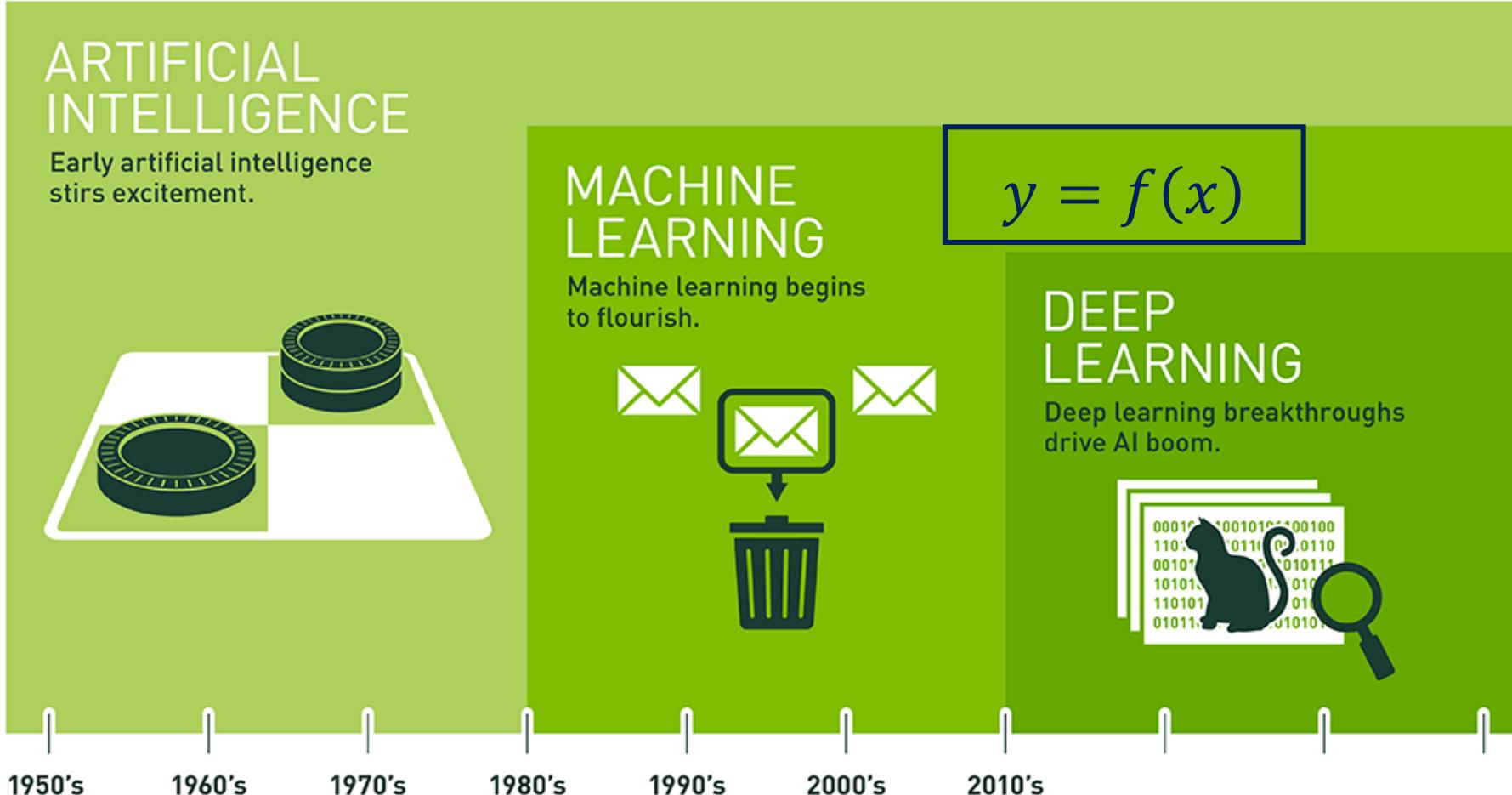


Regression vs Classification

y learned is continuous → Regression
y learned is categorical → Classification



Notations

 x_i

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	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	x_i^n	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

Mechanism for computer to learn 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 $\mathcal{L}(f)$

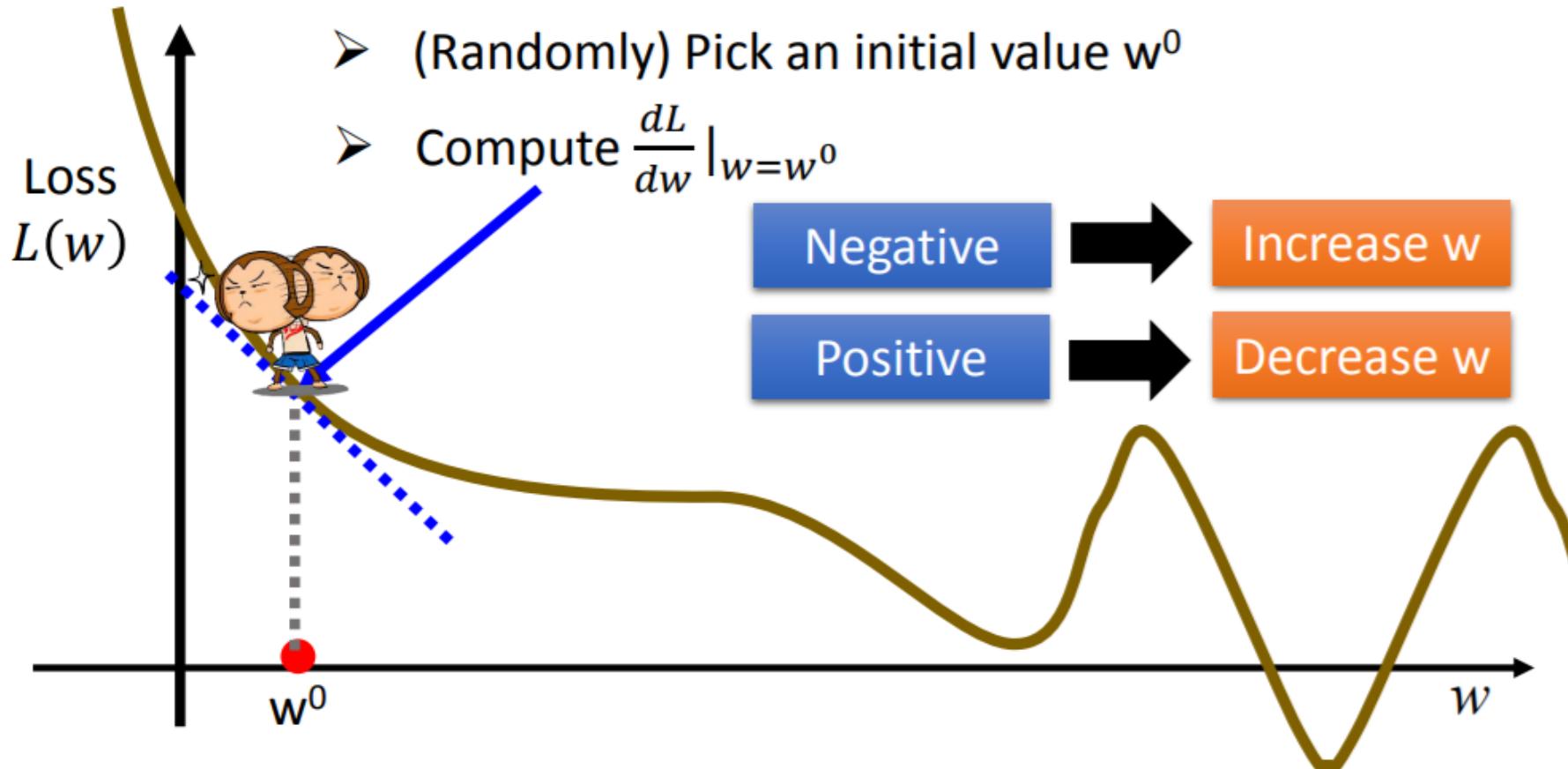
ML model (1) – Linear regression

- 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 optimal parameters

$$w^* = \arg \min_w L(w)$$

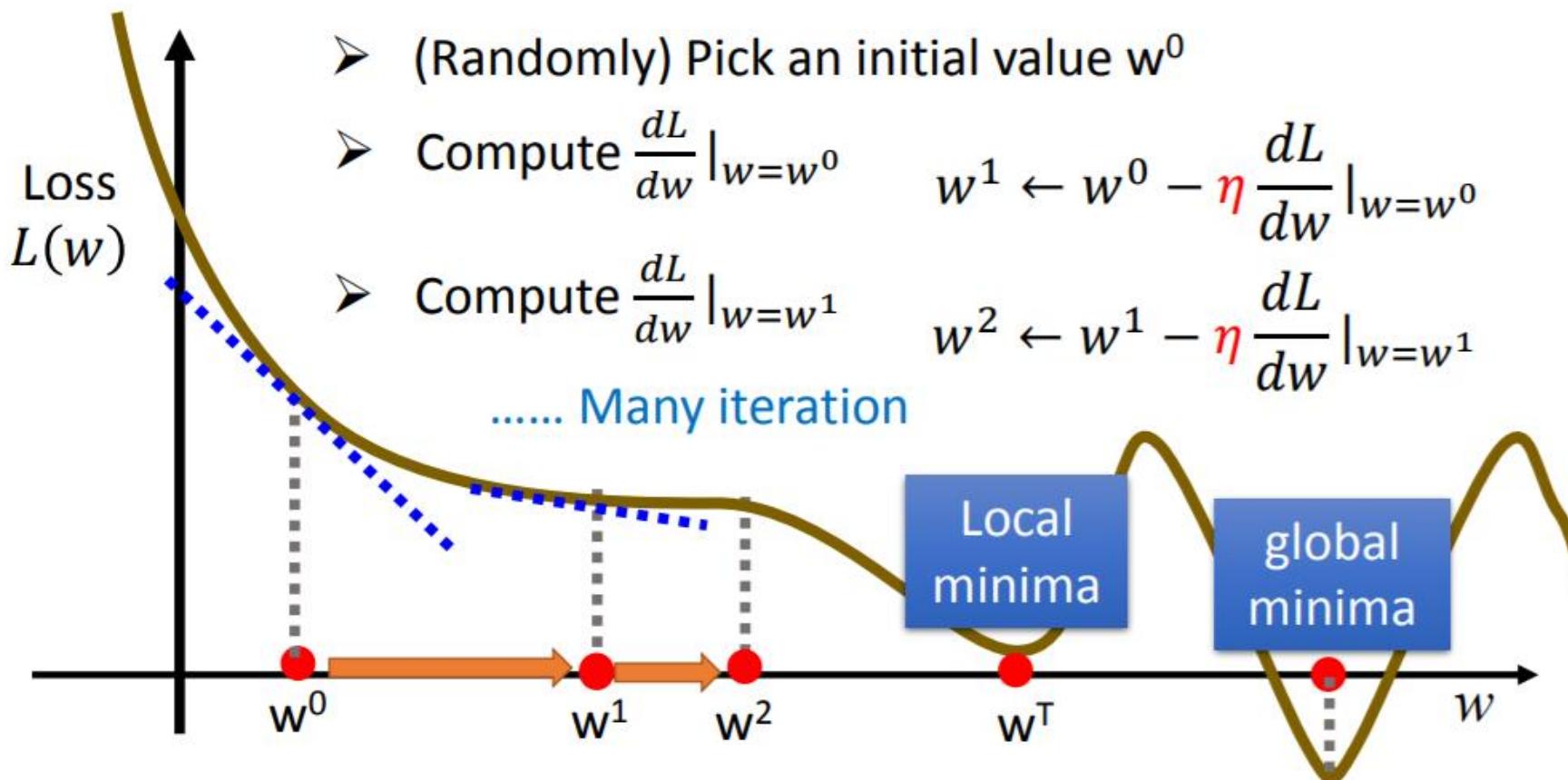
- Consider loss function $L(w)$ with one parameter w :



Gradient decent

$$w^* = \arg \min_w L(w)$$

- Consider loss function $L(w)$ with one parameter w :



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 $\frac{\partial L}{\partial w} |_{w=w^0, b=b^0}, \frac{\partial L}{\partial b} |_{w=w^0, b=b^0}$

$$\left[\begin{array}{c} \frac{\partial L}{\partial w} \\ \frac{\partial L}{\partial b} \end{array} \right] \text{gradient}$$

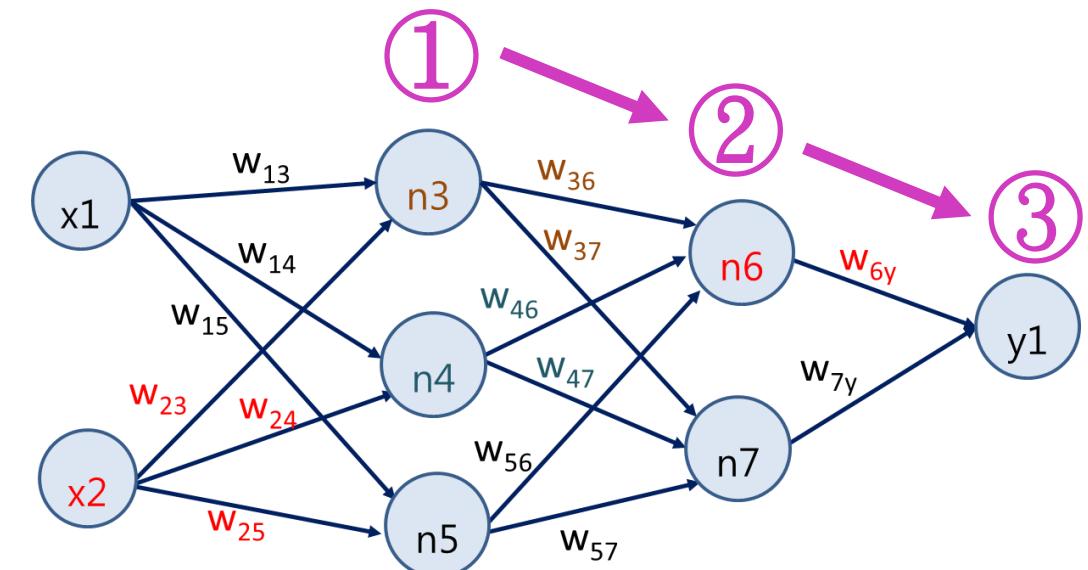
$$w^1 \leftarrow w^0 - \eta \frac{\partial L}{\partial w} |_{w=w^0, b=b^0} \quad b^1 \leftarrow b^0 - \eta \frac{\partial L}{\partial b} |_{w=w^0, b=b^0}$$

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

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

Machine learning model (2) – Deep learning

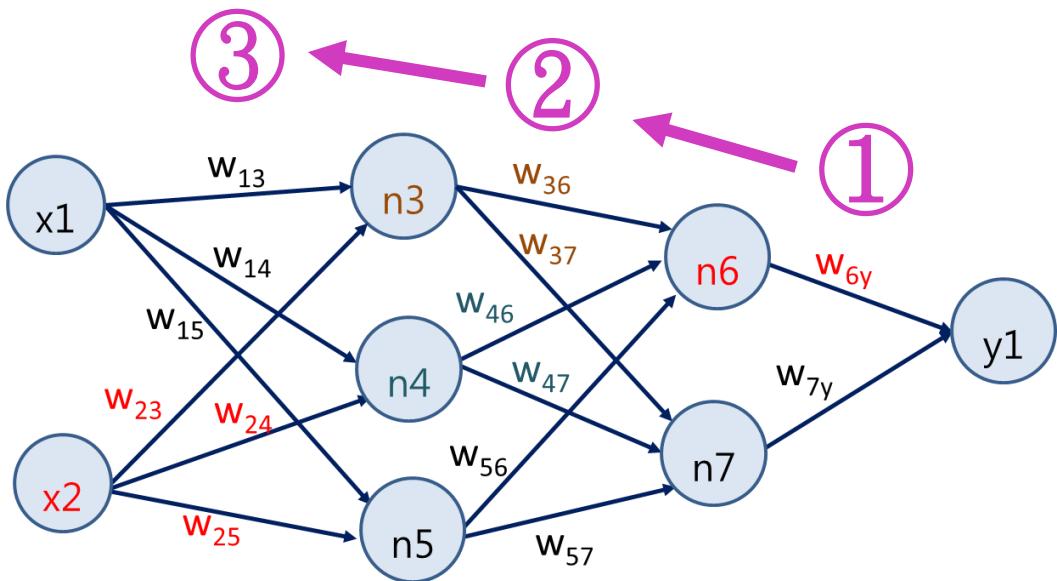
Define a function to be learned: $y^n = f(x^n)$



- ① $n_3 = \sigma(x_1 * w_{13} + x_2 * w_{23} + b_3)$
 $n_4 = \sigma(x_1 * w_{14} + x_2 * w_{24} + b_4)$
 $n_5 = \sigma(x_1 * w_{15} + x_2 * w_{25} + b_5)$
- ② $n_6 = \sigma(n_3 * w_{36} + n_4 * w_{46} + n_5 * w_{56} + b_6)$
 $n_7 = \sigma(n_3 * w_{37} + n_4 * w_{47} + n_5 * w_{57} + b_7)$
- ③ $y_1 = \sigma(n_6 * w_{6y} + n_7 * w_{7y} + b_y)$

Machine learning model (2) – Deep learning

Use gradient decent to find optimal parameters



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

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

① $w_{6y} \leftarrow w_{6y} - \eta \frac{\partial L}{\partial w_{6y}} \quad \frac{\partial L}{\partial w_{6y}} = \frac{\partial L}{\partial y} \frac{\partial y}{\partial w_{6y}}$

② $w_{7y} \leftarrow w_{7y} - \eta \frac{\partial L}{\partial w_{7y}} \quad \frac{\partial L}{\partial w_{7y}} = \frac{\partial L}{\partial y} \frac{\partial y}{\partial w_{7y}}$

③ $w_{57} \leftarrow w_{57} - \eta \frac{\partial L}{\partial w_{57}} \quad \frac{\partial L}{\partial w_{57}} = \frac{\partial L}{\partial y} \frac{\partial y}{\partial n_7} \frac{\partial n_7}{\partial w_{57}}$

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

Jeffery Hinton



Geoffrey Hinton spent 30 years hammering away at an idea most other scientists dismissed as nonsense. Then, one day in 2012, he was proven right. Canada's most influential thinker in the field of artificial intelligence is far too classy to say I told you so

<https://torontolife.com/tech/ai-superstars-google-facebook-apple-studied-guy/>

For more than 30 years, Geoffrey Hinton hovered at the edges of artificial intelligence research, an outsider clinging to a simple proposition: that computers could think like humans do—using intuition rather than rules.

Geoffrey Hinton 多年來堅持着一個簡單的觀點：電腦可以像人類一樣思考-用直覺而不是規則。Hinton 一直好奇的是，電腦能不能像人類大腦一樣的工作：信息通過一個巨大的，由神經元圖譜連接起來的細胞網絡傳播，在多達十億條的路徑上發射、連接和傳輸。

Practice – MLP regression

The screenshot shows a Google Colaboratory interface with a modal dialog for GitHub integration. The dialog has a yellow header bar with tabs: 範例, 最近, Google 雲端硬碟, GitHub (which is highlighted with a red circle), and 上傳. Below the tabs is a search bar labeled "輸入 GitHub 網址或依機構或使用者搜尋" and a checkbox for "包括私人存放區". The main area displays a list of GitHub repositories under the heading "TienLungSun". A red circle highlights the repository "TienLungSun/2020-PyTorch-Colab". Underneath it, there are dropdown menus for "存放區:" (main) and "分支版本:" (main). The list of notebooks includes:

- 1. 1. Understand MLP.ipynb
- 1. 2. MLP regression.ipynb (highlighted with a red circle)
- 1. 3. MLP Classification.ipynb
- 2. 1. Understand CNN.ipynb

At the bottom right of the dialog is a "取消" (Cancel) button.

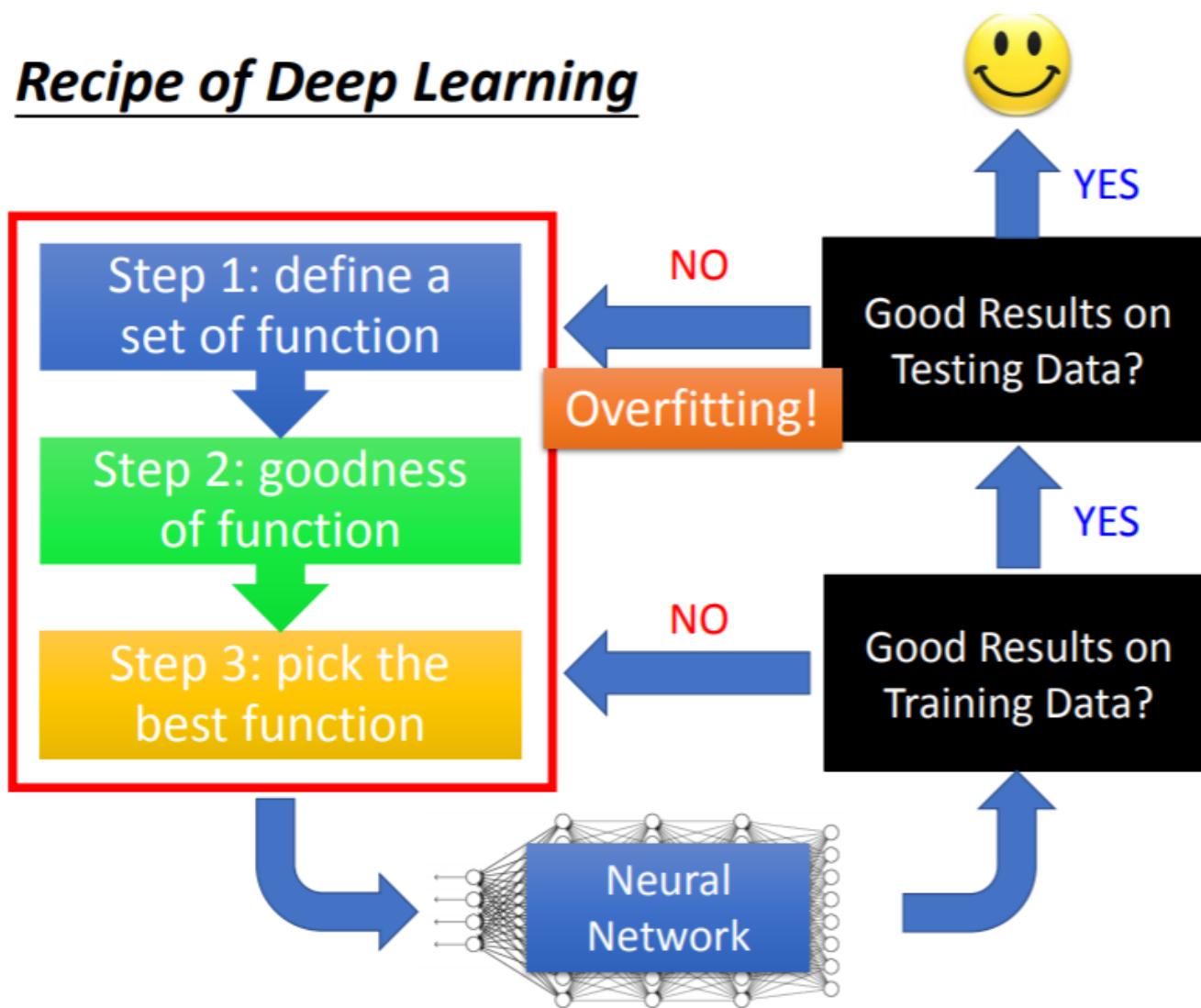
At the very bottom of the screen, there is a taskbar with various icons and a system tray showing the date and time (下午 09:10 2021/2/25).

Practice – Read data from file

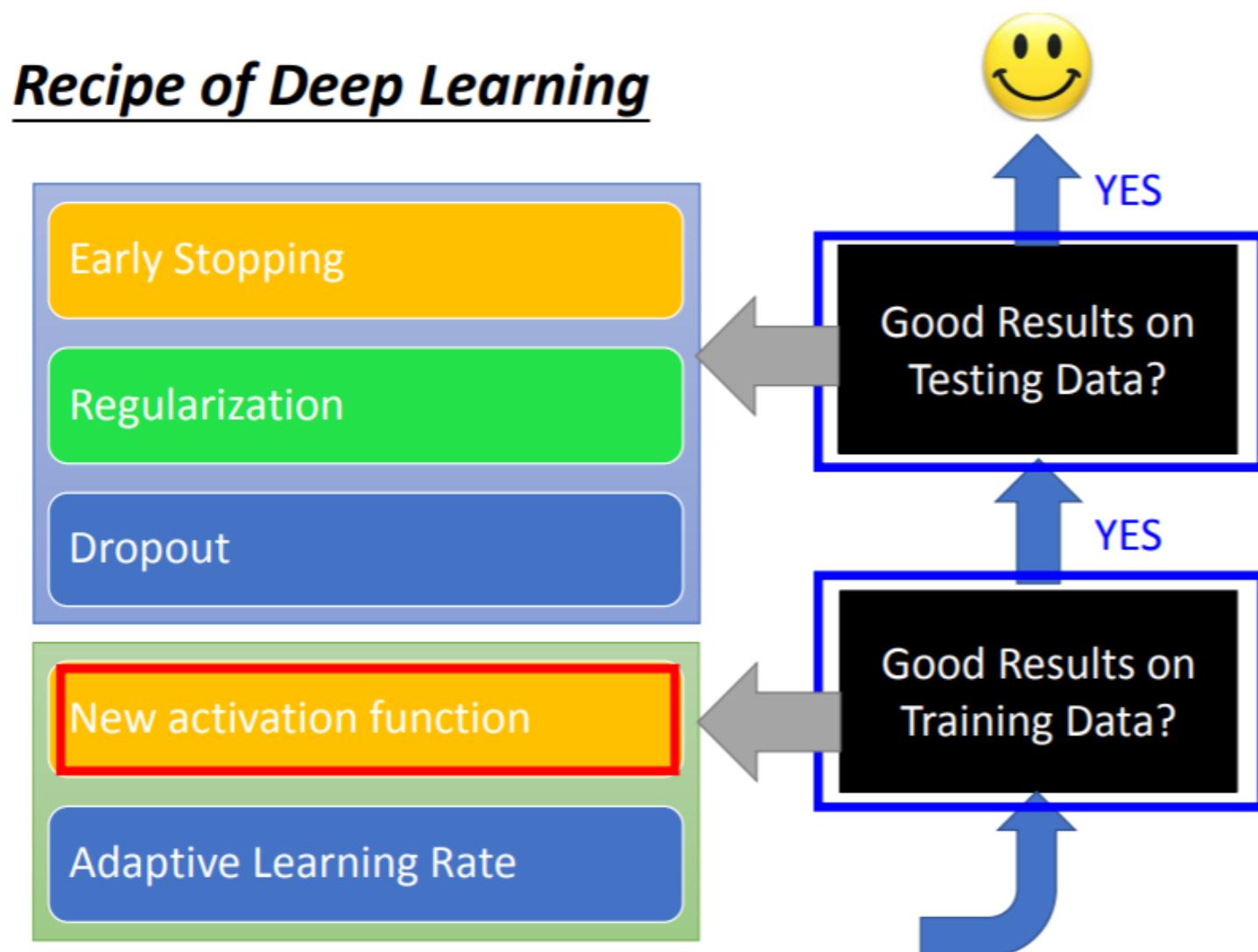
- Run "1. 2. MLP regression (Read Excel data file)"



Recipe of deep learning



When training result is not good

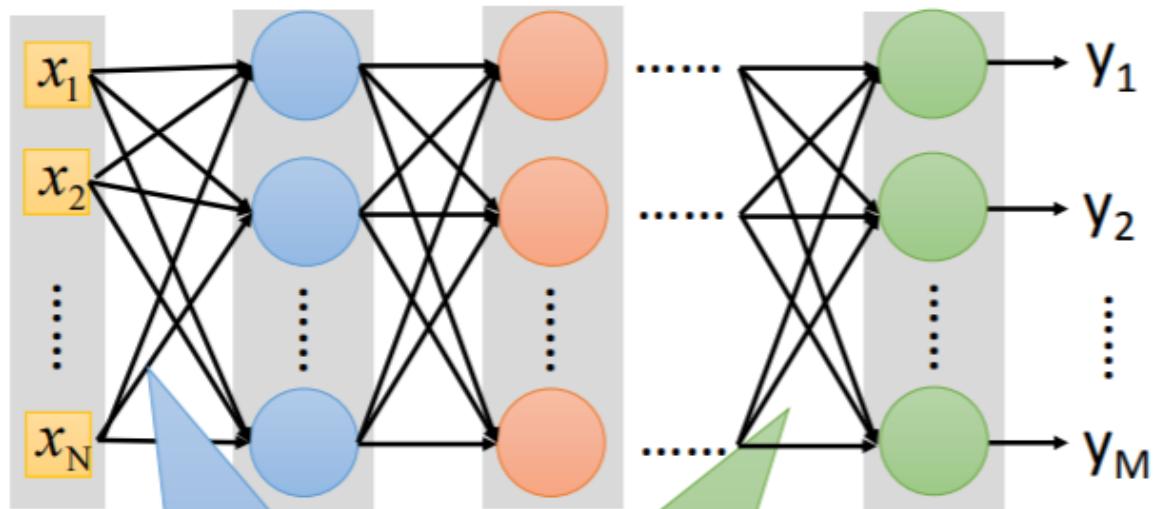


Practice – Activation function

- 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

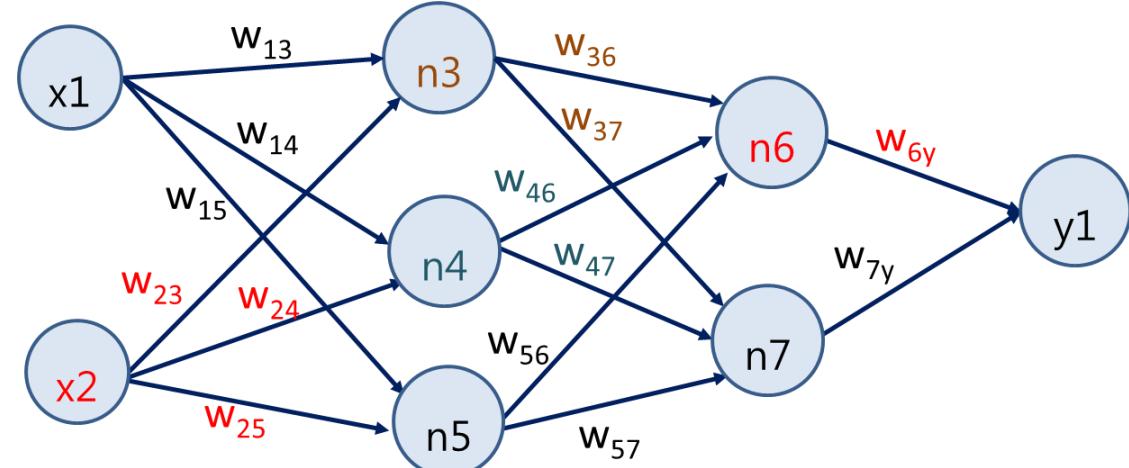
Almost random

Larger gradients

Learn very fast

Already converge

based on random!?

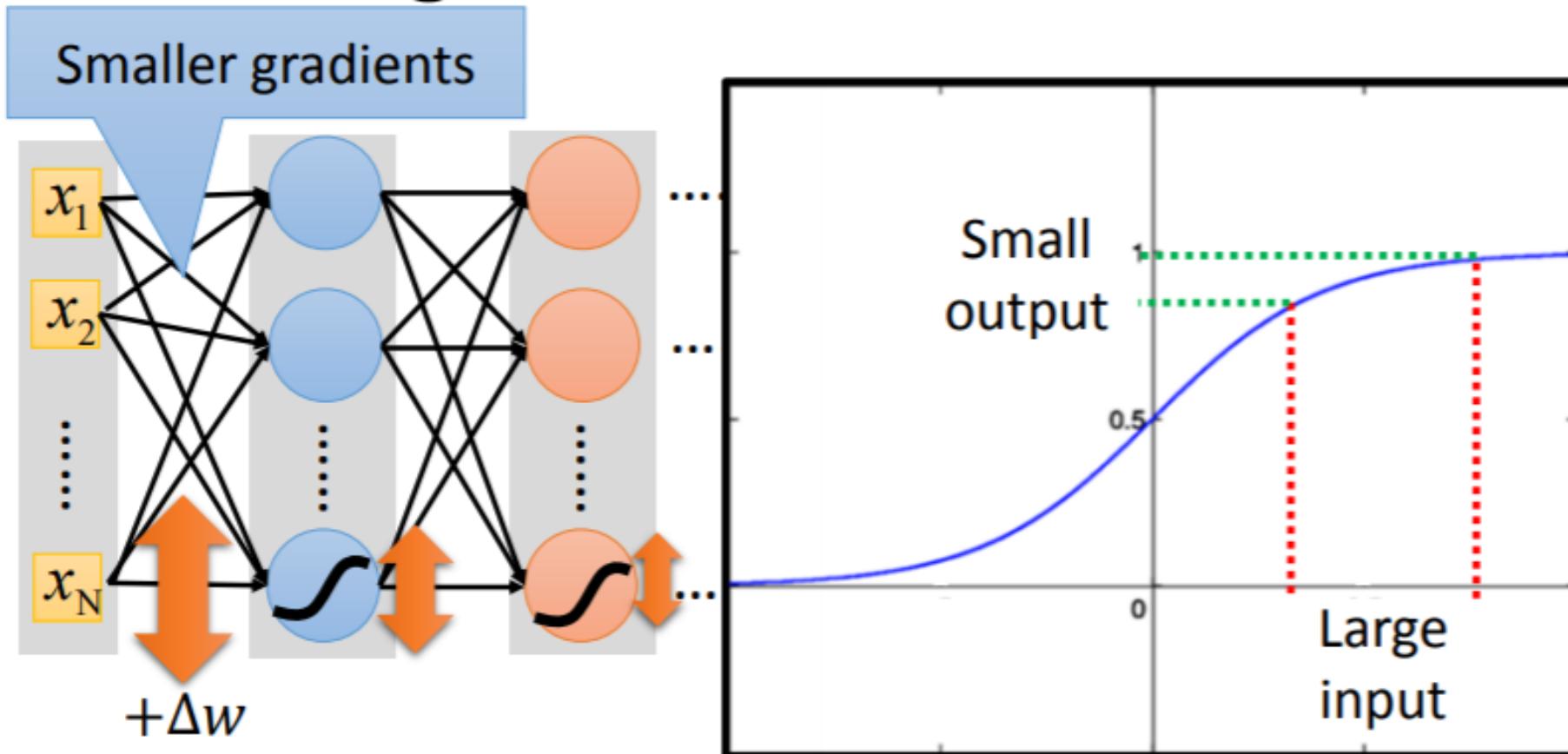


$$\frac{\partial L}{\partial w_{6y}} = \frac{\partial L}{\partial y_1} \frac{\partial y_1}{\partial w_{6y}}$$

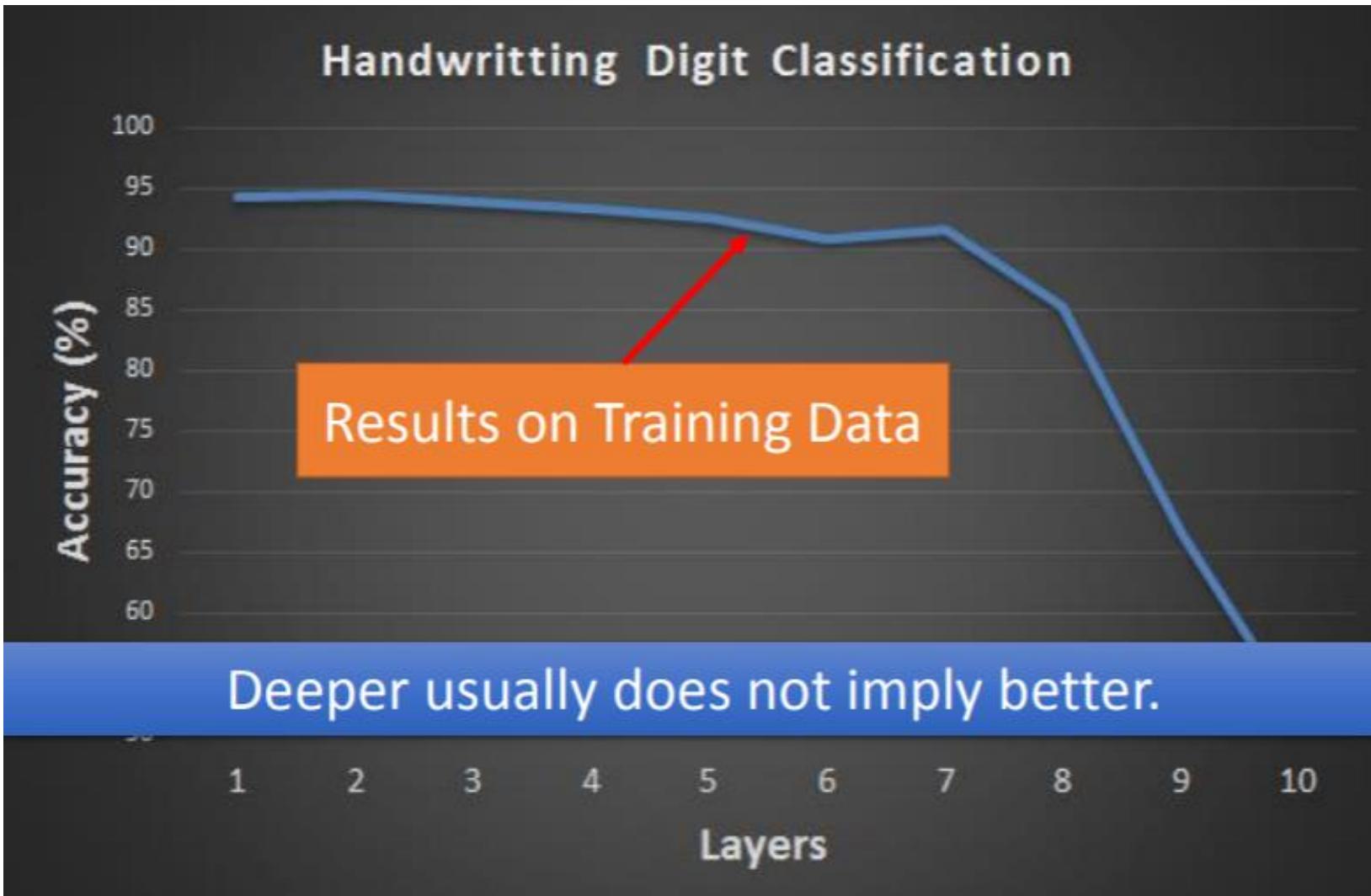
$$\frac{\partial L}{\partial w_{57}} = \frac{\partial L}{\partial y_1} \frac{\partial y_1}{\partial n_7} \frac{\partial n_7}{\partial w_{57}}$$

Vanishing gradient problem

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

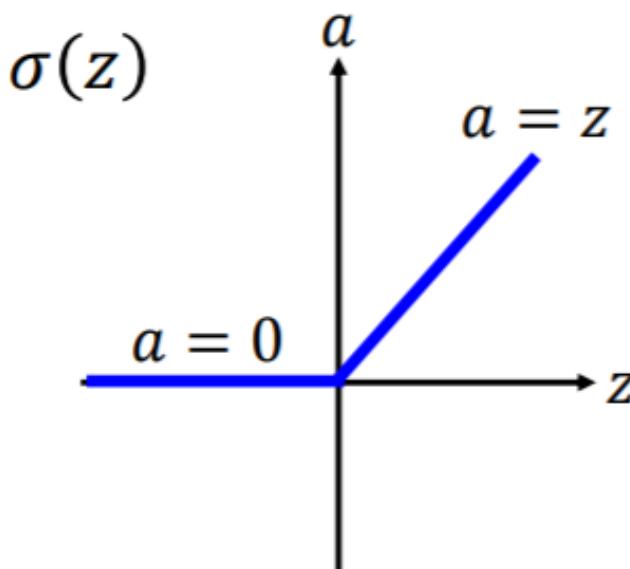


Sigmoid is hard to get the power of deep



ReLU

- Rectified Linear Unit (ReLU)



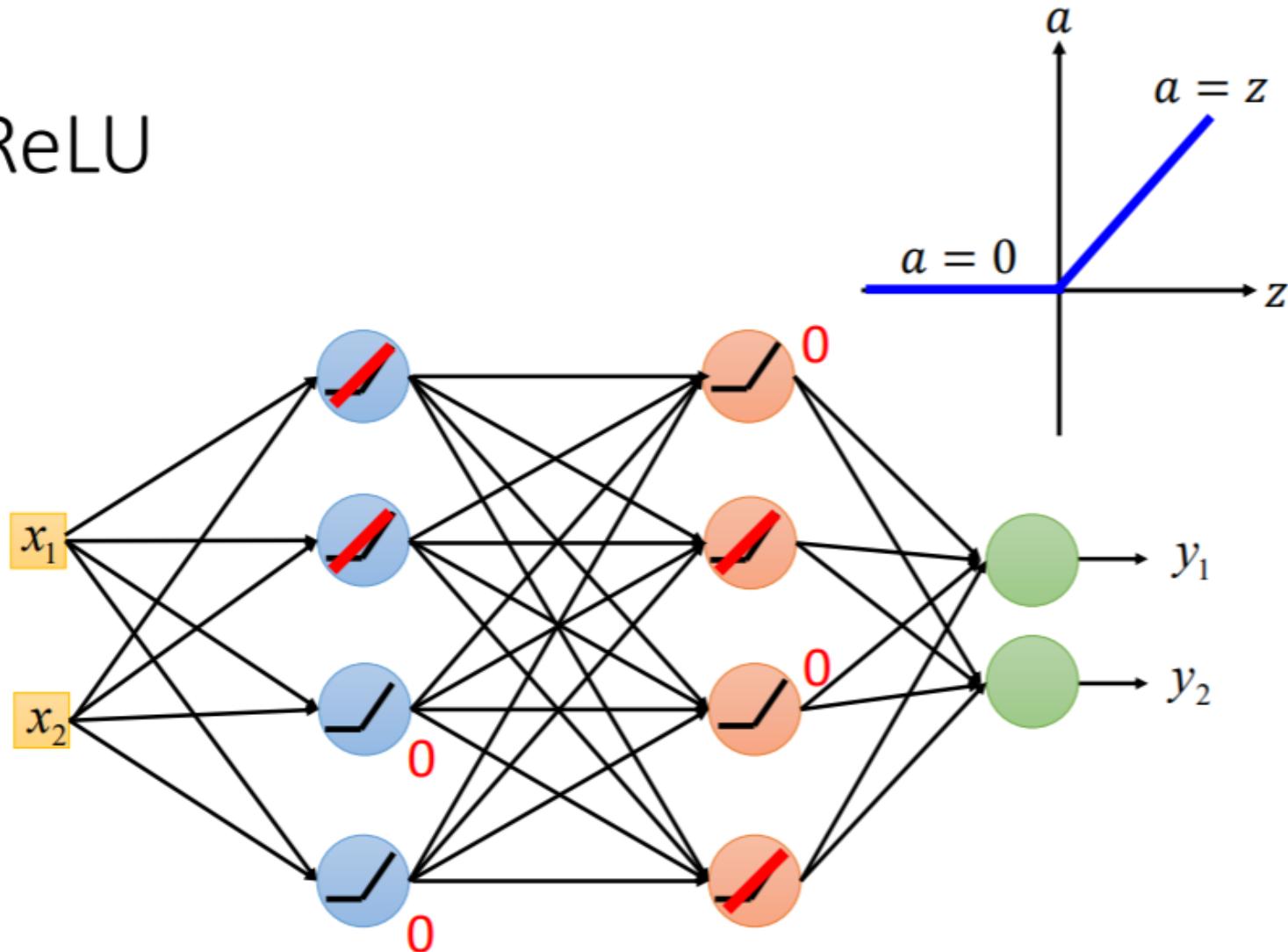
[Xavier Glorot, AISTATS'11]
[Andrew L. Maas, ICML'13]
[Kaiming He, arXiv'15]

Reason:

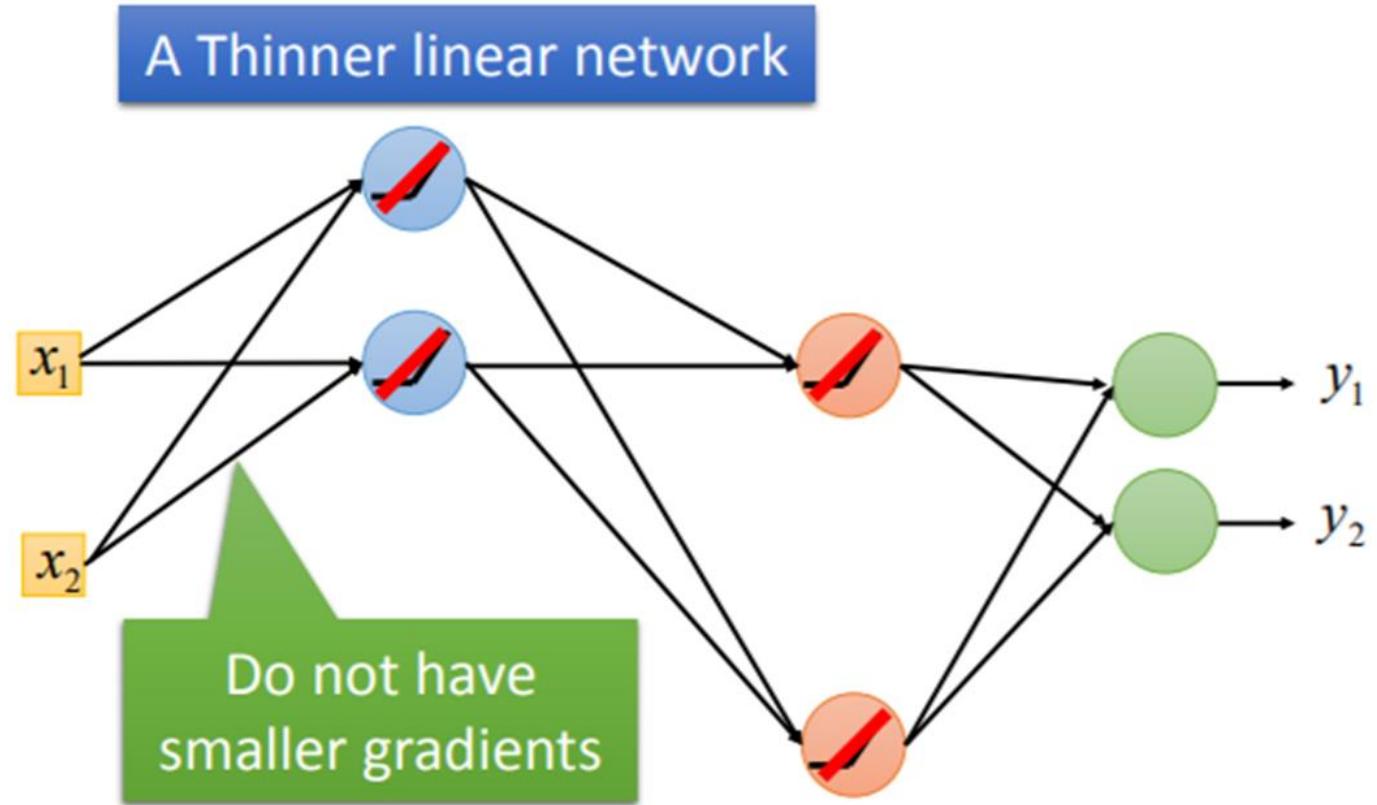
1. Fast to compute
2. Biological reason
3. Infinite sigmoid with different biases
4. Vanishing gradient problem

ReLU

ReLU



ReLU



Practice – When training result is not good

- Run "1. 2.1. Learn from sparse data.ipynb".



HW3 (1)

- Based on "1. 2.1. Learn from sparse data.ipynb", design your own training data and function between x and y , i.e., $y = f(x)$.
Experiment with different NN designs.

	No. of parameters	No. of parameters
Deep and thin	Loss on training data	
Shallow and fat		
In-between version		



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

	Underfitting	Just right	Overfitting
Symptoms	<ul style="list-style-type: none"> • High training error • Training error close to test error • High bias 	<ul style="list-style-type: none"> • Training error slightly lower than test error 	<ul style="list-style-type: none"> • Very low training error • Training error much lower than test error • High variance
Regression illustration			
Classification illustration			
Deep learning illustration			
Possible remedies	<ul style="list-style-type: none"> • Complexify model • Add more features • Train longer 		<ul style="list-style-type: none"> • Perform regularization • Get more data

Practice – Overfitting

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



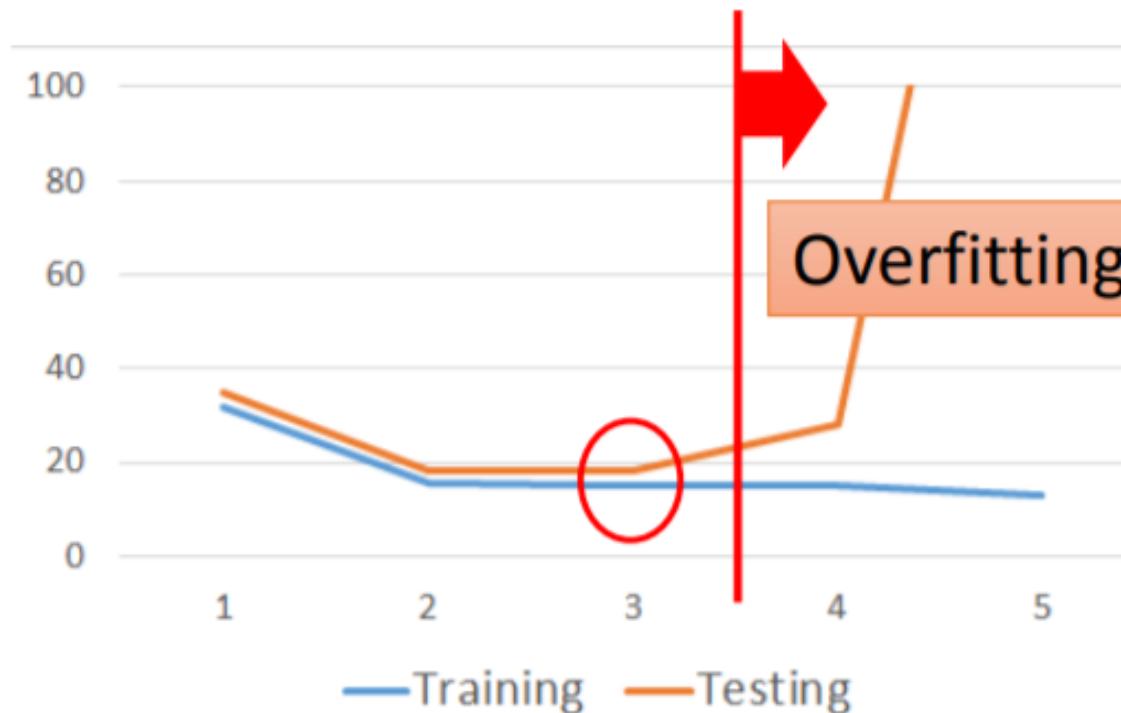
HW3 (2)

- Extend HW3(1) to report overfitting problem.

		Training	Testing
No of parameters =	Deep and thing		
	Shallow and fat		
	In-between version		
No of parameters =	Deep and thing		
	Shallow and fat		
	In-between version		



Overfitting problem

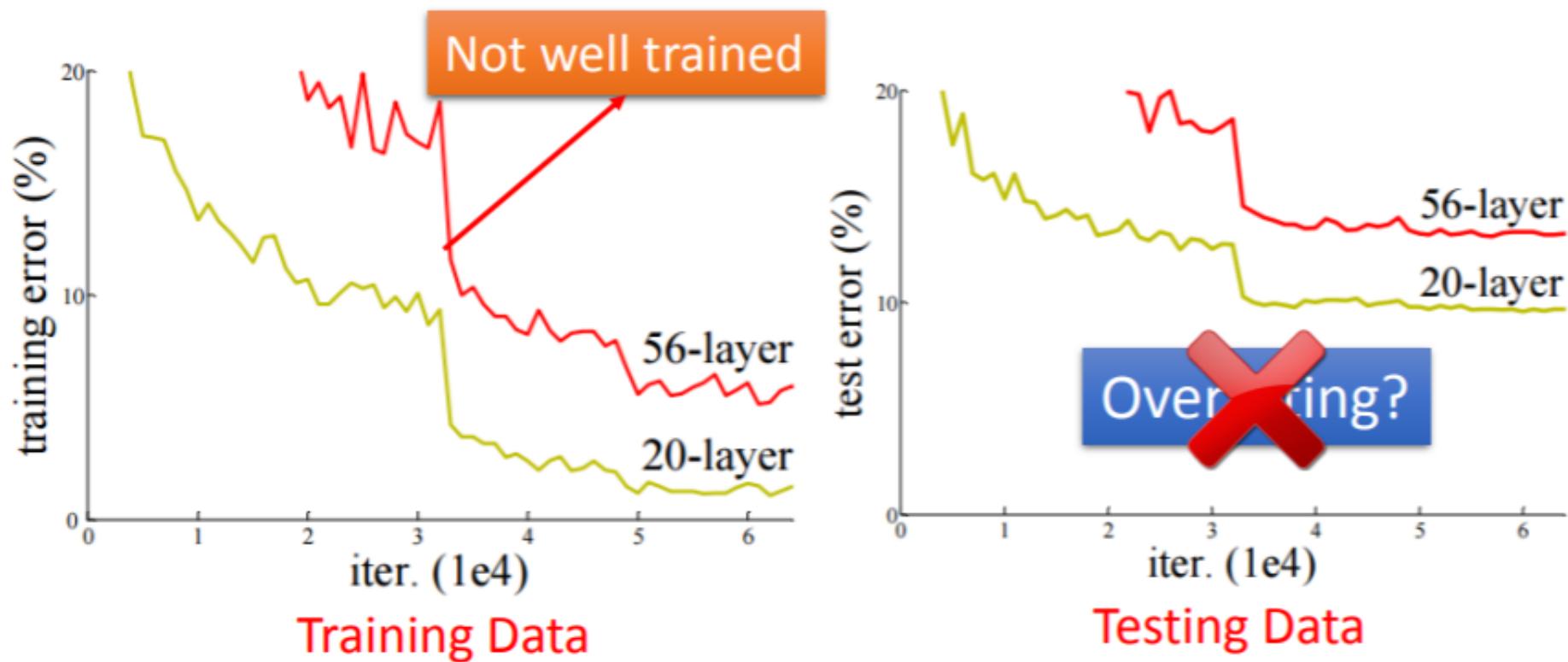


	Training	Testing
1	31.9	35.0
2	15.4	18.4
3	15.3	18.1
4	14.9	28.2
5	12.8	232.1

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

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

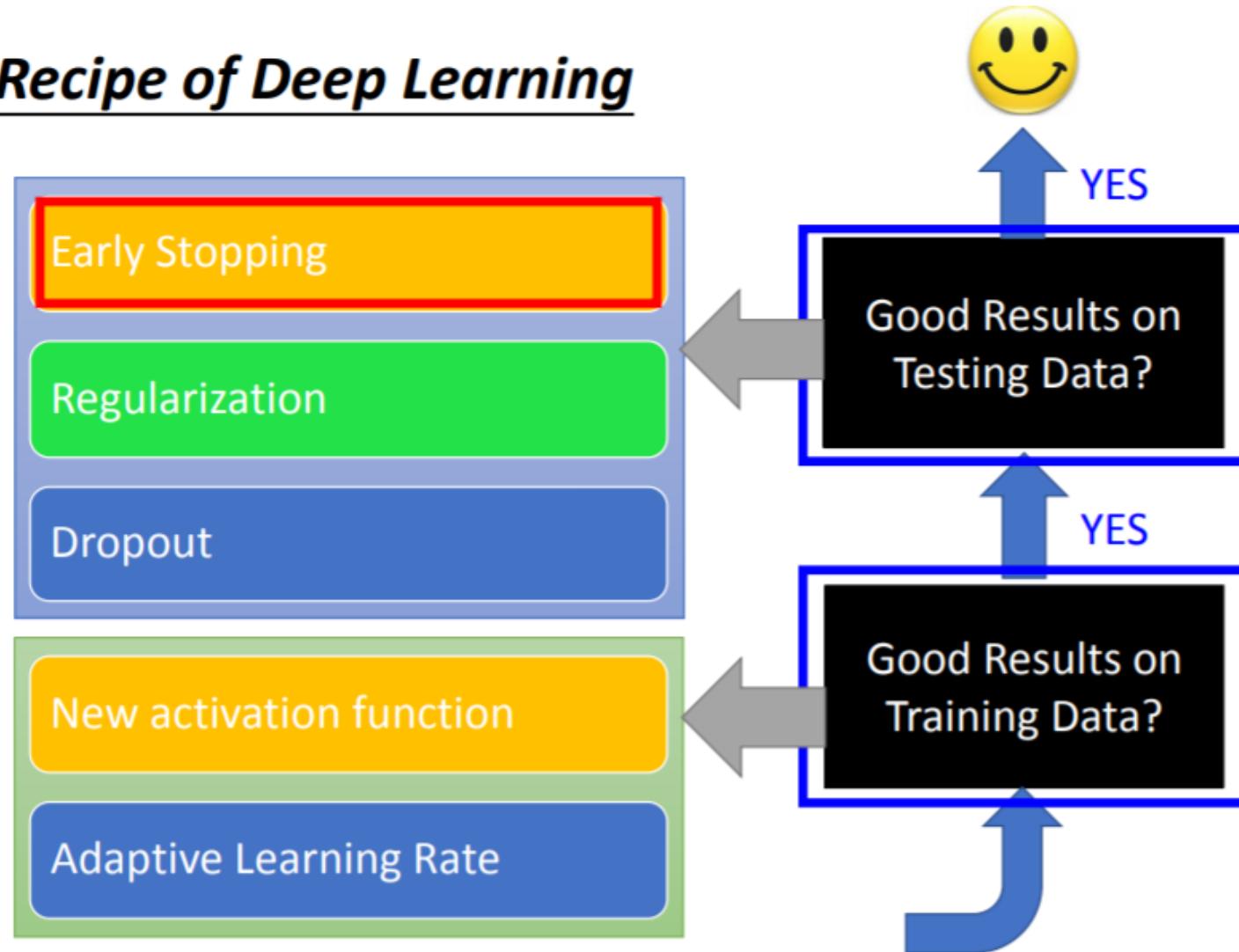
Do not always blame overfitting



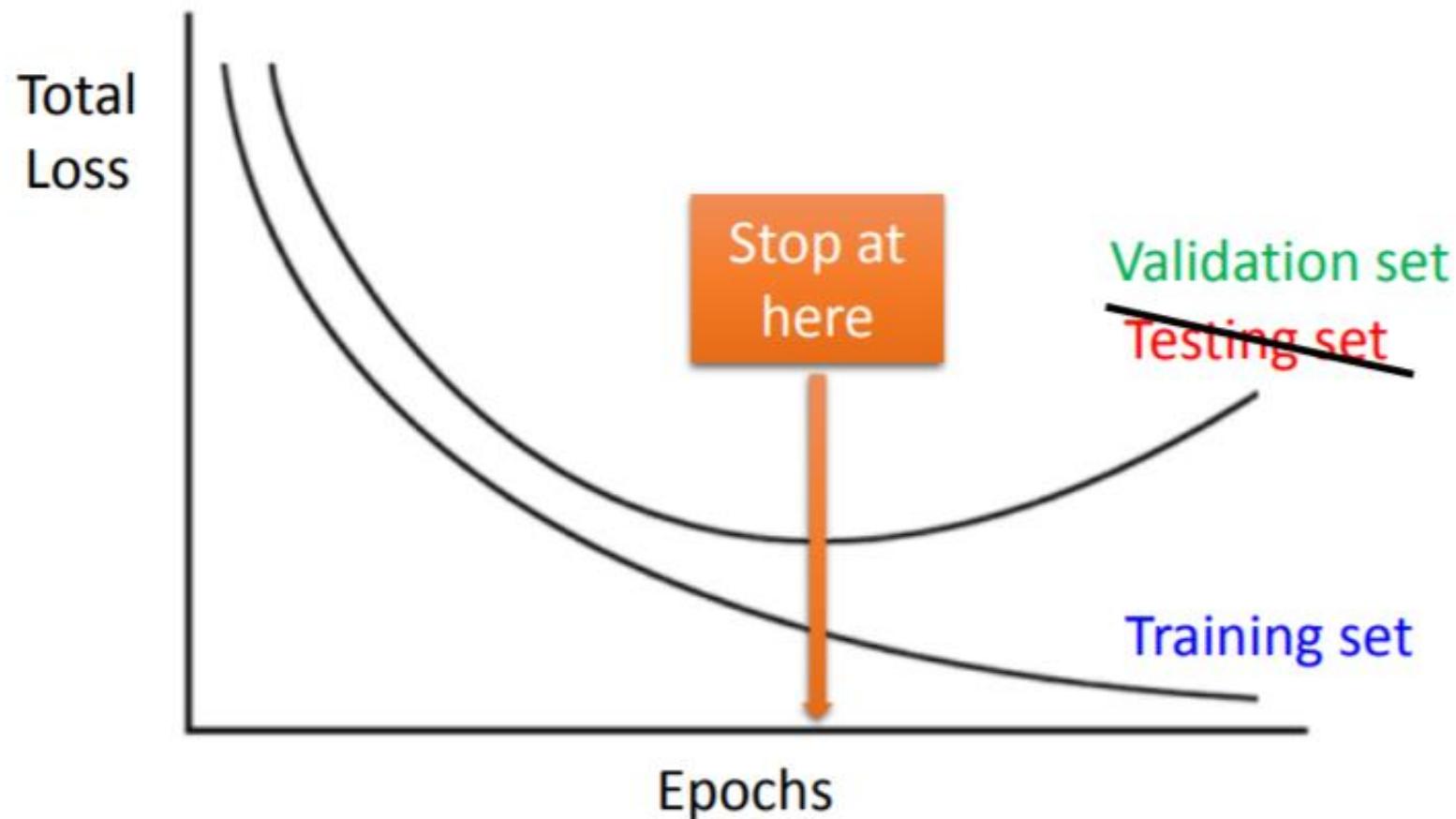
Deep Residual Learning for Image Recognition
<http://arxiv.org/abs/1512.03385>

What to do if overfitting?

Recipe of Deep Learning



Early stopping



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

Practice – Early stop

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



HW3 (3)

- Based on HW3(2), experiment the effect of early stop on resolving overfitting.

		Training with early stop	Testing
No of parameters =	Deep and thing		
	Shallow and fat		
	In-between version		
No of parameters =	Deep and thing		
	Shallow and fat		
	In-between version		



Regularization – L2

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

$$L'(\theta) = \underline{L(\theta)} + \lambda \frac{1}{2} \|\theta\|_2 \rightarrow \text{Regularization term}$$

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

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

L2 regularization:

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

(usually not consider biases)

L2 regularization

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

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

$$= \underbrace{(1 - \eta \lambda)w^t}_{\downarrow} - \eta \underbrace{\frac{\partial L}{\partial w}}_{\text{Weight Decay}}$$

Closer to zero

Practice – L2 regularization

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



HW3 (4)

- Based on HW3(2), experiment the effect of L2 regularization on resolving overfitting.

		Train with L2 regularization	Testing
No of parameters =	Deep and thing		
	Shallow and fat		
	In-between version		
No of parameters =	Deep and thing		
	Shallow and fat		
	In-between version		



L1 regularization

L1 regularization:

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

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

Update:

$$\begin{aligned} w^{t+1} &\rightarrow w^t - \eta \frac{\partial L'}{\partial w} = w^t - \eta \left(\frac{\partial L}{\partial w} + \lambda \operatorname{sgn}(w^t) \right) \\ &= w^t - \eta \frac{\partial L}{\partial w} - \underline{\eta \lambda \operatorname{sgn}(w^t)} \quad \text{Always delete} \\ &= (1 - \eta \lambda) w^t - \eta \frac{\partial L}{\partial w} \quad \dots \dots \text{L2} \end{aligned}$$

Practice – L1 regularization

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



HW3 (5)

- Based on HW3(2), experiment the effect of L1 regularization on resolving overfitting.

		Train with L1 regularization	Testing
No of parameters =	Deep and thing		
	Shallow and fat		
	In-between version		
No of parameters =	Deep and thing		
	Shallow and fat		
	In-between version		



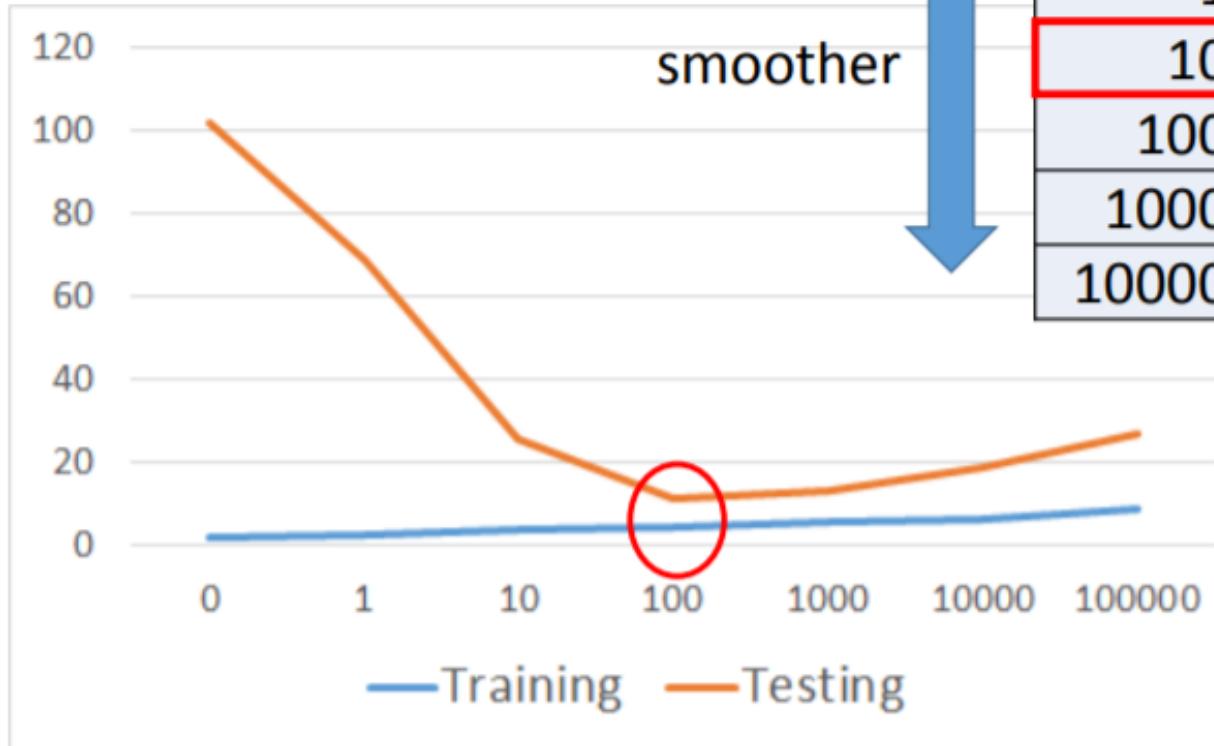
Practice – Small initial weights

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



Regularization

Regularization

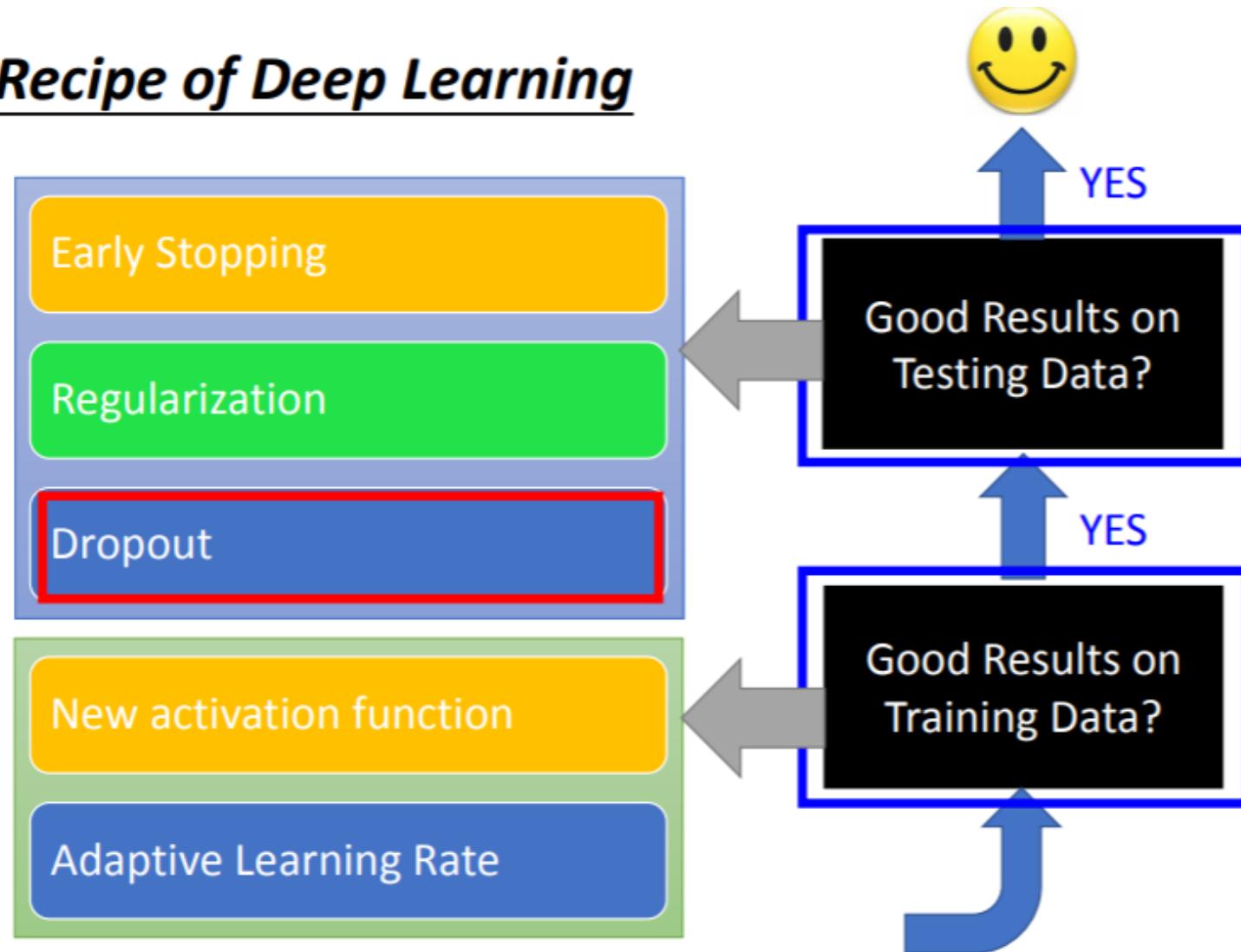


λ	Training	Testing
0	1.9	102.3
1	2.3	68.7
10	3.5	25.7
100	4.1	11.1
1000	5.6	12.8
10000	6.3	18.7
100000	8.5	26.8

How smooth?
Select λ obtaining
the best model

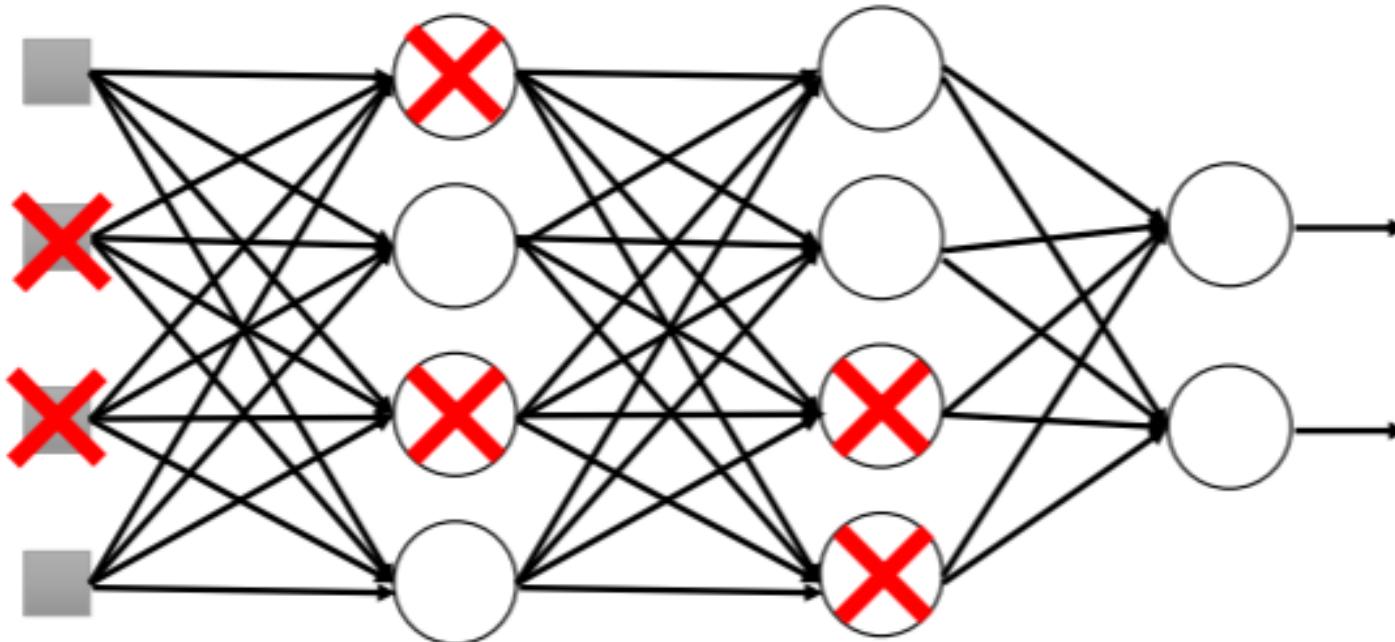
Drop out

Recipe of Deep Learning



Drop out

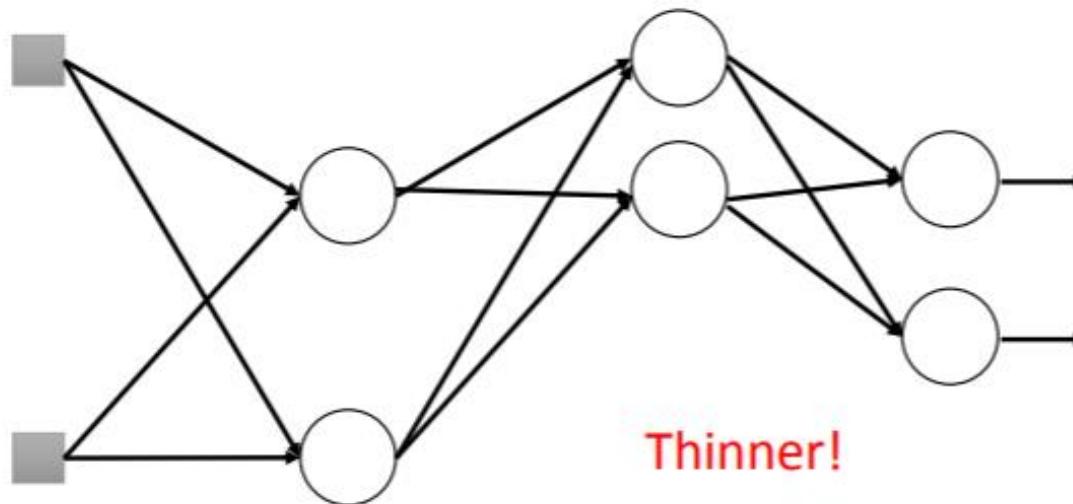
Training:



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

Drop out

Training:

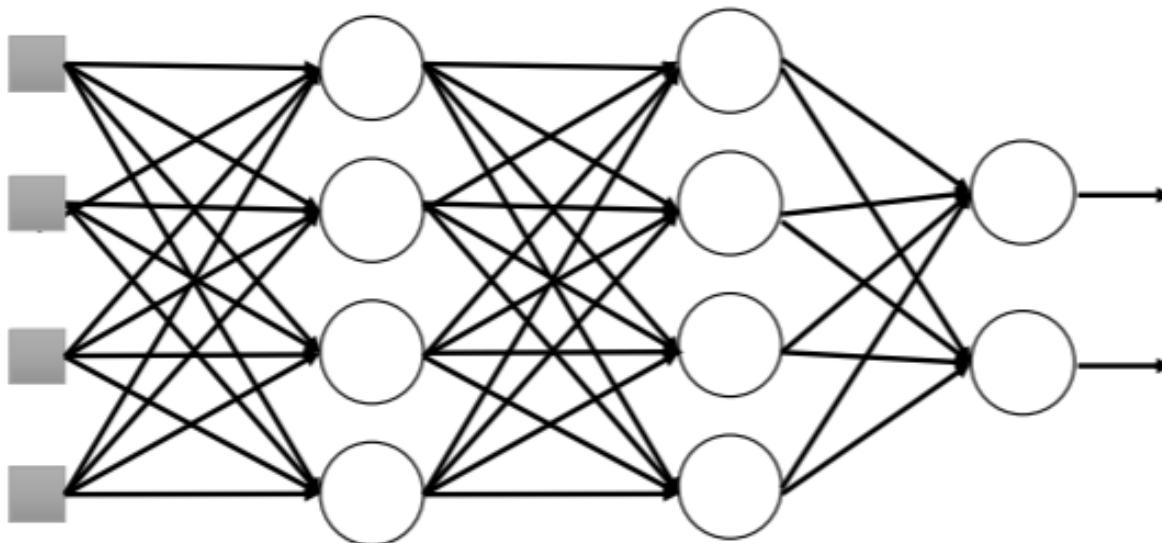


- **Each time before updating the parameters**
 - Each neuron has p% to dropout
 - ➡ **The structure of the network is changed.**
 - Using the new network for training

For each mini-batch, we resample the dropout neurons

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.

Practice – Drop out

- Run “1. 2.3. Dropout.ipynb” .



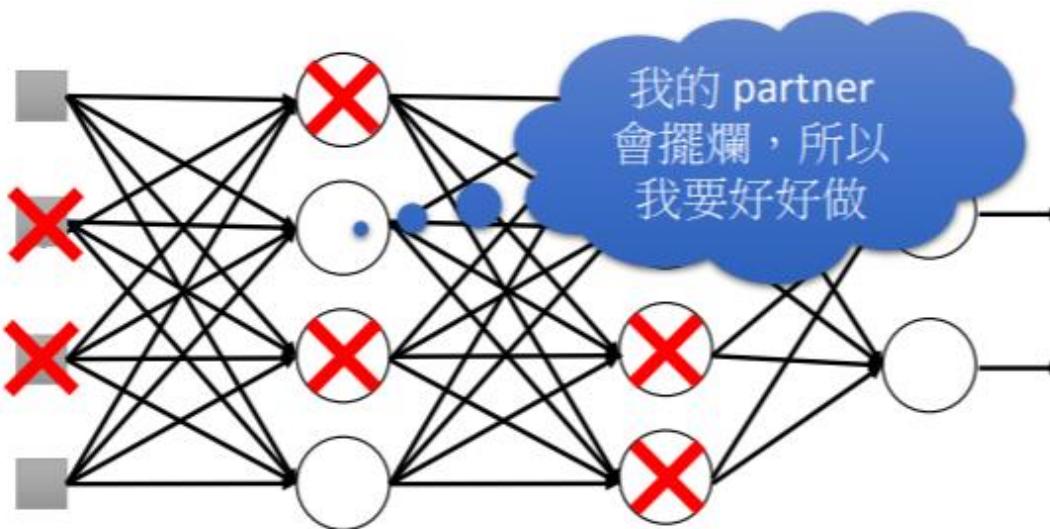
HW3 (6)

- Based on HW3(2), experiment the effect of drop out on resolving overfitting.

		Train using drop out	Testing
No of parameters =	Deep and thin		
	Shallow and fat		
	In-between version		
No of parameters =	Deep and thin		
	Shallow and fat		
	In-between version		



Why drop out makes NN perform better?



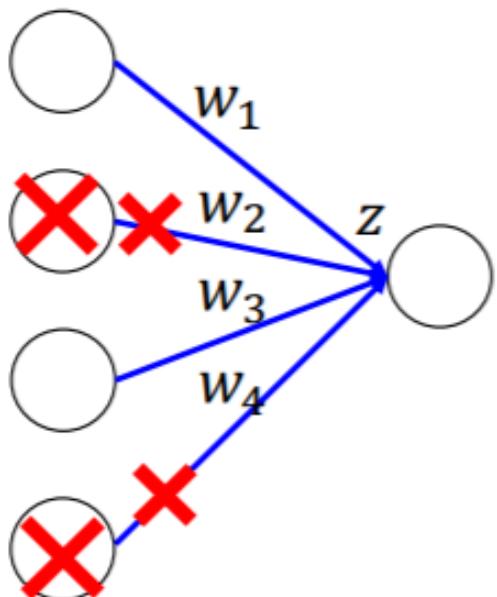
- When teams up, if everyone expect the partner will do the work, nothing will be done finally.
- However, if you know your partner will dropout, you will do better.
- When testing, no one dropout actually, so obtaining good results eventually.

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

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

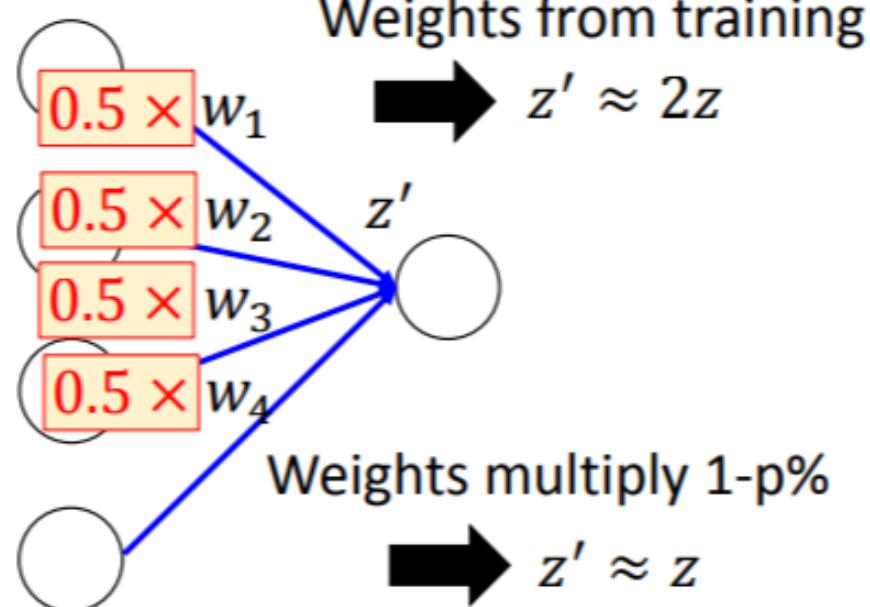
Training of Dropout

Assume dropout rate is 50%

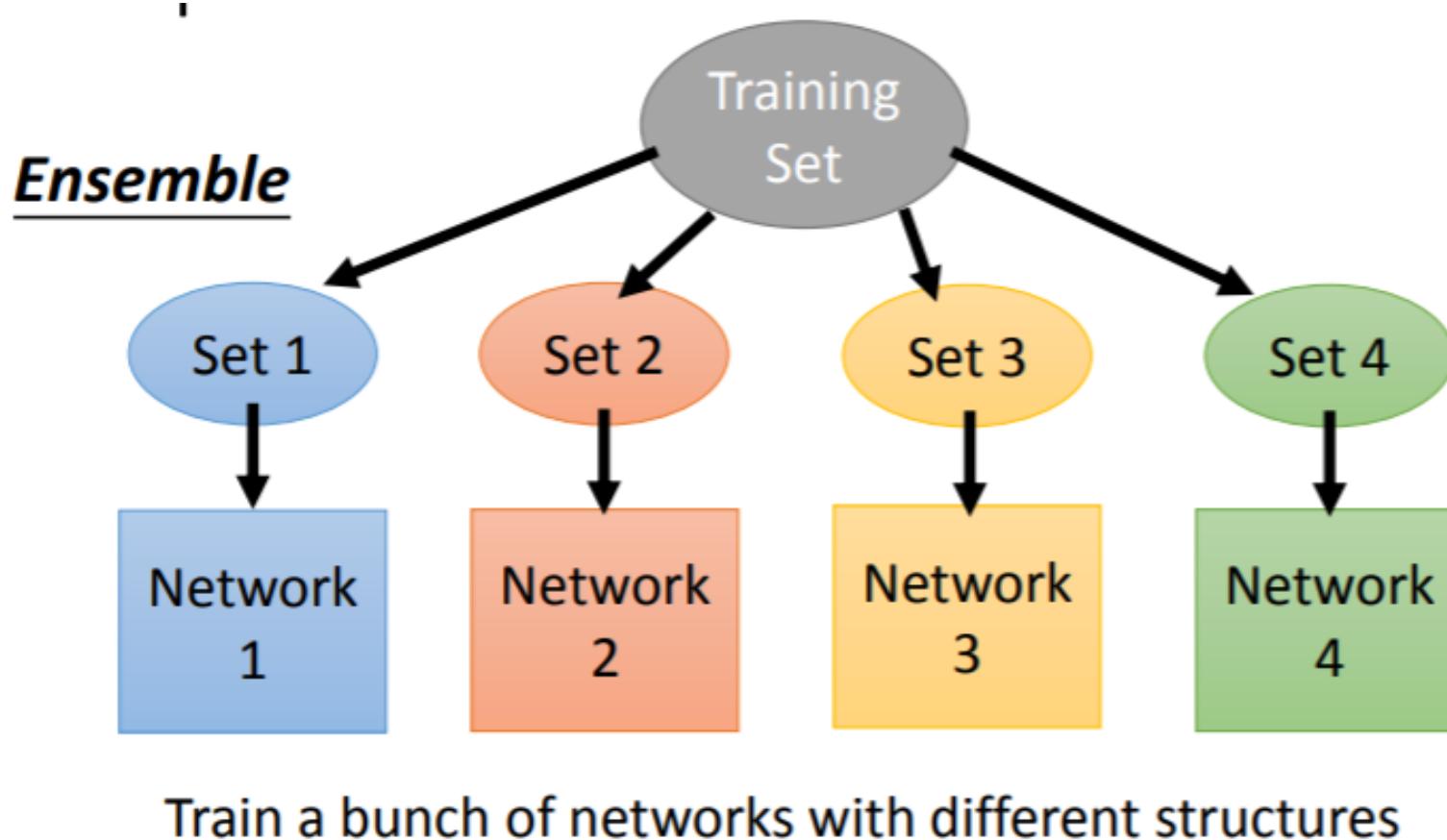


Testing of Dropout

No dropout

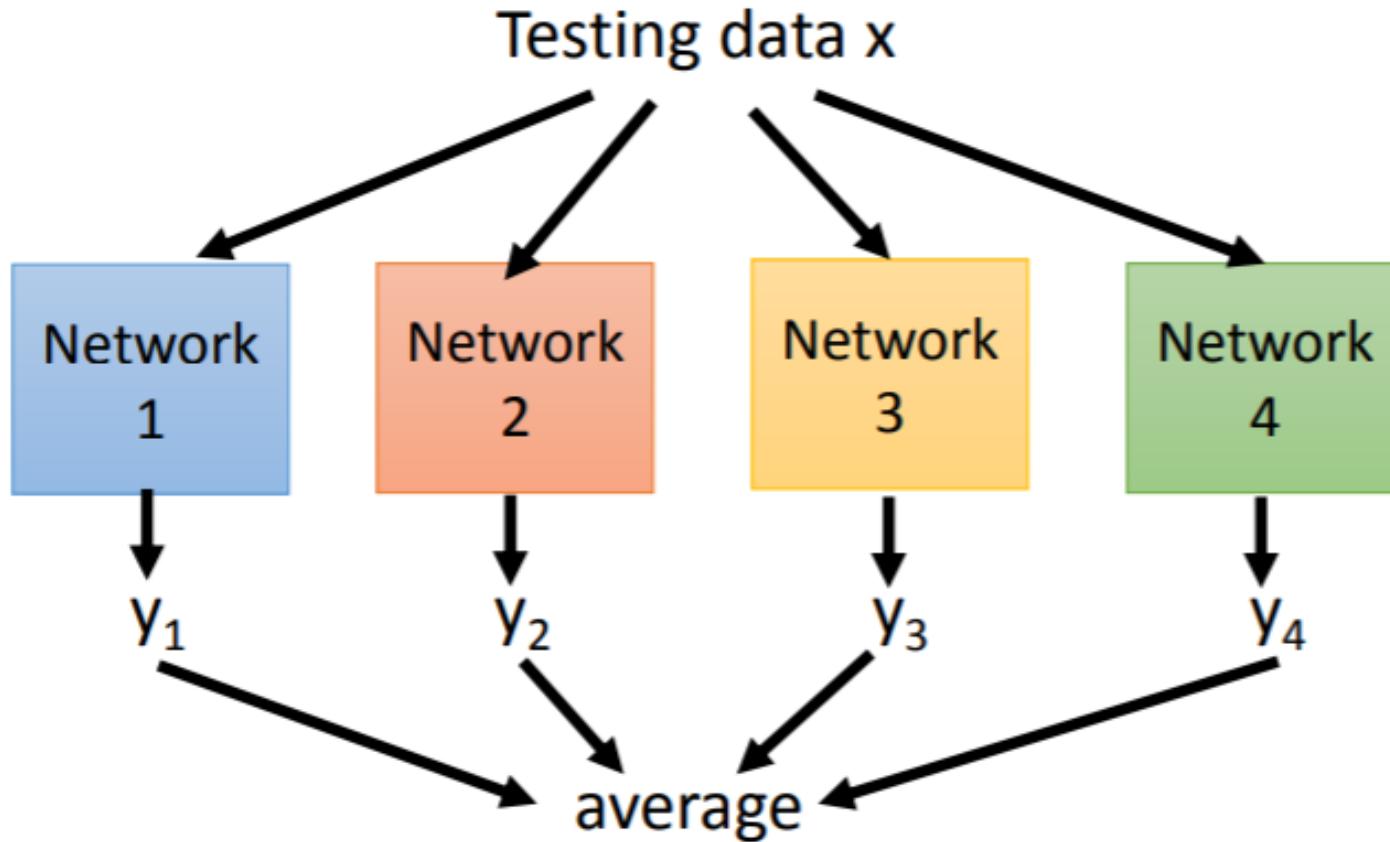


Why drop out makes NN performs better?

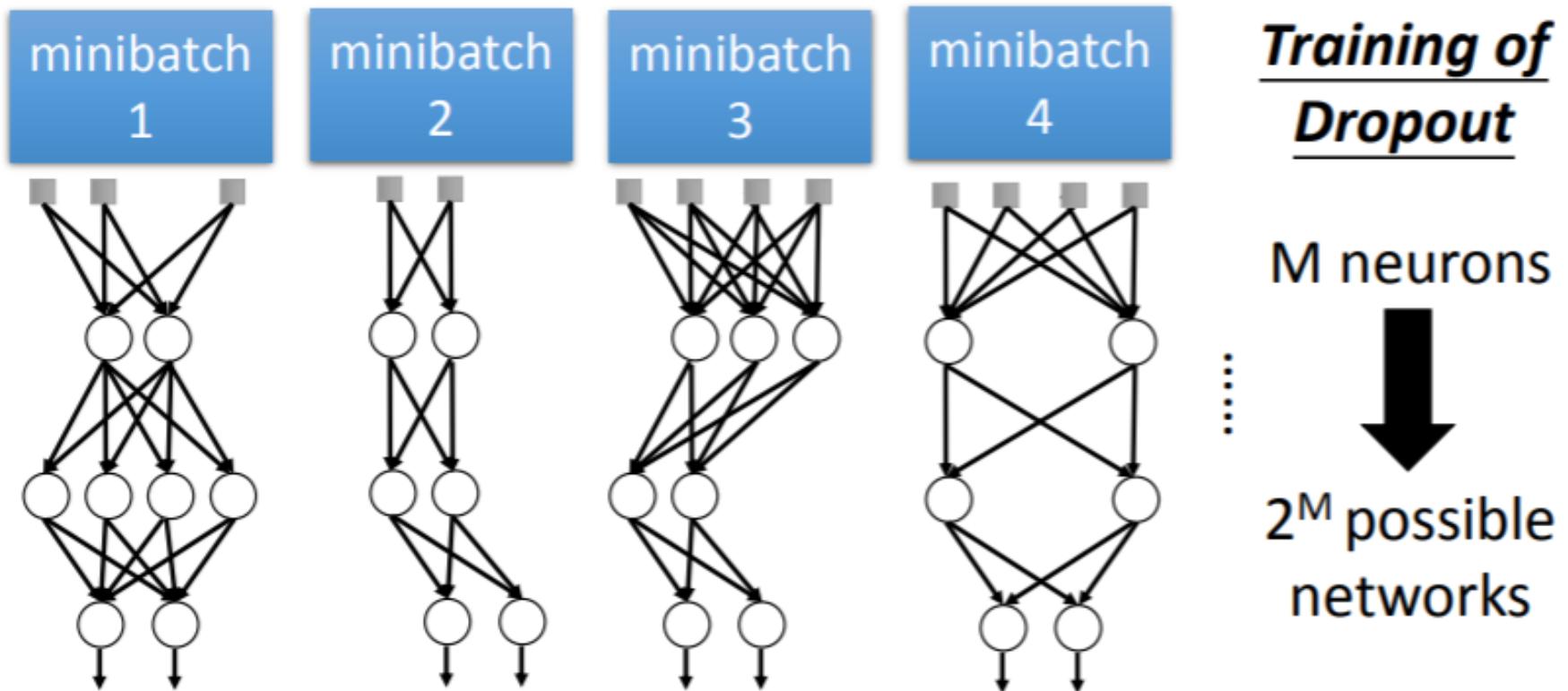


Why drop out makes NN performs better?

Ensemble

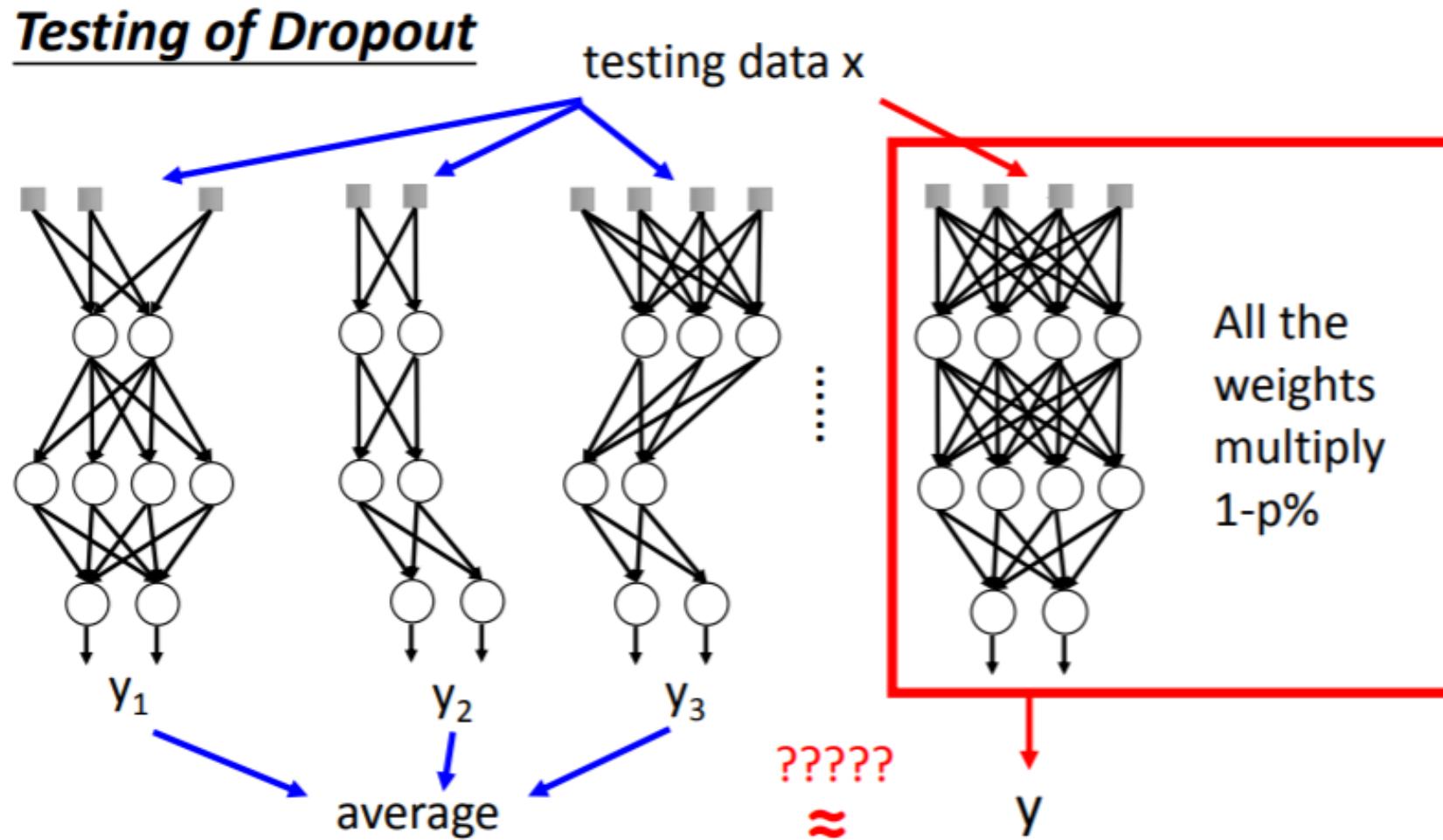


Why drop out makes NN performs better?



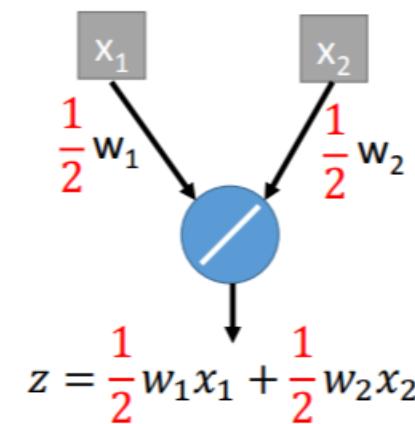
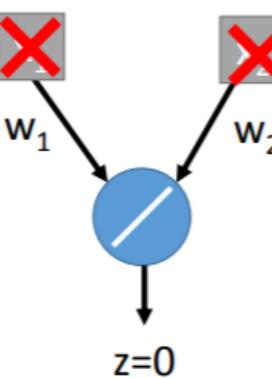
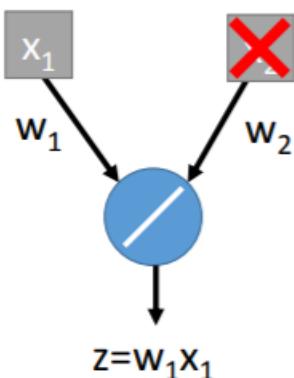
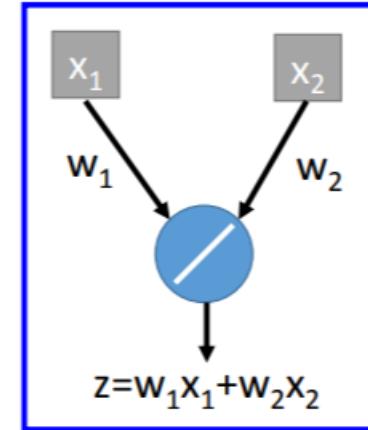
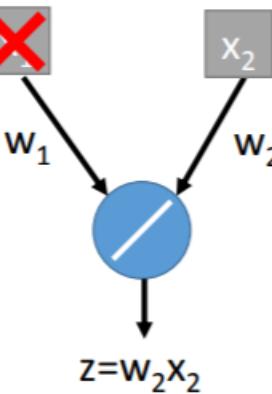
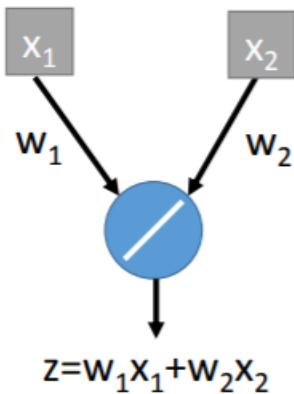
- Using one mini-batch to train one network
- Some parameters in the network are shared

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



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

Testing of Dropout



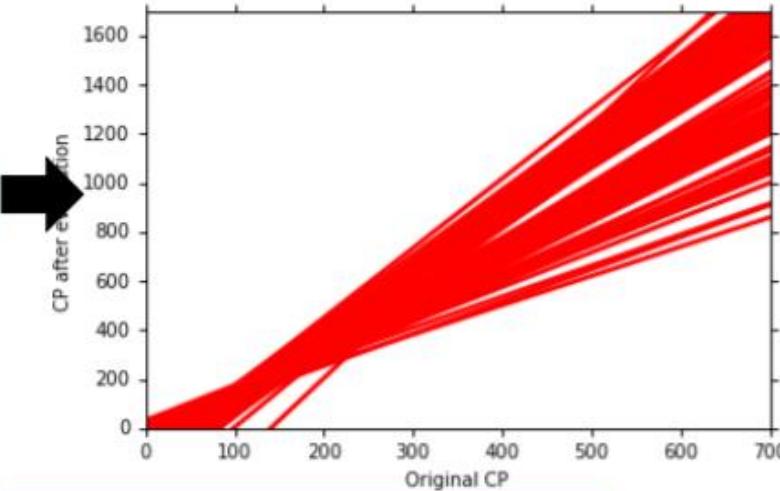
Errors of ML models

ML models learned from training data will have bias and variances

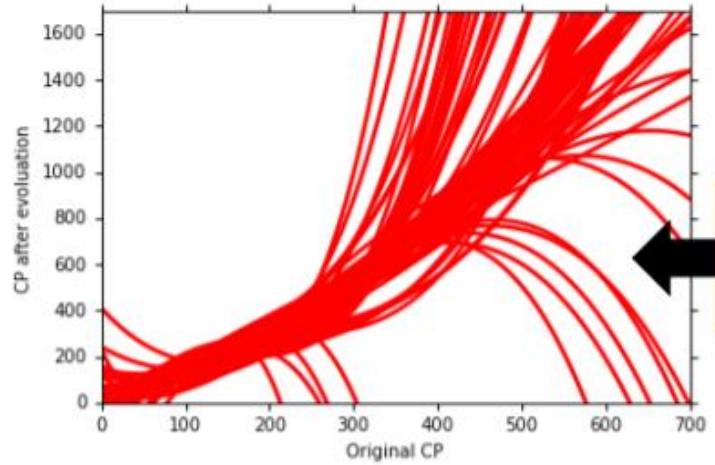
Variances of ML models

Each model is learned from 100 sampled data.

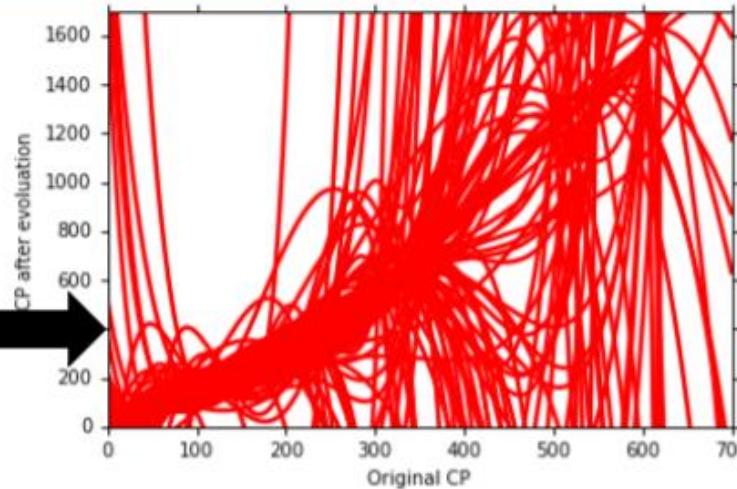
$$y = b + w \cdot x_{cp}$$



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

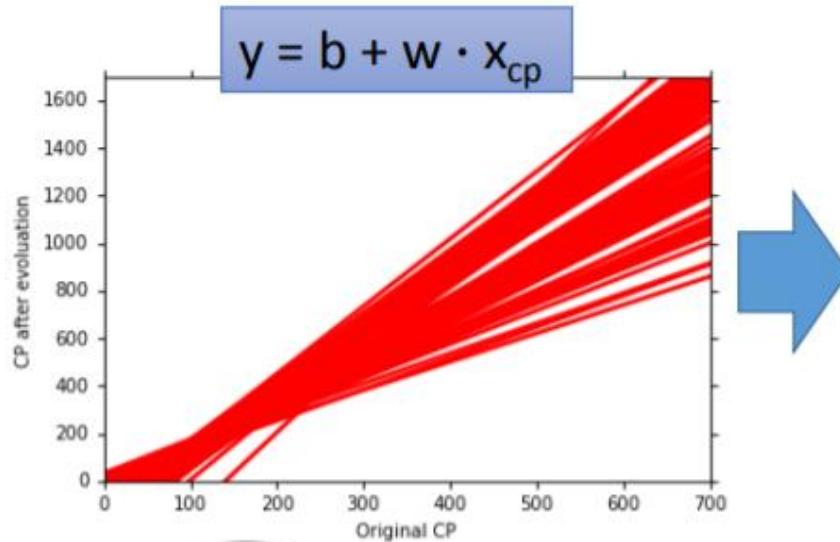


$$y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2 + w_3 \cdot (x_{cp})^3 + w_4 \cdot (x_{cp})^4 + w_5 \cdot (x_{cp})^5$$



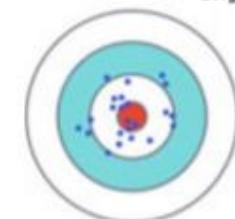
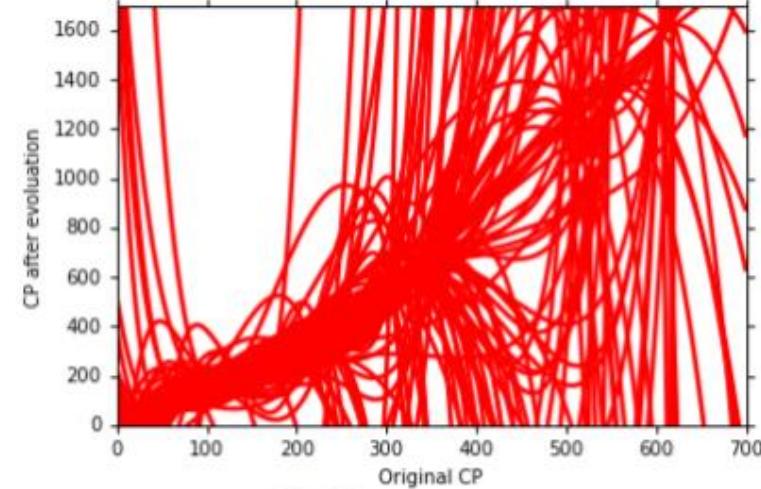
Variance of ML models

Variance



Small
Variance

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



Large
Variance

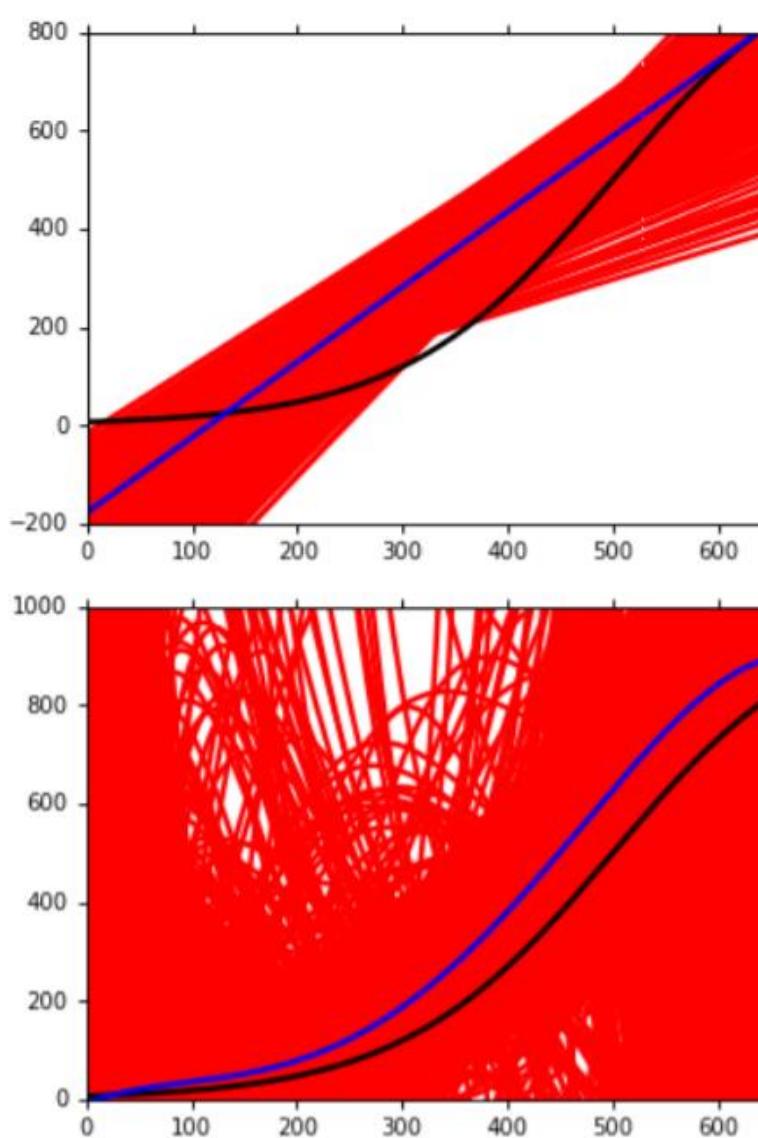
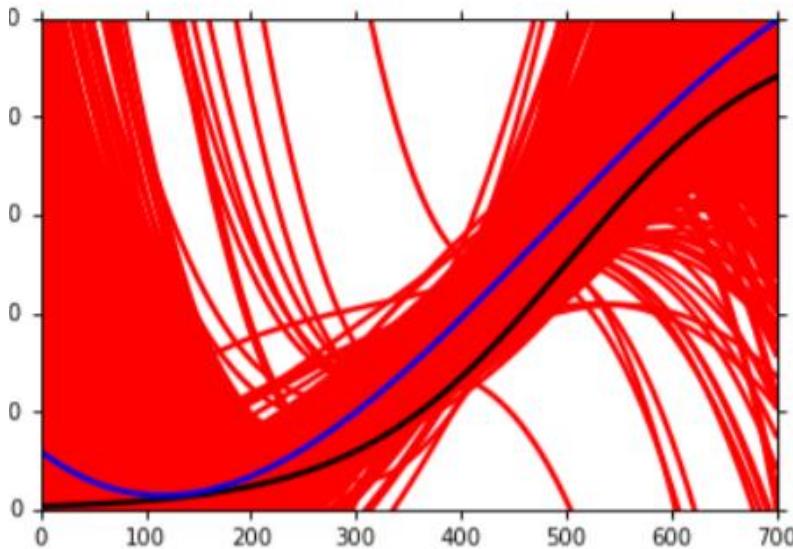
Simpler model is less influenced by the sampled data

Bias and variance of ML models

Black curve: the true function \hat{f}

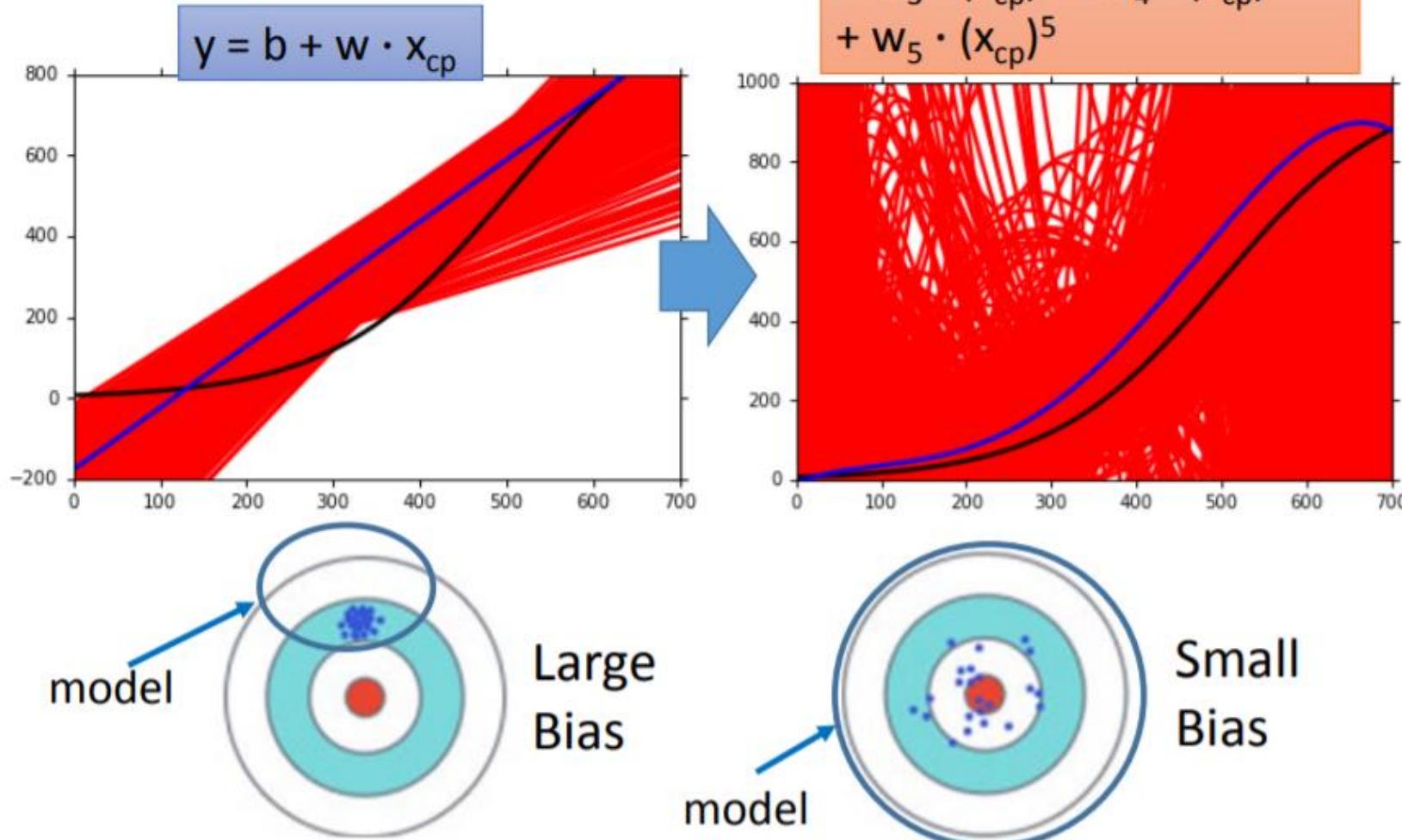
Red curves: 5000 f^*

Blue curve: the average of 5000 f^*
 $= \bar{f}$



Bias and variance of ML models

Bias



Practice – Variance of model prediction errors

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

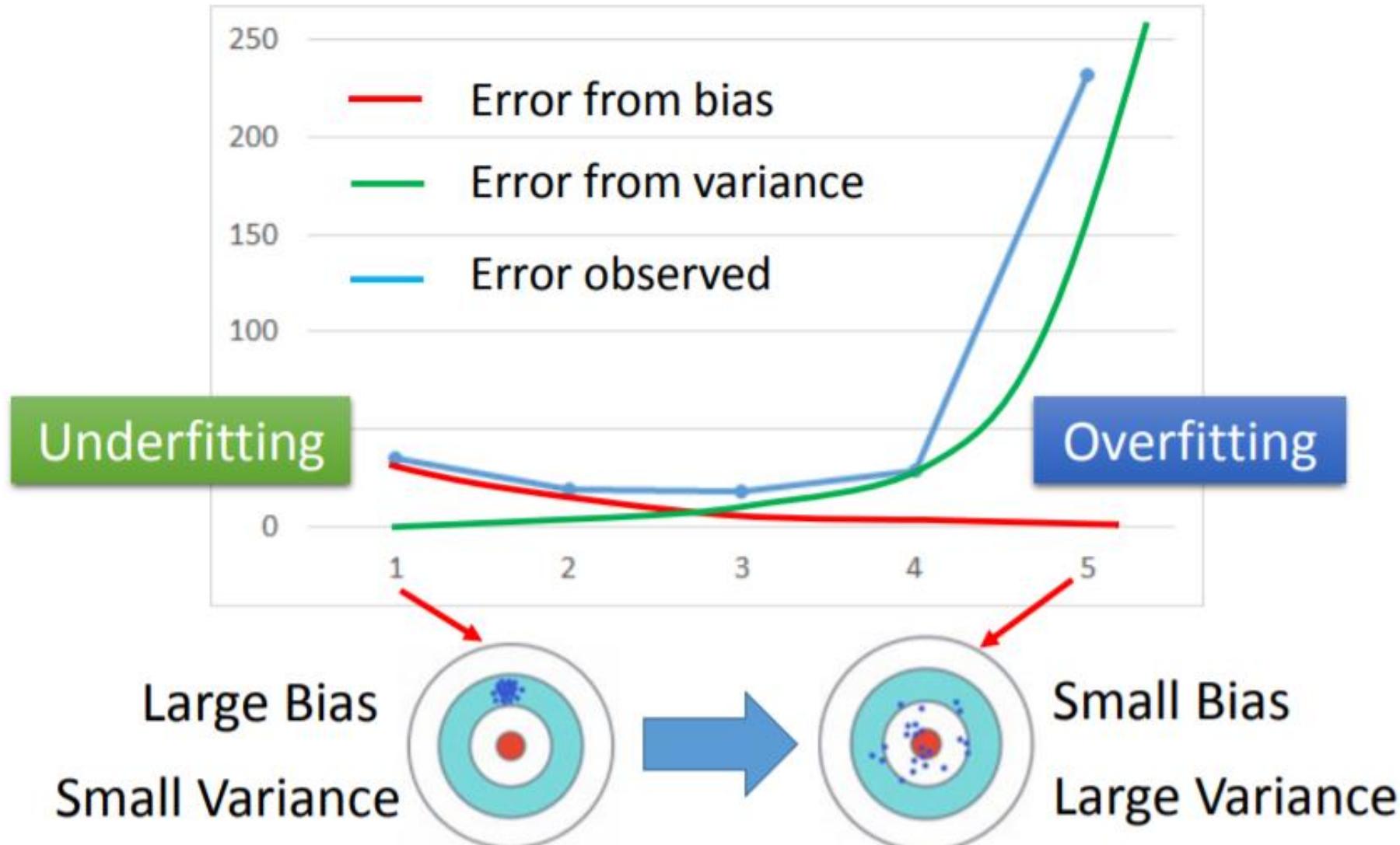


HW3 (7)

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



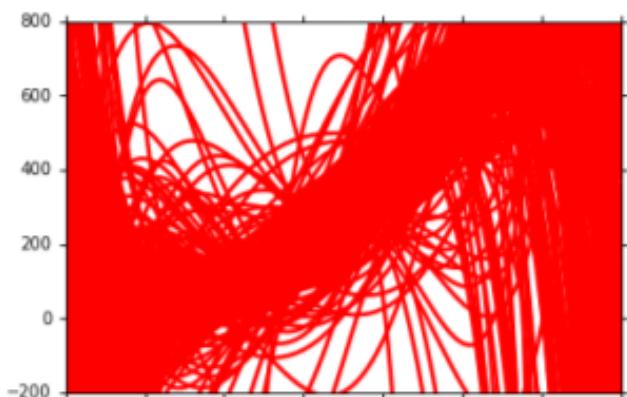
Errors of ML model



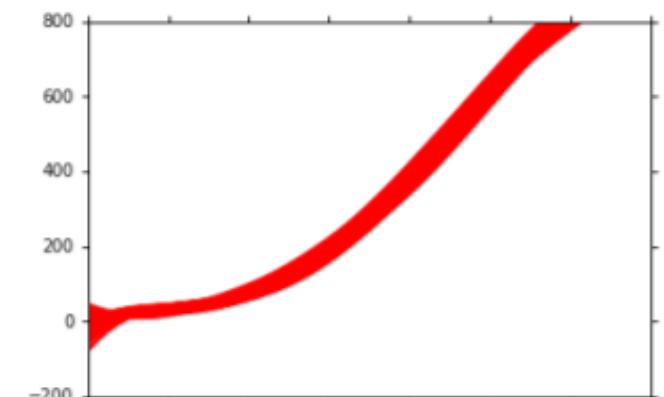
Errors of ML model → Reduce variances

- More data

Very effective,
but not always
practical

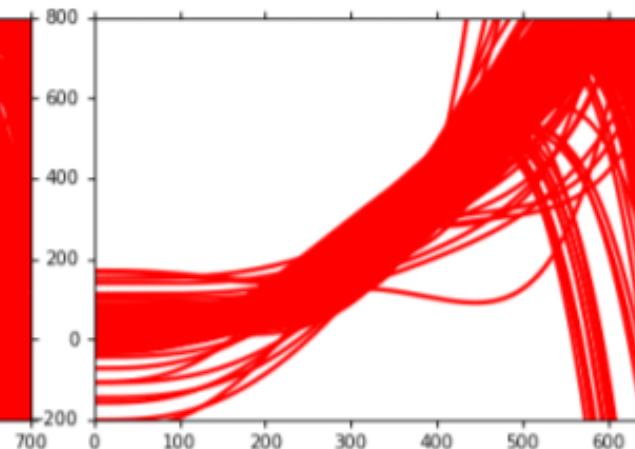
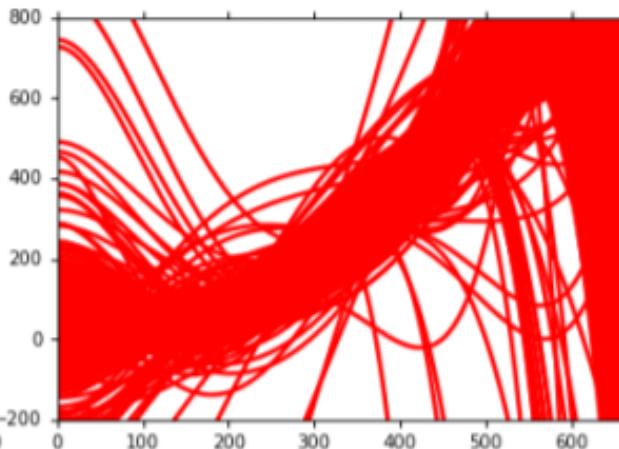
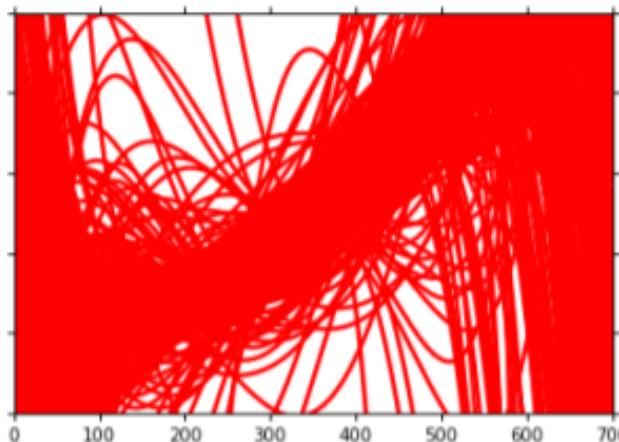


10 examples



100 examples

- Regularization



Errors of ML model → Cross validation

