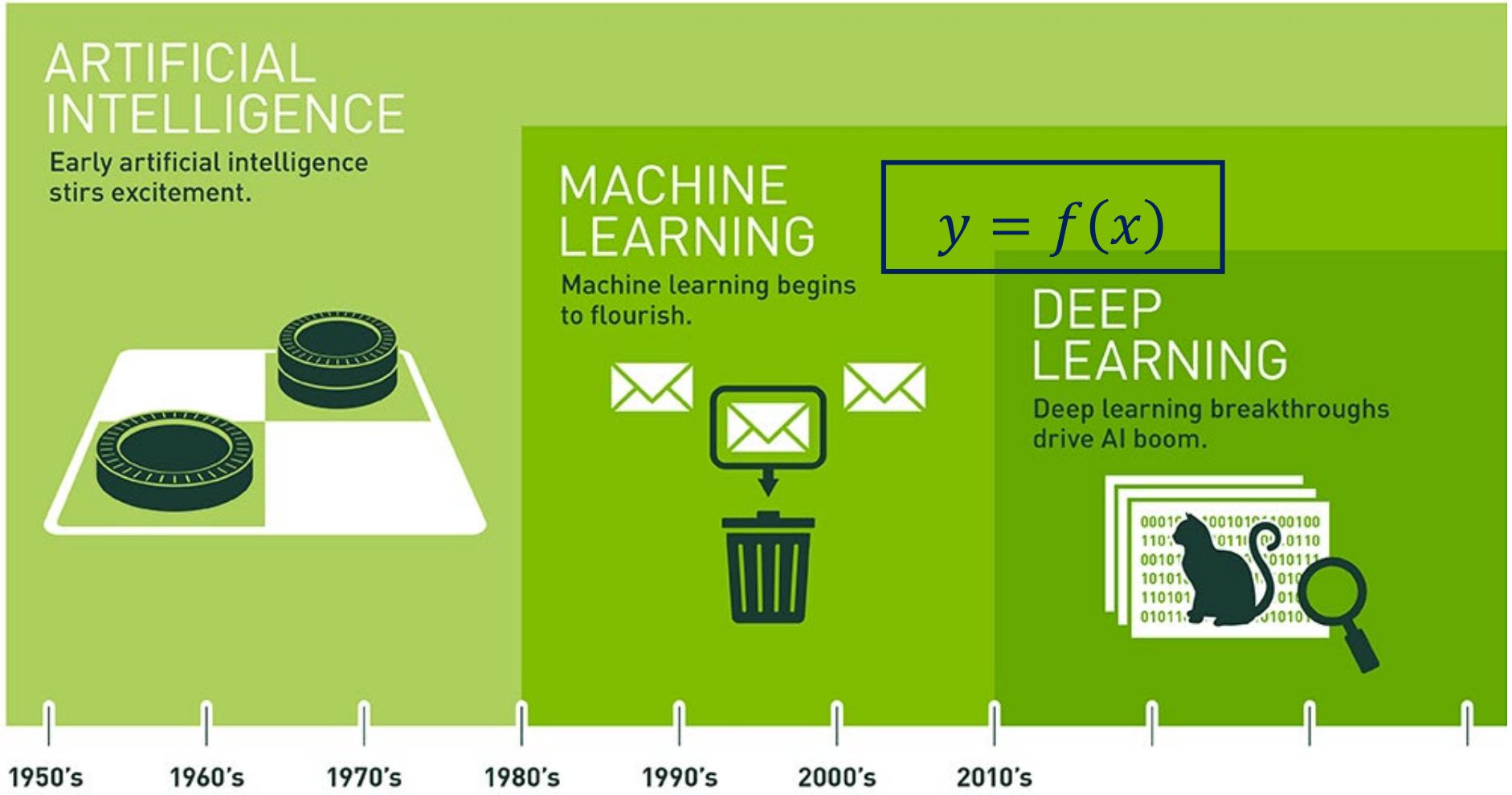
ML tasks

y learned is continuous → Regression

y learned is categorical → Classification



https://blogs.nvidia.com/blog/2016/07/29/whats-difference-artificial-intelligence-machine-learning-deep-learning-ai/

Notations

x_i

x_i^n

x^n

$\hat{y}^n$

No	age	t1	t2	t3	t4	t5	t6	time	Step frequency	n1	n2	n3	n4	n5	n6	px	py	pz	Steps	Gender	TUG	y1	BBS	y2
1	70	1.76	2.64	6.24	7.02	10	12.8	11	2.285	80	120	282	317	453	575	11.67	1.809	-1.99	13	F	11	0	26	0
2	86	1.64	2.6	5.82	7.27	10.4	12.6	11	1.934	75	118	263	328	470	570	11.14	2.302	-4.651	12	F	11	0	24	0
3	76	1.76	2.93	6.27	7.04	10.3	12.8	11	2.109	80	133	283	318	465	575	11.53	2.169	-3.253	14	F	11	0	22	1
4	70	2.38	3.29	5.58	6.47	9.02	10.4	8	2.461	108	149	252	292	407	468	11.6	1.838	-3.138	12	F	8	0	24	0
5	66	3.09	4.07	6.6	7.4	10.2	12.1	9	2.461	140	184	298	334	462	545	11.55	2.531	-2.742	12	F	9	0	26	0
6	79	1.76	2.91	5.87	6.6	10.2	12.8	11	2.109	80	132	265	298	462	575	11.5	1.788	-1.349	13	F	11	0	26	0
7	85	1.2	2.33	5.42	8.31	12.1	17.2	16	2.988	55	106	245	375	545	775	11.1	2.203	-4.89	17	M	16	1	18	1
8	81	1.64	2.93	5.98	7.47	10.9	13.6	12	1.758	75	133	270	337	493	615	11.1	2.667	-4.594	10	F	12	0	24	0
9	82	0.64	1.47	4.76	5.76	9.36	11.6	11	2.109	30	67	215	260	422	525	11.26	4.1	-2.693	14	M	11	0	24	0
10	69	1.64	2.49	5.02	5.98	9.82	12.6	11	2.637	75	113	227	270	443	570	11.27	3.292	-3.522	13	F	11	0	20	1
11	84	0.64	1.4	5.67	7.29	11.5	14.6	14	1.934	30	64	256	329	520	660	11.53	2.335	-2.999	15	M	14	1	26	0
12	69	1.09	1.98	5	5.62	8.38	10.1	9	2.109	50	90	226	254	378	455	11.15	1.919	-4.608	11	M	9	0	26	0
13	73	1.09	2.13	6.78	8.38	12.4	17.1	16	3.691	50	97	306	378	558	770	11.46	2.264	-3.333	16	F	16	1	14	1
14	81	0.64	1.87	9.24	11.2	19	22.6	22	1.934	30	85	417	507	857	1020	11.58	2.511	-2.157	27	M	22	1	24	0
15	80	0.76	1.71	3.98	5	7.58	9.76	9	2.109	35	78	180	226	342	440	11.33	2.821	-3.595	10	M	9	0	26	0
16	88	0.98	2.13	6.31	7.44	11.5	14	13	1.934	45	97	285	336	518	630	11.38	2.498	-3.702	16	M	14	1	26	0
17	81	1.09	2.09	4.18	5.16	7.76	10.1	9	2.285	50	95	189	233	350	455	11.21	2.241	-4.337	10	M	9	0	28	0
18	76	1.76	2.64	5.87	6.98	9.98	12.8	11	1.406	80	120	265	315	450	575	11.33	2.679	-3.736	10	M	11	0	26	0
19	69	0.36	3.76	13.3	16.7	24.2	29.4	29	3.691	17	170	598	753	1090	1322	11.31	1.361	-4.171	28	F	29	1	10	1
20	75	1.98	2.93	5.98	7.91	12.2	15	13	1.934	90	133	270	357	551	675	11.5	2.202	-1.495	14	M	13	0	28	0
21	87	1.53	3.2	10.9	13.8	21.3	26.5	25	2.9	70	145	492	624	960	1195	11.6	2.199	-2.54	19	F	25	1	16	1
22	72	0.2	1.02	3.36	4.11	7.42	10.2	10	1.758	10	47	152	186	335	460	11.52	2.658	-2.081	9	M	10	0	28	0
23	109	0.64	1.93	5.04	5.71	9.13	10.6	10	2.285	30	88	228	258	412	480	11.51	2.056	-3.158	15	F	10	0	28	0

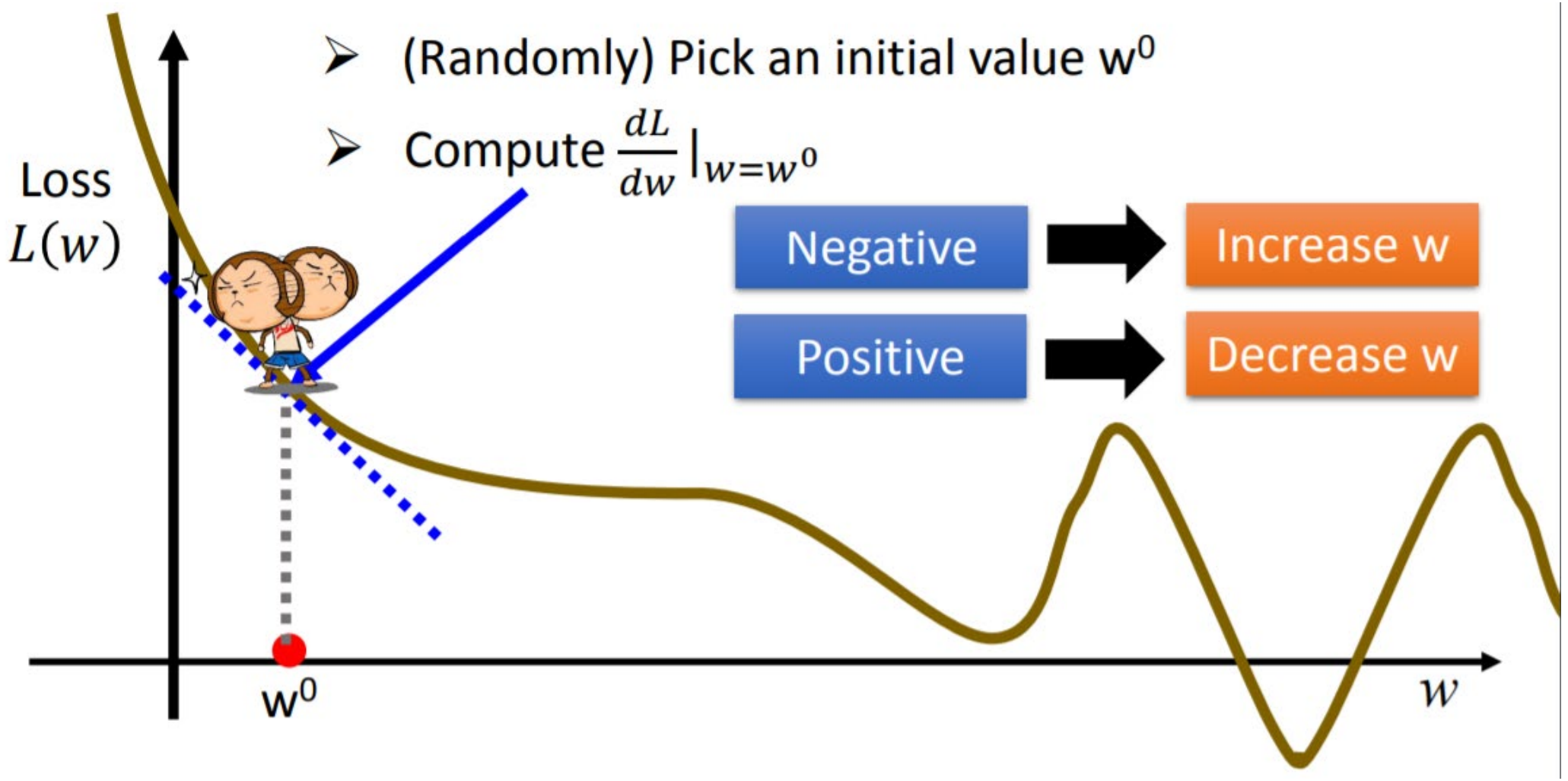
How machine learns from data?

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

Linear regression

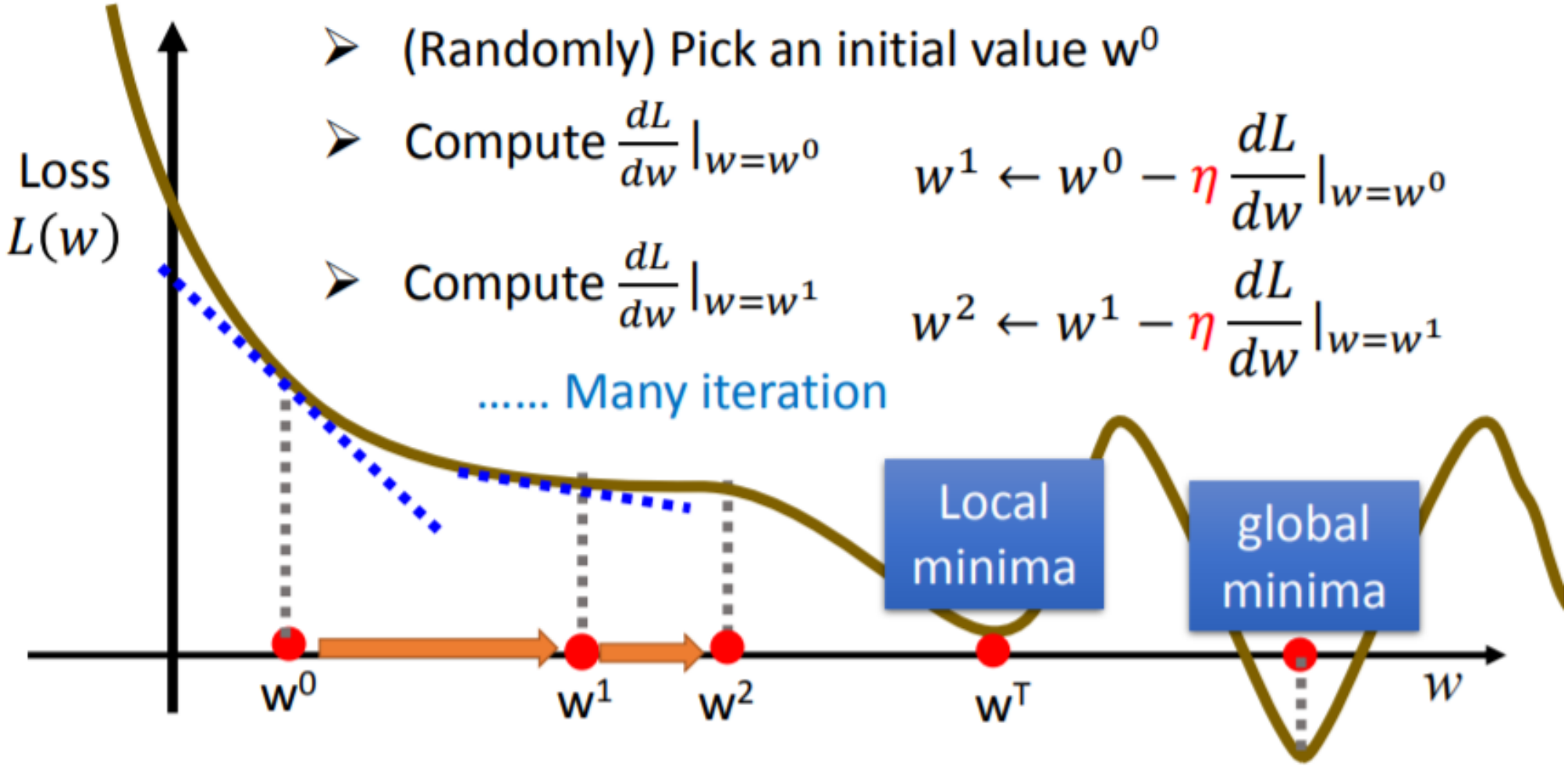
- Linear model: $y^n = \sum_i (w_i x_i^n) + b$
- Loss function: $L(w,b) = \sum_{n=1}^{N} (\hat{y}^n - y^n)^2 = \sum_{n=1}^{N} (\hat{y}^n - (\sum_i (w_i x_i^n) + b))^2$
- Find the optimal parameters that minimize loss: $\arg \min_{w,\, b} L(w,b)$

Use gradient decent to find w^*



Reference: 李弘毅 ML Lecture 1 https://youtu.be/CXgbekl66jc

Gradient decent



Reference: 李弘毅 ML Lecture 1 https://youtu.be/CXgbekl66jc

Gradient decent to find two parameters w^* and b^*

- How about two parameters? $w^*, b^* = arg \min_{w,b} L(w,b)$
  - (Randomly) Pick an initial value w^0, b^0
  - Compute $\frac{\partial L}{\partial w}|_{w=w^0,b=b^0}$, $\frac{\partial L}{\partial b}|_{w=w^0,b=b^0}$

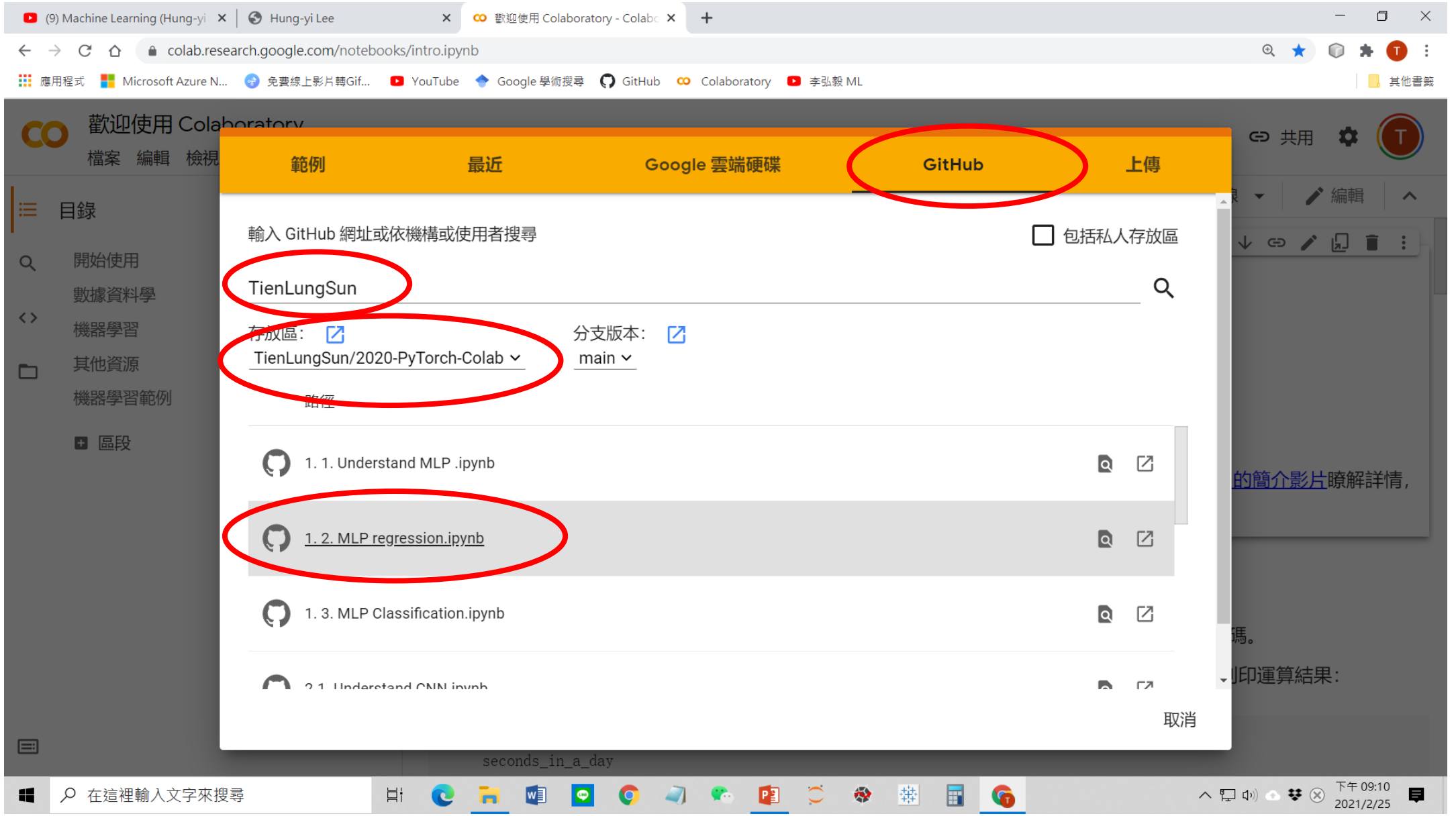
$$w^1 \leftarrow w^0 - \eta \frac{\partial L}{\partial w}|_{w=w^0,b=b^0} \qquad b^1 \leftarrow b^0 - \eta \frac{\partial L}{\partial b}|_{w=w^0,b=b^0}$$

  - Compute $\frac{\partial L}{\partial w}|_{w=w^1,b=b^1}$, $\frac{\partial L}{\partial b}|_{w=w^1,b=b^1}$

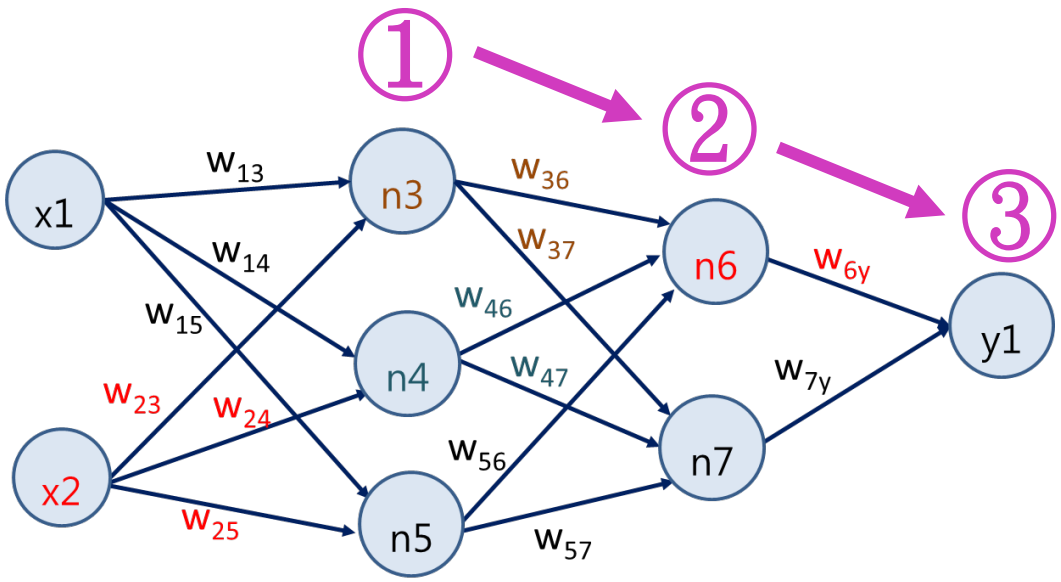
$$w^2 \leftarrow w^1 - \eta \frac{\partial L}{\partial w}|_{w=w^1,b=b^1} \qquad b^2 \leftarrow b^1 - \eta \frac{\partial L}{\partial b}|_{w=w^1,b=b^1}$$

Reference: 李弘毅 ML Lecture 1 https://youtu.be/CXgbekl66jc

Practice – MLP regression



Model = neural network



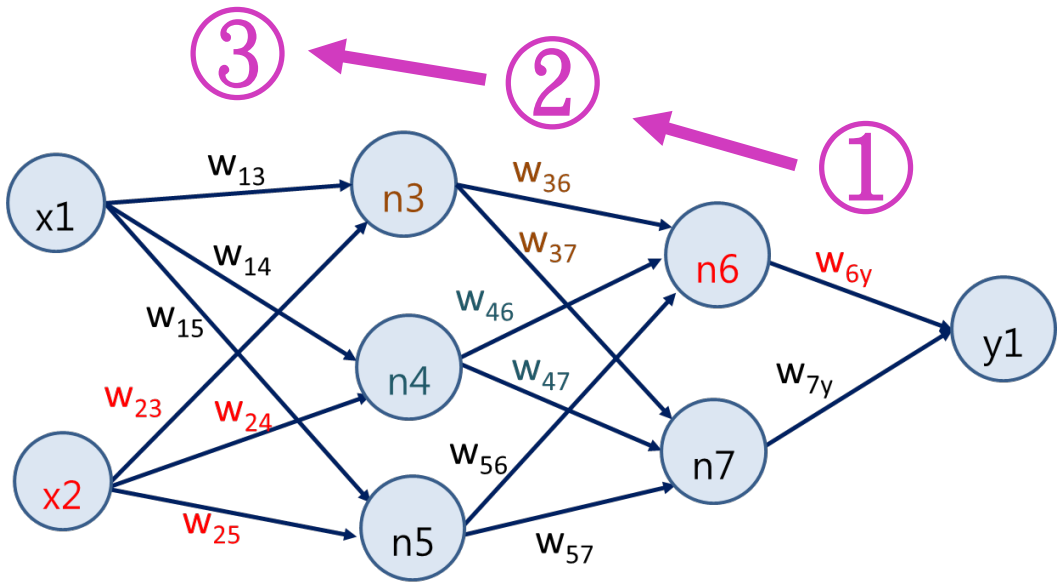
① $n_3 = \sigma(x_1 * w_{13} + x_2 * w_{23} + b_3)$
① $n_4 = \sigma(x_1 * w_{14} + x_2 * w_{24} + b_4)$
① $n_5 = \sigma(x_1 * w_{15} + x_2 * w_{25} + b_5)$

② $n_6 = \sigma(n_3 * w_{36} + n_4 * w_{46} + n_5 * w_{56} + b_6)$
② $n_7 = \sigma(n_3 * w_{37} + n_4 * w_{47} + n_5 * w_{57} + b_7)$

③ $y_1 = \sigma(n_6 * w_{6y} + n_7 * w_{7y} + b_y)$

Comparison: linear model in this case only have 3 parameters $y = \sum_i (w_i x_i) + b$

Gradient decent to find optimal parameters



$$e = g(y - y_1) \quad y_1 = \sigma(n_6 * w_{6y} + n_7 * w_{7y} + b_y)$$

①

$$w_{6y} \leftarrow w_{6y} - \eta \frac{\partial e}{\partial w_{6y}} \qquad \frac{\partial e}{\partial w_{6y}} = \frac{\partial e}{\partial y_1} \frac{\partial y_1}{\partial w_{6y}}$$

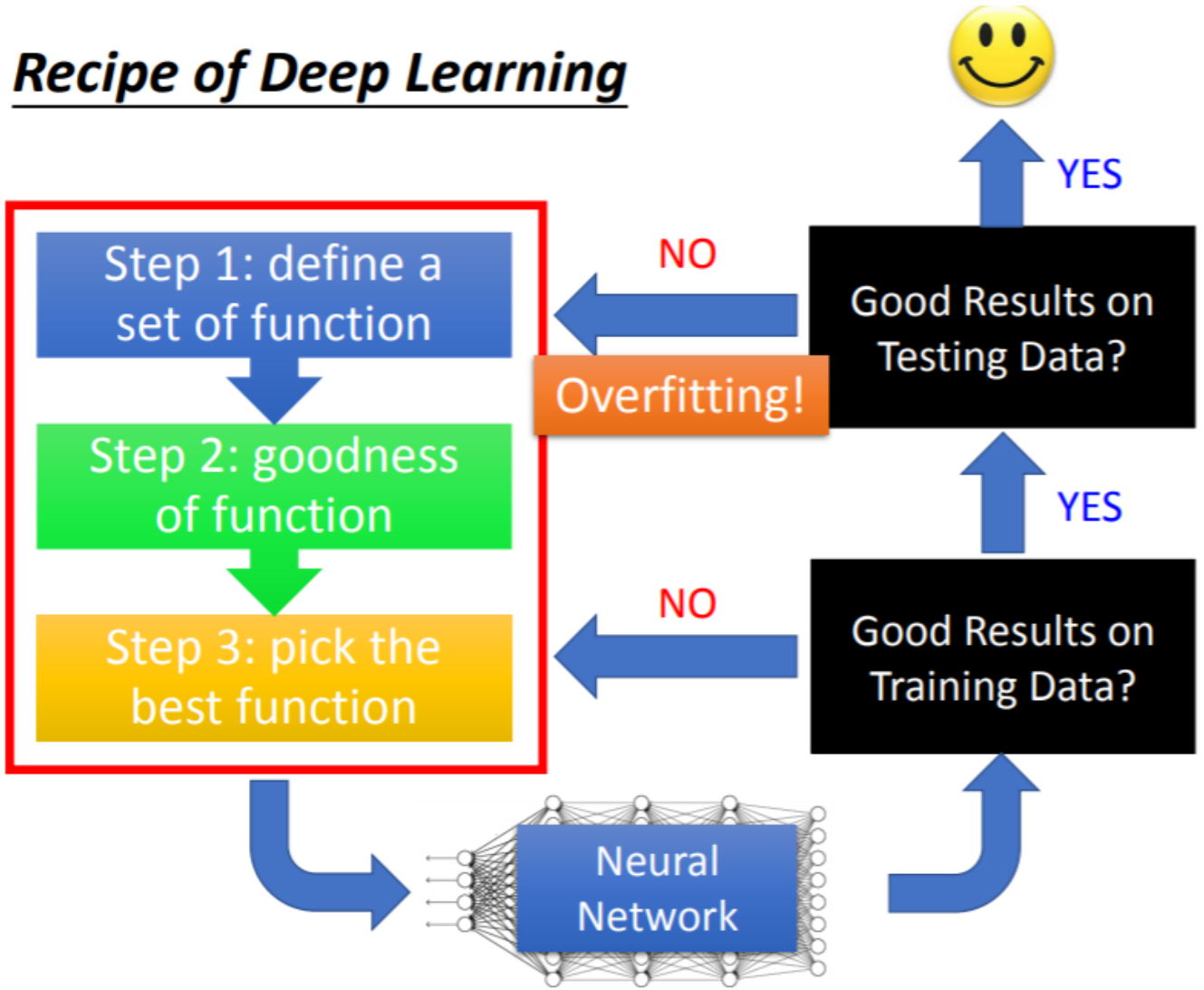
$$w_{7y} \leftarrow w_{7y} - \eta \frac{\partial e}{\partial w_{7y}} \qquad \frac{\partial e}{\partial w_{7y}} = \frac{\partial e}{\partial y_1} \frac{\partial y_1}{\partial w_{7y}}$$

$$w_i \leftarrow w_i - \eta \frac{\partial e}{\partial w_i}$$

② $$w_{57} \leftarrow w_{57} - \eta \frac{\partial e}{\partial w_{57}} \qquad \frac{\partial e}{\partial w_{57}} = \frac{\partial e}{\partial y_1} \frac{\partial y_1}{\partial n_7} \frac{\partial n_7}{\partial w_{57}}$$

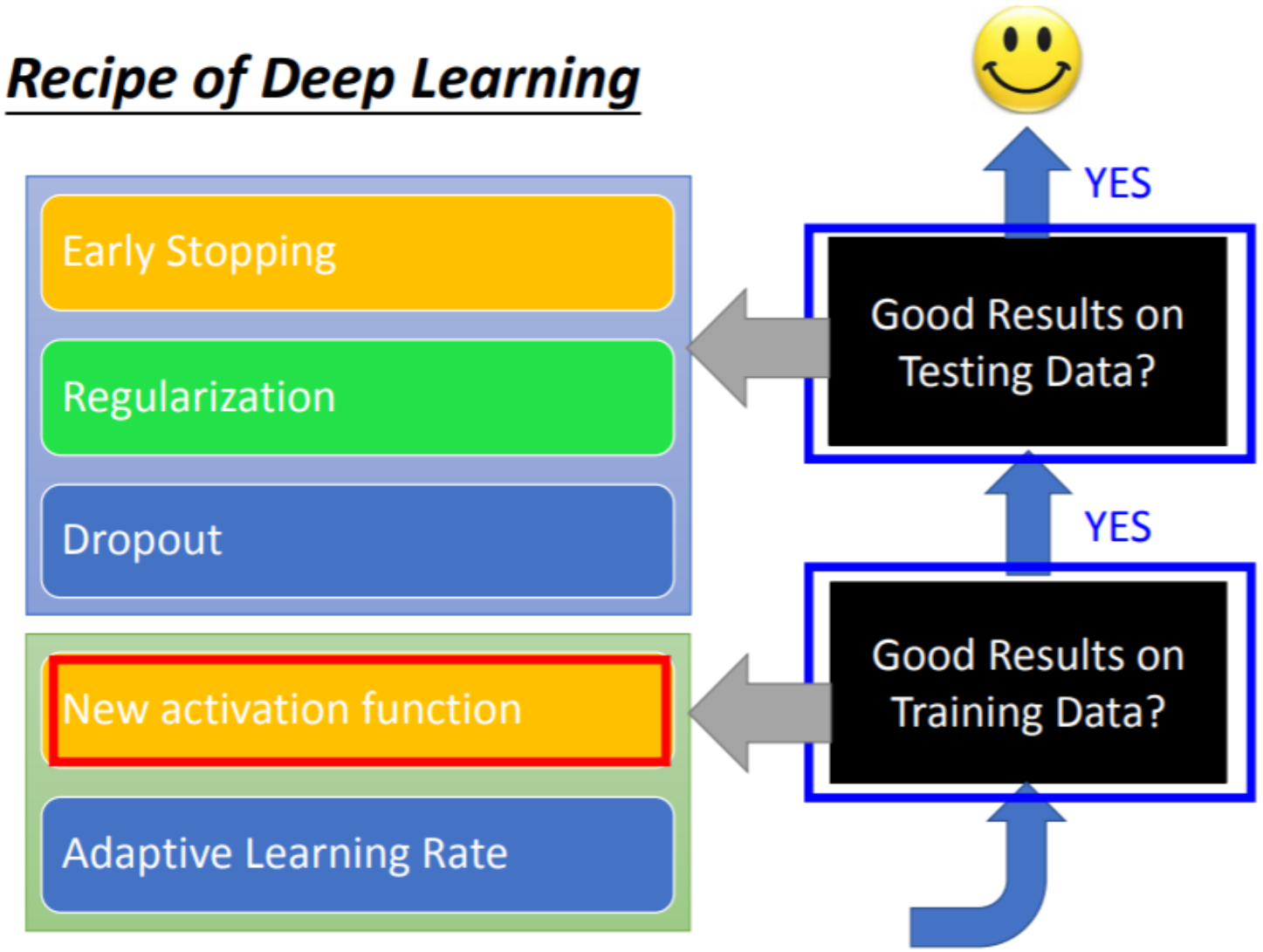
$$n_7 = f(n_3 * w_{37} + n_4 * w_{47} + n_5 * w_{57} + b_7)$$

Recipe of deep learning



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

What to do if the training result is not good?

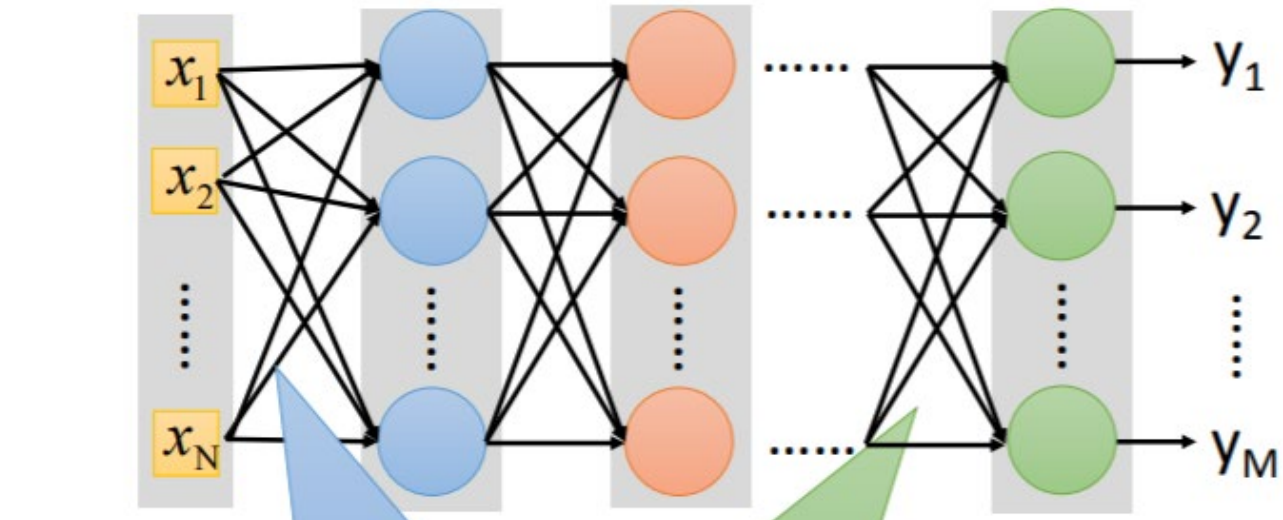


Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

Practice – Activation function

- Run "1.2 MLP regression.ipynb", change the activation function from ReLU to Sigmoid and explain why the results become worse?

Vanishing gradient problem



Smaller gradients

Learn very slow

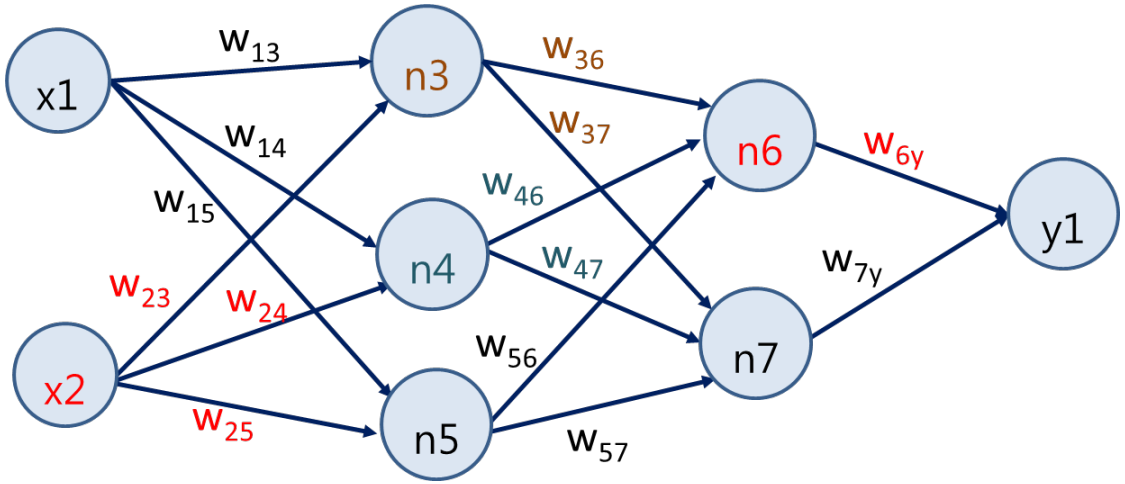
Almost random

Larger gradients

Learn very fast

Already converge

based on random!?



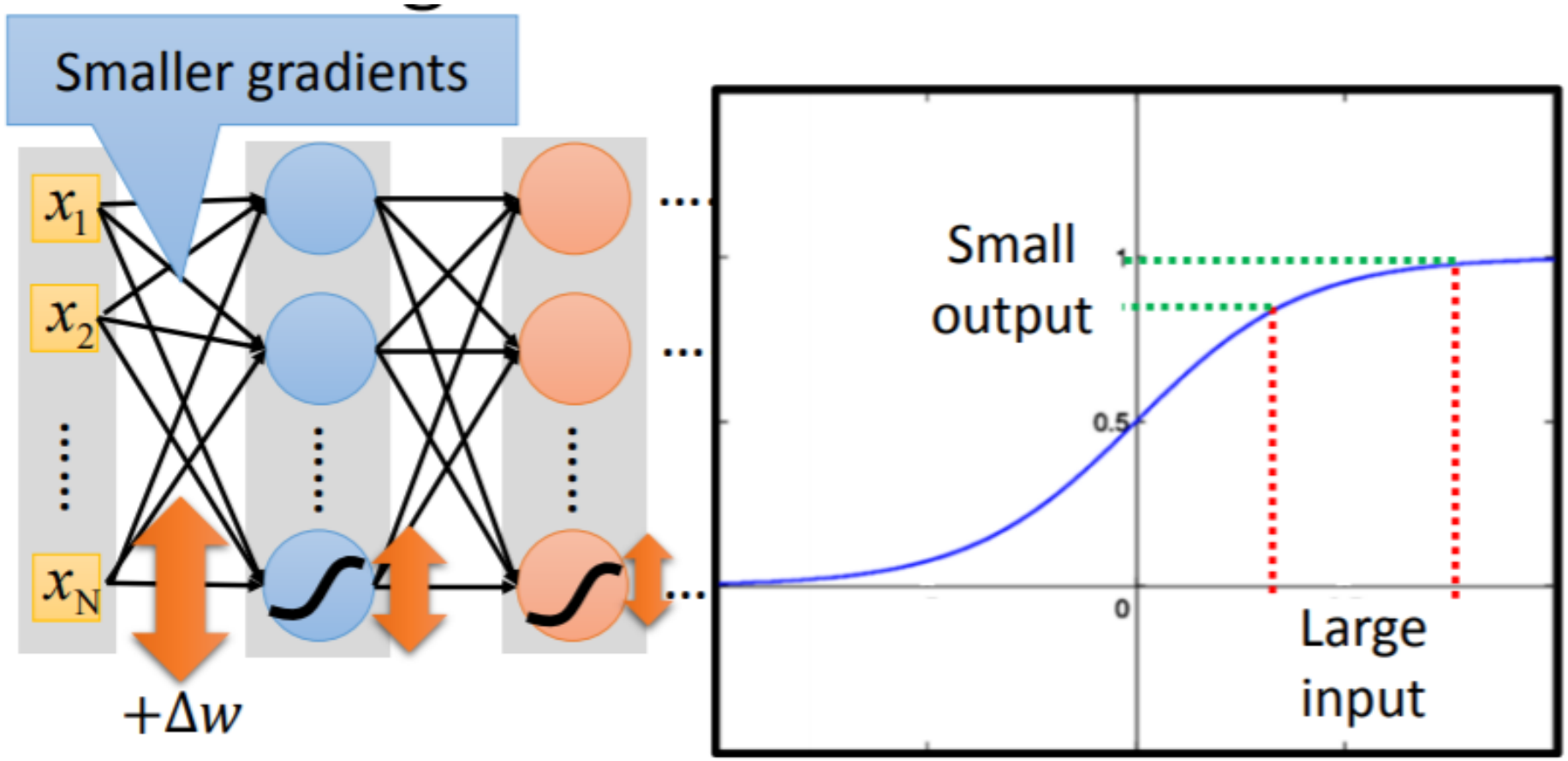
$$\frac{\partial L}{\partial w_{6y}} = \frac{\partial L}{\partial y_1}\frac{\partial y_1}{\partial w_{6y}}$$

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

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

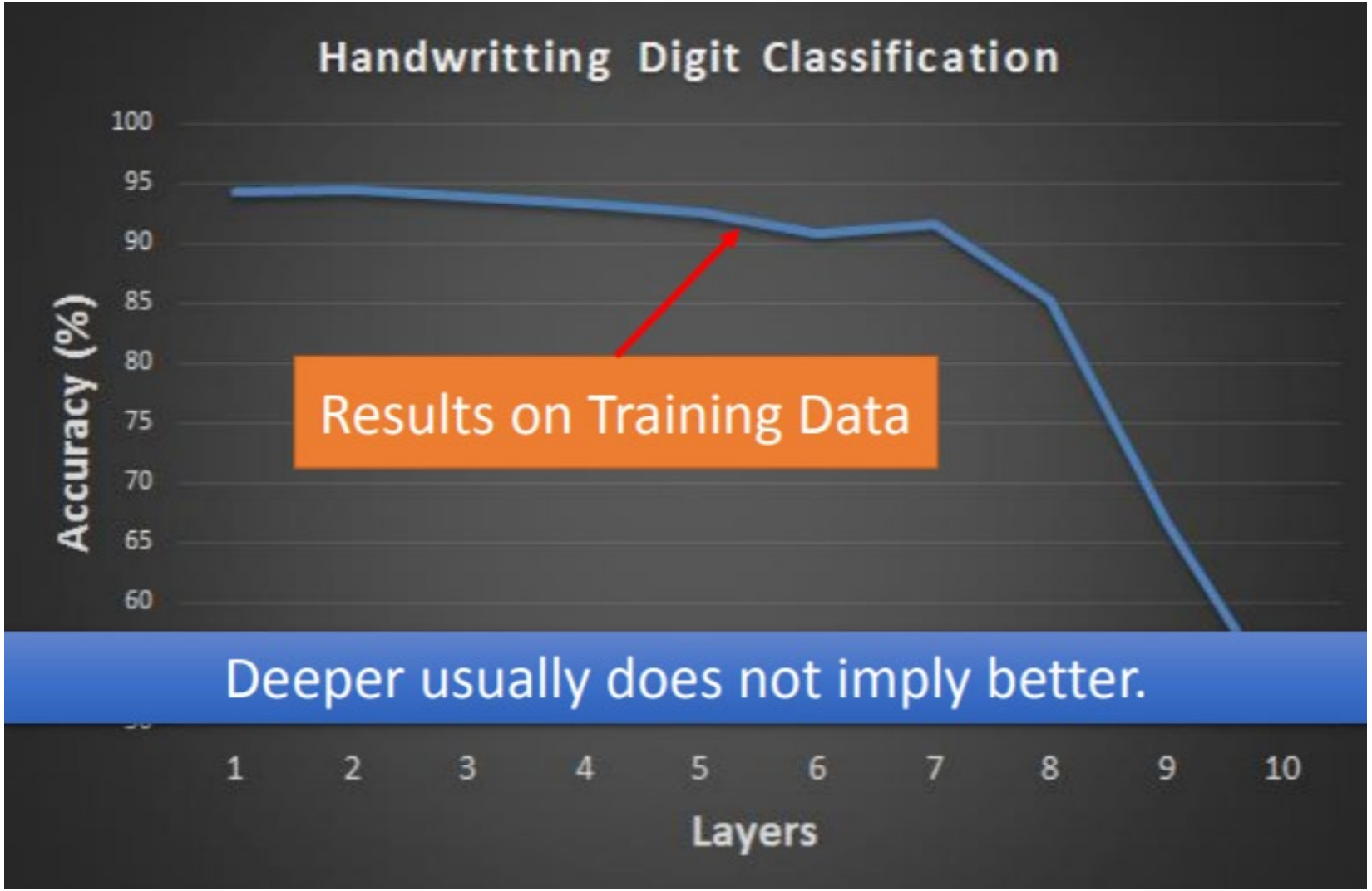
Vanishing gradient problem

$n_7 = \sigma(n_3 * w_{37} + n_4 * w_{47} + n_5 * w_{57} + b_7)$



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

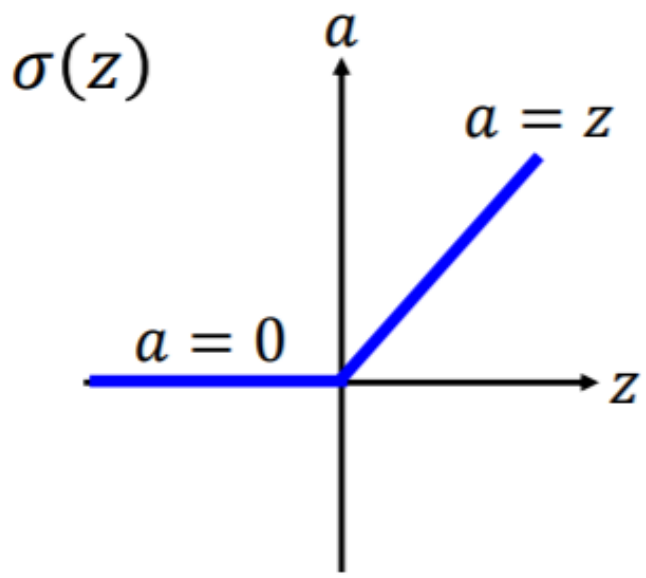
Sigmoid is hard to get the power of deep



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

ReLU

- Rectified Linear Unit (ReLU)



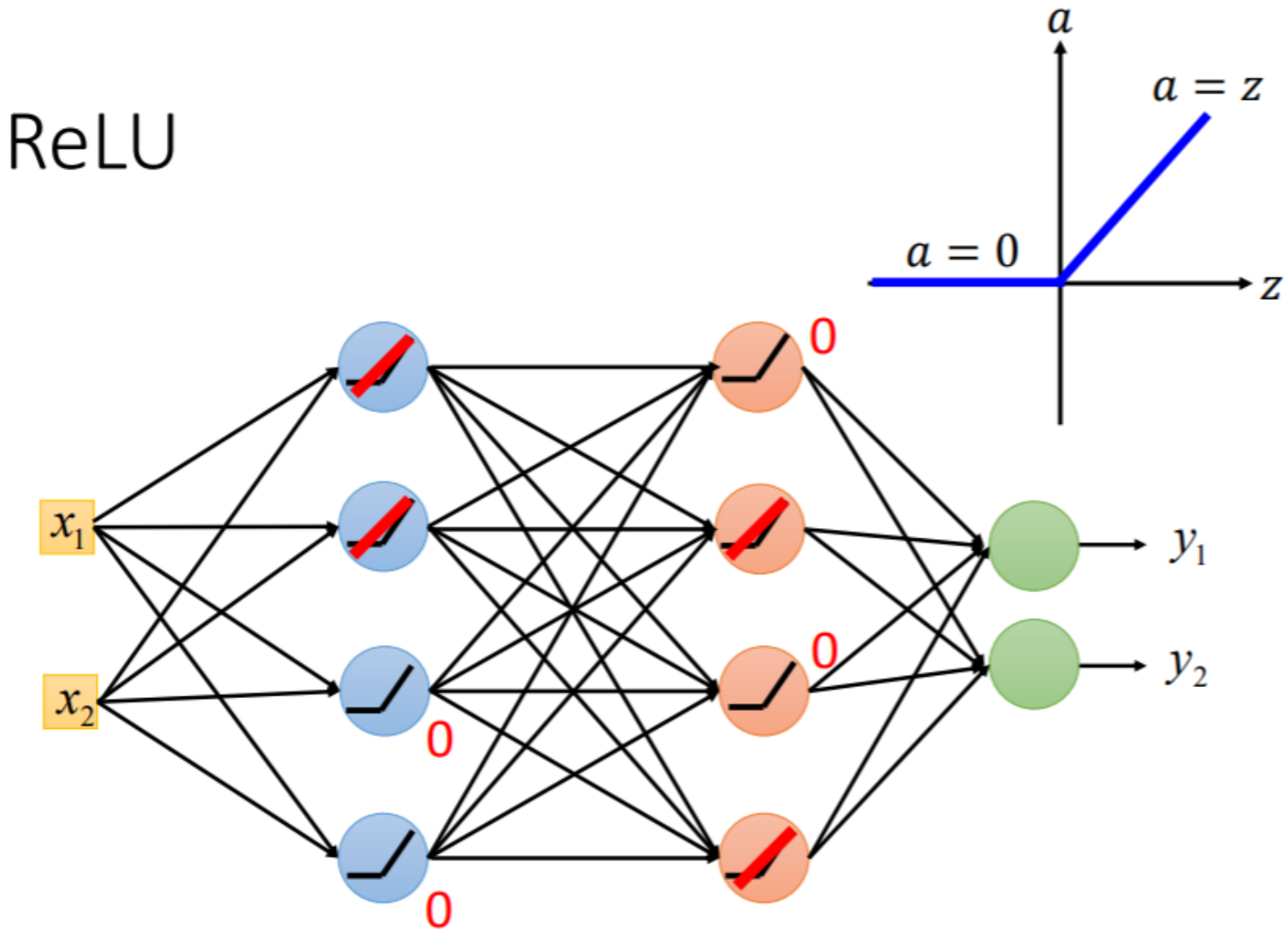
[Xavier Glorot, AISTATS'11]
[Andrew L. Maas, ICML'13]
[Kaiming He, arXiv'15]

Reason:

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

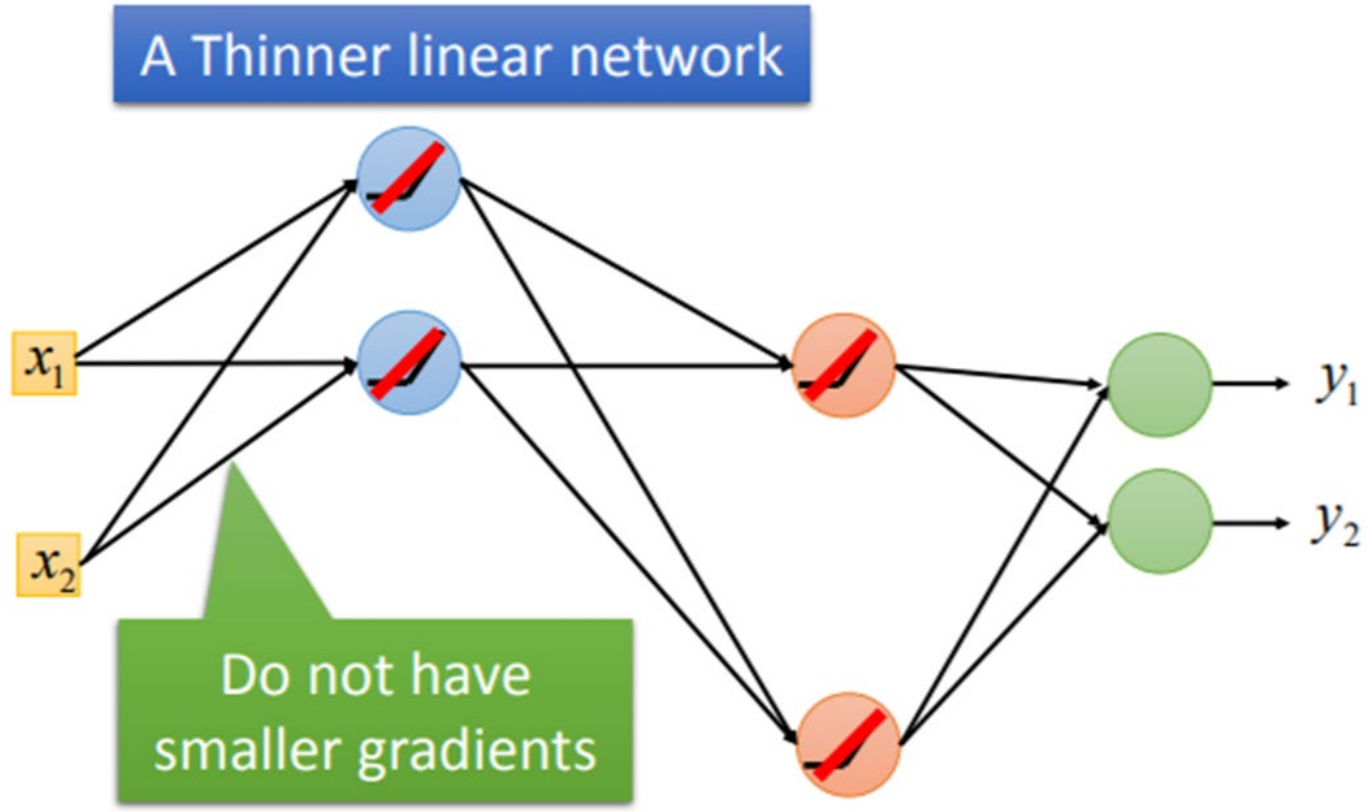
Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

ReLU



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

ReLU



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

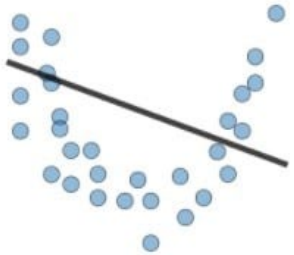
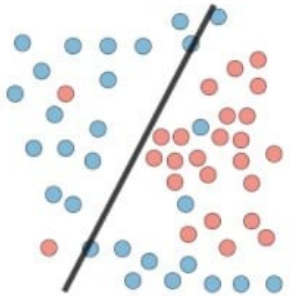
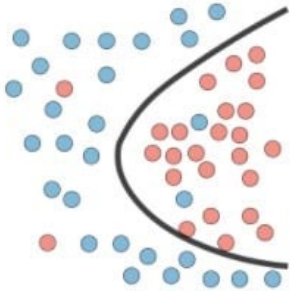
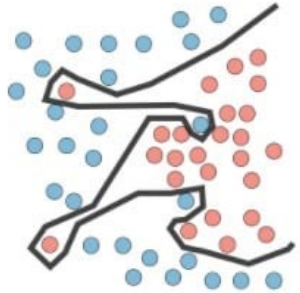
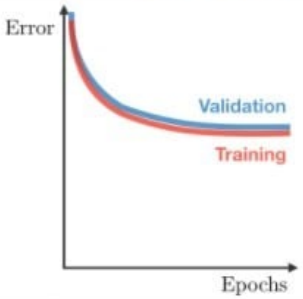
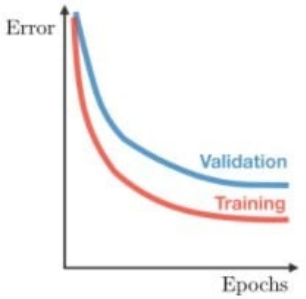
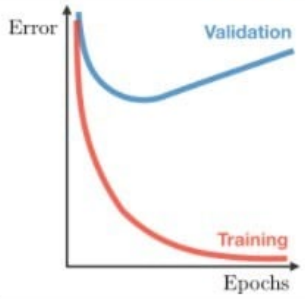
Practice – Learn from sparse data

- Run "1. 2.1. Learn from sparse data.ipynb", try to improve the training results.

HW3 (1)

- Change the linear equation in "1. 2.1. Learn from sparse data.ipynb" to quadratic or cubic equation. Sample sparse data and build a MLP to learn the mapping $y = f(x)$.
- Name your code as "HW3.ipynb"

Overfitting problem – NN performs well on training data but not good on test data

	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/

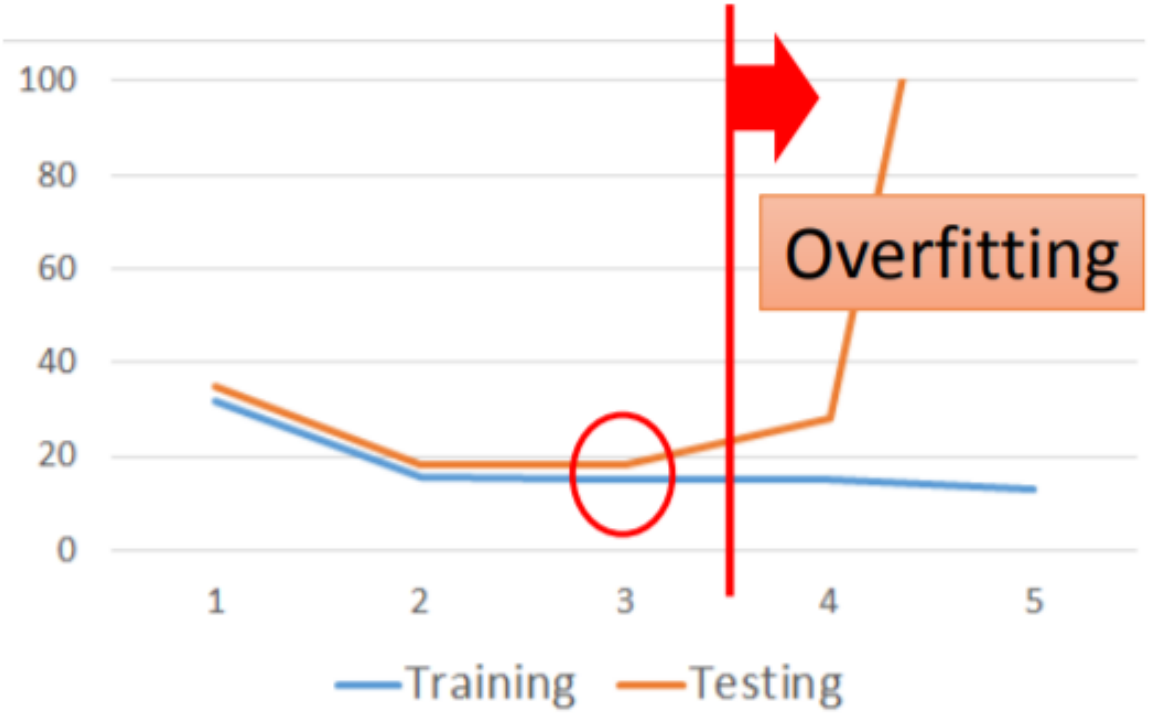
Practice – Overfitting

- Run "1. 2.2. Overfitting.ipynb", observe the overfitting problem.

HW3 (2)

- Study the overfitting problem in "HW3.ipynb".

Overfitting problem



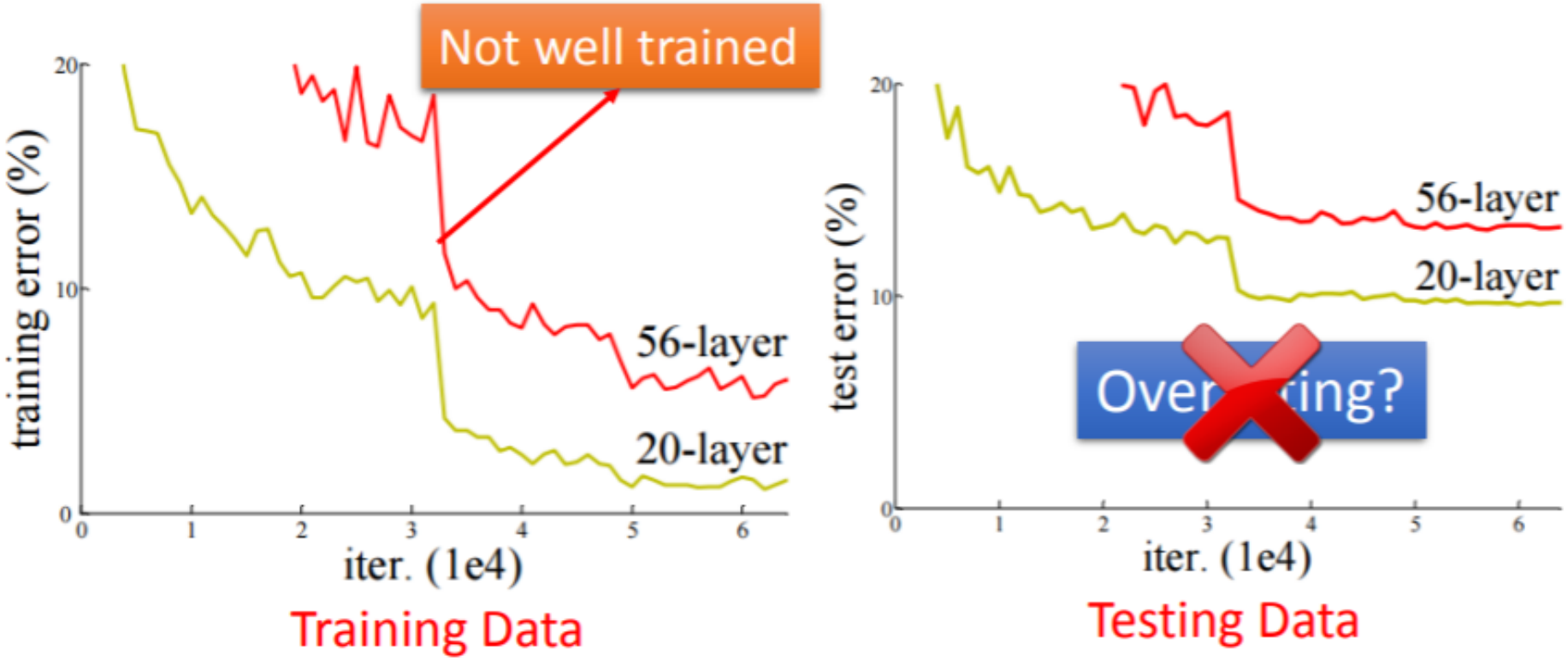
	Training	Testing
1	31.9	35.0
2	15.4	18.4
3	15.3	18.1
4	14.9	28.2
5	12.8	232.1

A more complex model does not always lead to better performance on ***testing data***.

This is ***Overfitting***. → Select suitable model

Reference: 李弘毅 ML Lecture 1 https://youtu.be/CXgbekl66jc

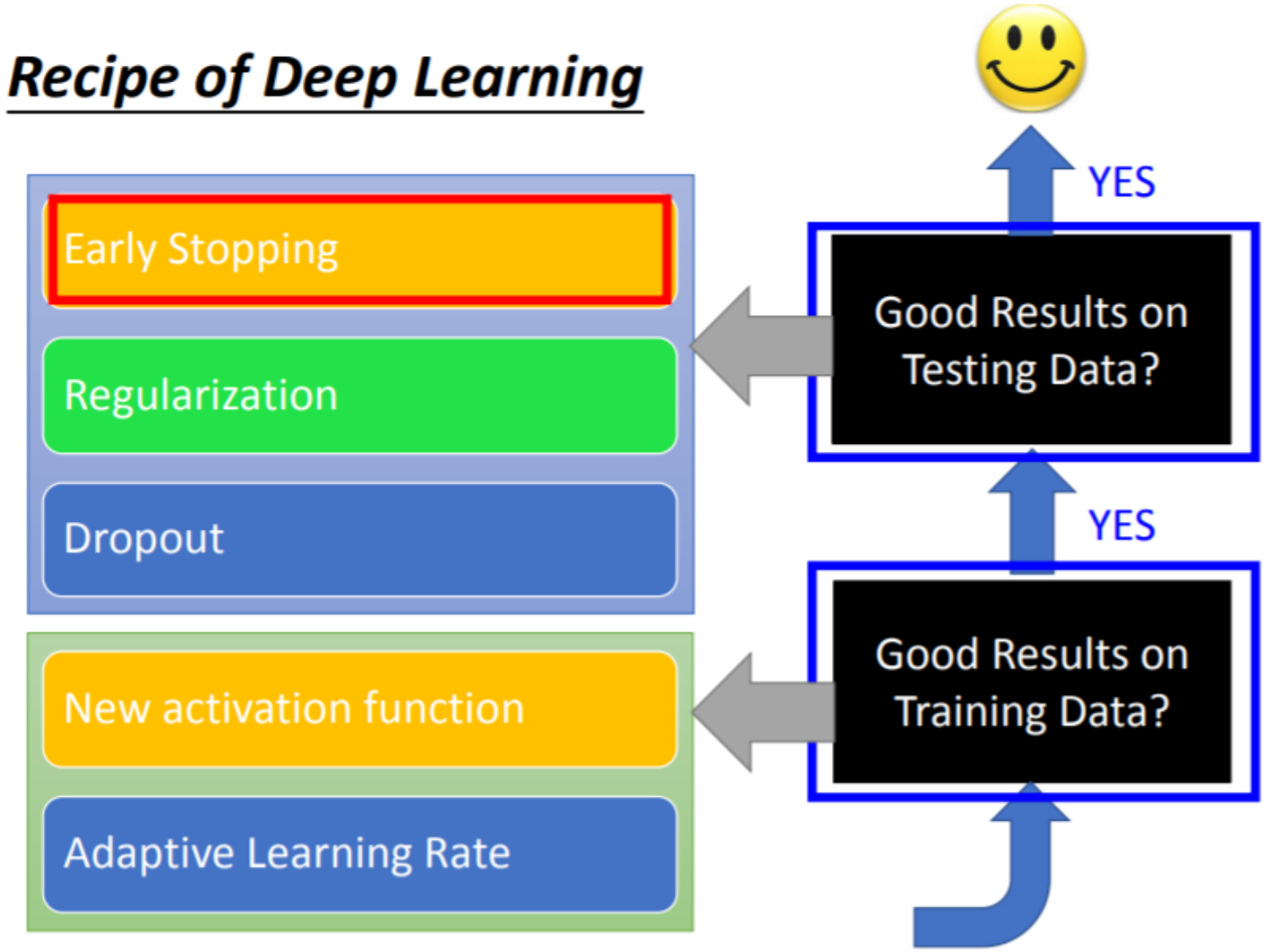
Do not always blame overfitting



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

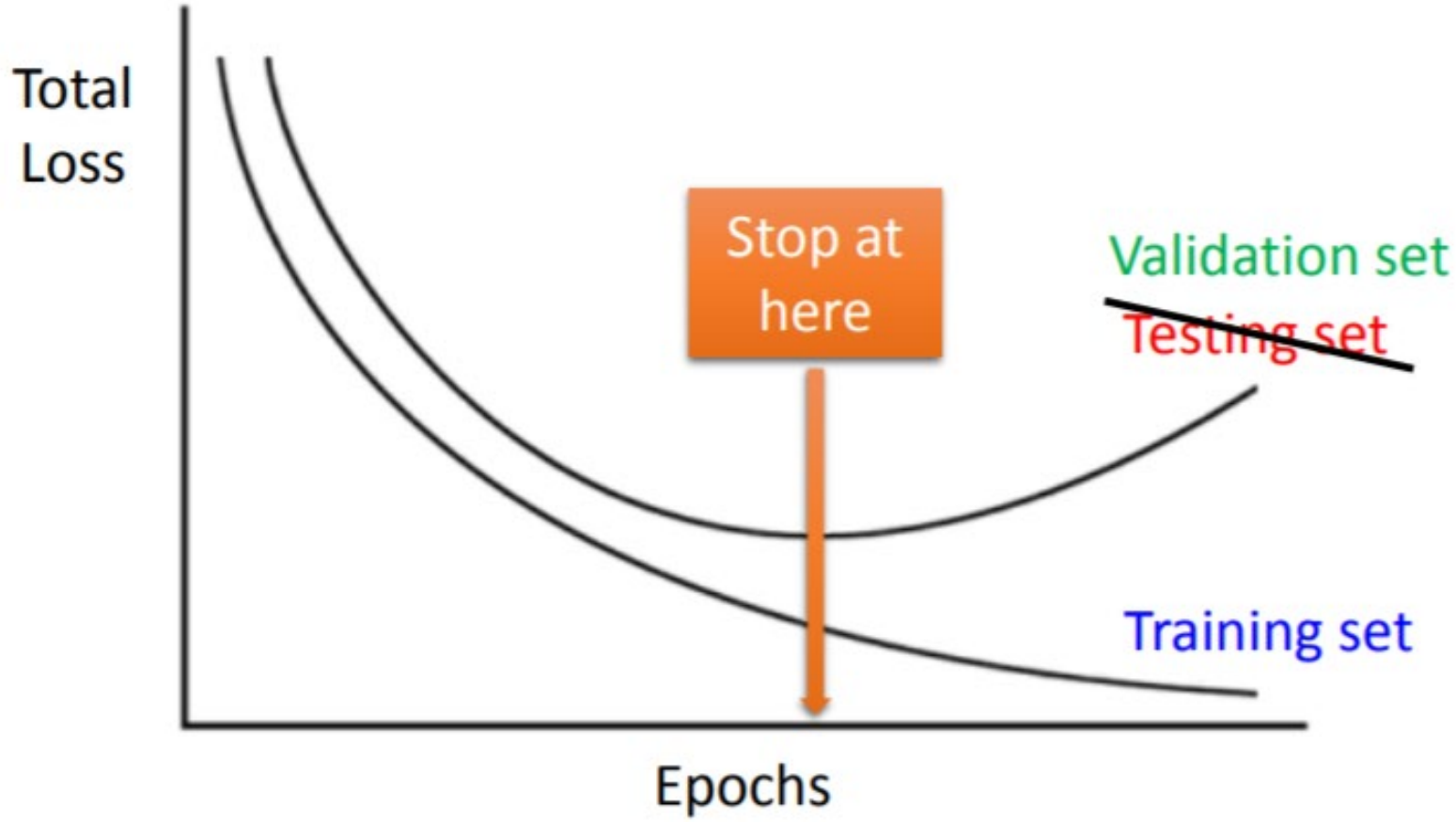
Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

What to do if overfitting?



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

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

Practice – Early stop

- Run "1. 2.3. Early stop.ipynb", observe how the overfitting problem is reduced.

HW3 (3)

- Implement early stop in "HW3.ipynb" and study whether the overfitting problem can be reduced.

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

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

Original loss
(e.g. minimize square error, cross entropy …)

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

L2 regularization

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

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

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

Practice – L2 regularization

- Run "1. 2.3. L2_Regularization.ipynb", observe the overfitting problem.

HW3 (4)

- Apply L2 regularization in "HW3.ipynb" and study whether the overfitting problem can be reduced.

L1 regularization

L1 regularization:

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

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

Update:

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

$$= w^t - \eta \frac{\partial L}{\partial w} - \eta\lambda \,\mathrm{sgn}\left(w^t\right)$$ 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

Practice – L1 regularization

- Run "1. 2.3. L1_Regularization.ipynb", observe the overfitting problem.

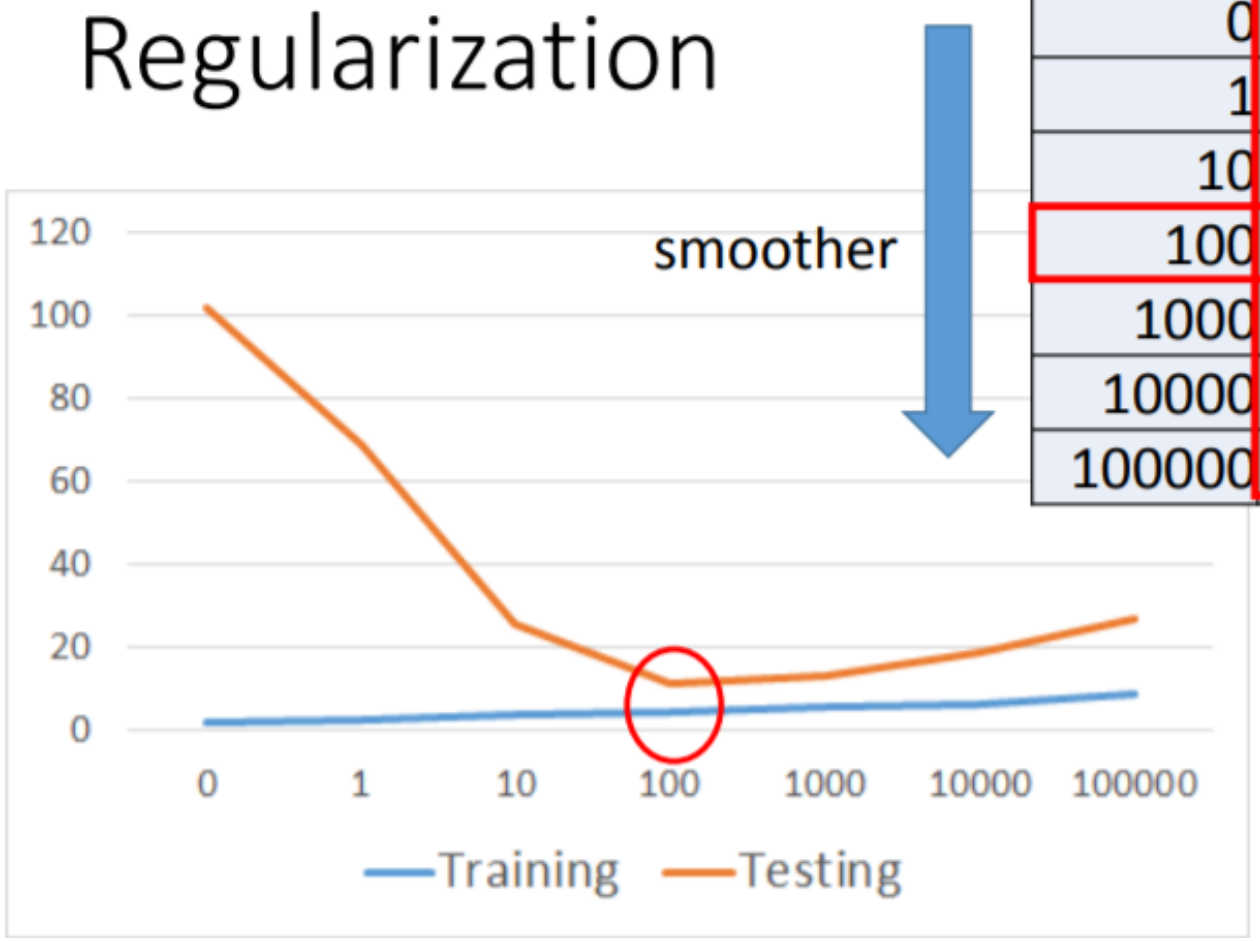
HW3 (5)

- Apply L1 regularization in "HW3.ipynb" and study whether the overfitting problem can be reduced.

Practice – Regularization with small initial weights

- Run "1. 2.3. Initialize_small_weights.ipynb". By initializing NN weight using small values we can also do regularization.

Regularization



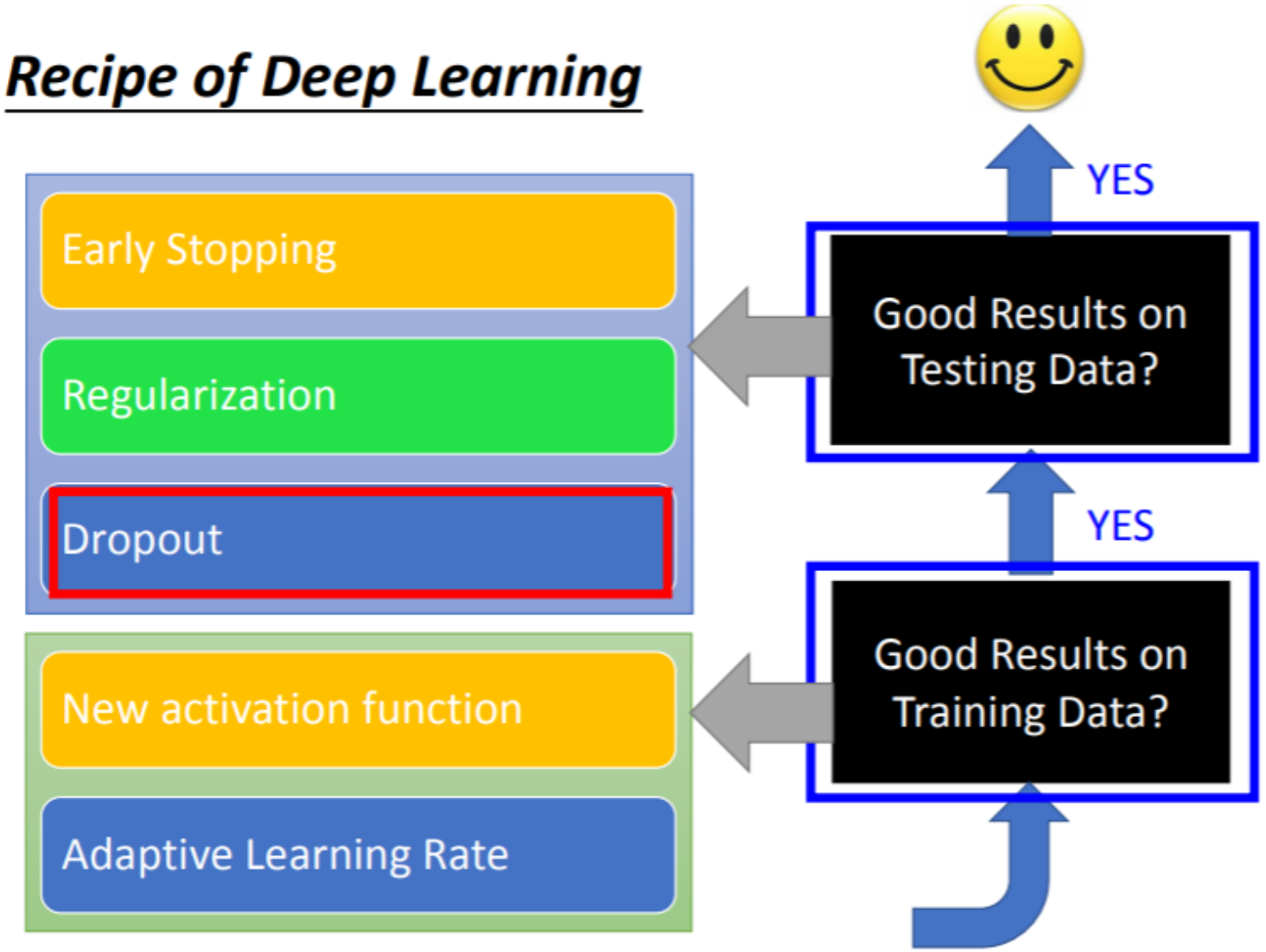
λ	Training	Testing
0	1.9	102.3
1	2.3	68.7
10	3.5	25.7
100	4.1	11.1
1000	5.6	12.8
10000	6.3	18.7
100000	8.5	26.8

How smooth?

Select λ obtaining the best model

Reference: 李弘毅 ML Lecture 1 https://youtu.be/CXgbekl66jc

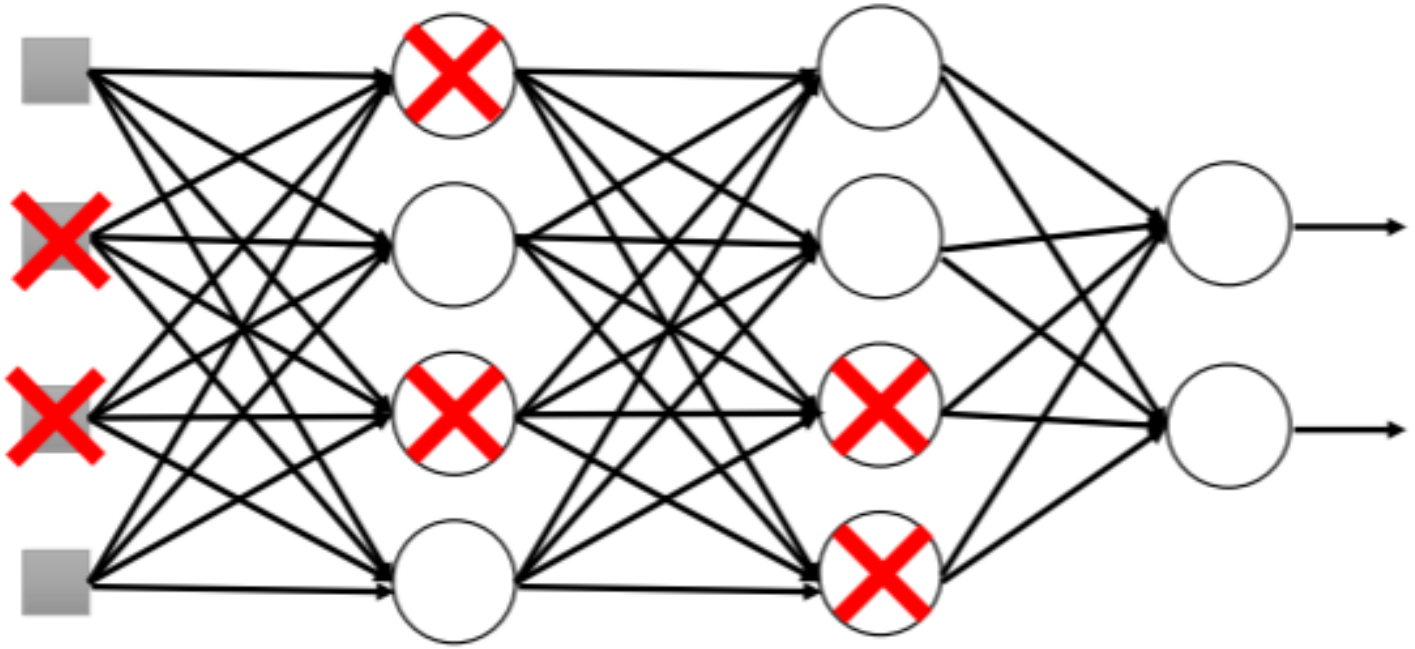
Drop out



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

Drop out

Training:

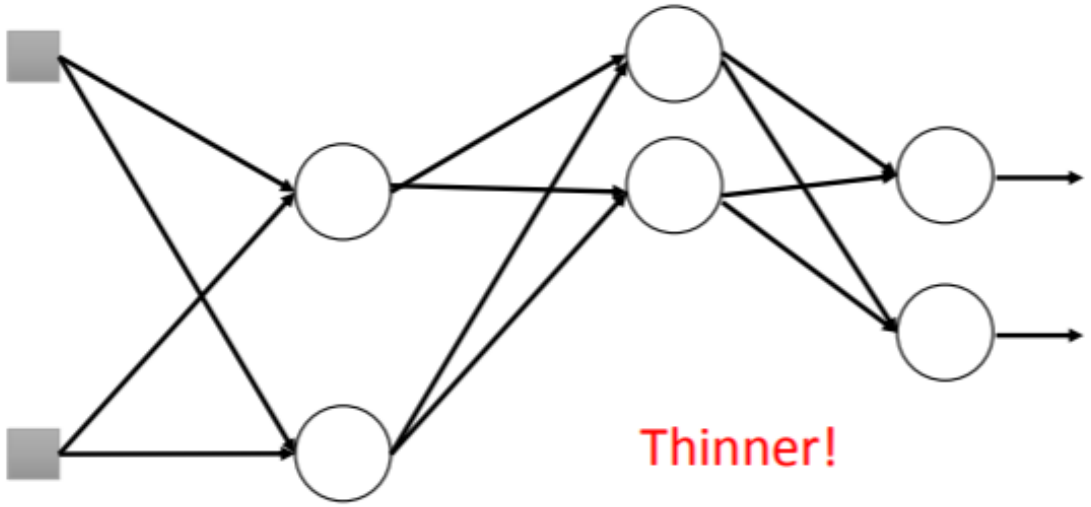


- **Each time before updating the parameters**
  - Each neuron has p% to dropout

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

Drop out

Training:



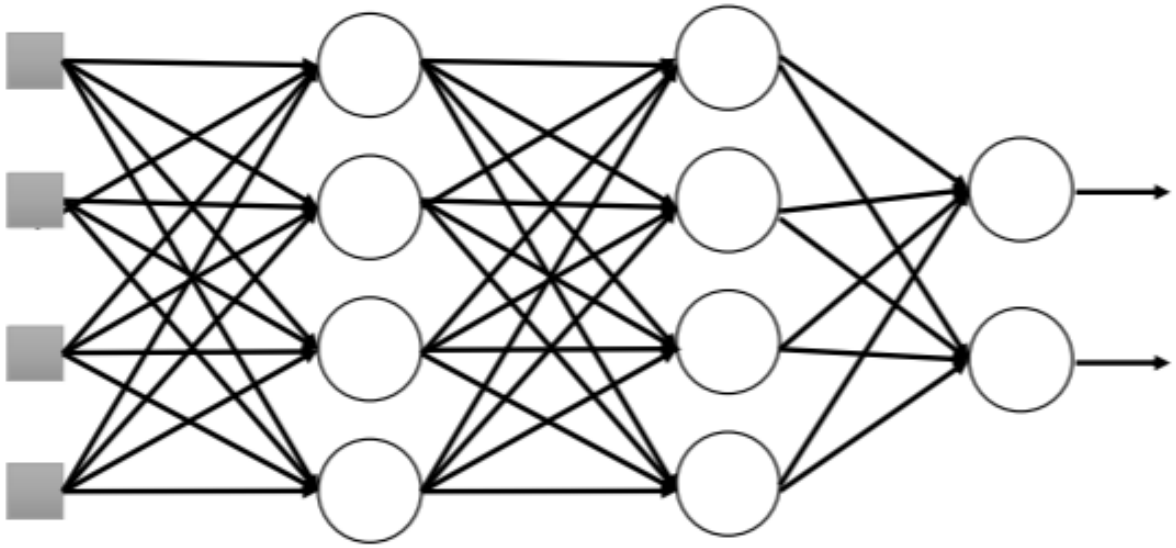
- **Each time before updating the parameters**
  - Each neuron has p% to dropout
    - **The structure of the network is changed.**
  - Using the new network for training

For each mini-batch, we resample the dropout neurons

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

Drop out

Testing:



- **No dropout**
  - If the dropout rate at training is p%, all the weights times 1-p%
  - Assume that the dropout rate is 50%. If a weight $w = 1$ by training, set $w = 0.5$ for testing.

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

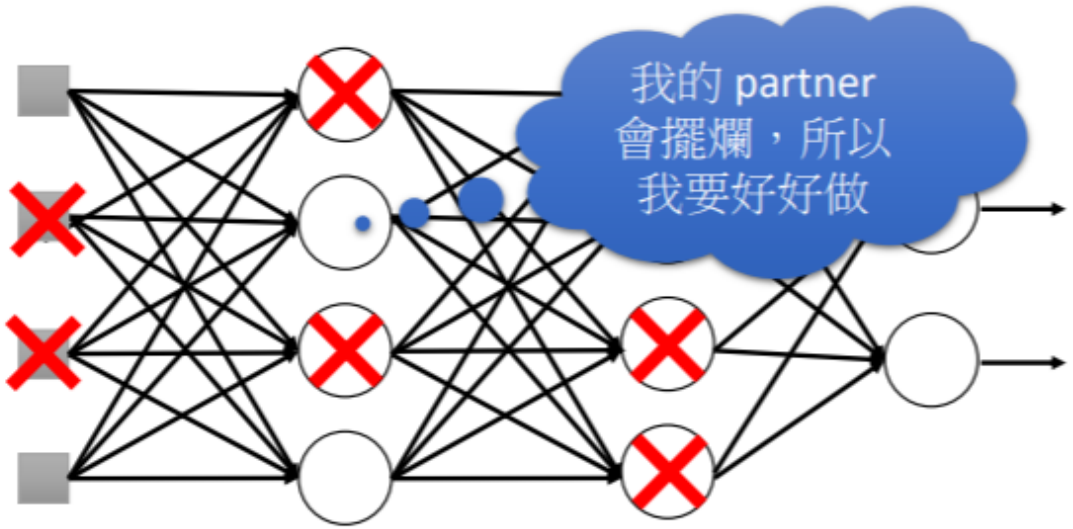
Practice – Drop out

- Run “1. 2.3. Dropout.ipynb” .

HW3 (6)

- Apply drop out to the neural network in "HW3.ipynb" and study whether the overfitting problem can be reduced.

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.

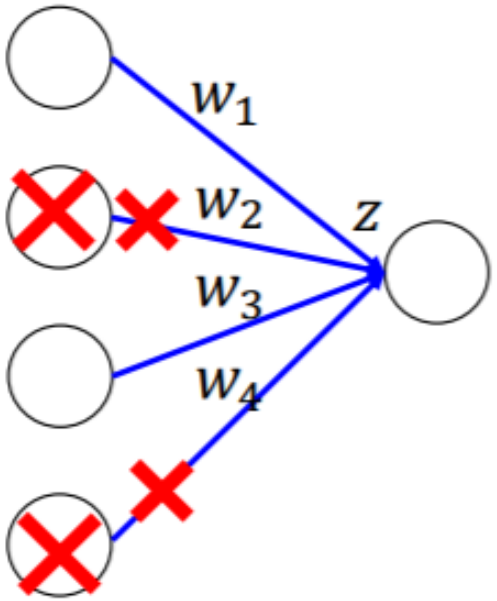
Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

Why 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%

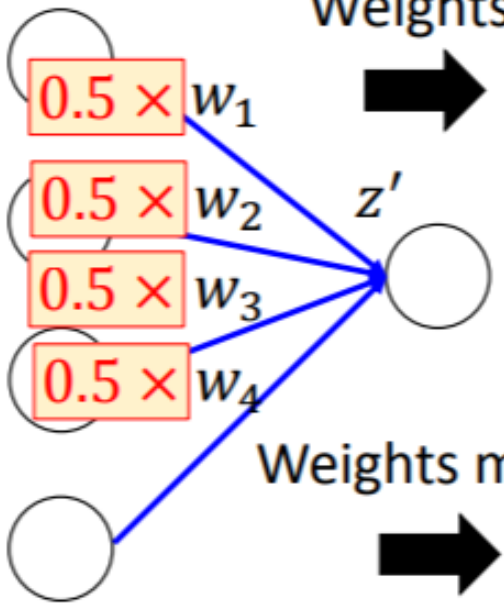


Testing of Dropout

No dropout

Weights from training

$z' \approx 2z$

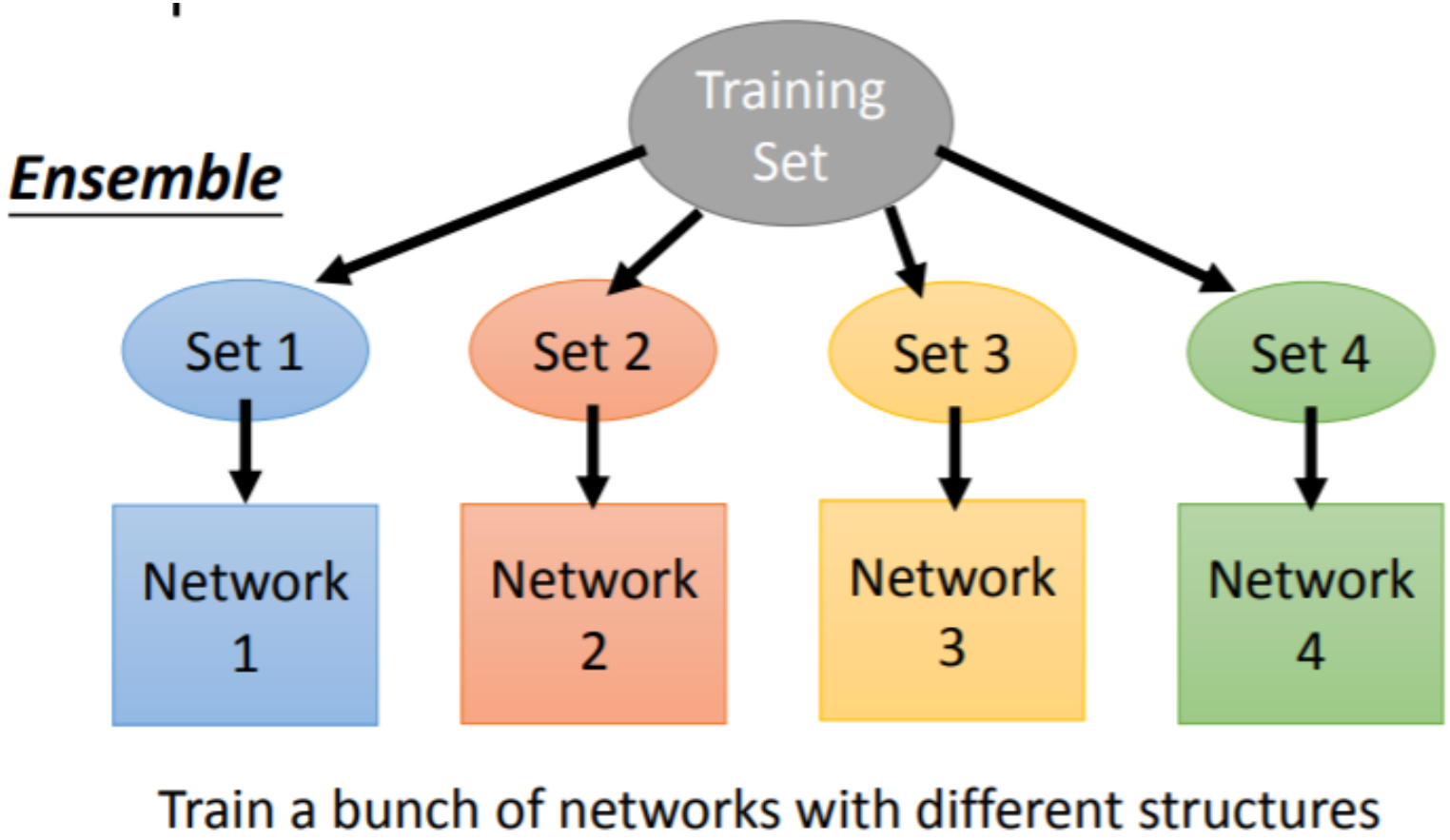


Weights multiply 1-p%

$z' \approx z$

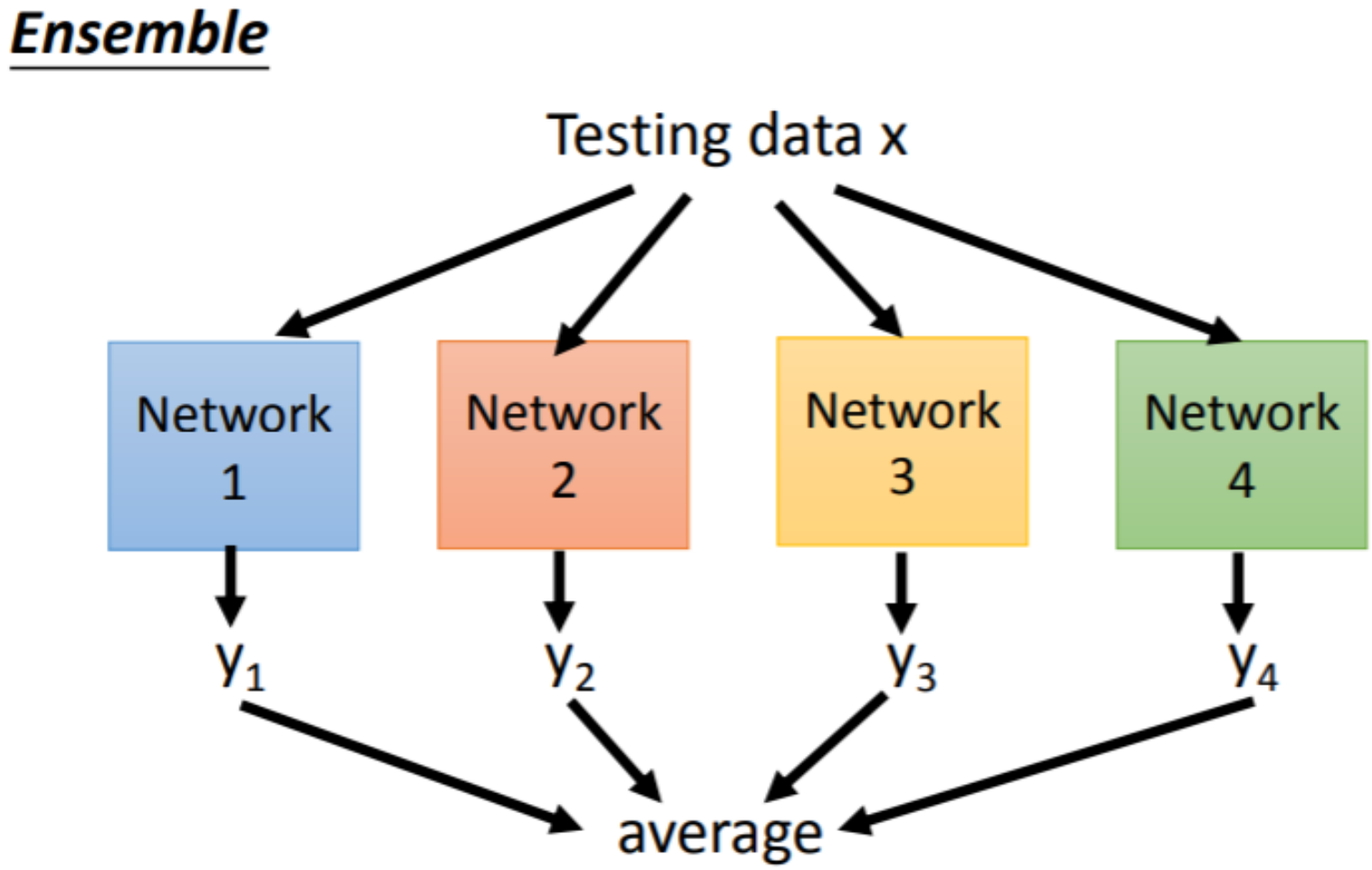
Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

Why drop out makes NN performs better?



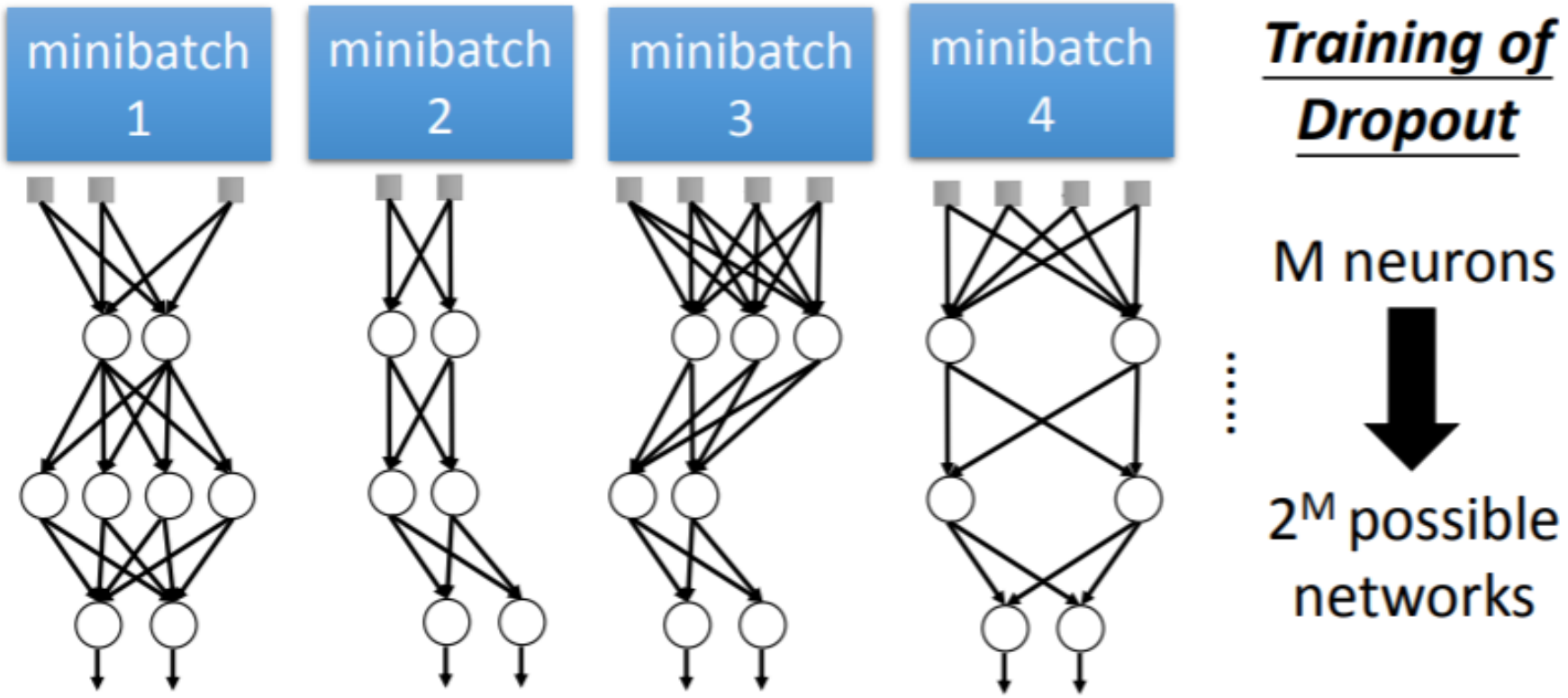
Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

Why drop out makes NN performs better?



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

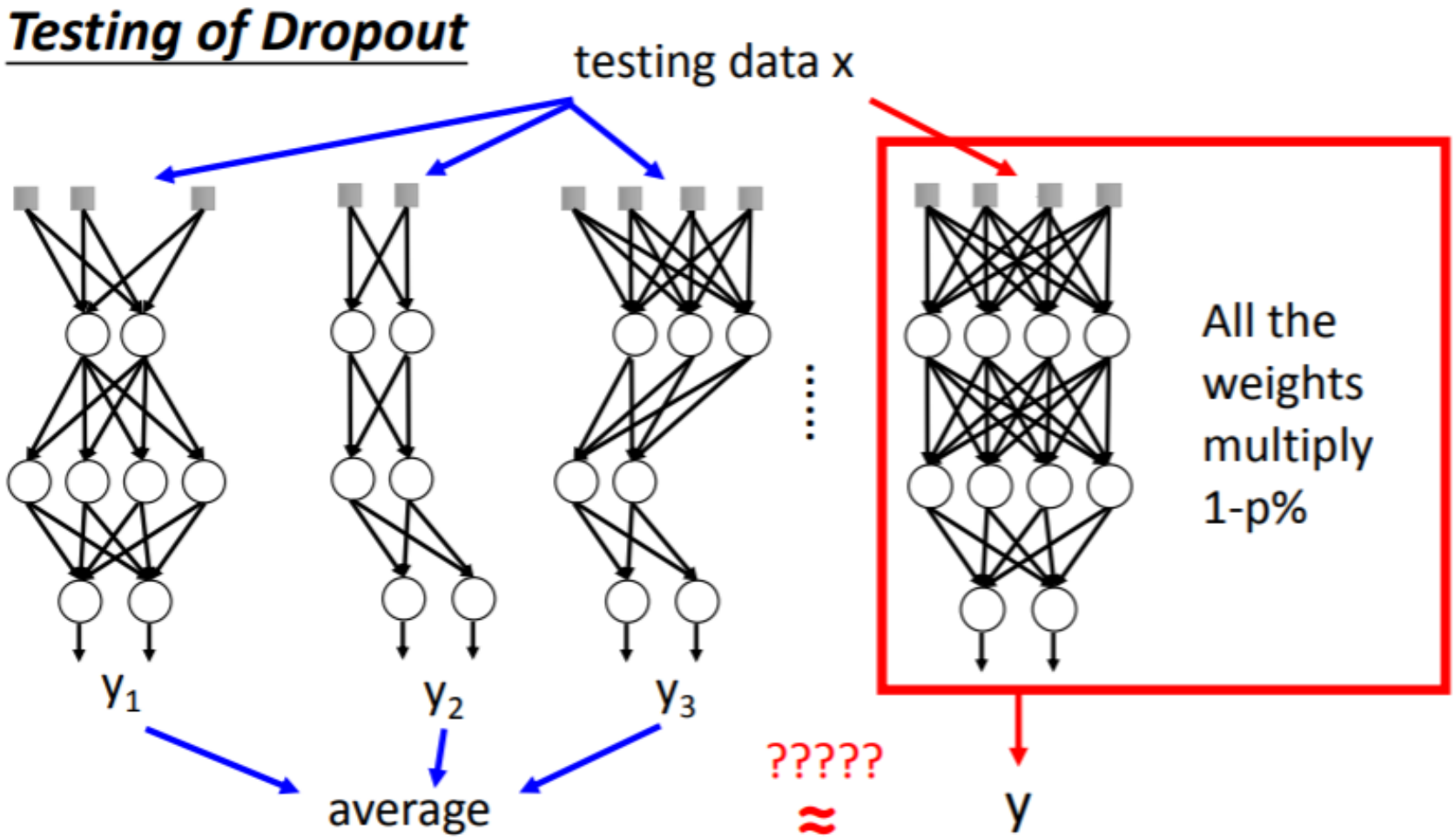
Why drop out makes NN performs better?



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

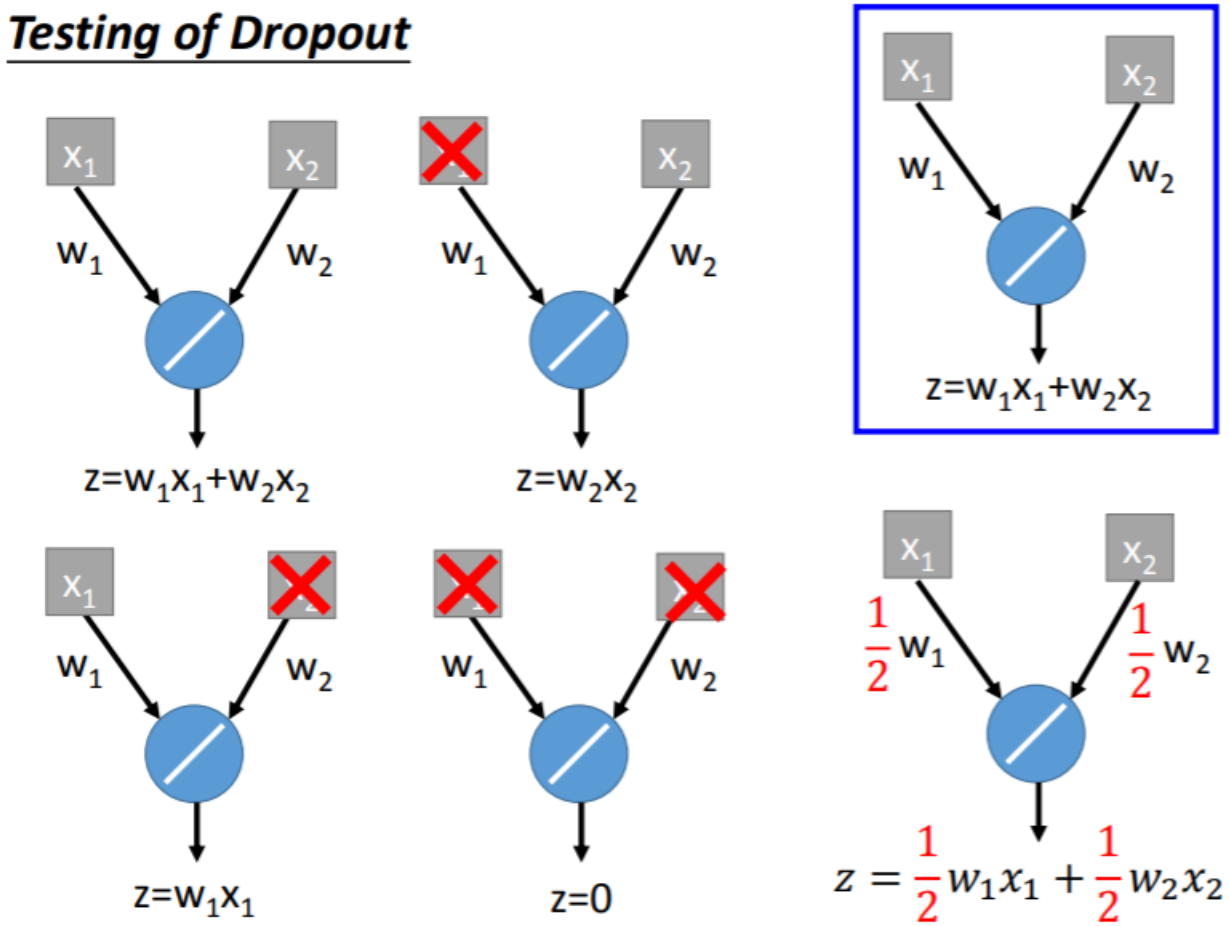
Reference: 李弘毅 ML Lecture 9-1 https://youtu.be/xki61j7z-30

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



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

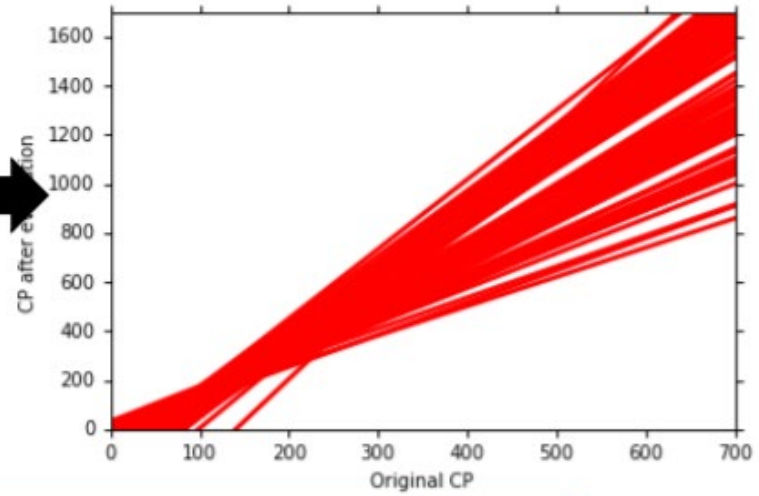
Errors of ML models

ML models learned from training data will have bias and variances

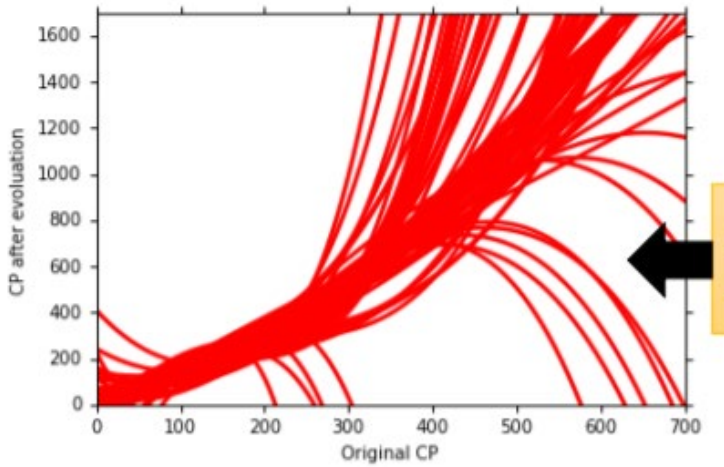
Variances of ML models

Each model is learned from 100 sampled data.

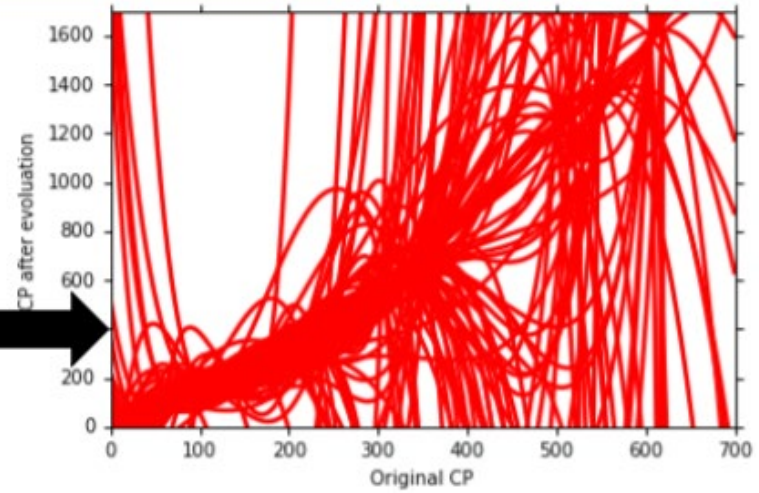
$y = b + w \cdot x_{cp}$



$y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2 + w_3 \cdot (x_{cp})^3$

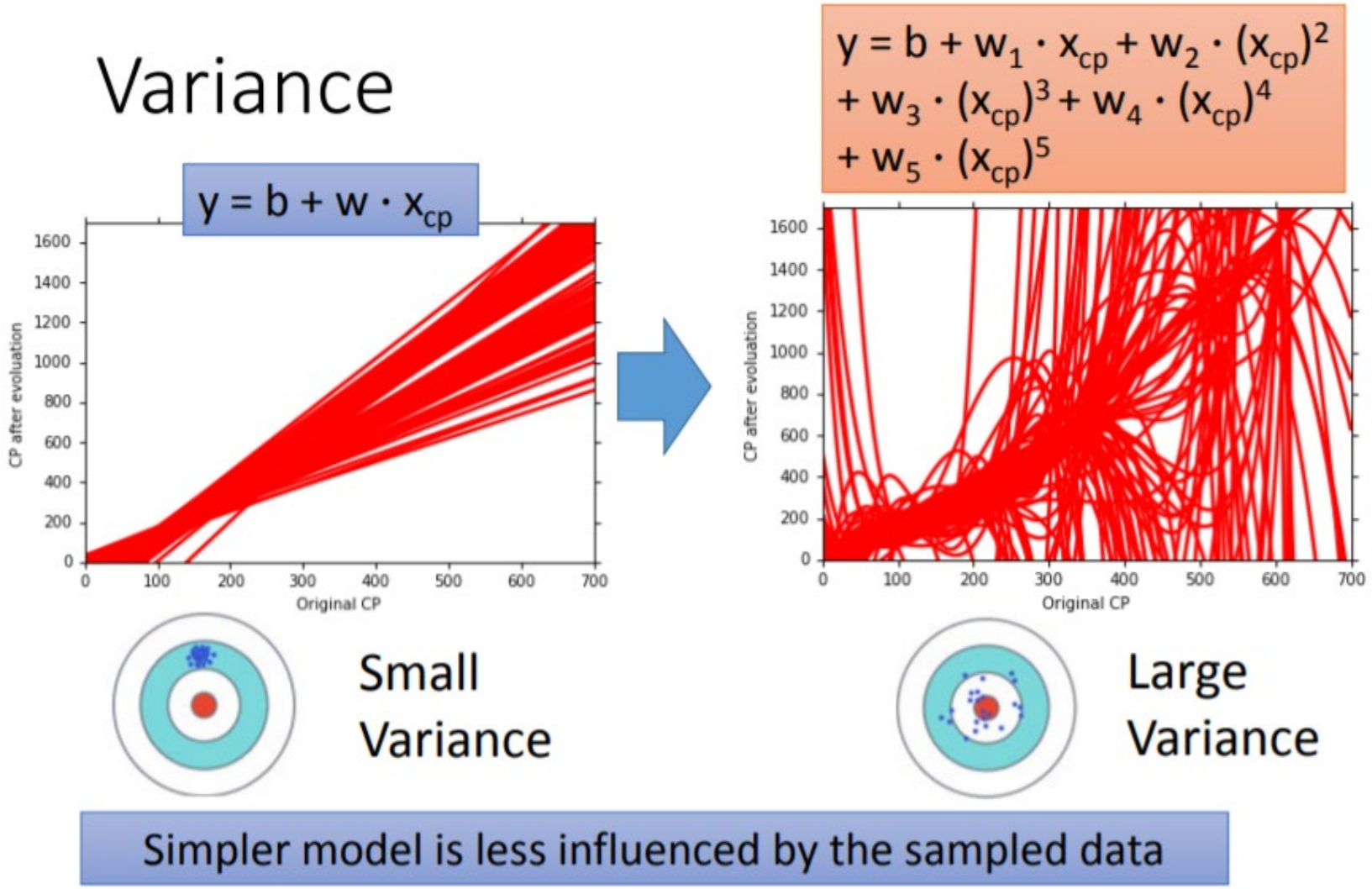


$y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2 + w_3 \cdot (x_{cp})^3 + w_4 \cdot (x_{cp})^4 + w_5 \cdot (x_{cp})^5$



Reference: 李弘毅 ML Lecture 2 https://youtu.be/CXgbekl66jc

Variance of ML models



Reference: 李弘毅 ML Lecture 2 https://youtu.be/CXgbekl66jc

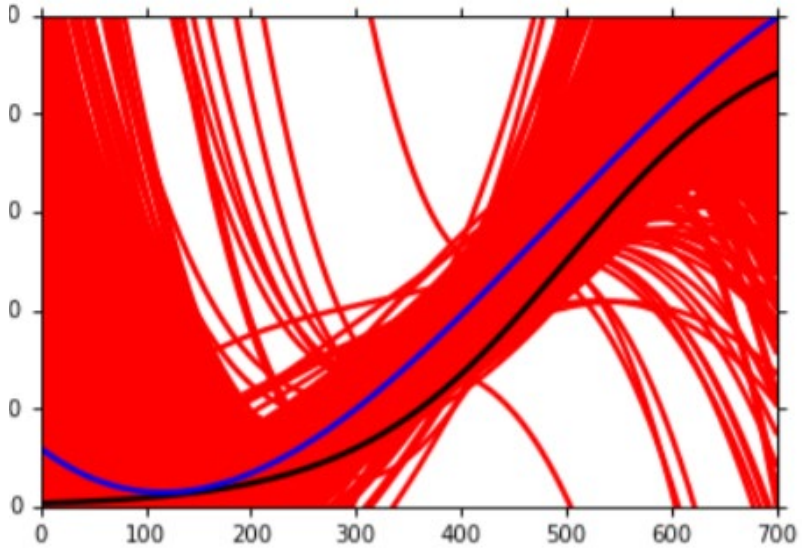
Bias and variance of ML models

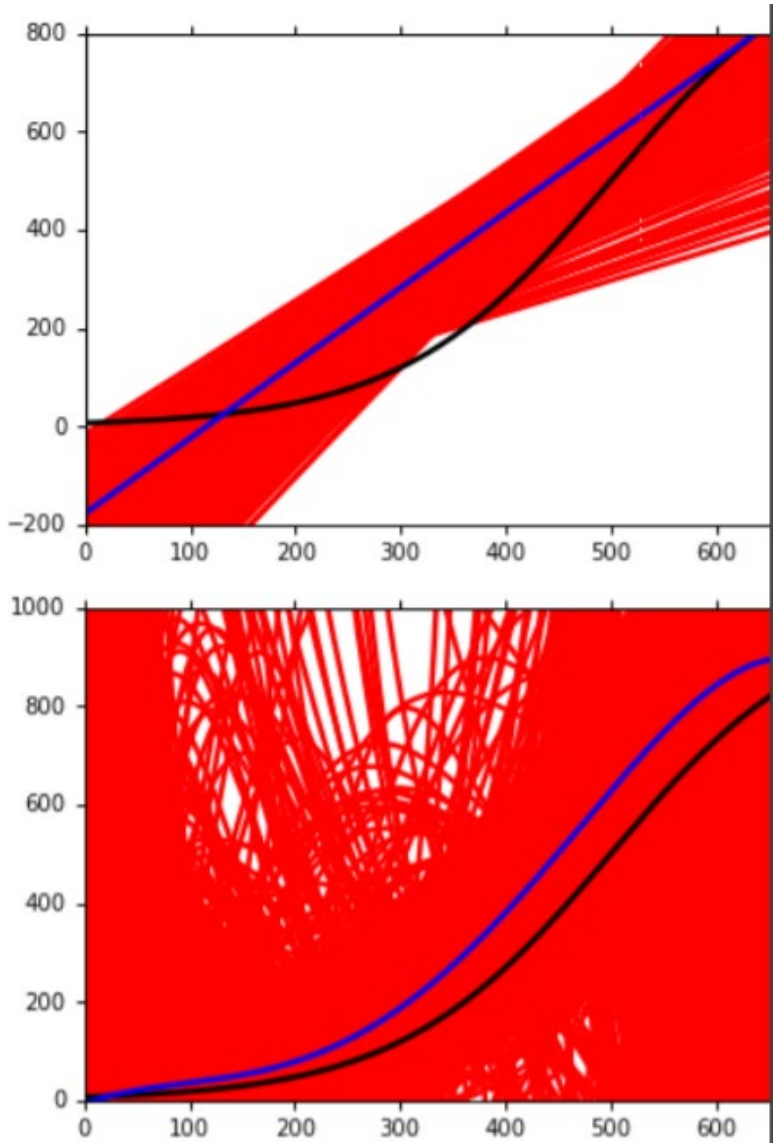
Black curve: the true function $\hat{f}$

Red curves: 5000 f^*

Blue curve: the average of 5000 f^*

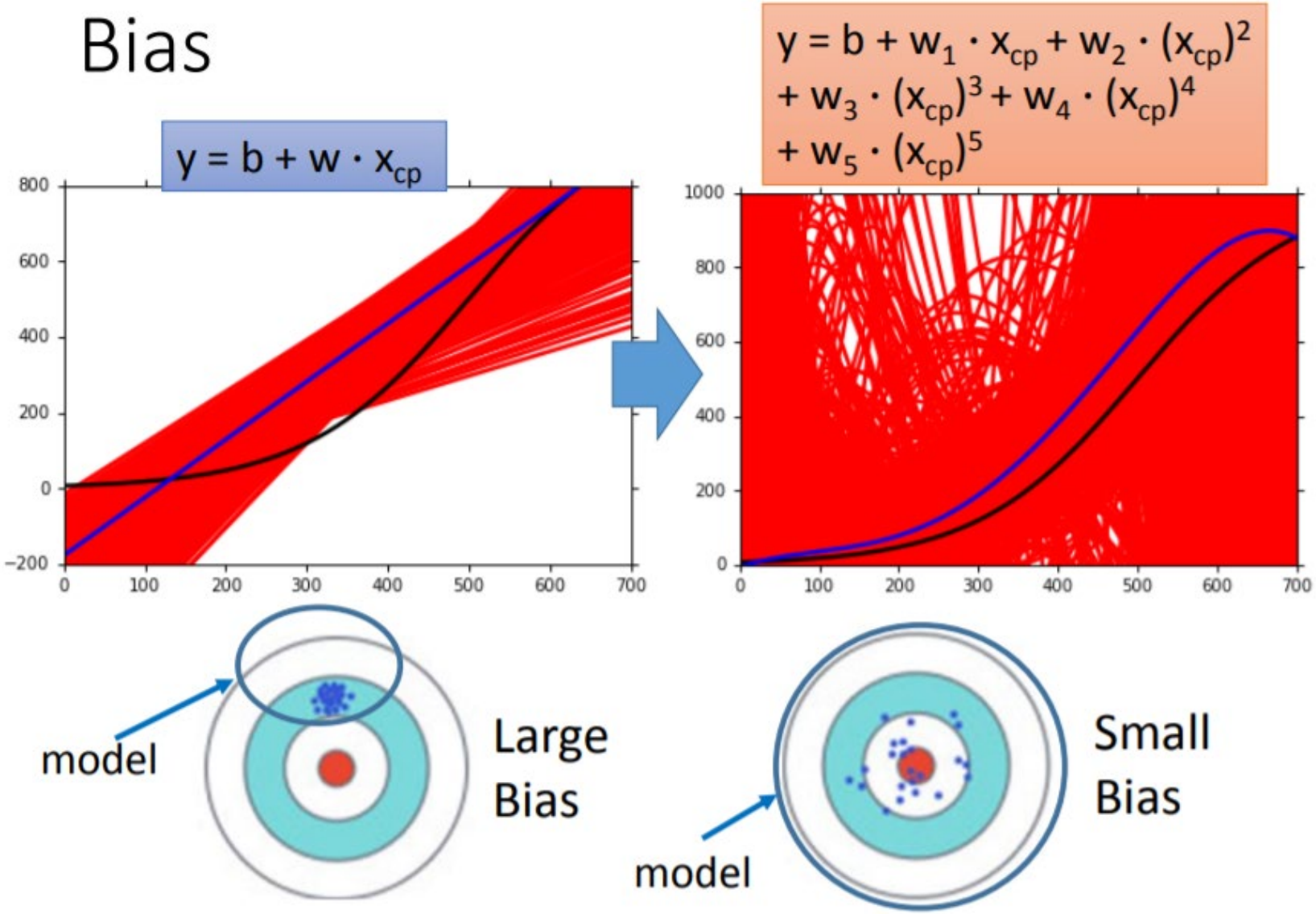
$= \bar{f}$





Reference: 李弘毅 ML Lecture 2 https://youtu.be/CXgbekl66jc

Bias and variance of ML models



Reference: 李弘毅 ML Lecture 2 https://youtu.be/CXgbekl66jc

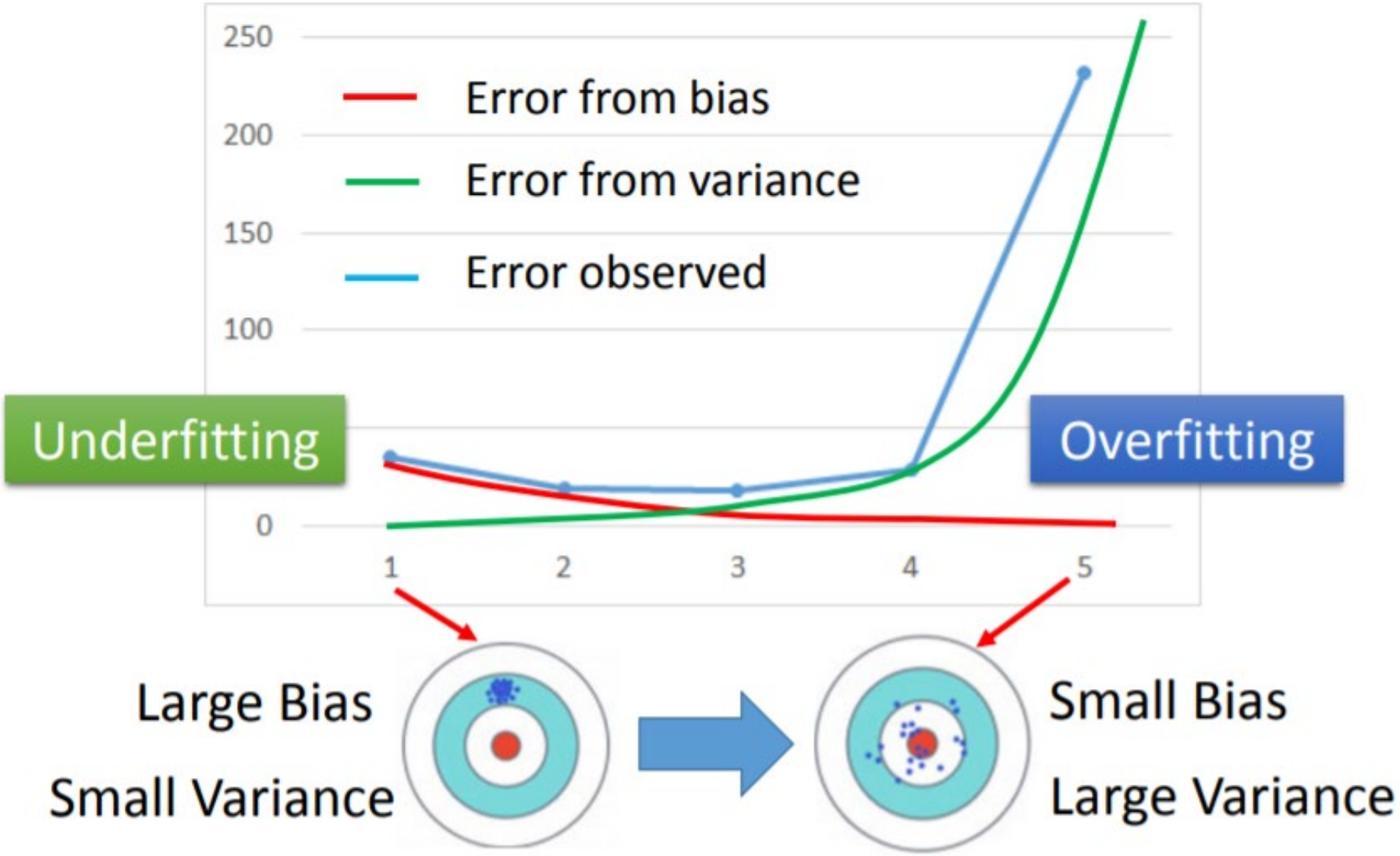
Practice – Variance of model prediction errors

- Run “1. 2.4. Variance of predicting error.ipynb” .

HW3 (7)

- Modify "HW3.ipynb" to study the variance of model prediction errors.

Errors of ML model

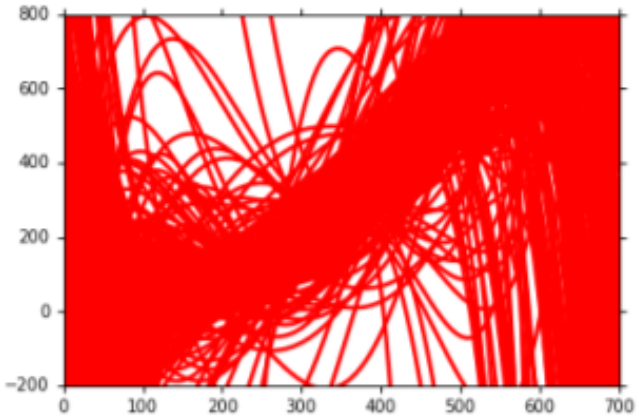


Reference: 李弘毅 ML Lecture 2 https://youtu.be/CXgbekl66jc

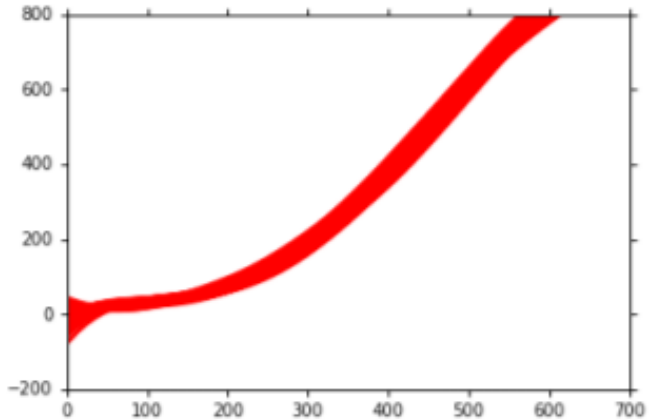
Errors of ML model → Reduce variances

- More data

Very effective, but not always practical

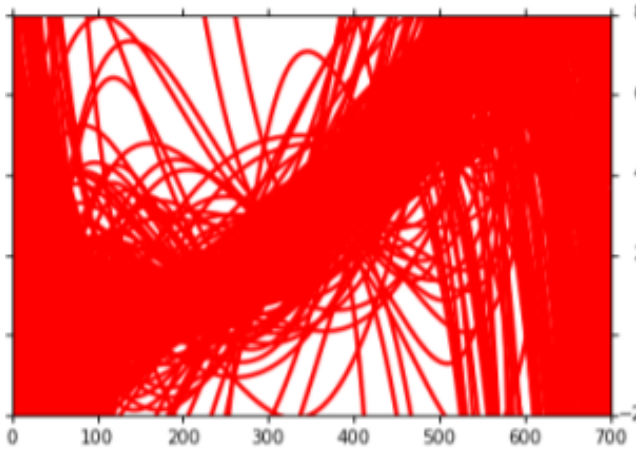


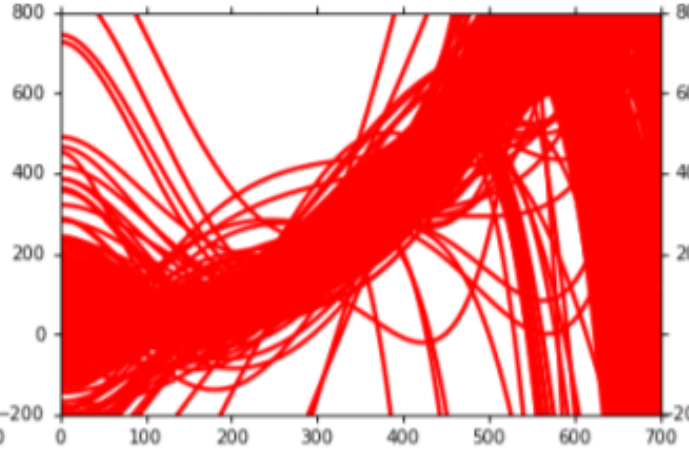
10 examples

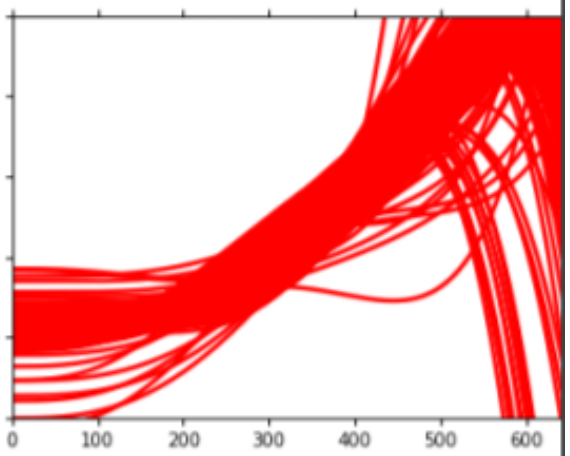


100 examples

- Regularization

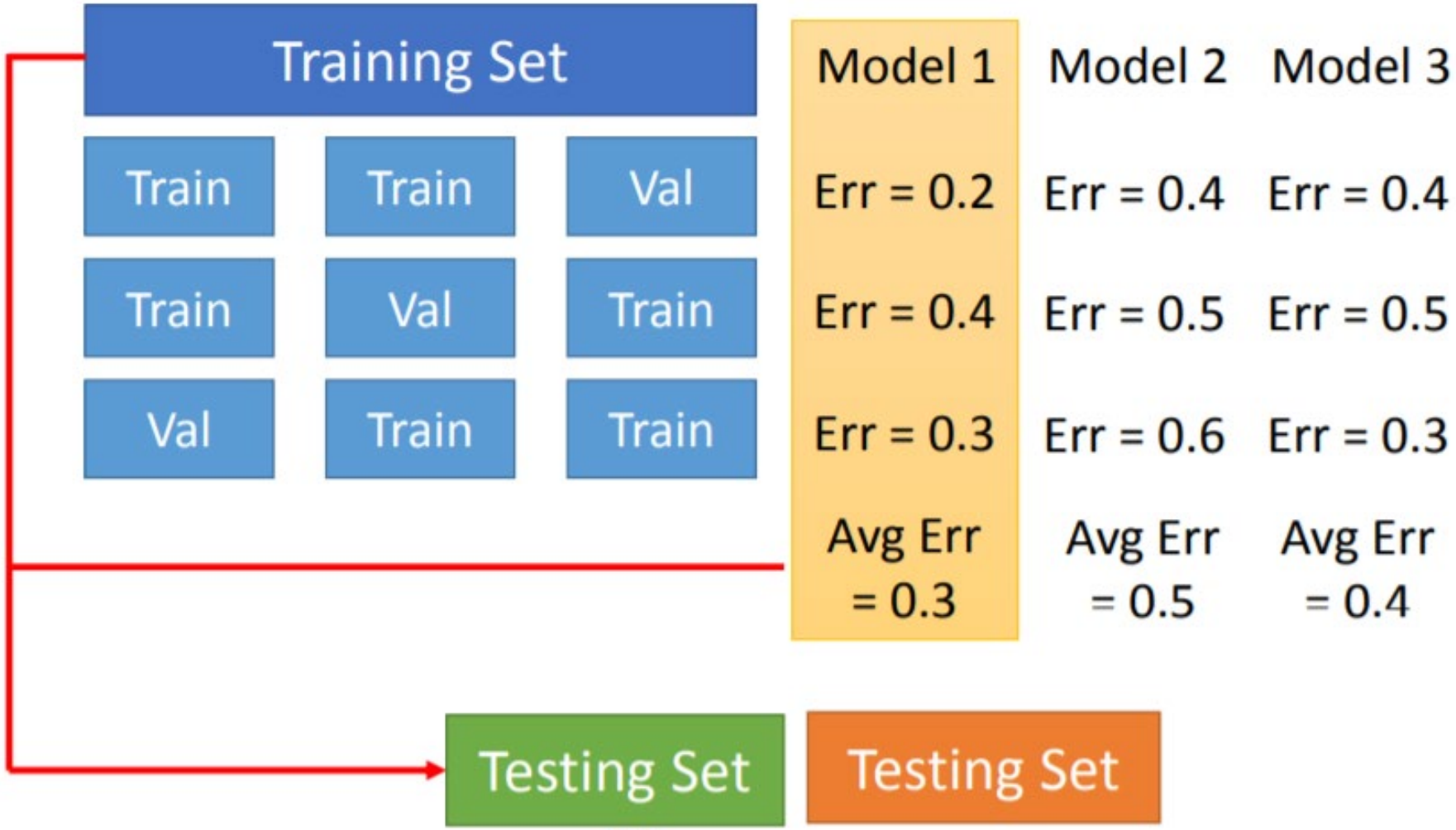






Reference: 李弘毅 ML Lecture 2 https://youtu.be/CXgbekl66jc

Errors of ML model → Cross validation



Reference: 李弘毅 ML Lecture 2 https://youtu.be/CXgbekl66jc