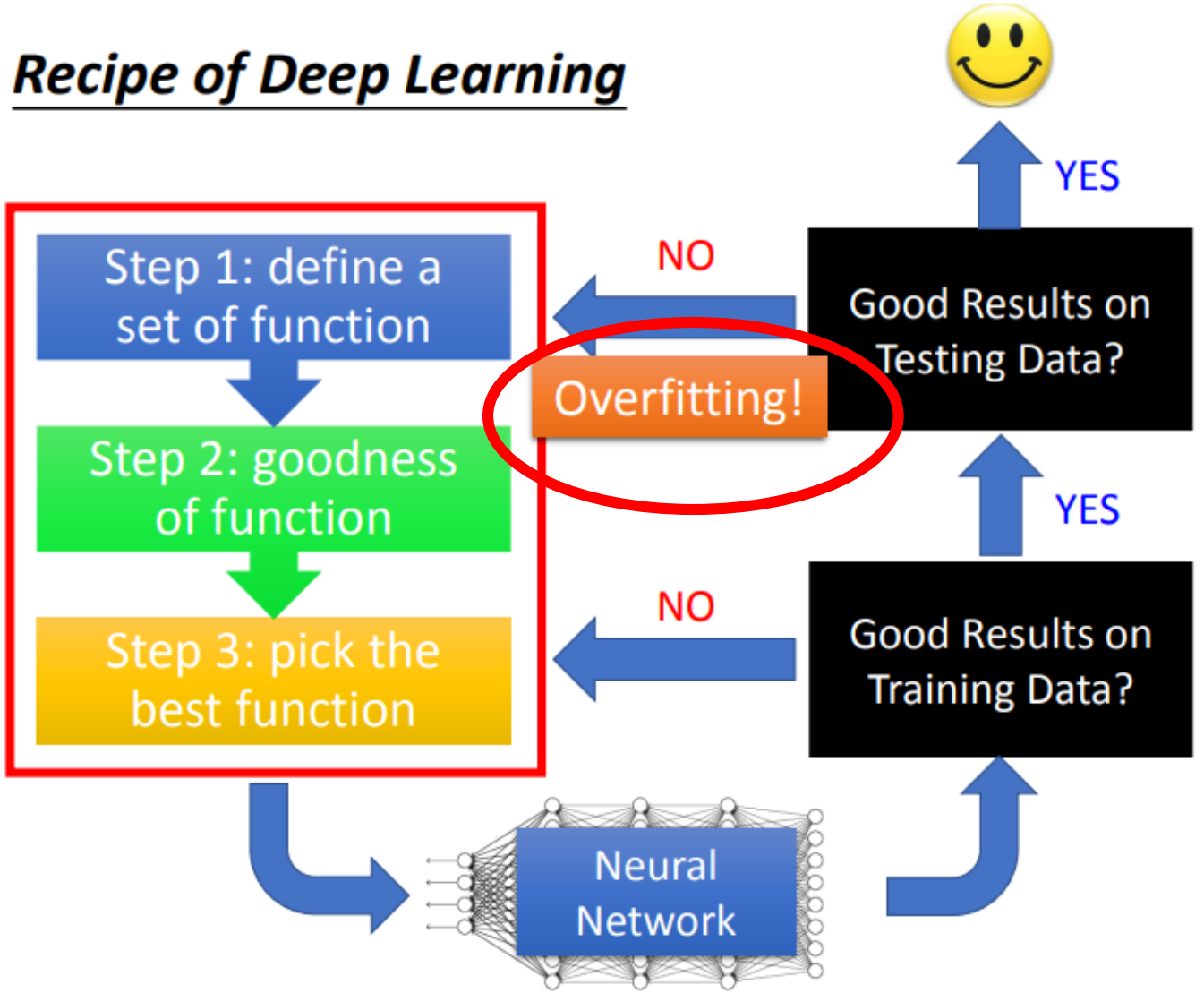
- Good results on training data?
- Good results on test data?

Overfitting

	Underfitting	Just right	Overfitting
Symptoms	• High training error • Training error close to test error • High bias	• Training error slightly lower than test error	• Very low training error • Training error much lower than test error • High variance
Regression illustration			
Classification illustration			
Deep learning illustration			
Possible remedies	• Complexify model • Add more features • Train longer		• Perform regularization • Get more data

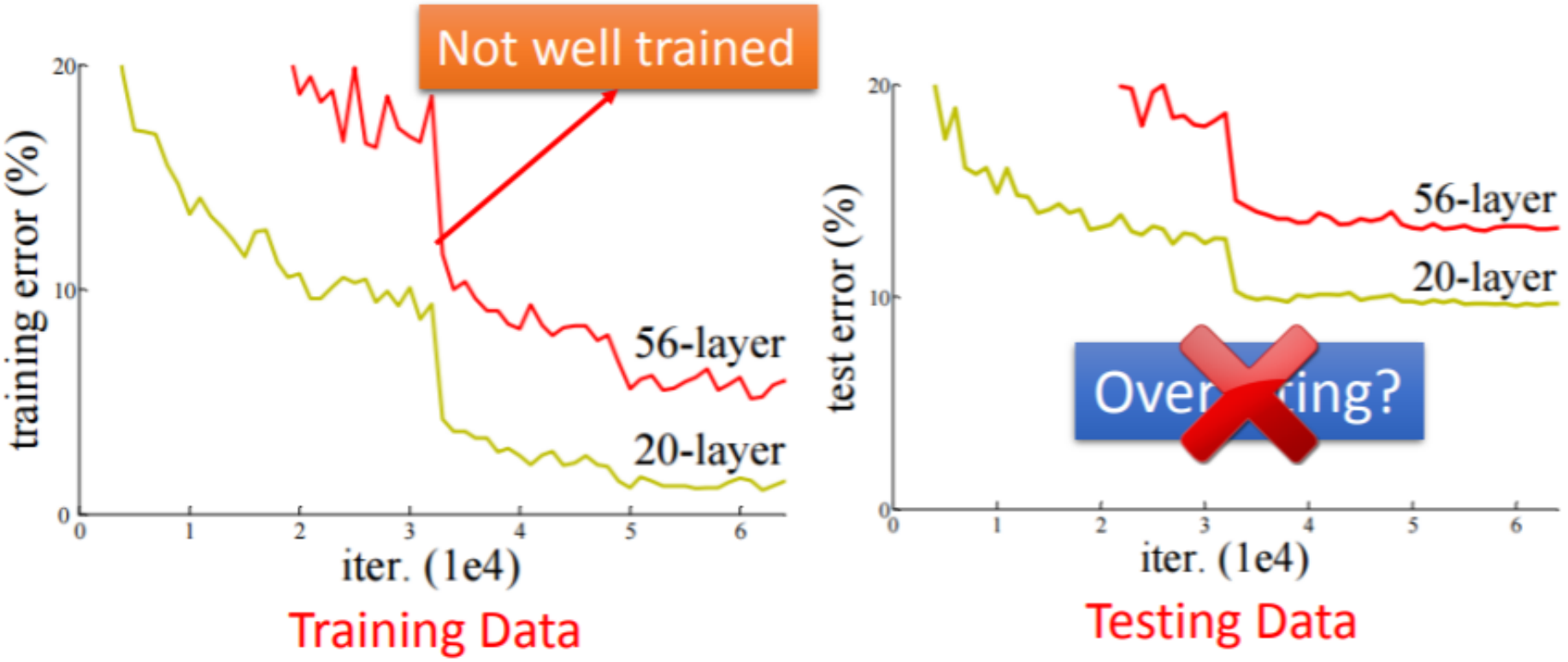
https://www.facebook.com/buggyprogrammers/photos/a.113230983855158/213140590530863/

How to know overfitting happens ?



Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

But be careful, do not always blame overfitting



Deep Residual Learning for Image Recognition
http://arxiv.org/abs/1512.03385

Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

Overfitting

2.2. Overfitting.ipynb

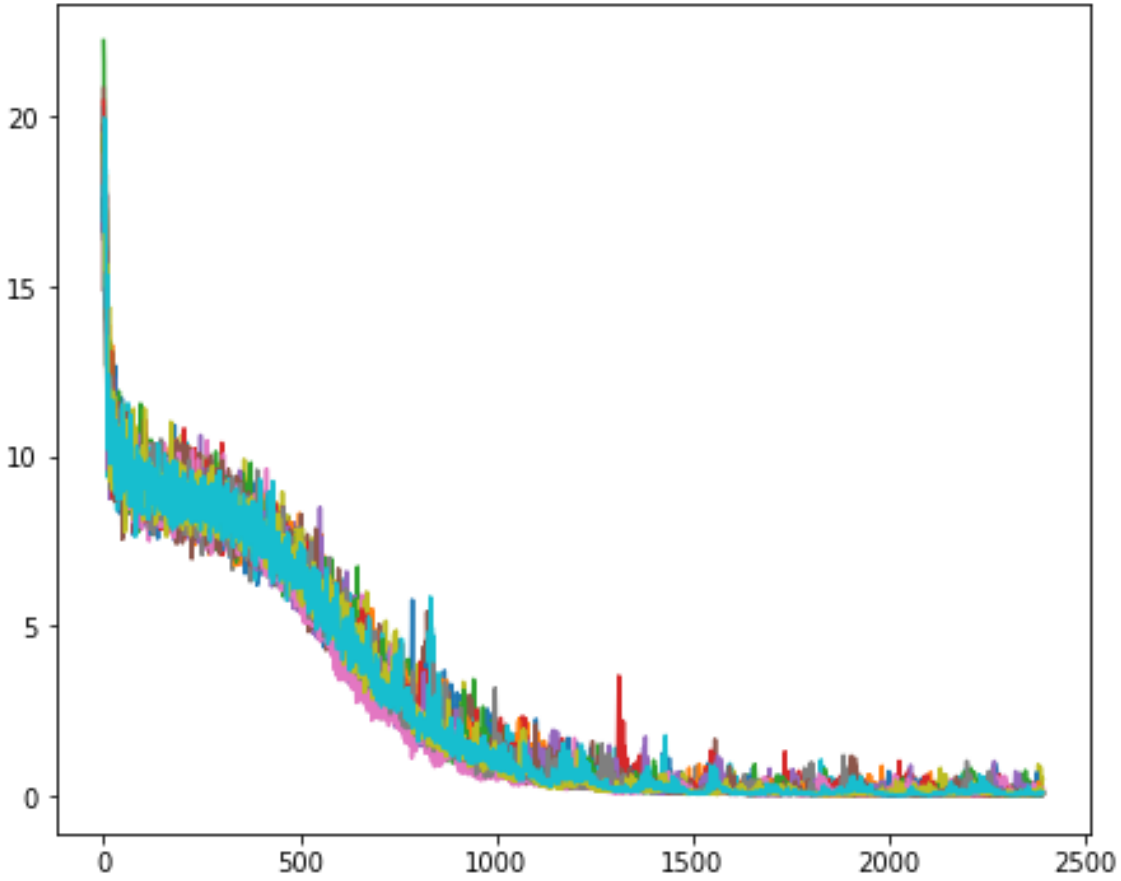
Add noises to y

$$y = 0.323{x_1}^2 + 0.586x_1x_2 + 0.4x_3 + 0.8972{x_5}^3 + 0.267{x_3}^2x_5x_6 + 0.78{x_7}^2 + \mathcal{N}(2,3)$$

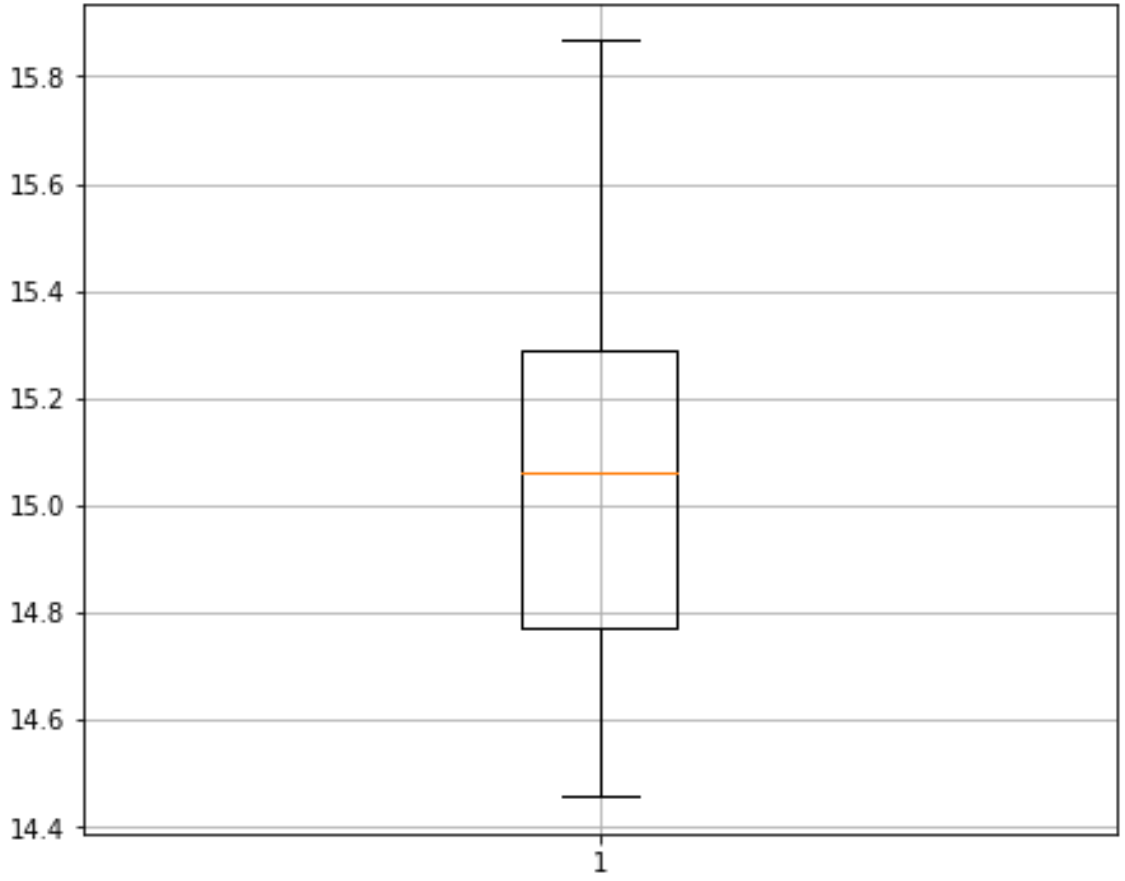
Use a complicated NN

7-1024-1024-1024-1024-1024-1

Overfitting

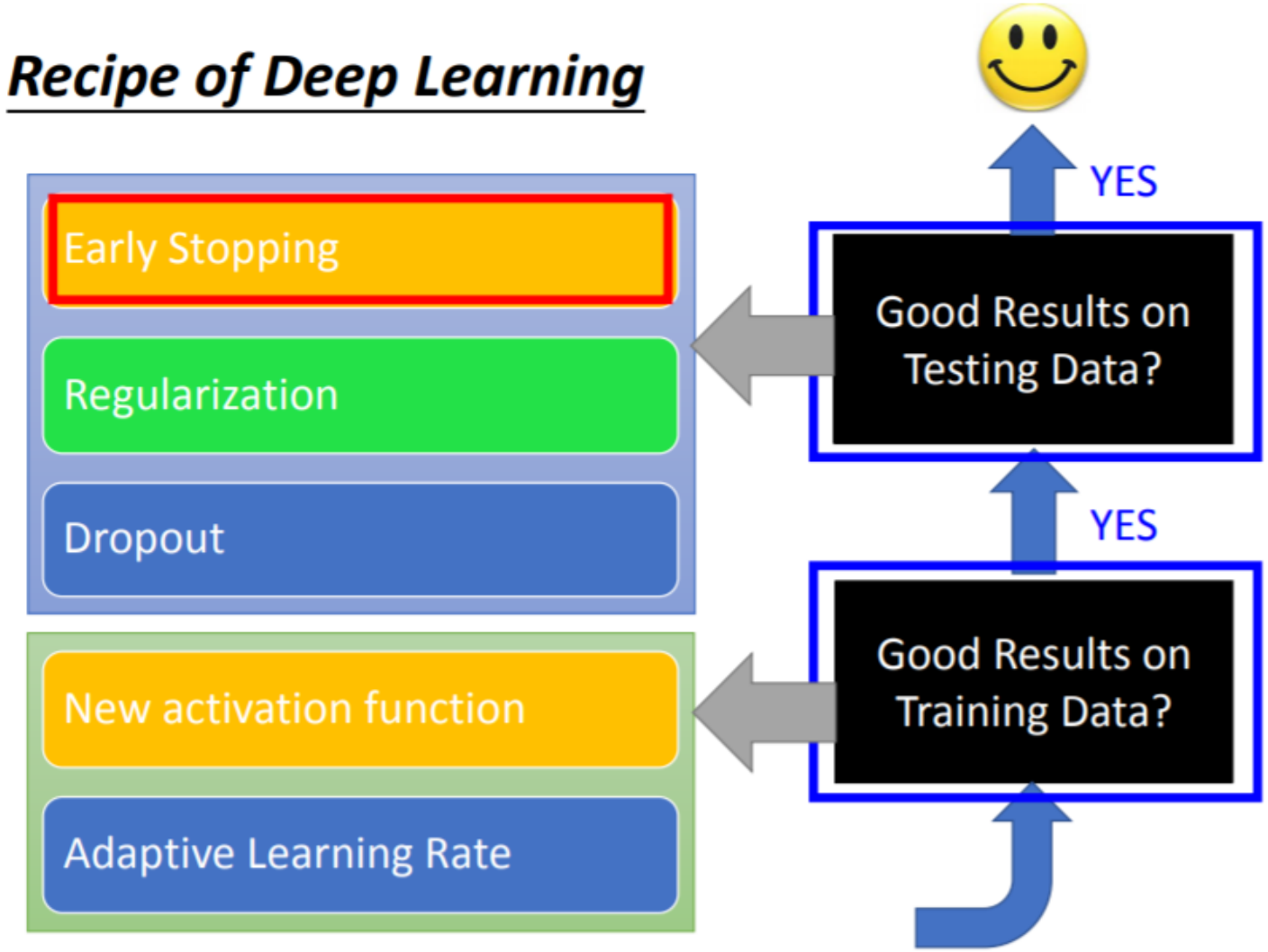


Good results on training data



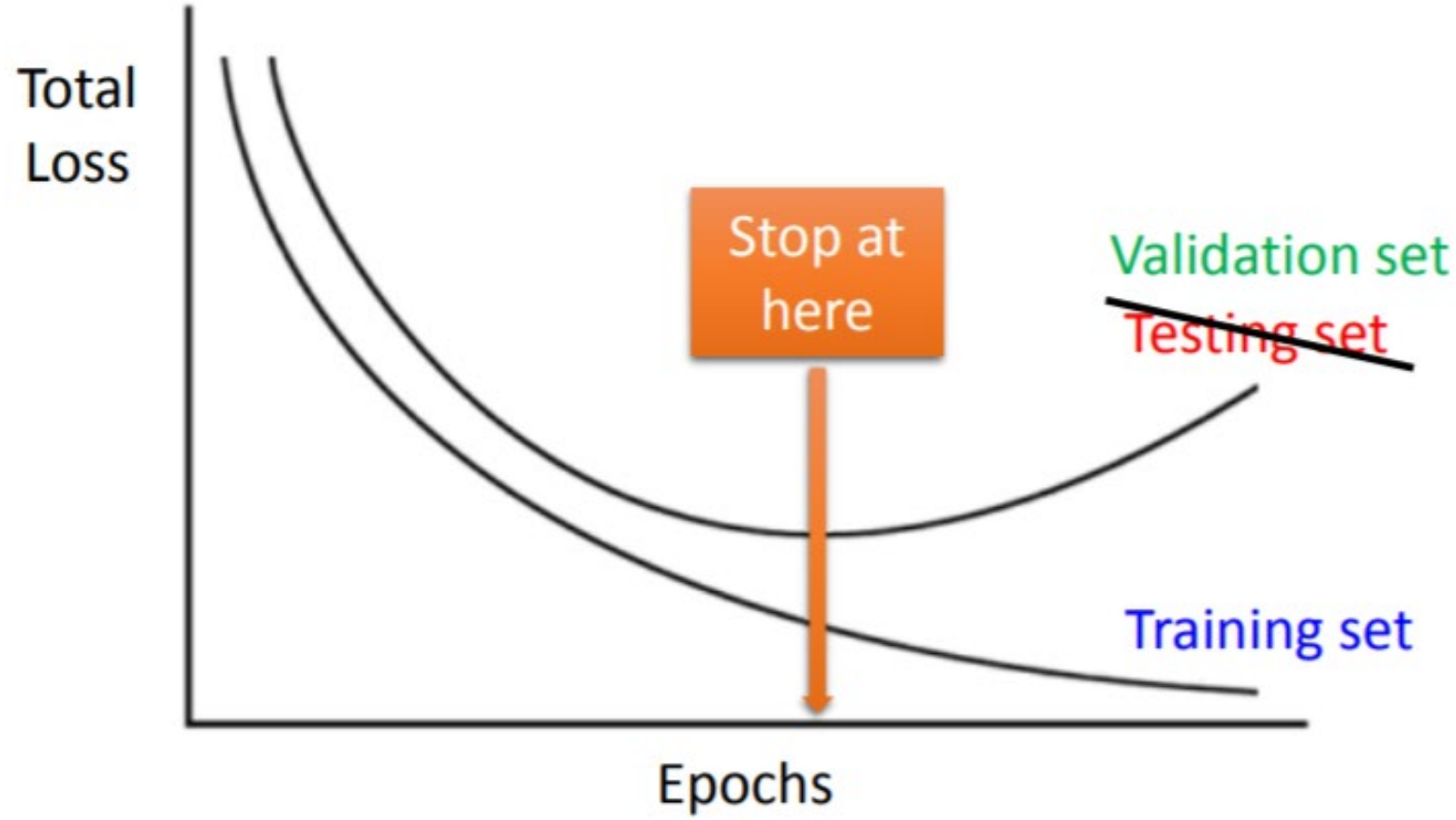
Bad results on test data

How to solve overfitting?



Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

(1) Early stopping



Keras: http://keras.io/getting-started/faq/#how-can-i-interrupt-training-when-the-validation-loss-isnt-decreasing-anymore

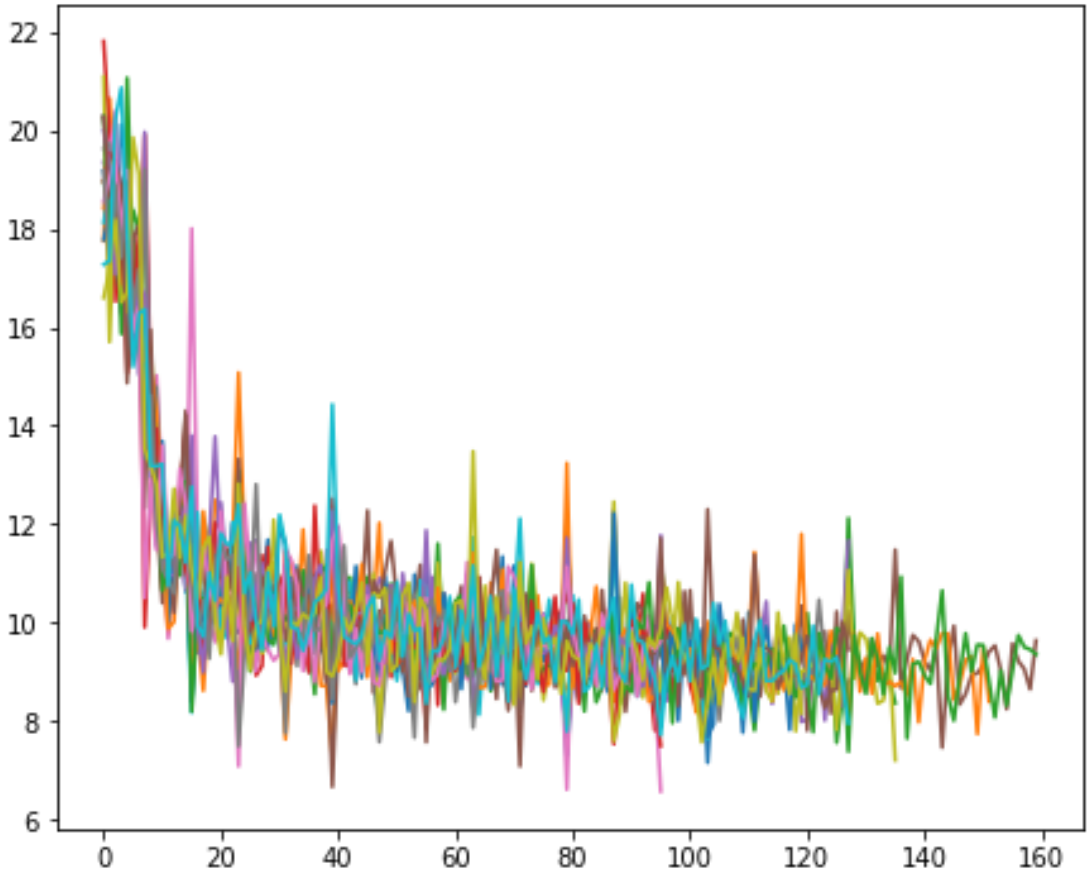
Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

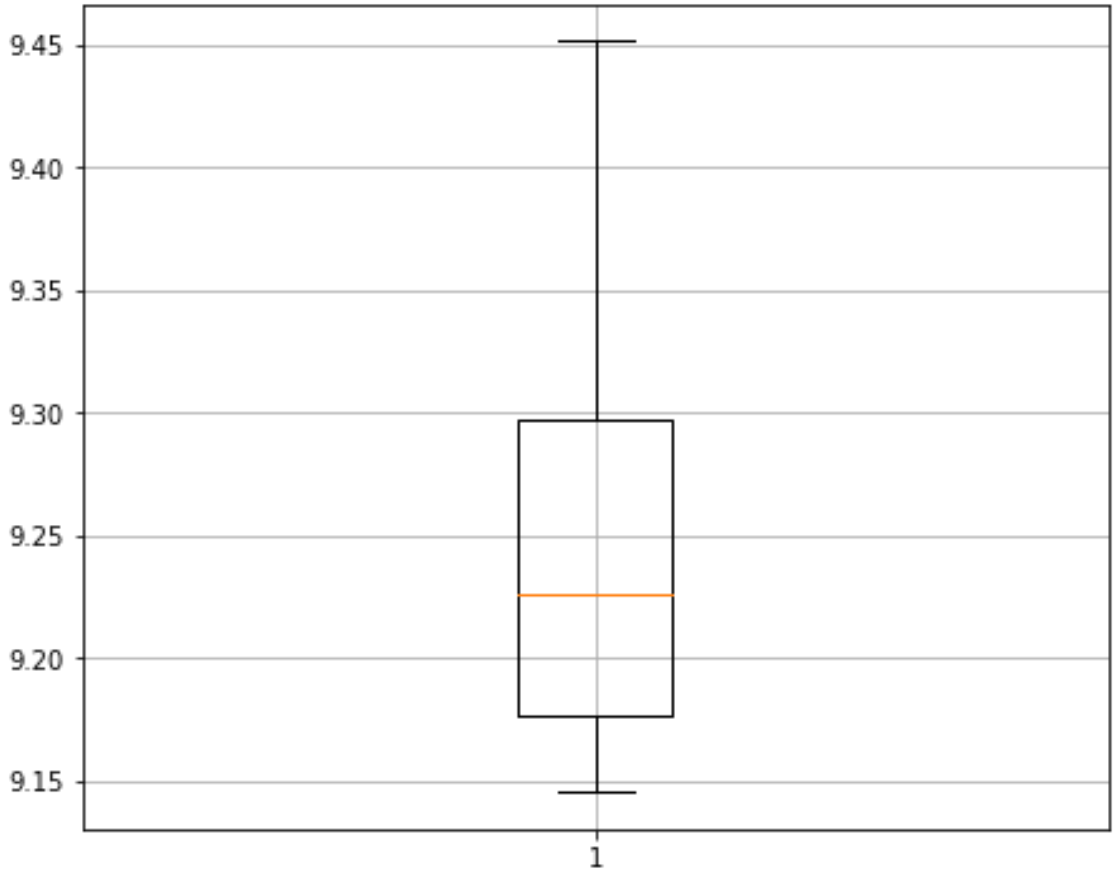
(1) Early stopping

```
  tensor_validationX = torch.FloatTensor(validationX).to(device)
  tensor_validationY = torch.FloatTensor(validationY).to(device)
  tensor_validationY_hat = MyNet(tensor_validationX)
  validatiion_loss = loss_func(tensor_validationY, tensor_validationY_hat)

  #early stop
  the_current_loss = float(validatiion_loss)
  if(the_current_loss > the_last_loss):
    trigger_times += 1
    print('trigger times:', trigger_times)
    if(trigger_times >= patience):
      print('Early stopping!')
      break  # early stop when validation loss increases 2 consective times
  elif(trigger_times >0):
    print('trigger times reset to 0')
    trigger_times = 0
  the_last_loss = the_current_loss
train_lossLst.append(epoch_lossLst)
```

(1) Early stopping

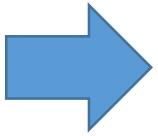




Try different NNs

Use your own $y = f(\vec{x})$ data

- 7-512-512-512-512-1
- 7-256-256-256-1
- 7-56-56-1



- Is the overfitting problem solved by early stop?

(2) Regularization – L2

- Find a set of weight not only minimizing original cost but also close to zero

$$L'(\theta) = L(\theta) + \lambda \frac{1}{2} \|\theta\|_2$$

→ Regularization term

Original loss

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

$$\theta = \{w_1, w_2, \ldots\}$$

L2 regularization:

$$\|\theta\|_2 = (w_1)^2 + (w_2)^2 + \ldots$$

(usually not consider biases)

Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

(2) Regularization – L2

$$L'(\theta) = L(\theta) + \lambda \frac{1}{2}\|\theta\|_2 \quad \text{Gradient:} \quad \frac{\partial L'}{\partial w} = \frac{\partial L}{\partial w} + \lambda w$$

Update:

$$w^{t+1} \rightarrow w^t - \eta \frac{\partial L'}{\partial w} = w^t - \eta\left(\frac{\partial L}{\partial w} + \lambda w^t\right)$$

$$= (1 - \eta\lambda) w^t - \eta \frac{\partial L}{\partial w}$$

Weight Decay

$(1 - \eta\lambda) w^t$: Closer to zero

Vanilla gradient decent update $w^{t+1} \rightarrow w^t - \eta \frac{\partial L}{\partial w}$

Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

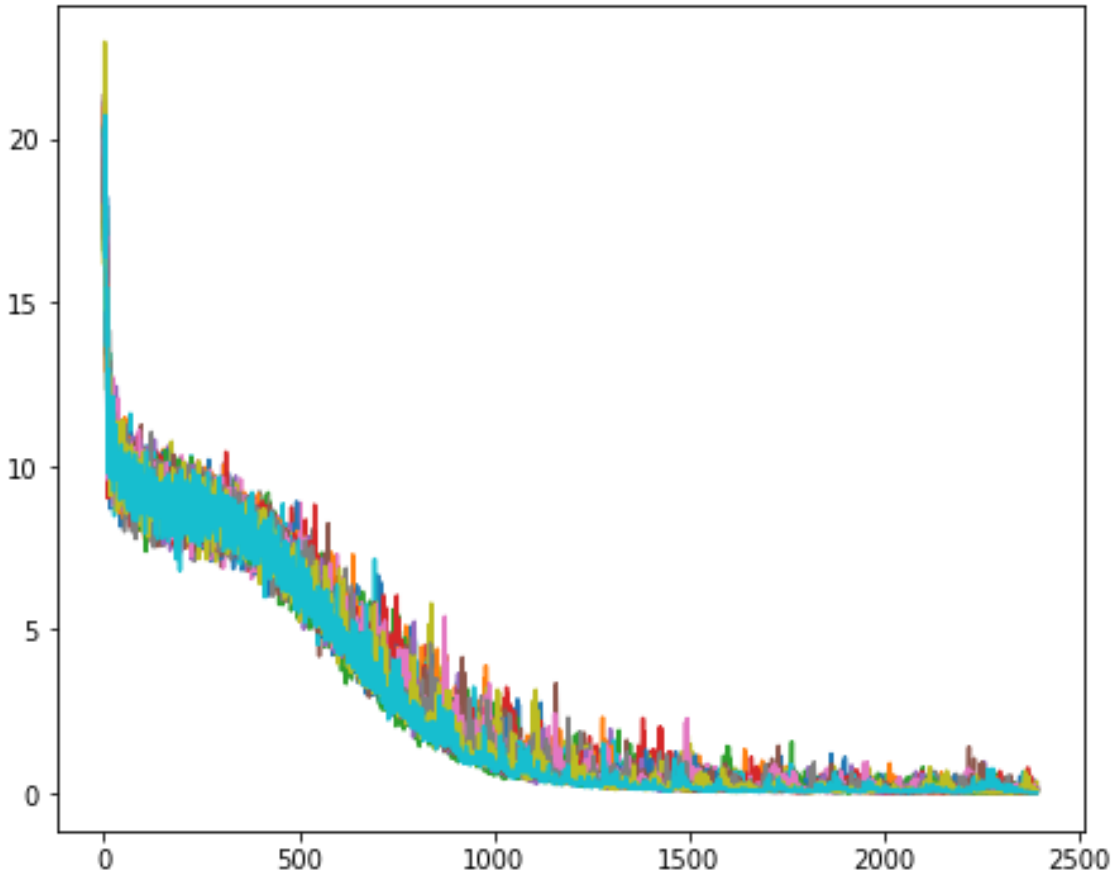
(2) Regularization – L2

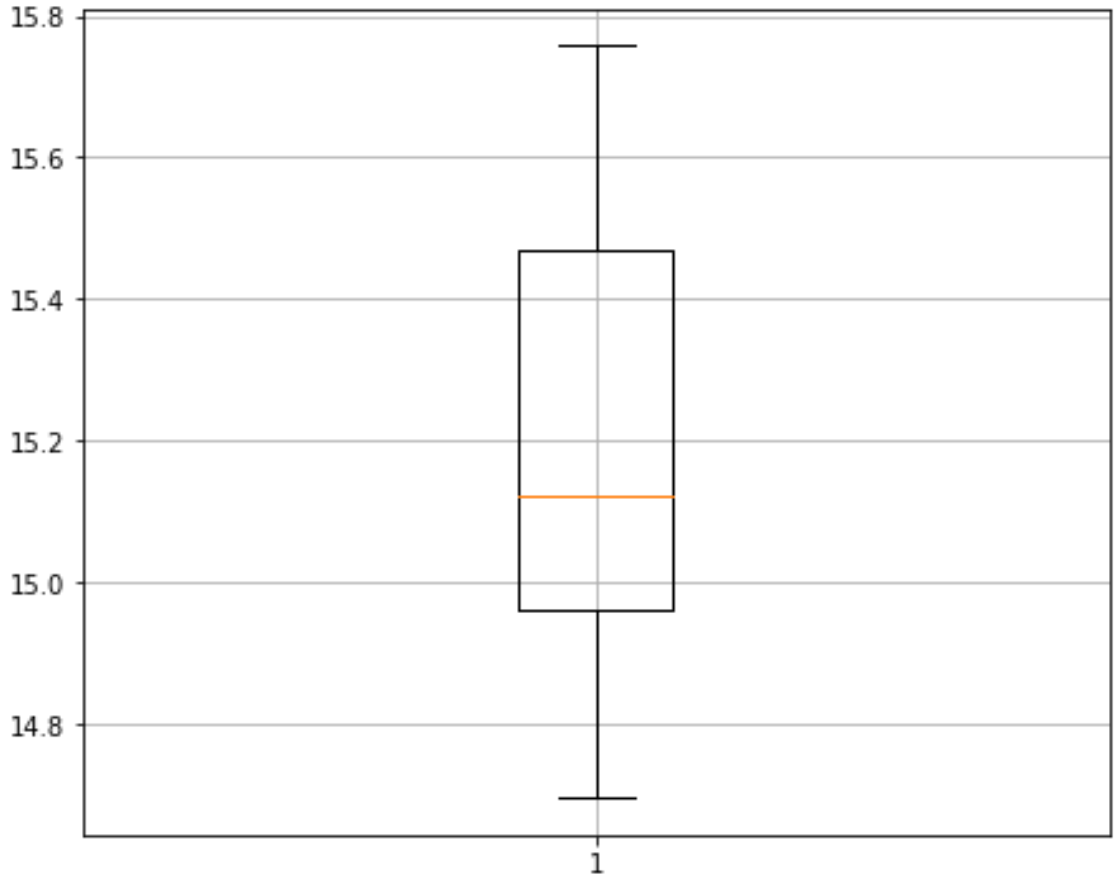
Regularization may not be that important in deep learning as in other machine learning algorithms like SVM.

```
# 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)
loss_func = torch.nn.MSELoss()
optimizer = torch.optim.Adam(MyNet.parameters(), lr=0.0003, weight_decay=0.0001)
```

(2) Regularization – L2

Regularization may not be that important in deep learning as in other machine learning algorithms like SVM.





(2) Regularization – L1

L1 regularization:

$$\|\theta\|_1 = |w_1| + |w_2| + \dots$$

$$L'(\theta) = L(\theta) + \lambda \frac{1}{2}\|\theta\|_1 \qquad \frac{\partial L'}{\partial w} = \frac{\partial L}{\partial w} + \lambda \operatorname{sgn}(w)$$

Update:

$$w^{t+1} \rightarrow w^t - \eta \frac{\partial L'}{\partial w} = w^t - \eta\left(\frac{\partial L}{\partial w} + \lambda \operatorname{sgn}(w^t)\right)$$

$$= w^t - \eta \frac{\partial L}{\partial w} - \underline{\eta\lambda \operatorname{sgn}(w^t)}$$ Always delete

$$= (1 - \eta\lambda) w^t - \eta \frac{\partial L}{\partial w}$$ L2

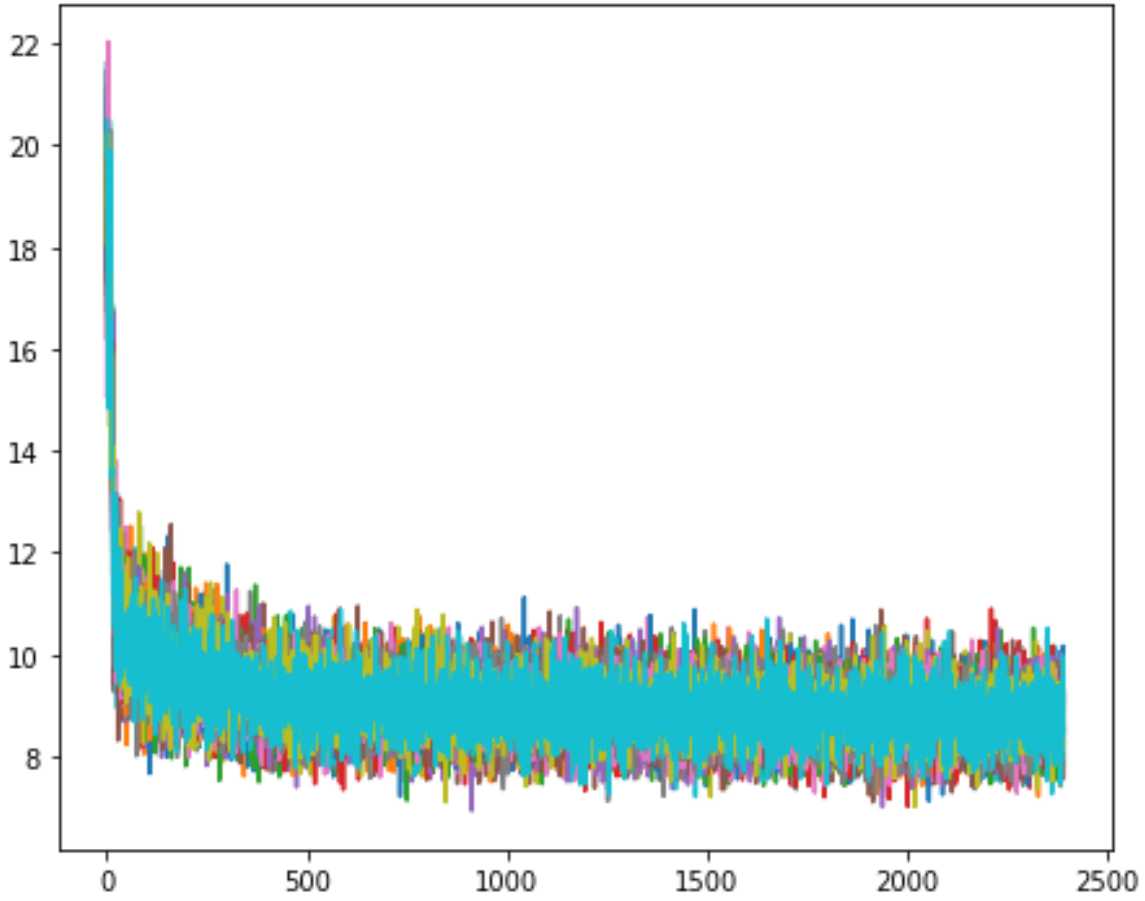
Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

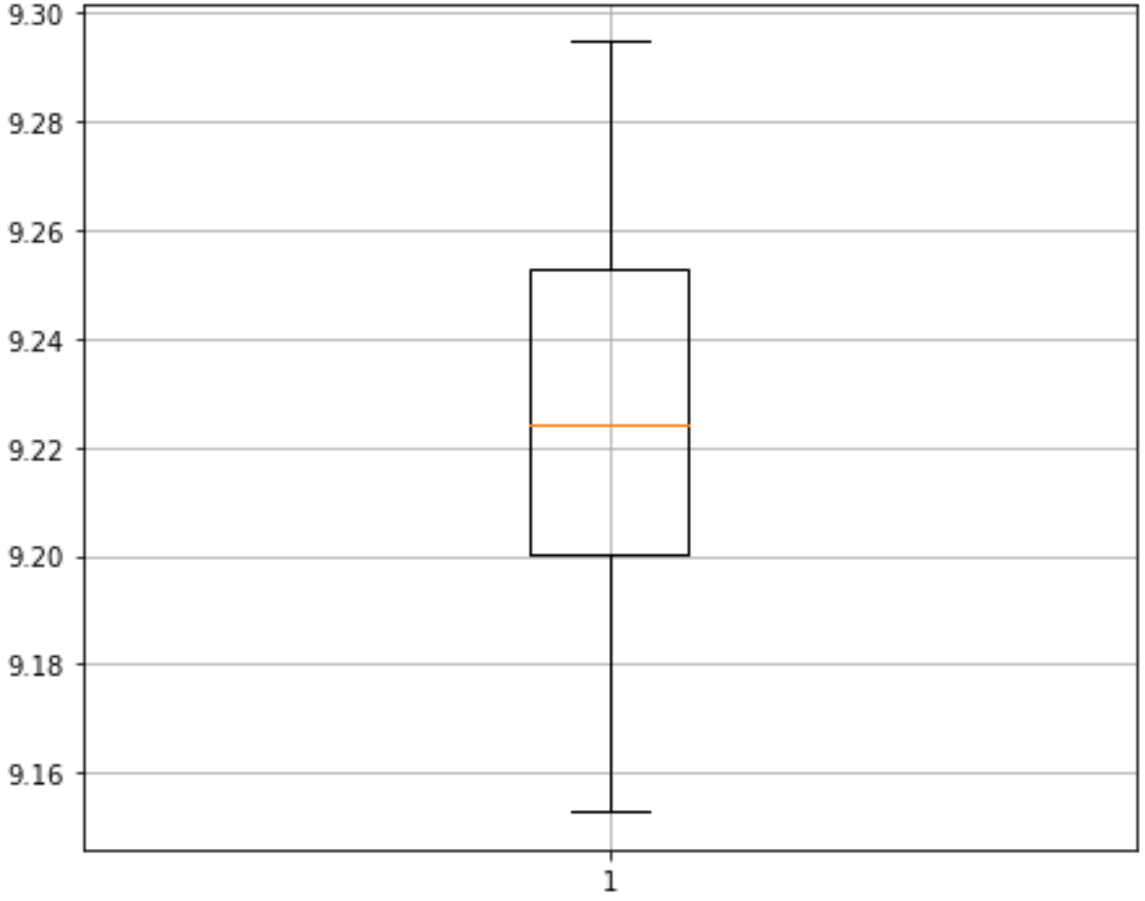
(2) Regularization – L1

```
for (batchX, batchY) in loader:
  batchY_hat = MyNet(batchX)
  loss = loss_func(batchY_hat, batchY)
  epoch_lossLst.append(float(loss))

  # add L1 regularization
  regularization_loss = 0
  for name, param in MyNet.named_parameters():
    if('weight' in name):
      regularization_loss += torch.sum(abs(param))
  loss = loss + lamda * regularization_loss
  optimizer.zero_grad()
  loss.backward()
  optimizer.step()
```

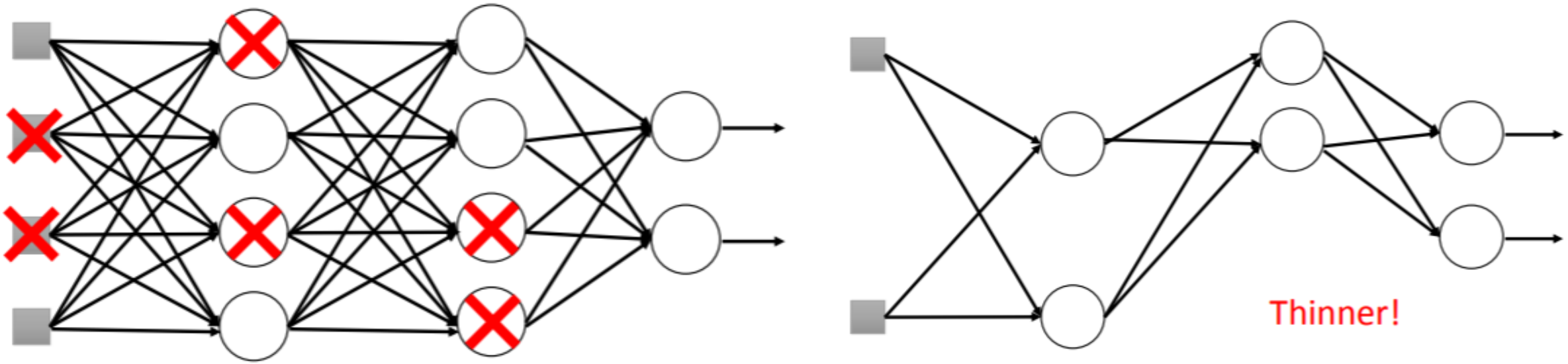
(2) Regularization – L1





(3) Drop out

Each time before updating θ, each neuron has $p\%$ to dropout. So the *NN* structure is changed (become thinner). That is, for each mini-batch, we resample the dropout neurons.

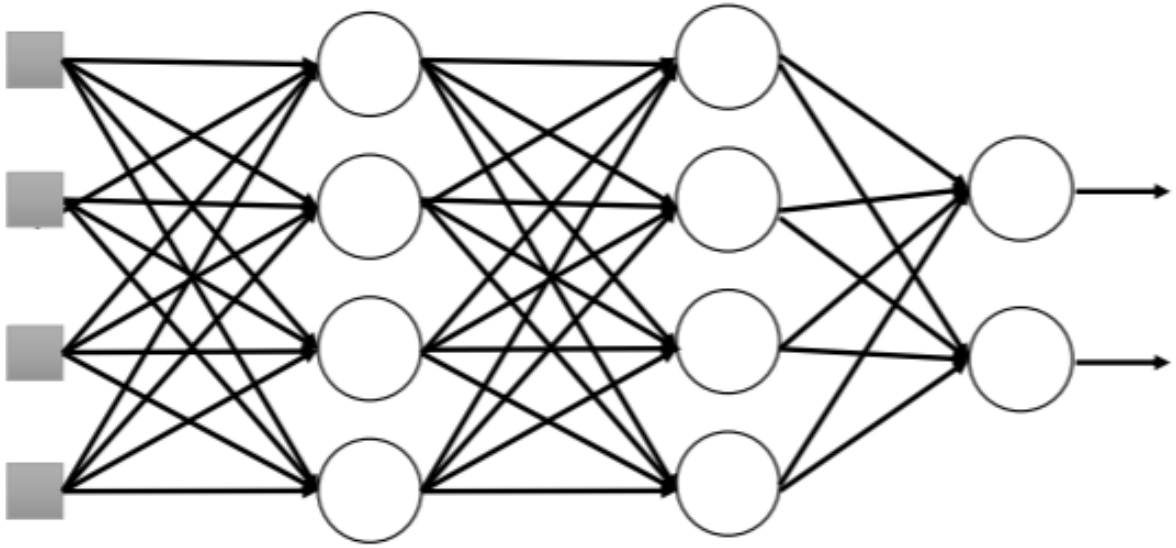


Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

(3) Drop out

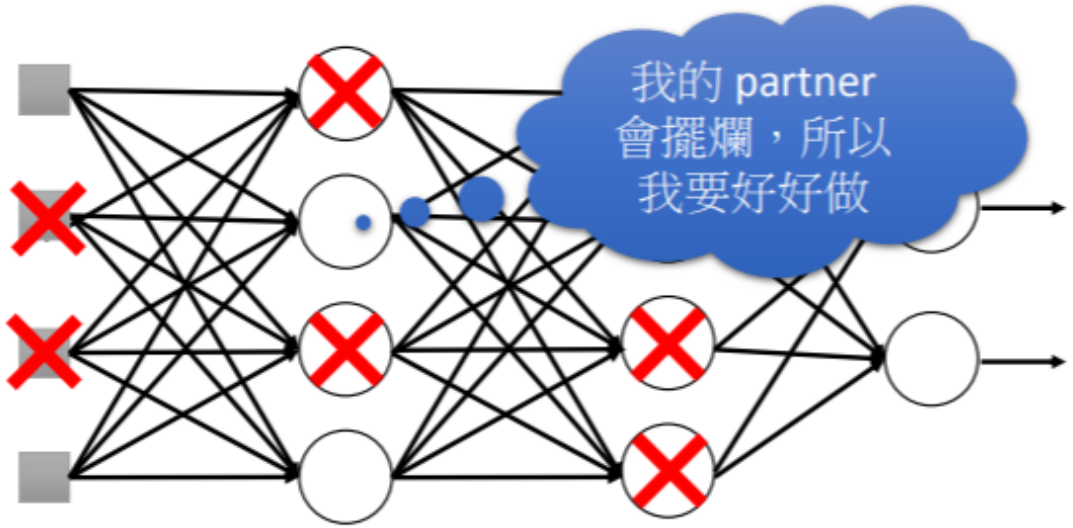
No neuron drop out at test stage. All weights time $1 - p\%$

Testing:



Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

Why drop out makes NN perform better?

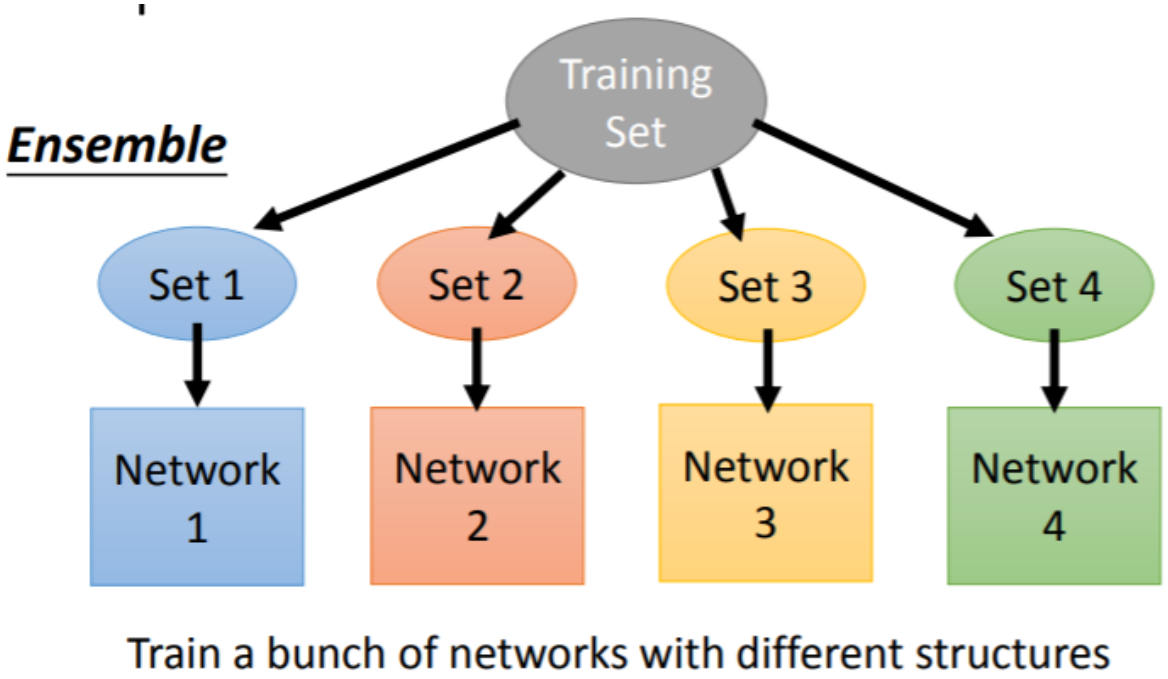


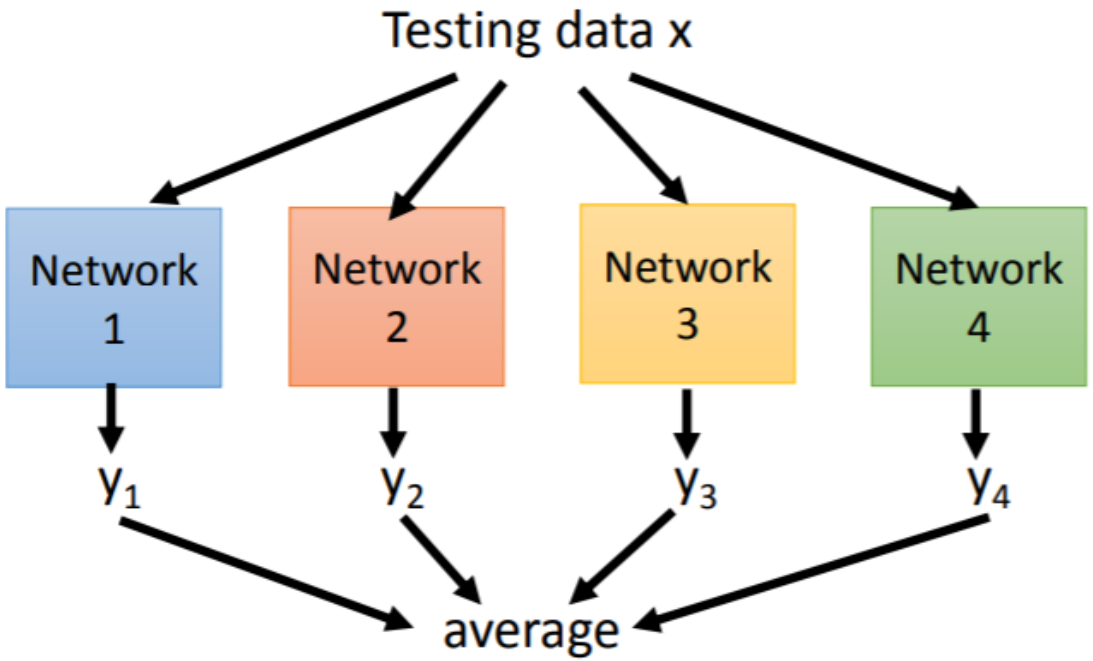
- When teams up, if everyone expect the partner will do the work, nothing will be done finally.
- However, if you know your partner will dropout, you will do better.
- When testing, no one dropout actually, so obtaining good results eventually.

Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

Why drop out makes NN perform better?

Drop out can be seen as an ensemble method.





Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

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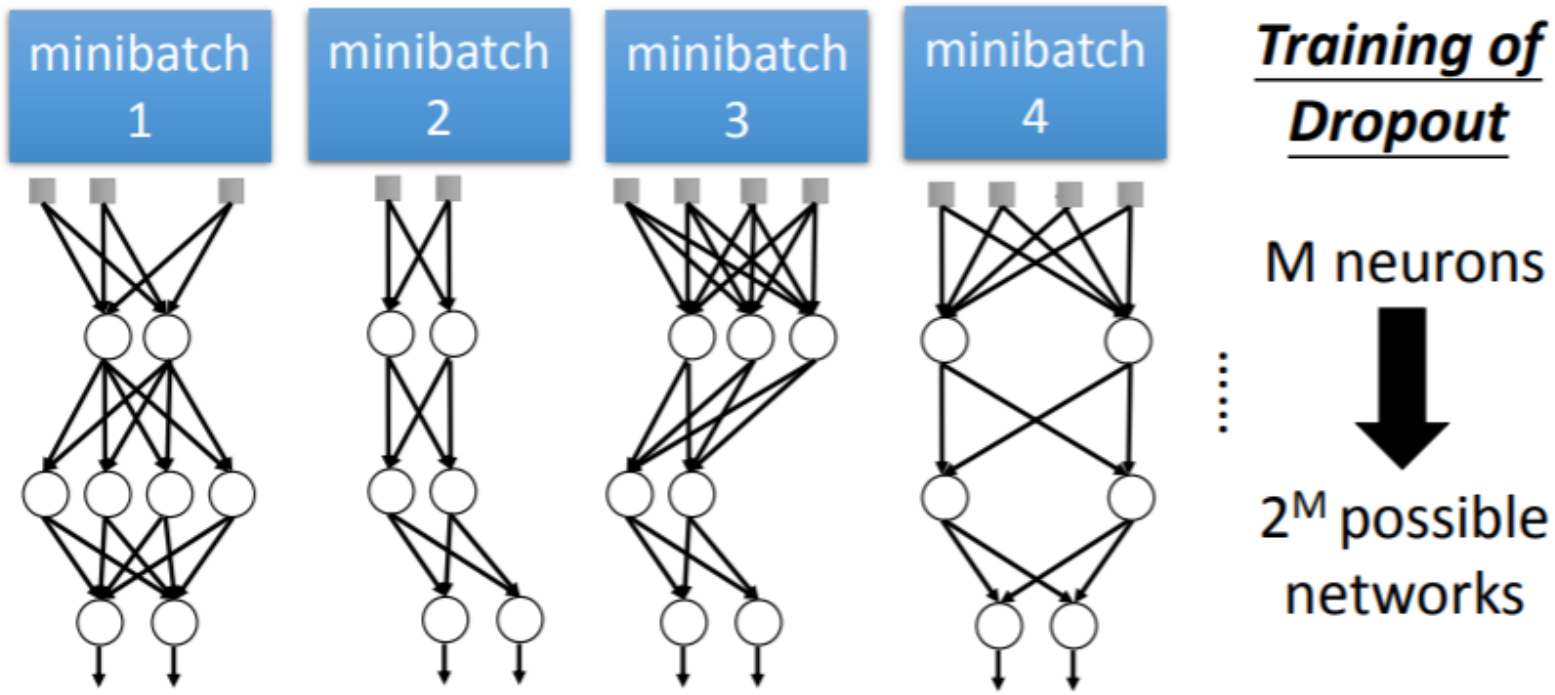


- Using one mini-batch to train one network
- Some parameters in the network are shared

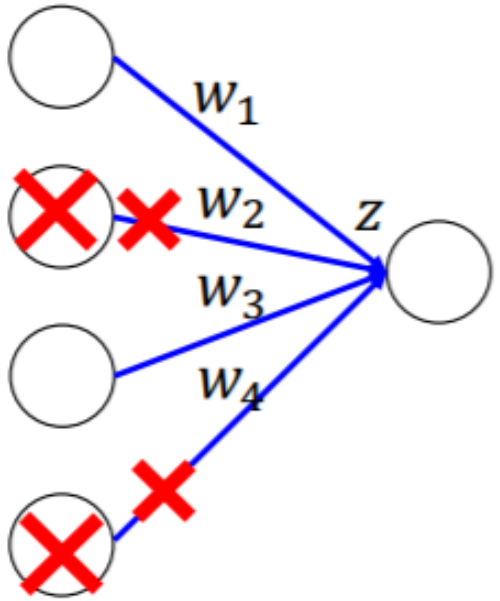
Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

Why multiply weights by (1-p)% during testing?

- Why the weights should multiply (1-p)% (dropout rate) when testing?

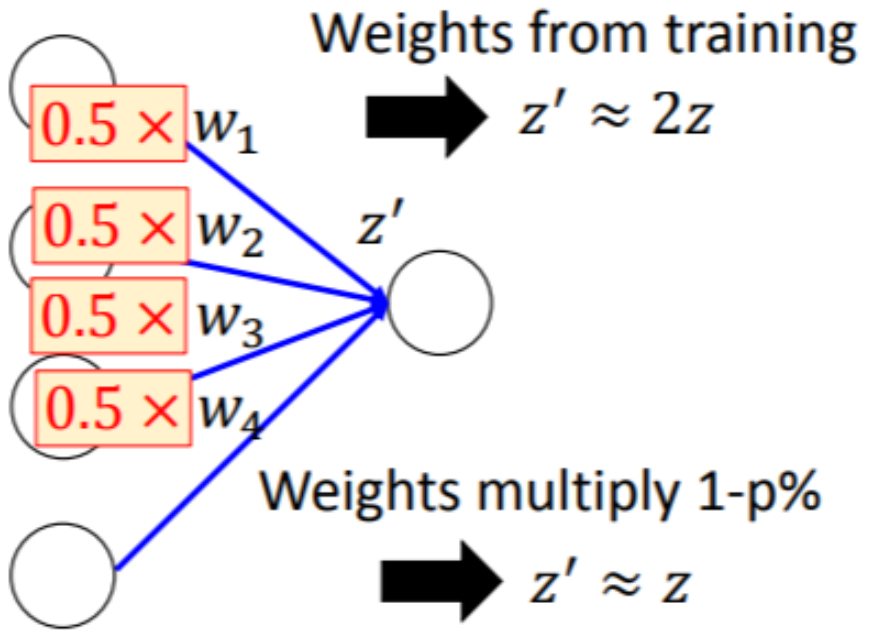
Training of Dropout

Assume dropout rate is 50%



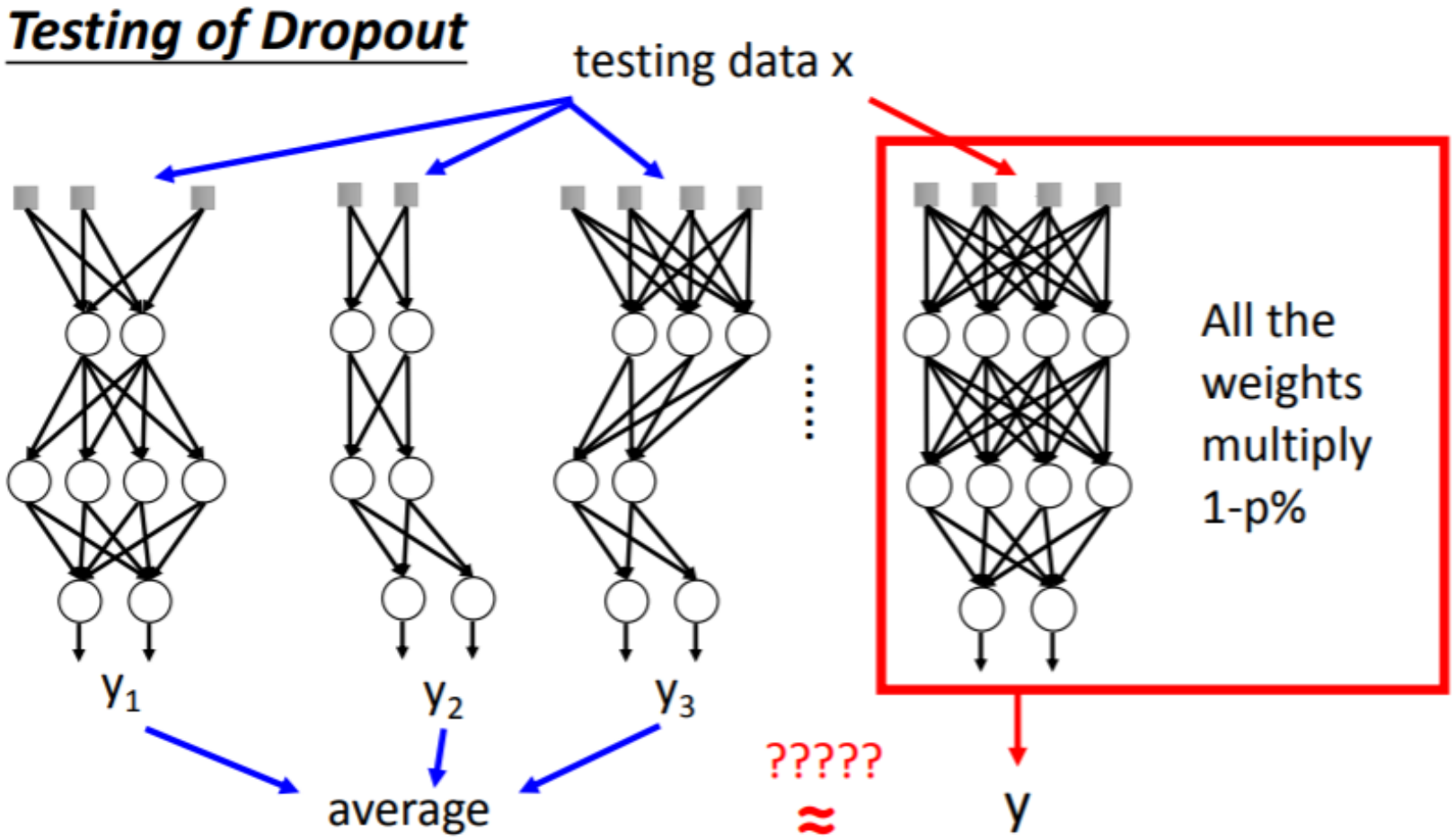
Testing of Dropout

No dropout



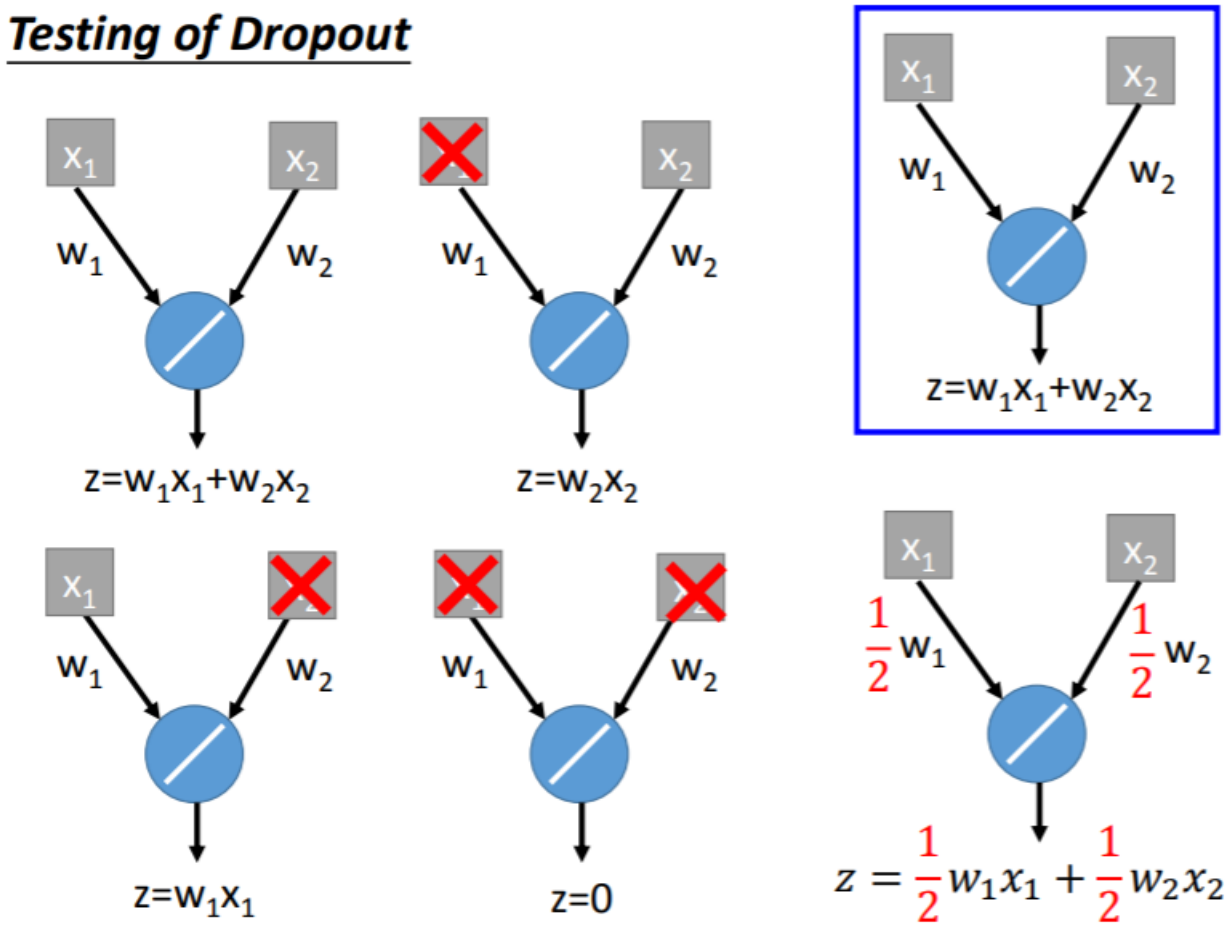
Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

Why multiply weights by (1-p)% during testing?



Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

Why multiply weights by (1-p)% during testing?



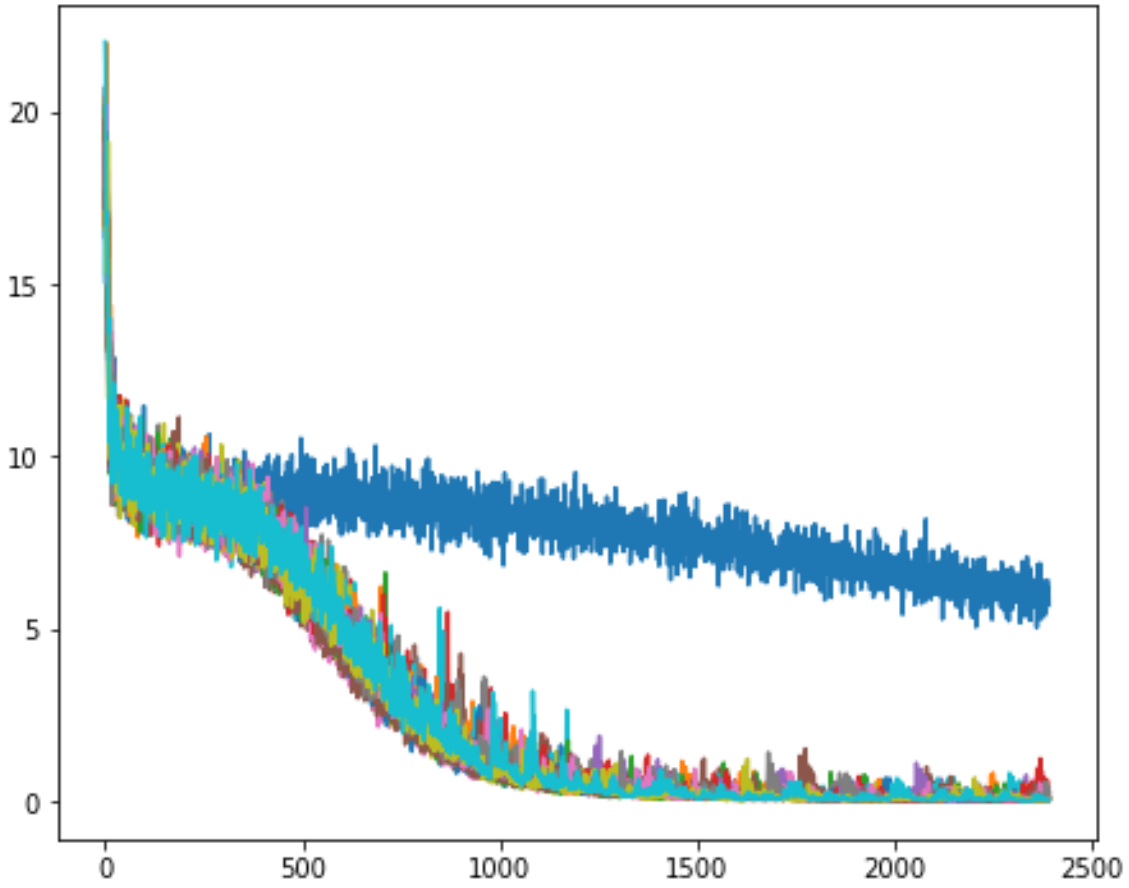
Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

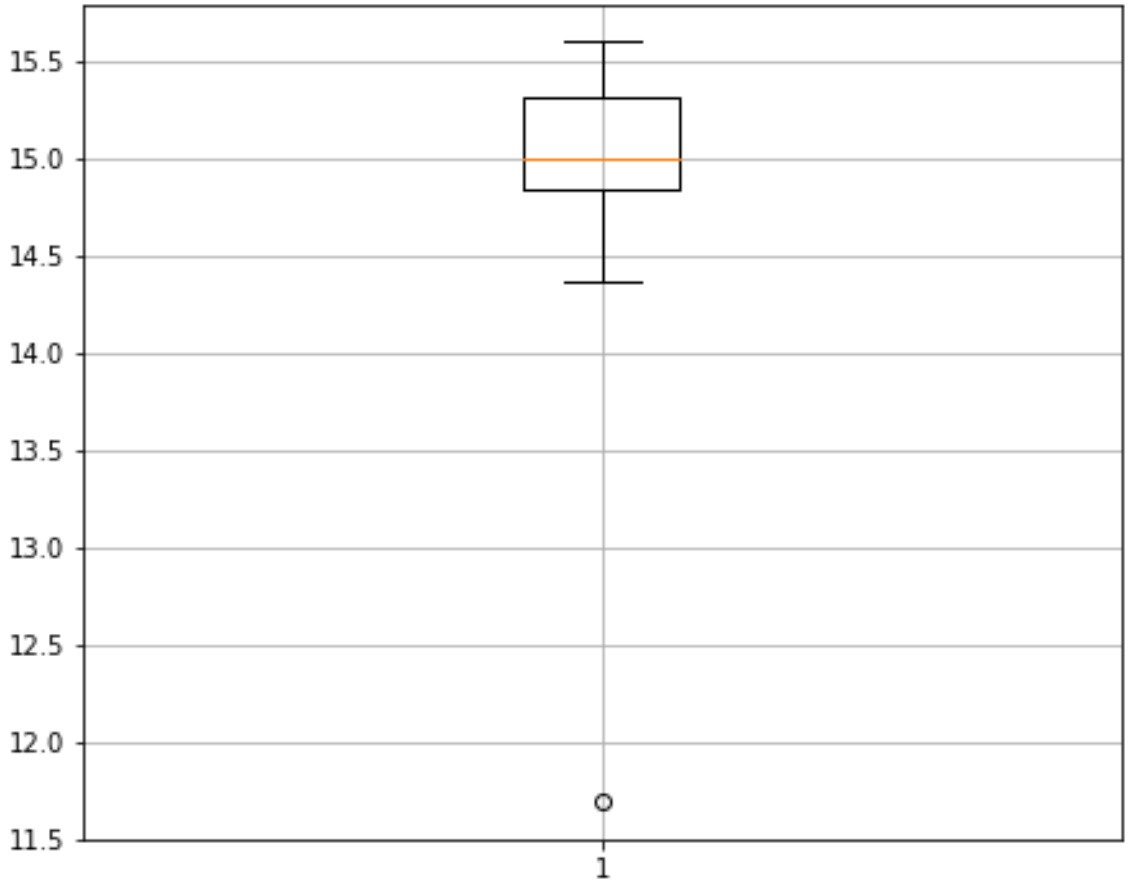
(3) Drop out

```
MyNet = nn.Sequential(
    nn.Linear(7, 1024),
    nn.ReLU(),
    nn.Dropout(p=0.5),
    nn.Linear(1024, 1024),
    nn.ReLU(),
    nn.Dropout(p=0.5),
    nn.Linear(1024, 1024),
    nn.ReLU(),
    nn.Dropout(p=0.5),
    nn.Linear(1024, 1024),
    nn.ReLU(),
    nn.Dropout(p=0.5),
    nn.Linear(1024, 1024),
    nn.ReLU(),
    nn.Dropout(p=0.2),
    nn.Linear(1024, 1),
)
MyNet.to(device)
print(MyNet)
```

```
#model.eval() will turn model to test mode and PyTorch will
# automatically handle weight scaling of the dropout layer
MyNet.eval()
tensorX = torch.FloatTensor(testX).to(device)
tensorY = torch.FloatTensor(testY).to(device)
tensorY_hat = MyNet(tensorX)
loss = loss_func(tensorY, tensorY_hat)
test_lossLst.append(float(loss))
```

(3) Drop out

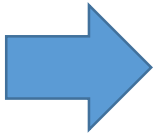

20
15
10
5
0
0
500
1000
1500
2000
2500


15.5
15.0
14.5
14.0
13.5
13.0
12.5
12.0
11.5
1

Try different NNs

Use your own $y = f(\vec{x})$ data

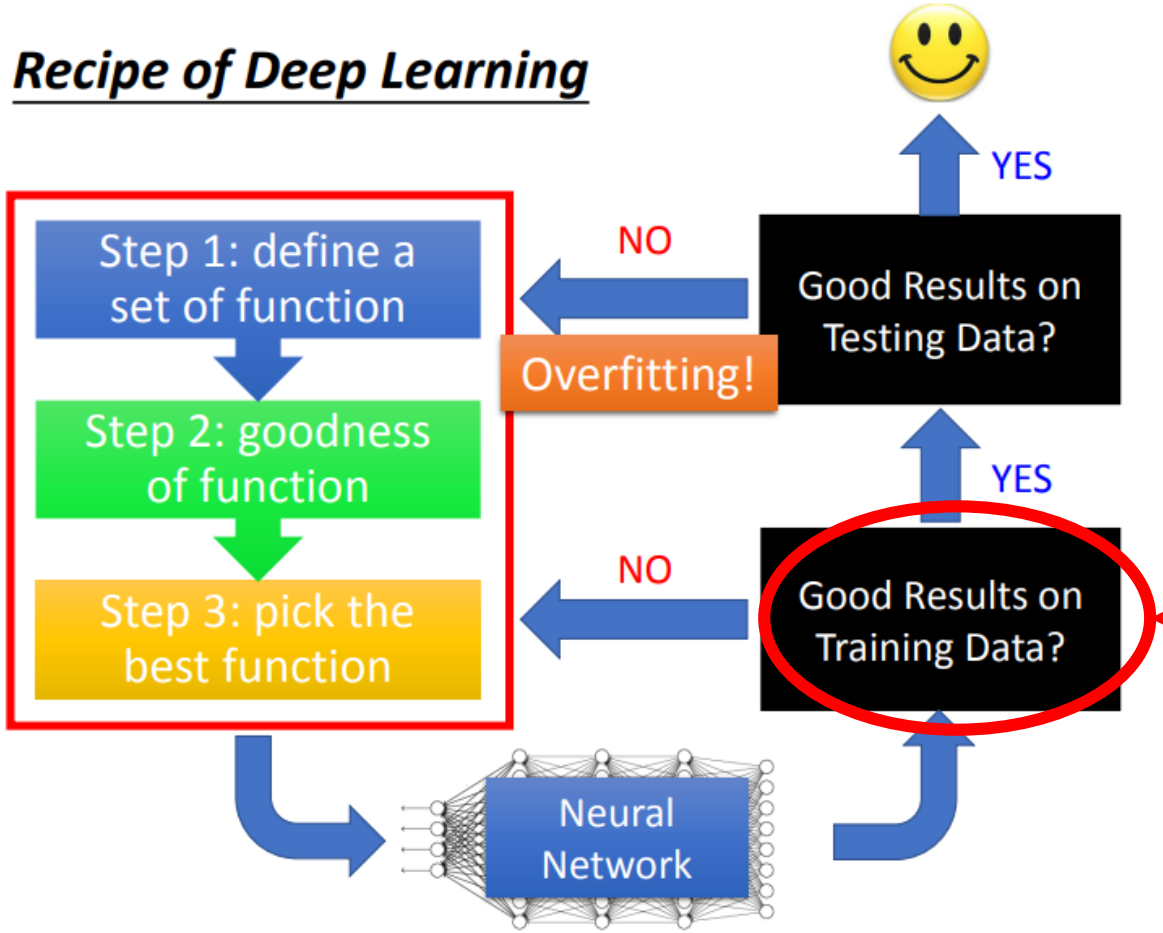
- 7-512-512-512-512-1
- 7-256-256-256-1
- 7-56-56-1

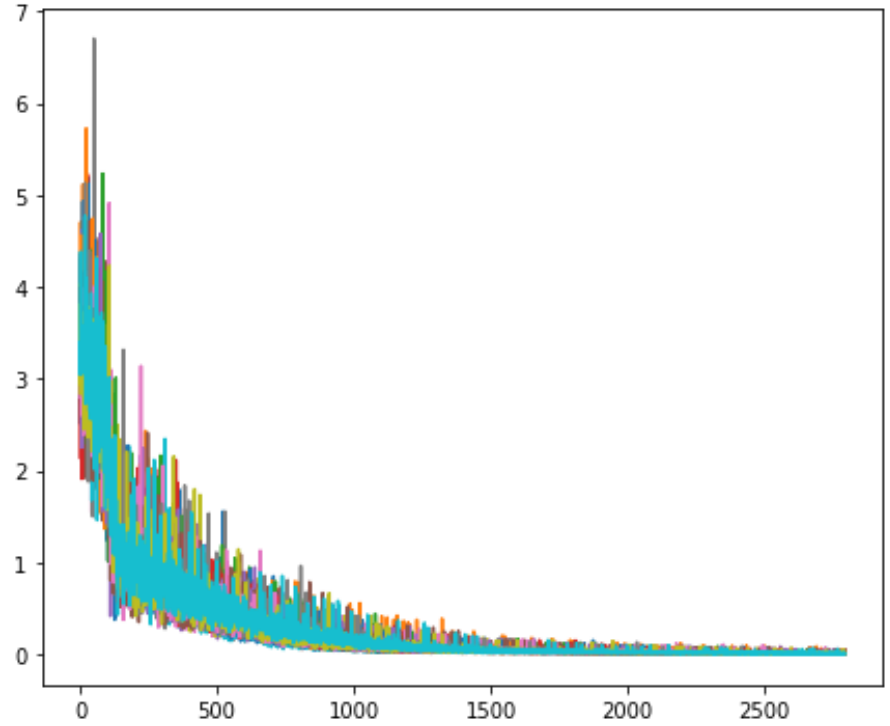


- Is the overfitting problem solved by drop out?

Class practice discussion

When data is generated from a formula $y = f(x) + \text{noises}$, NN can learn the mapping successfully (with 5000 data).

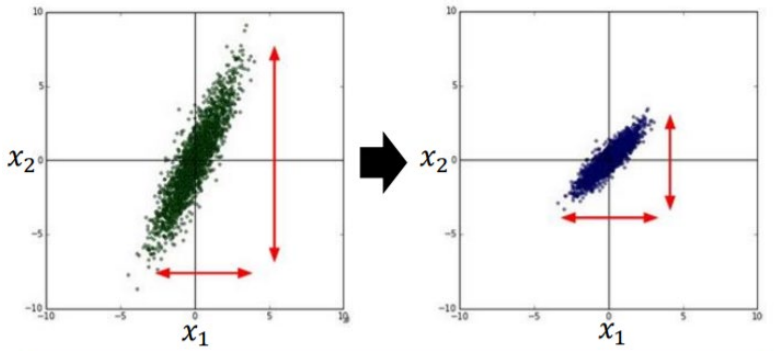




Class practice discussion

Feature scaling is OK

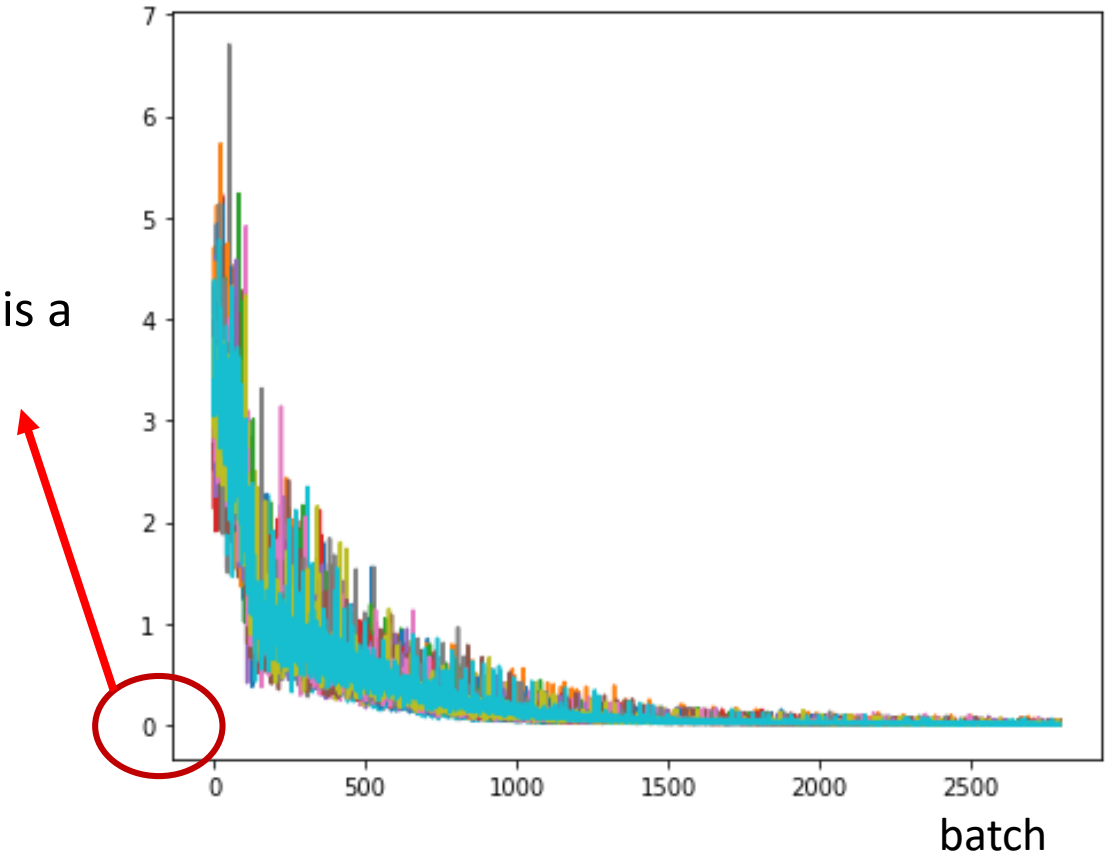
$$y = b + w_1 x_1 + w_2 x_2$$



Make different features have the same scaling

- Given the batch size and range of y, what is a good MSE value for successful training?

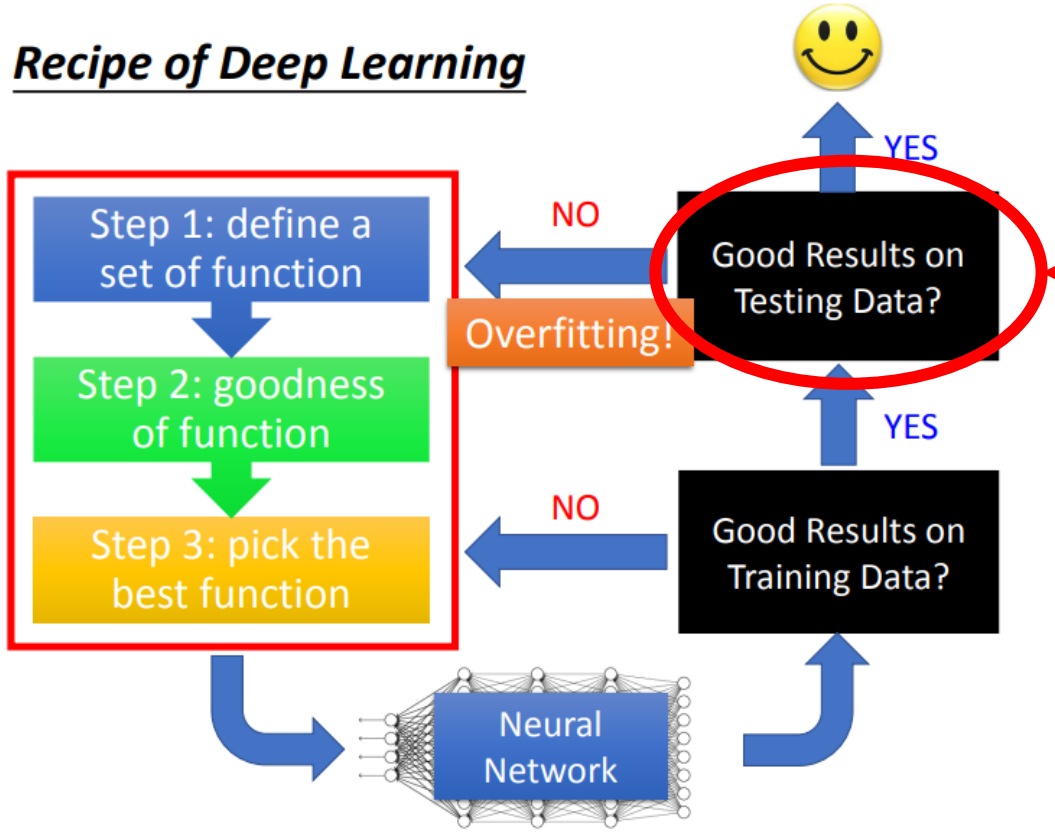
$$\sum_{n=1}^{N} (\hat{y}^n - y^n)^2$$



We add a noise to y, i.e., $y = f(x) + \text{noises}$. Normalization of y will reduce the variance again.

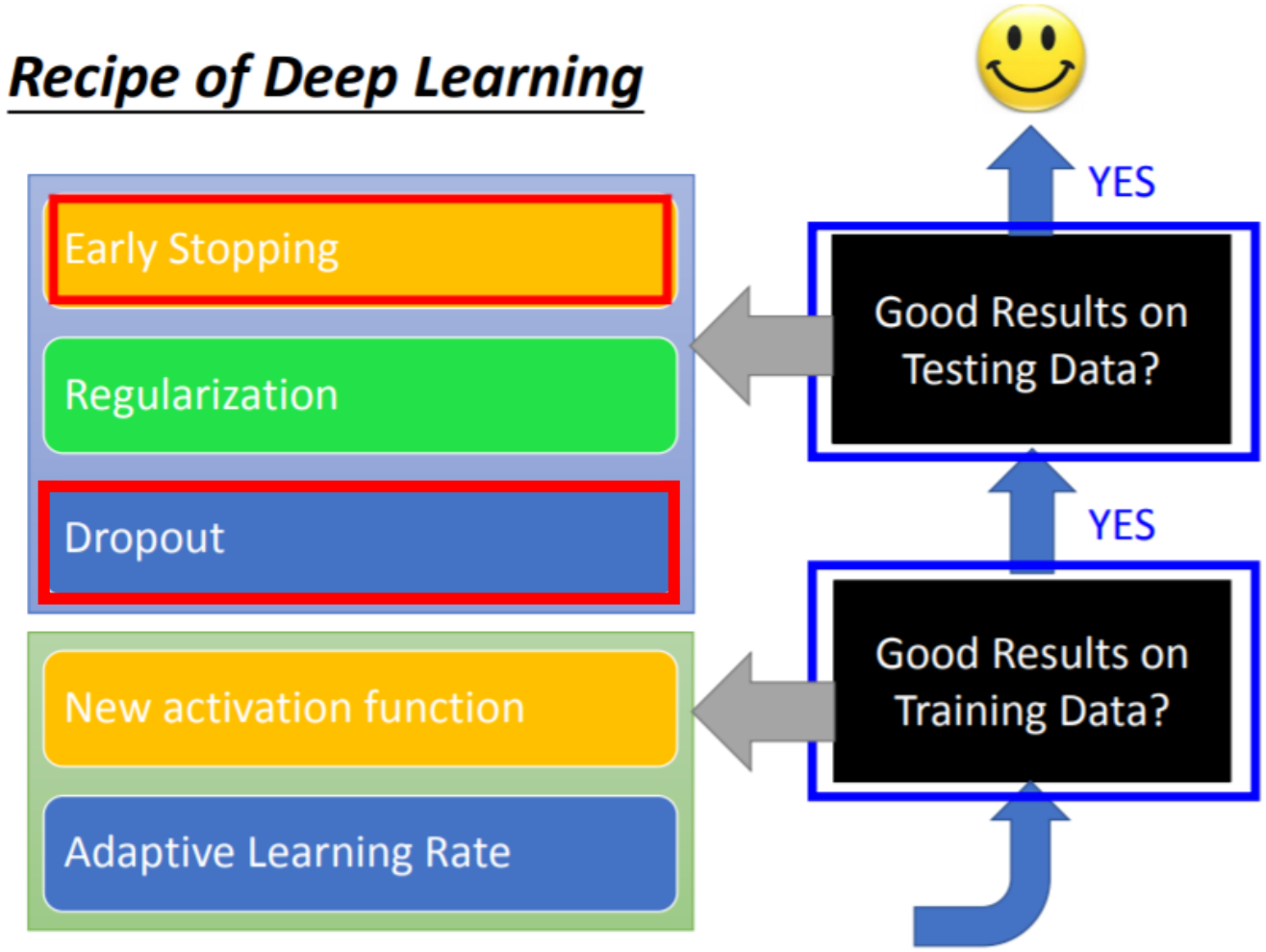
Class practice discussion

Overfitting can happen.



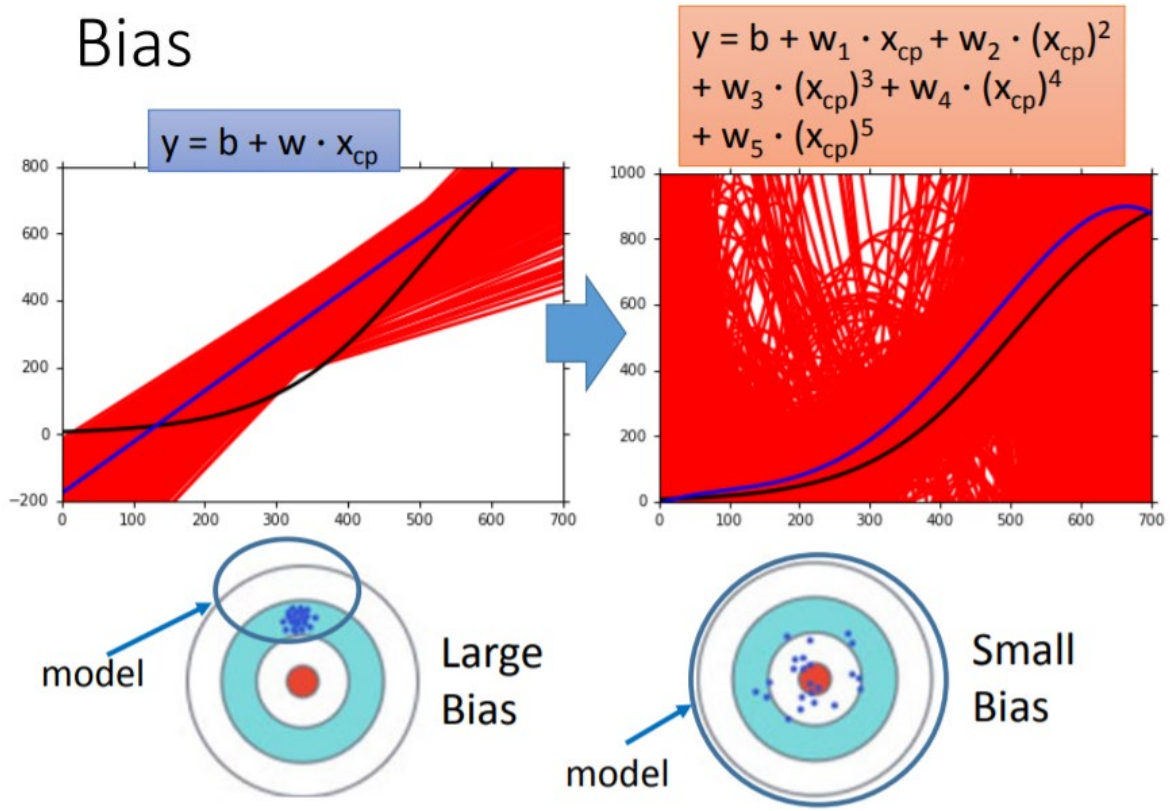
Class practice discussion

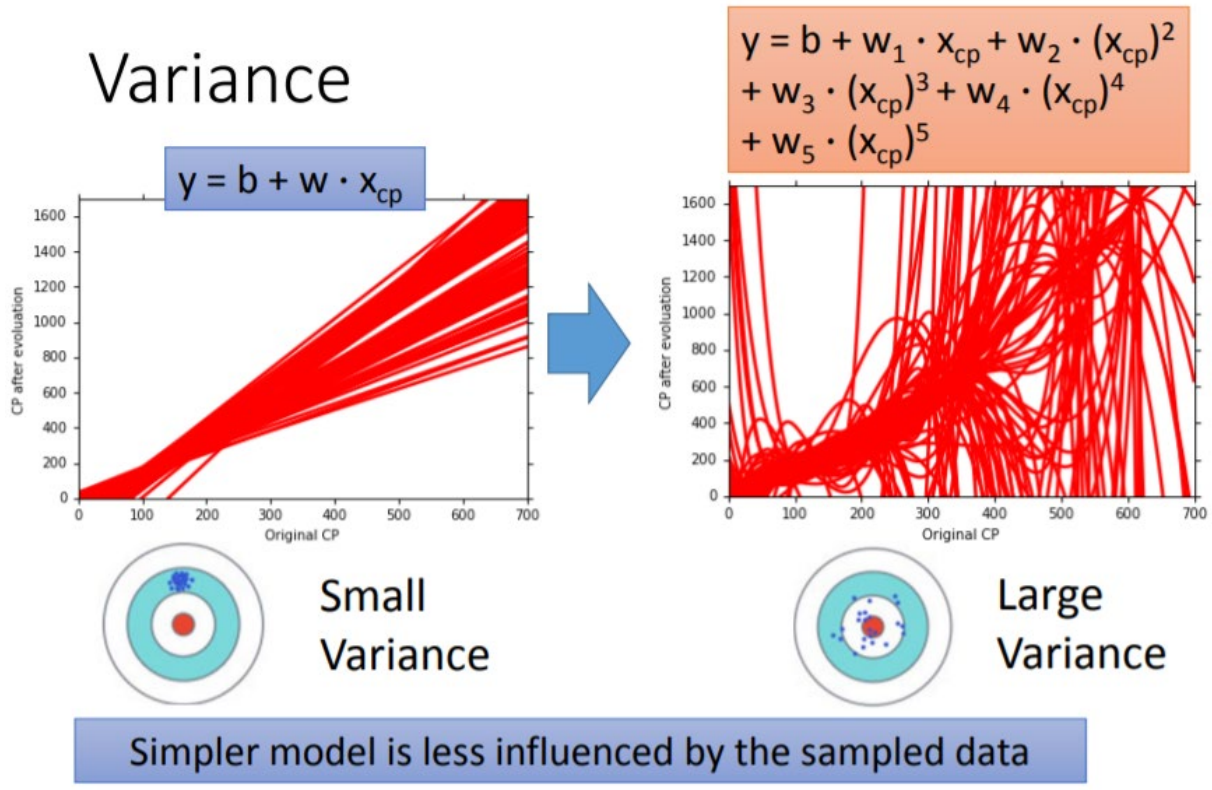
Early stop and drop out do not solve the overfitting problem?



Try different NNs

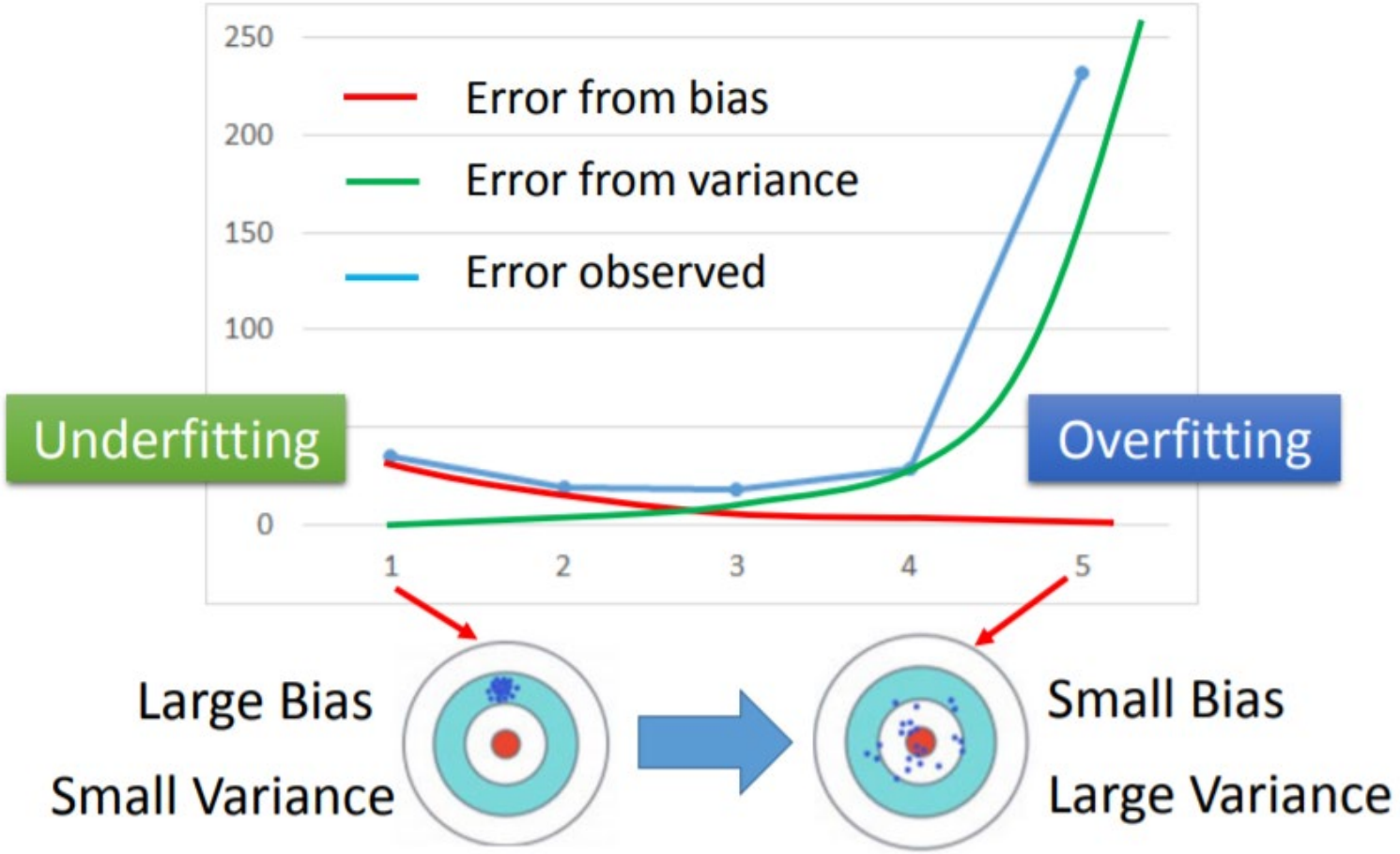
Simpler model is less influenced by the sampled data and has smaller variance





Reference: 李弘毅 ML Lecture 2 https://youtu.be/D_S6y0Jm6dQ

Try different NNs

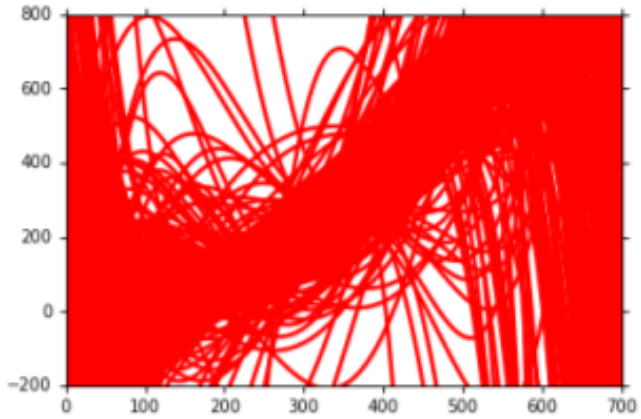


Reference: 李弘毅 ML Lecture 2 https://youtu.be/D_S6y0Jm6dQ

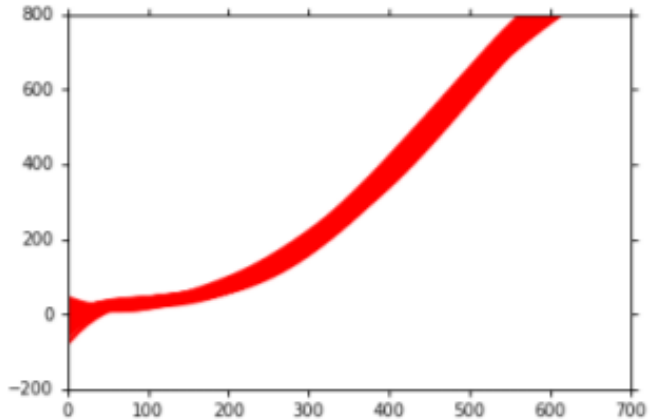
How number of data affect learning?

① More data

Very effective, but not always practical

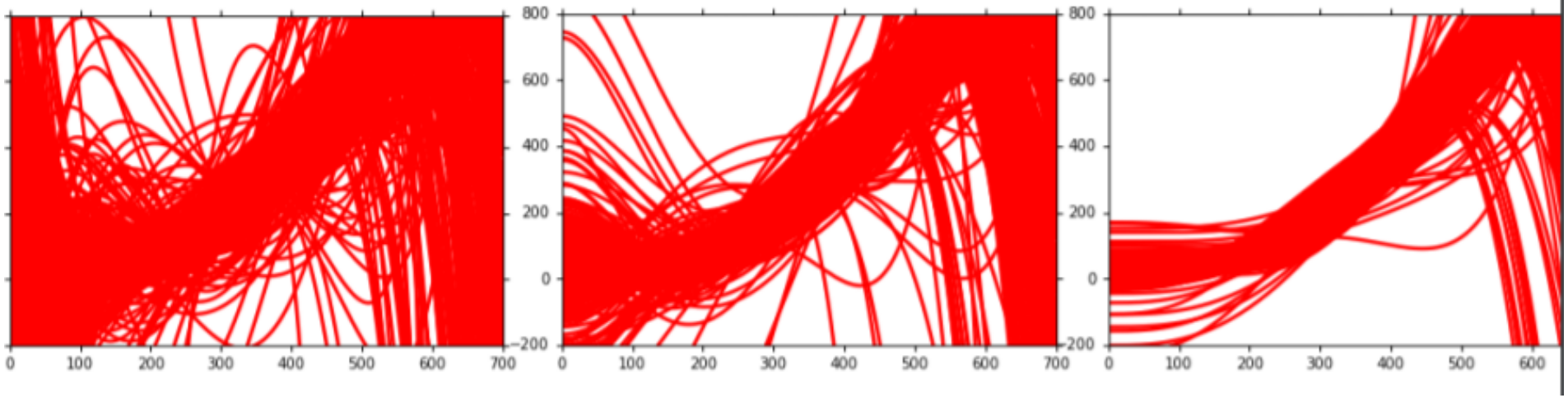


10 examples



100 examples

② Regularization



Reference: 李弘毅 ML Lecture 2 https://youtu.be/D_S6y0Jm6dQ