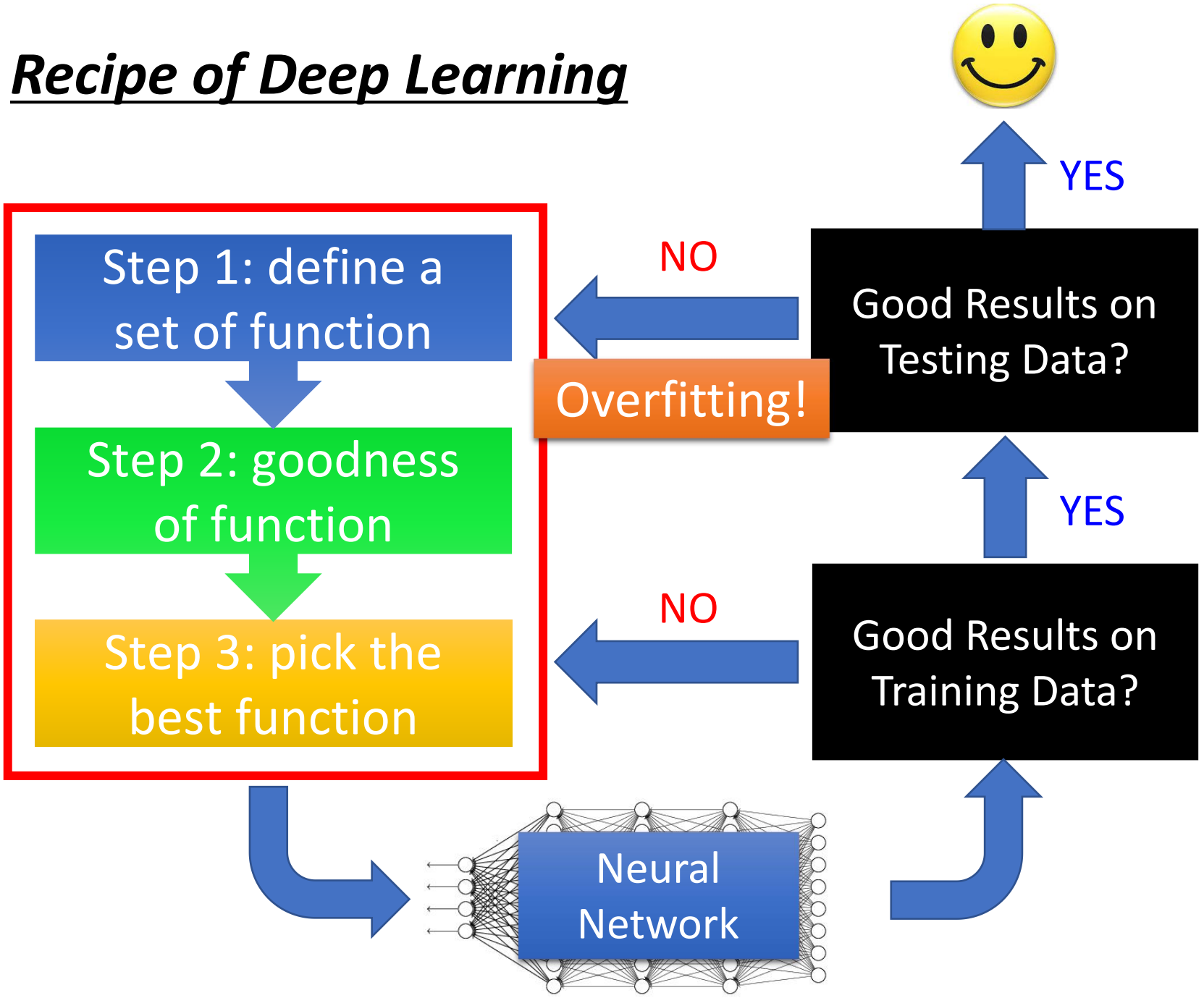
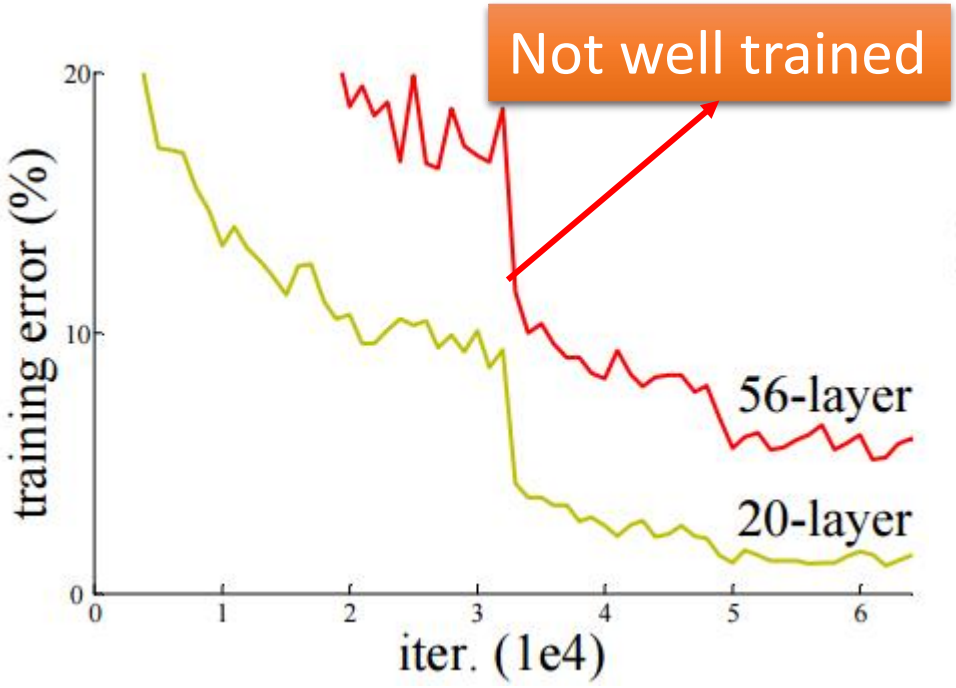
Tips for Deep Learning

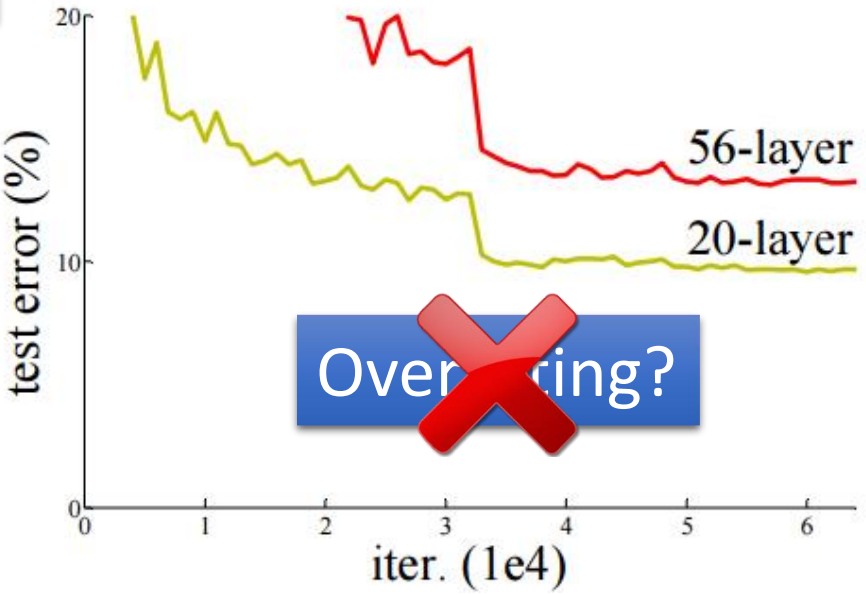
Recipe of Deep Learning



Do not always blame Overfitting



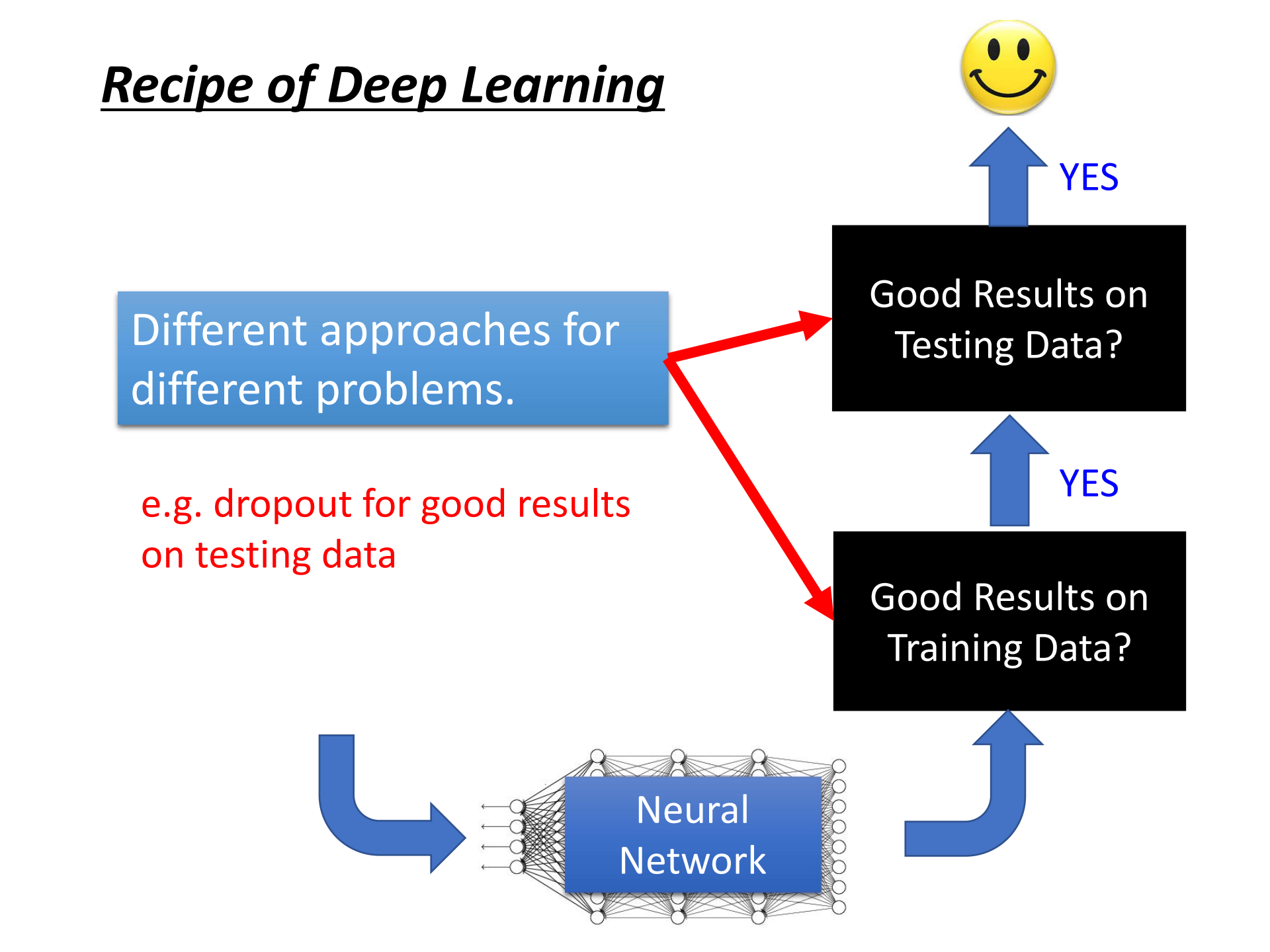
Training Data



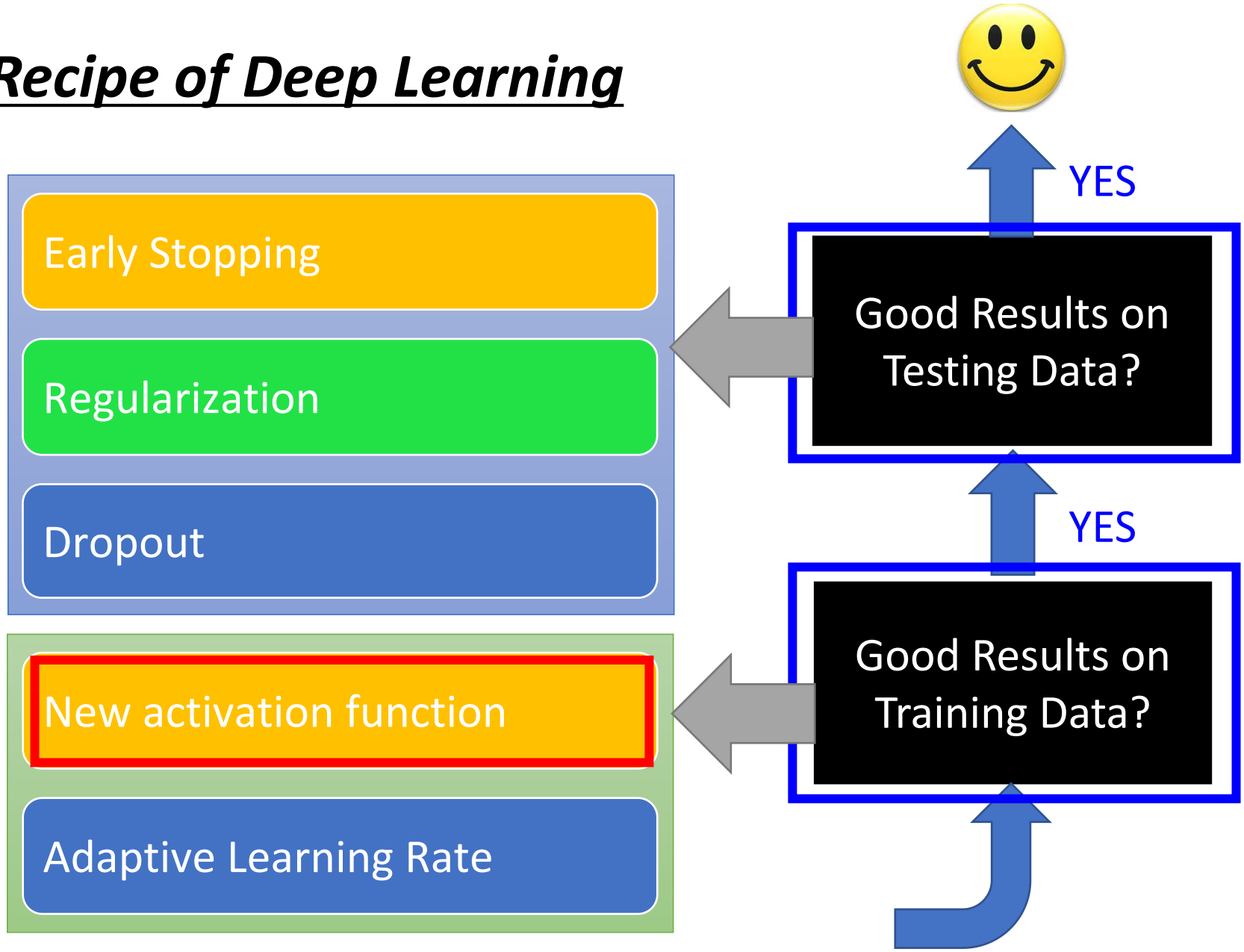
Testing Data

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

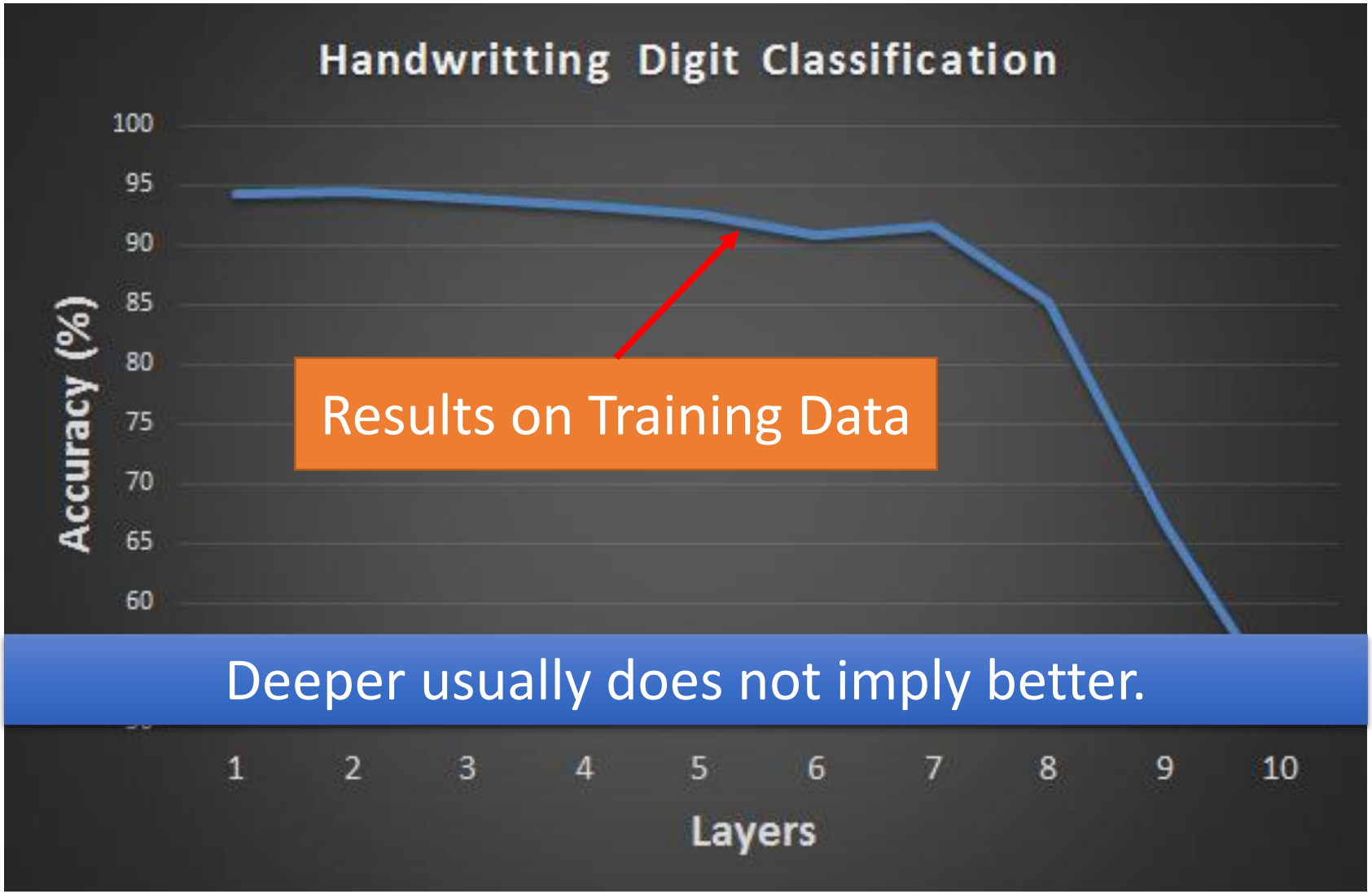
Recipe of Deep Learning



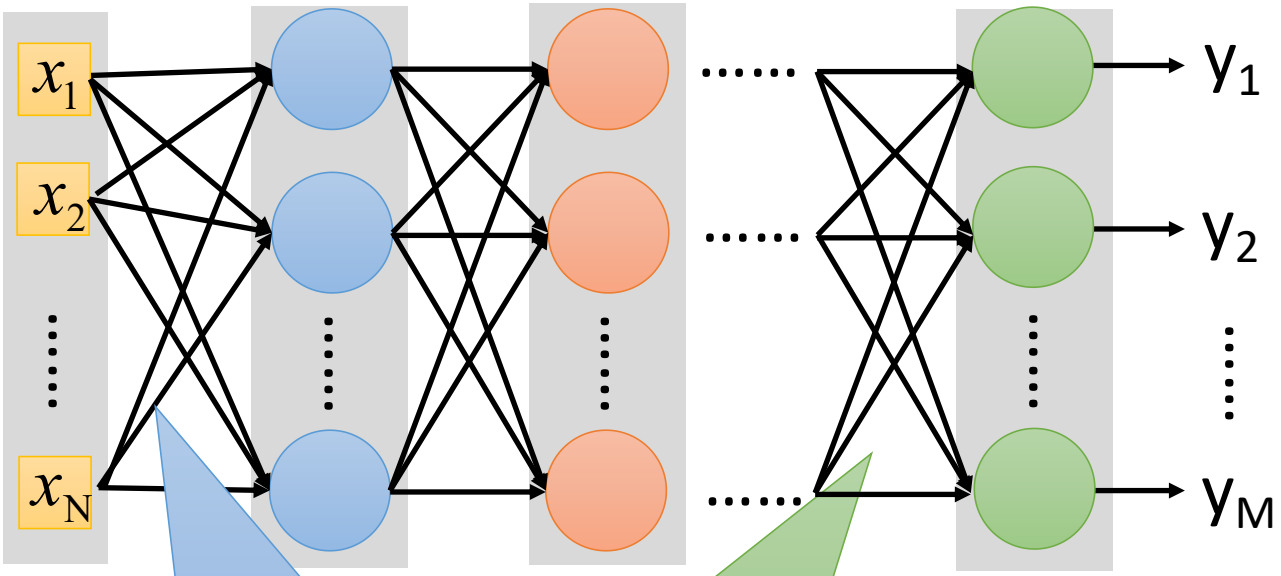
Recipe of Deep Learning



Hard to get the power of Deep …



Vanishing Gradient Problem



Smaller gradients

Learn very slow

Almost random

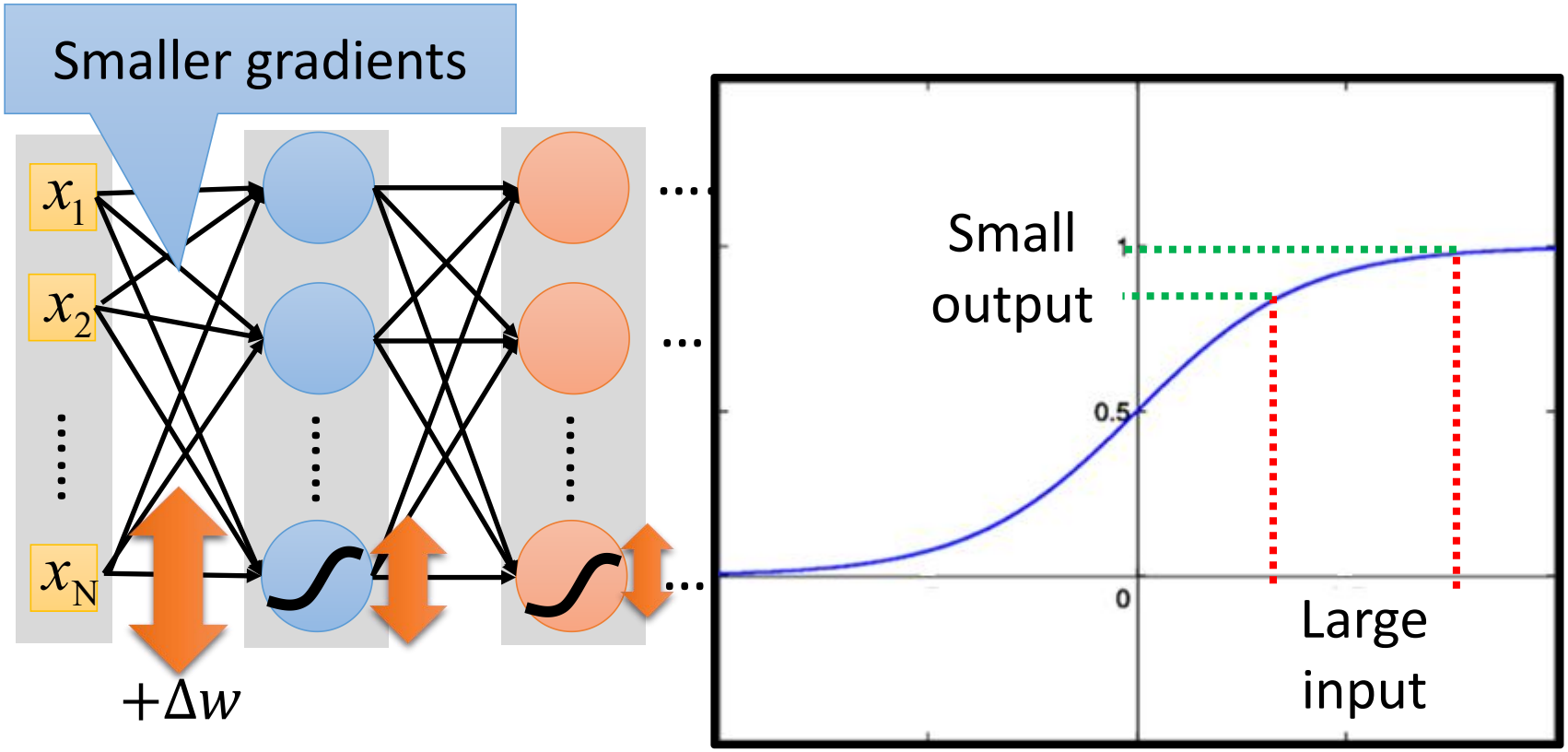
Larger gradients

Learn very fast

Already converge

based on random!?

Vanishing Gradient Problem

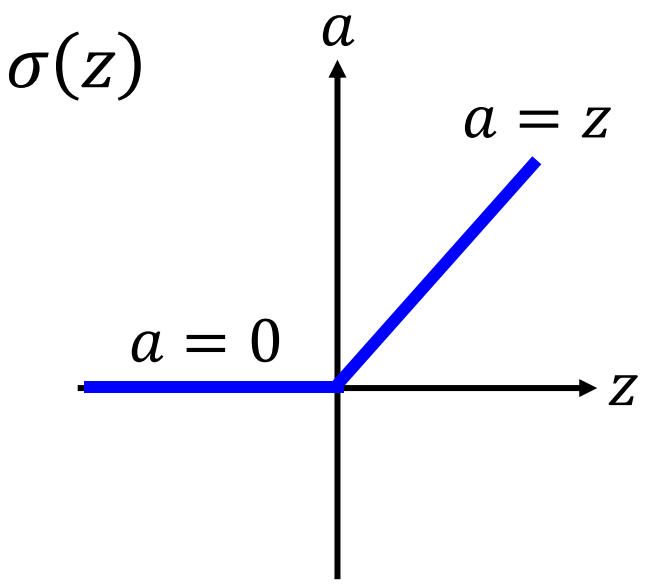


Intuitive way to compute the derivatives …

$$\frac{\partial l}{\partial w} = ? \frac{\Delta l}{\Delta w}$$

ReLU

- Rectified Linear Unit (ReLU)

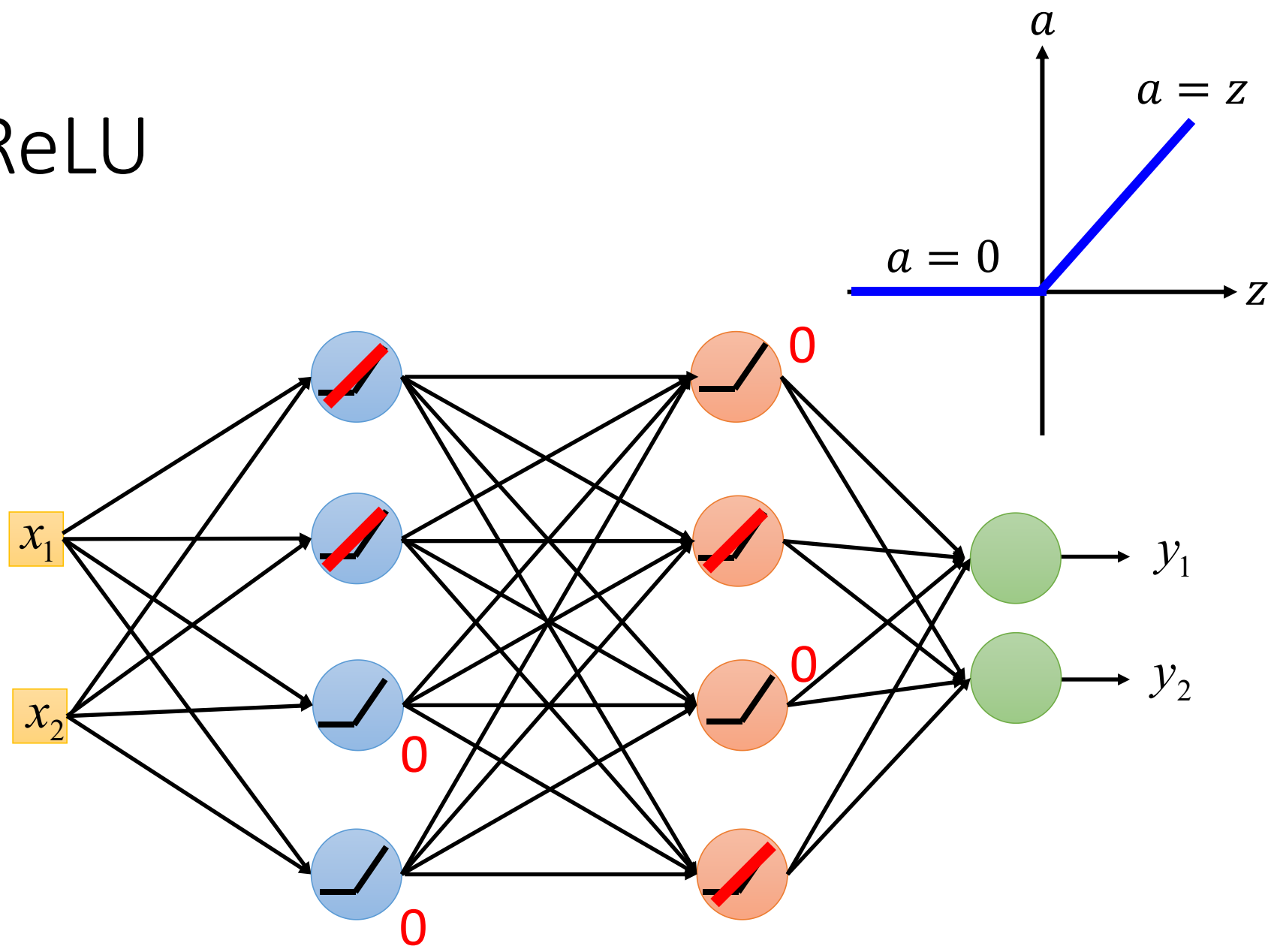


[Xavier Glorot, AISTATS'11]
[Andrew L. Maas, ICML'13]
[Kaiming He, arXiv'15]

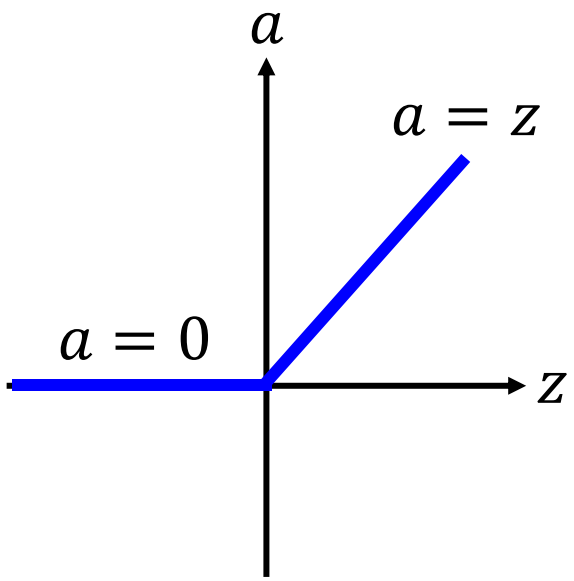
Reason:

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

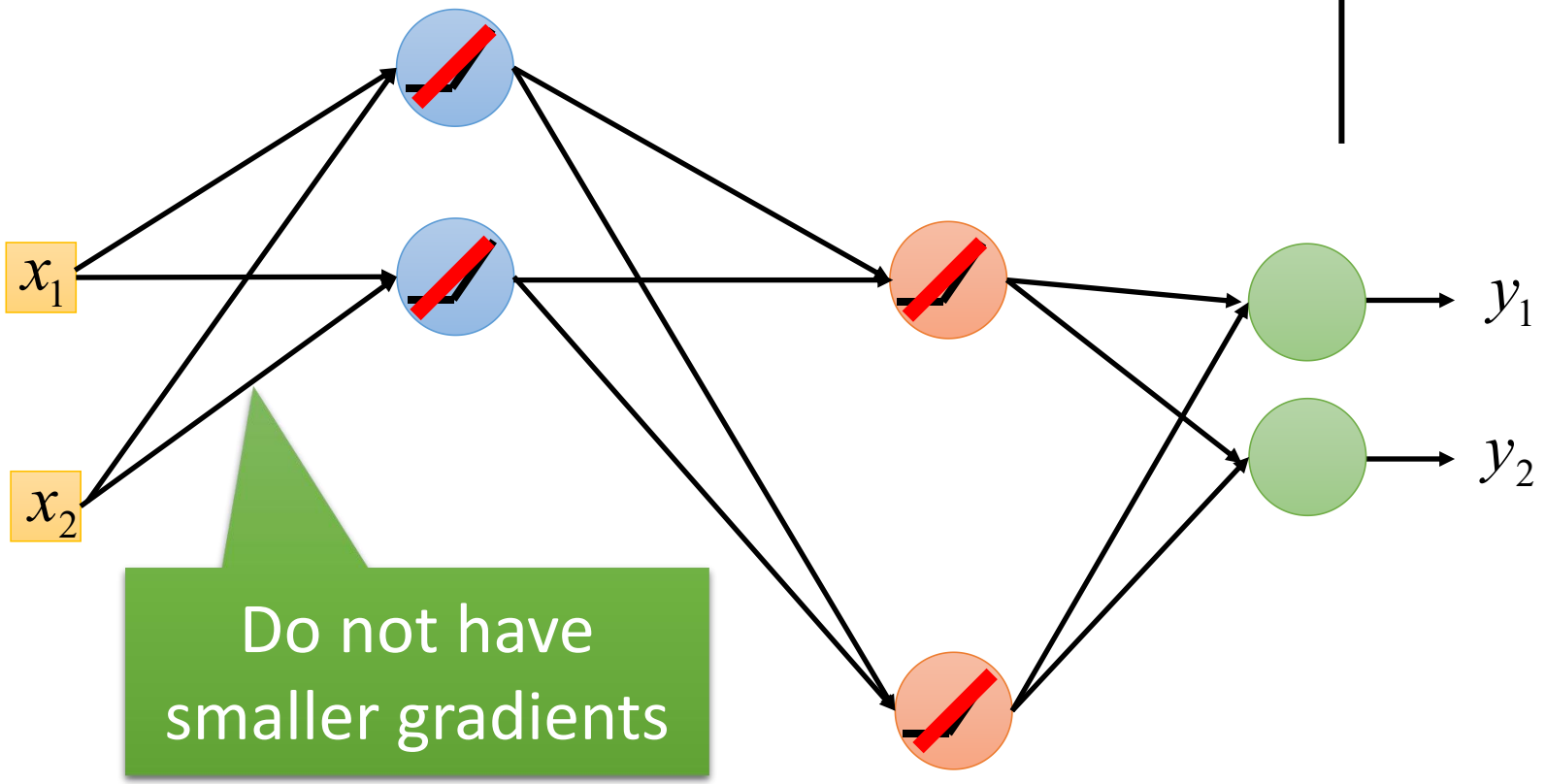
ReLU



ReLU



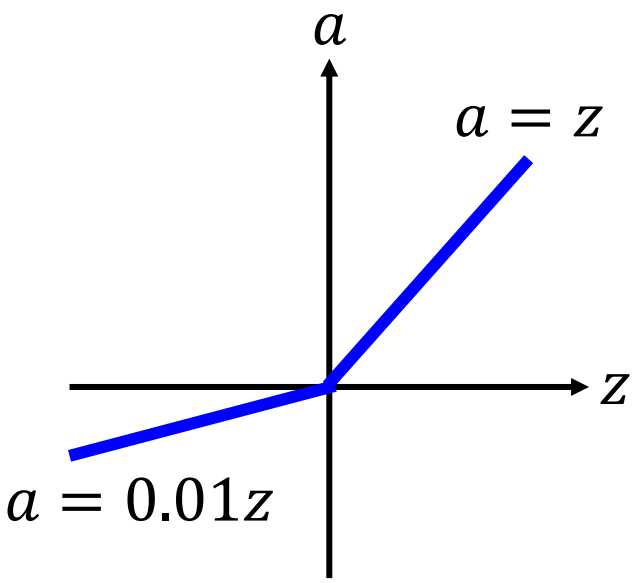
A Thinner linear network



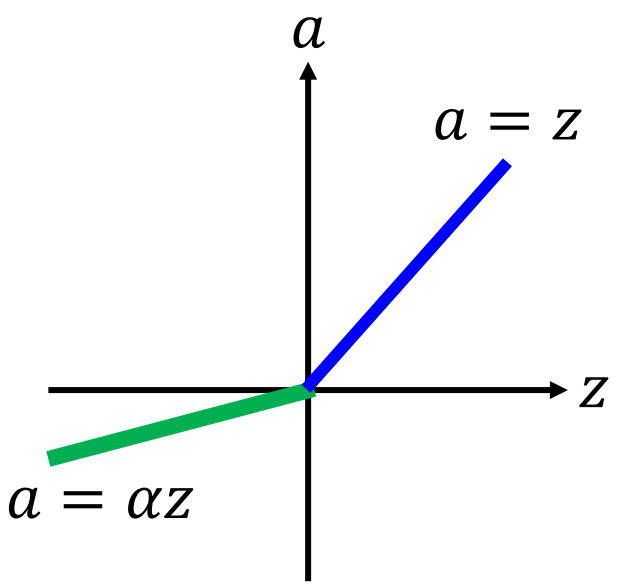
Do not have smaller gradients

ReLU - variant

Leaky ReLU



Parametric ReLU

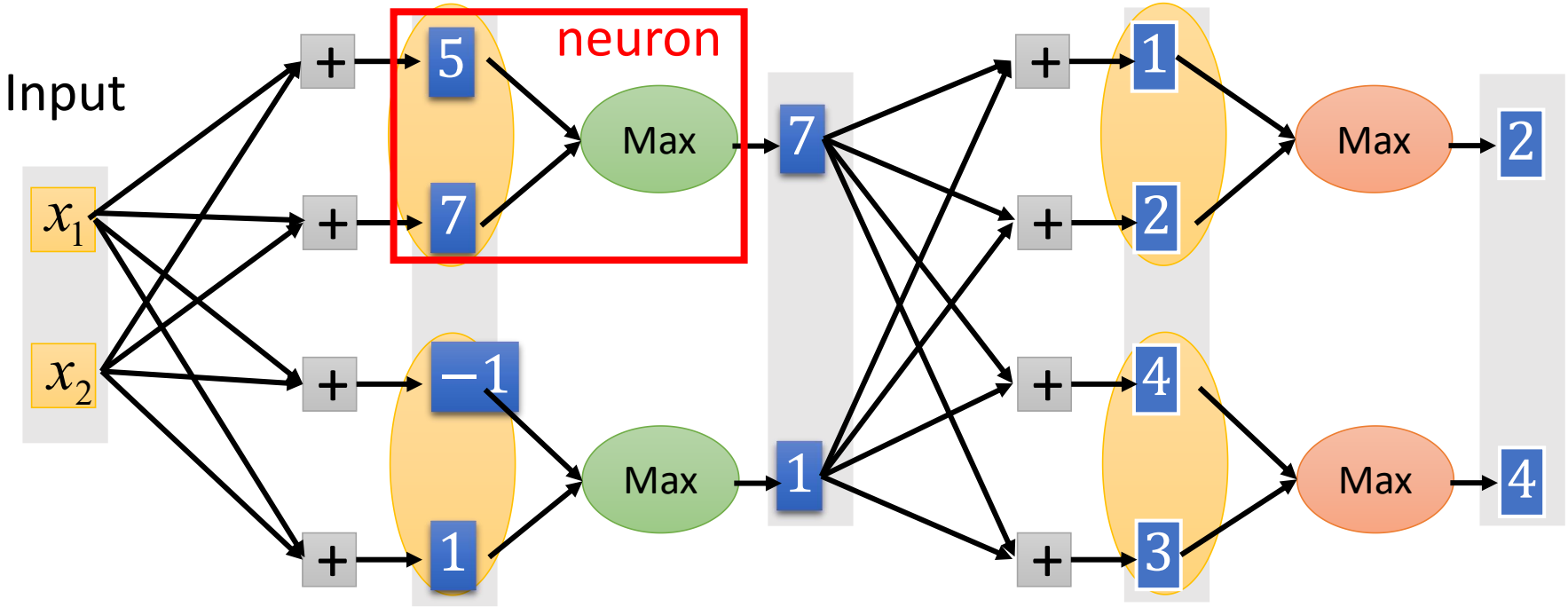


α also learned by gradient descent

Maxout

ReLU is a special cases of Maxout

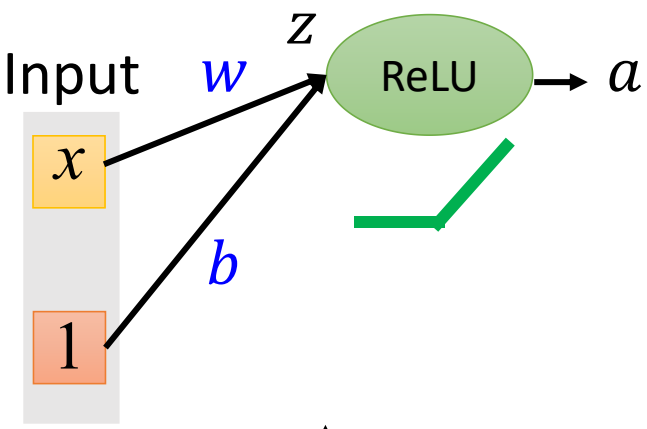
- Learnable activation function [Ian J. Goodfellow, ICML'13]

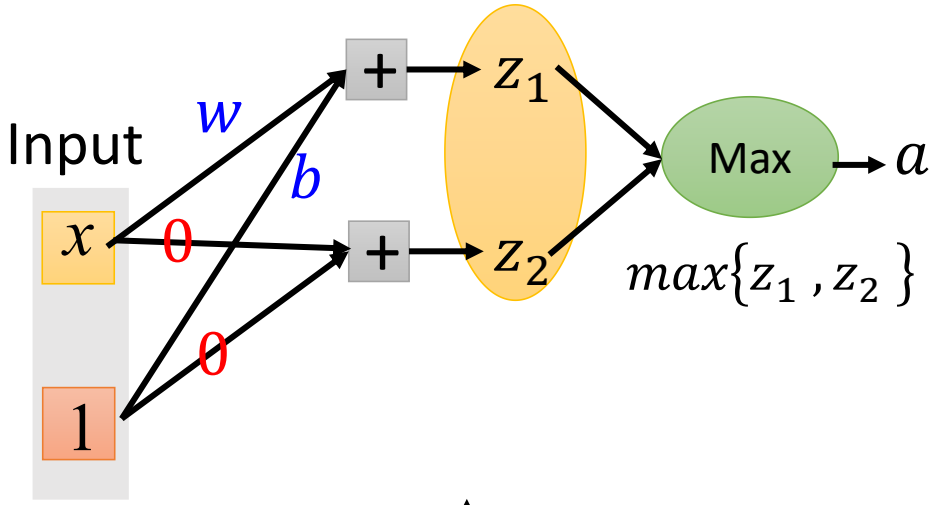


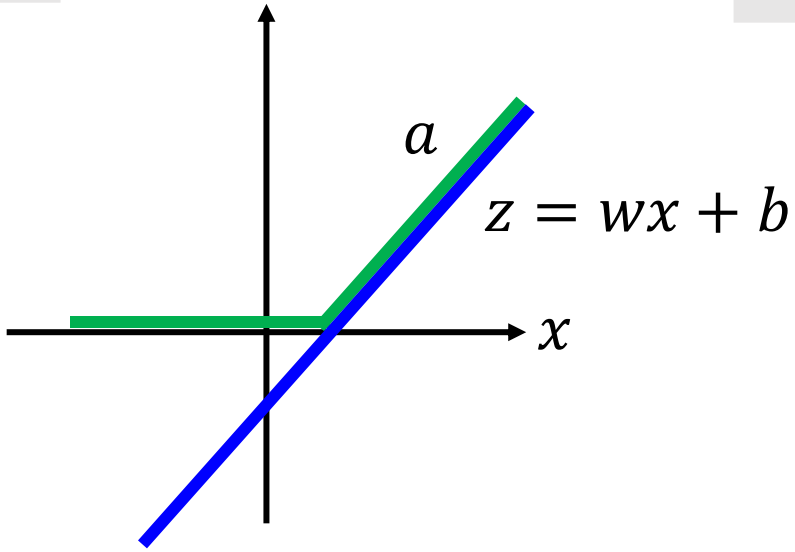
You can have more than 2 elements in a group.

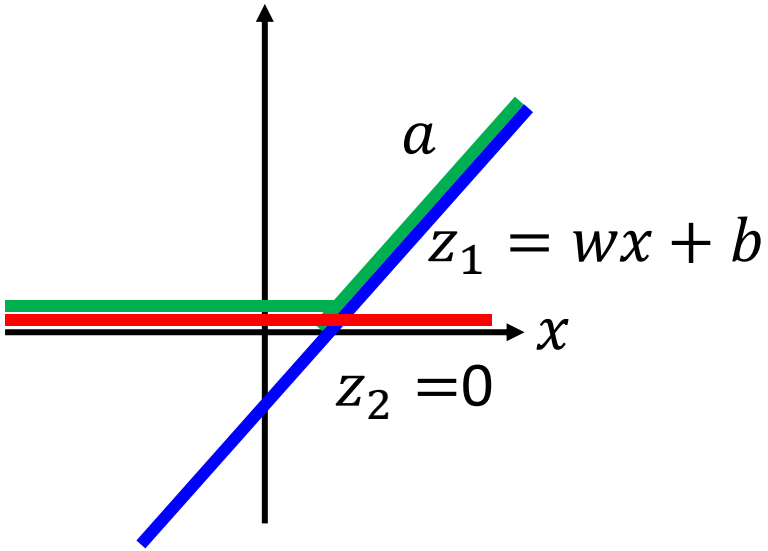
Maxout

ReLU is a special cases of Maxout



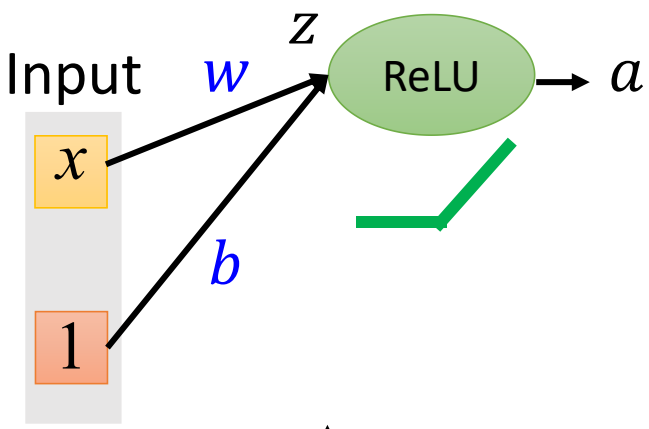


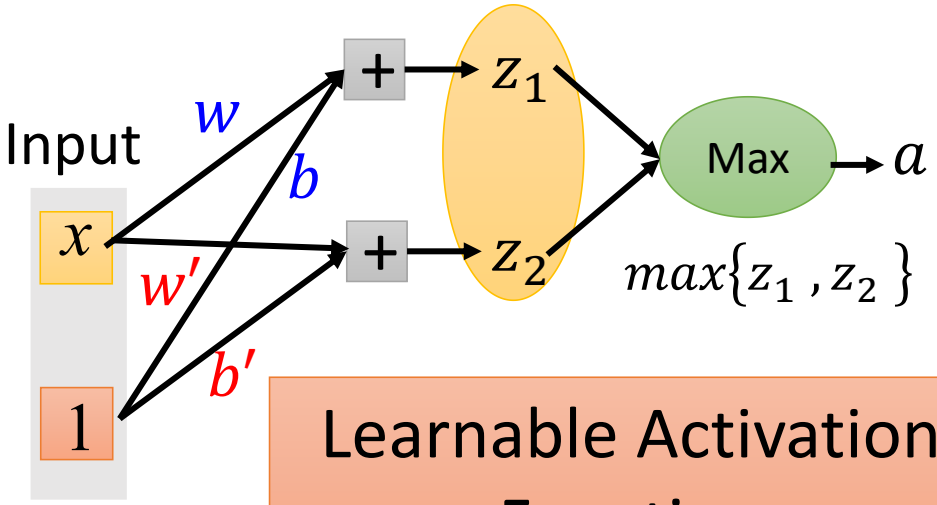




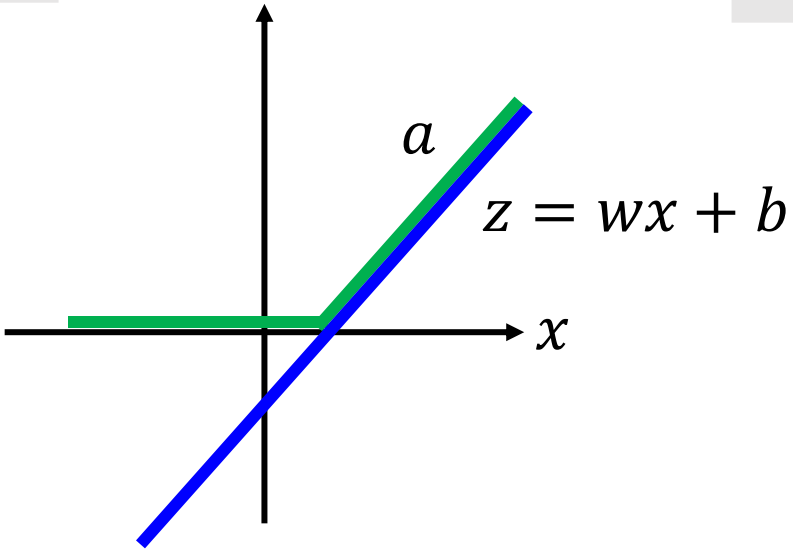
Maxout

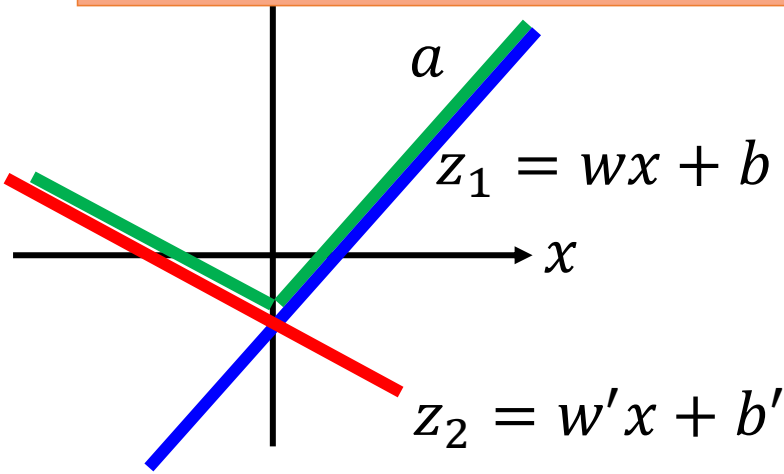
More than ReLU





Learnable Activation Function

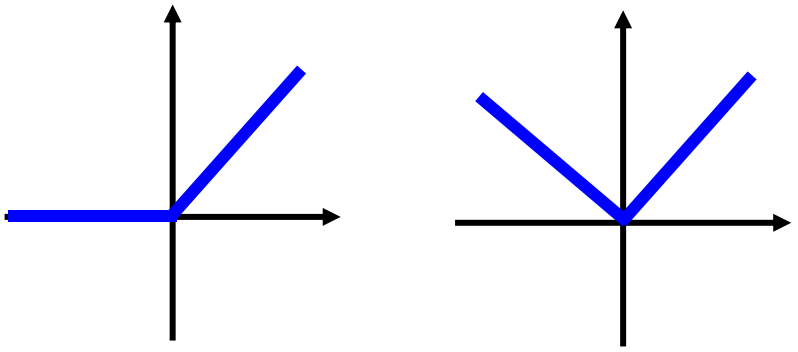




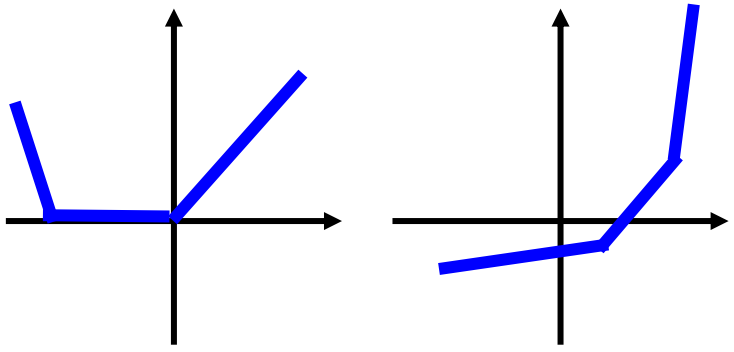
Maxout

- Learnable activation function [Ian J. Goodfellow, ICML'13]
  - Activation function in maxout network can be any piecewise linear convex function
  - How many pieces depending on how many elements in a group

2 elements in a group

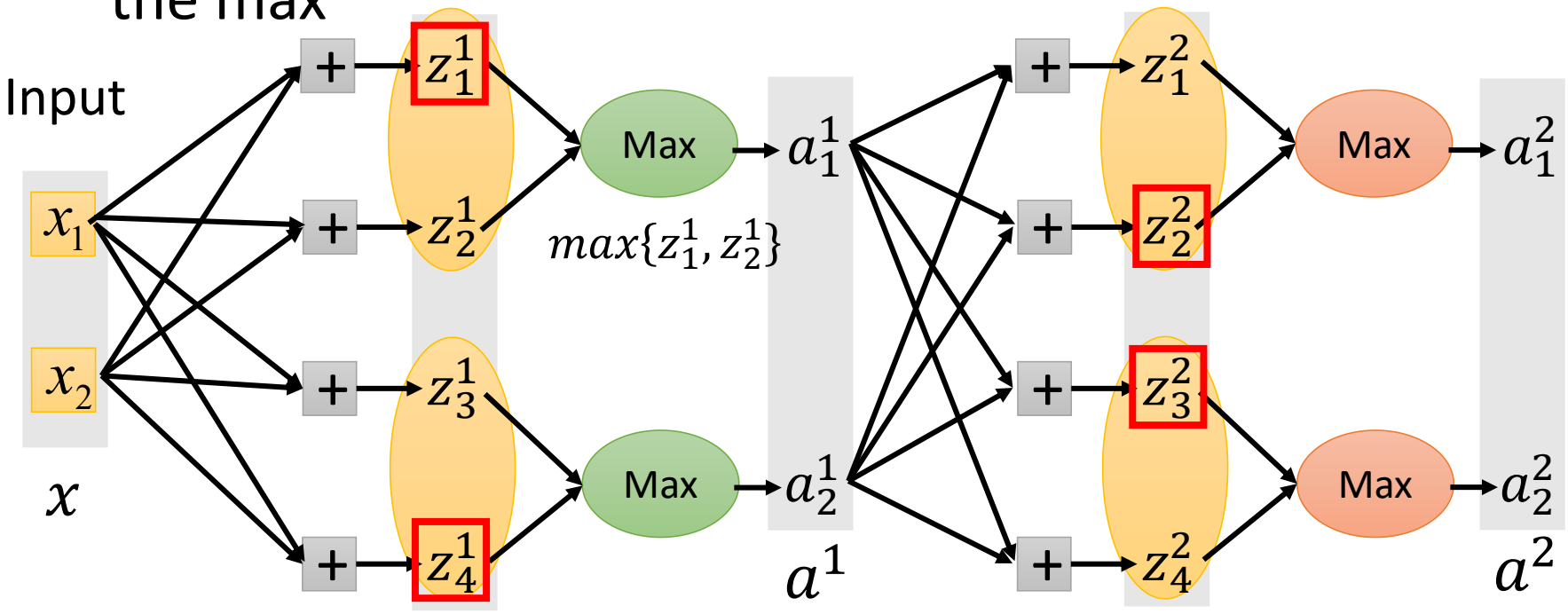


3 elements in a group



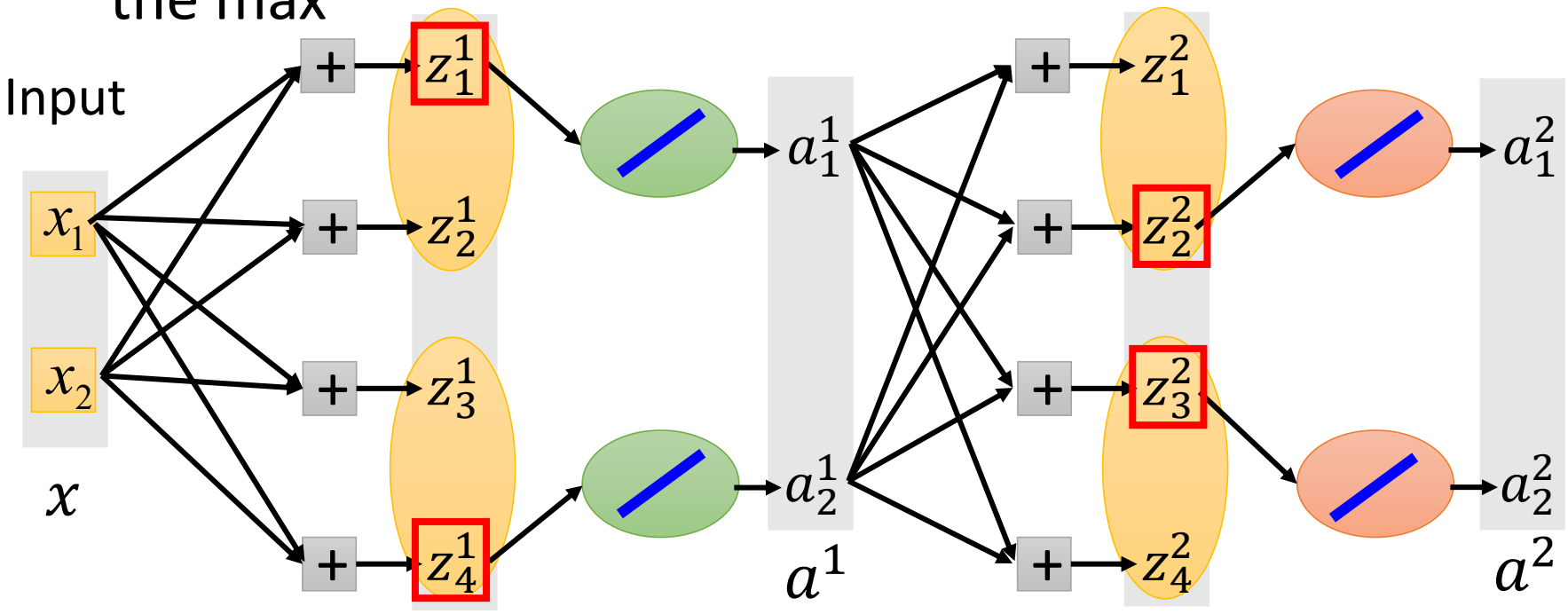
Maxout - Training

- Given a training data x, we know which z would be the max



Maxout - Training

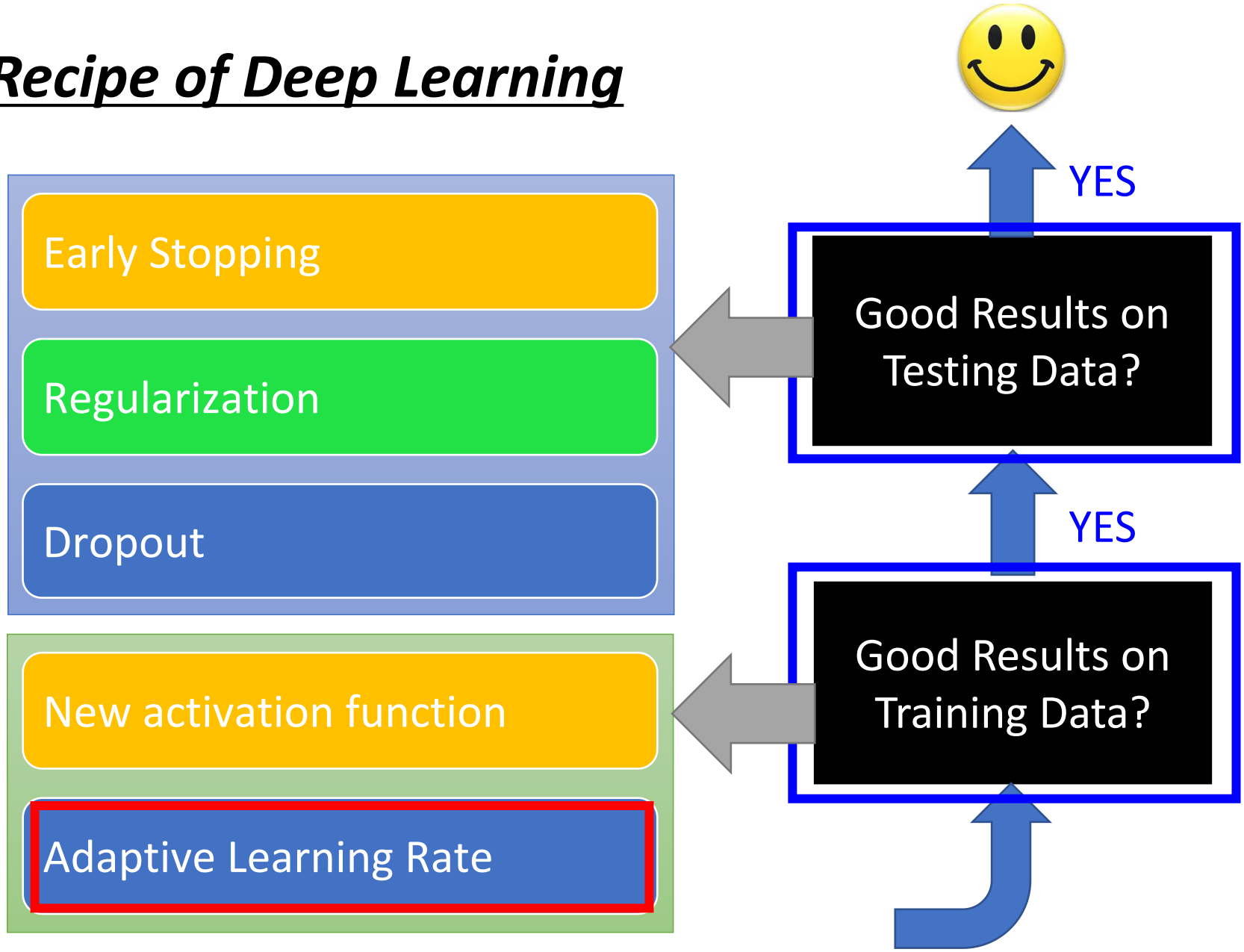
- Given a training data x, we know which z would be the max



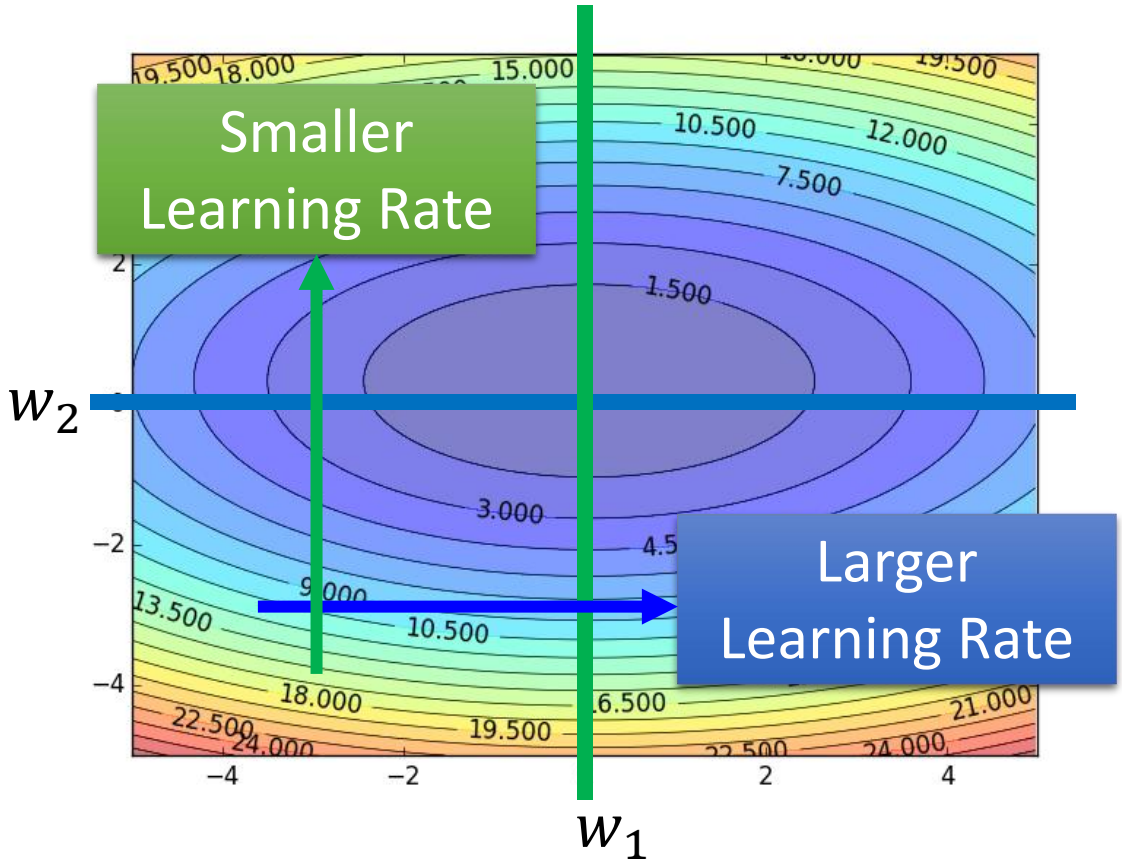
- Train this thin and linear network

Different thin and linear network for different examples

Recipe of Deep Learning



Review



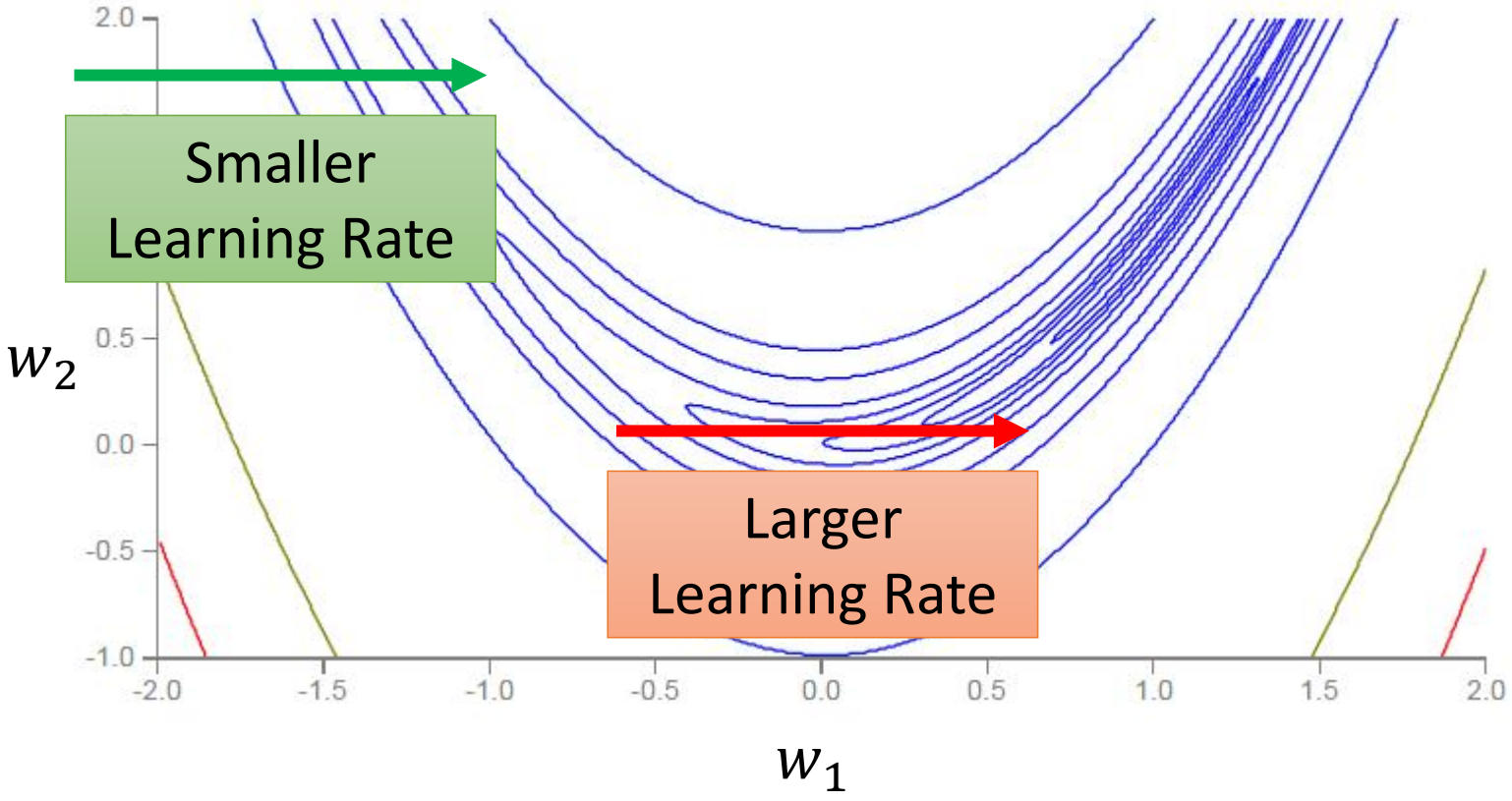
Adagrad

$$w^{t+1} \leftarrow w^t - \frac{\eta}{\sqrt{\sum_{i=0}^{t} (g^i)^2}} g^t$$

Use first derivative to estimate second derivative

RMSProp

Error Surface can be very complex when training NN.



RMSProp

$$w^1 \leftarrow w^0 - \frac{\eta}{\sigma^0} g^0 \qquad \sigma^0 = g^0$$

$$w^2 \leftarrow w^1 - \frac{\eta}{\sigma^1} g^1 \qquad \sigma^1 = \sqrt{\alpha(\sigma^0)^2 + (1-\alpha)(g^1)^2}$$

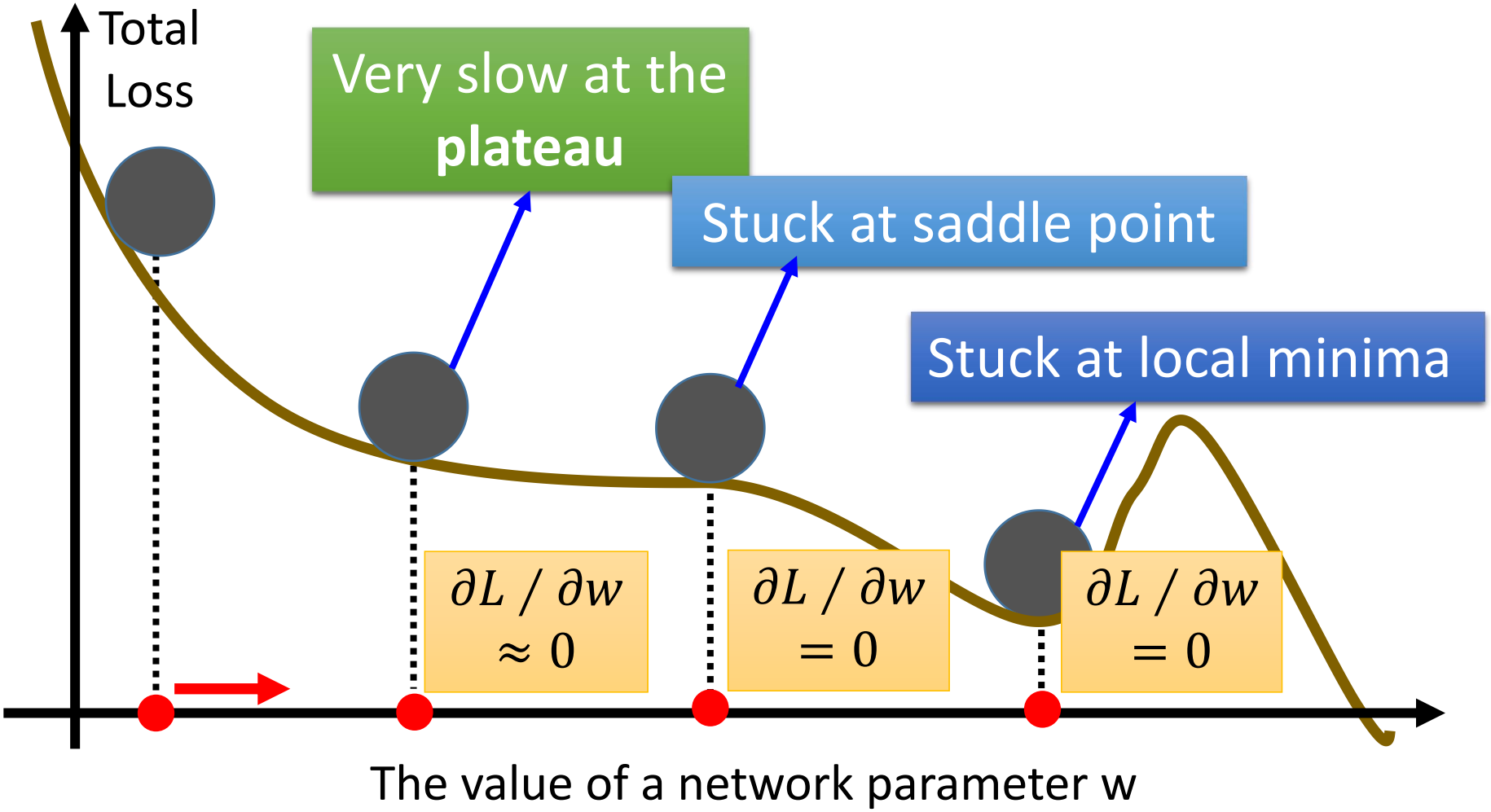
$$w^3 \leftarrow w^2 - \frac{\eta}{\sigma^2} g^2 \qquad \sigma^2 = \sqrt{\alpha(\sigma^1)^2 + (1-\alpha)(g^2)^2}$$

$$\vdots$$

$$w^{t+1} \leftarrow w^t - \frac{\eta}{\sigma^t} g^t \qquad \sigma^t = \sqrt{\alpha(\sigma^{t-1})^2 + (1-\alpha)(g^t)^2}$$

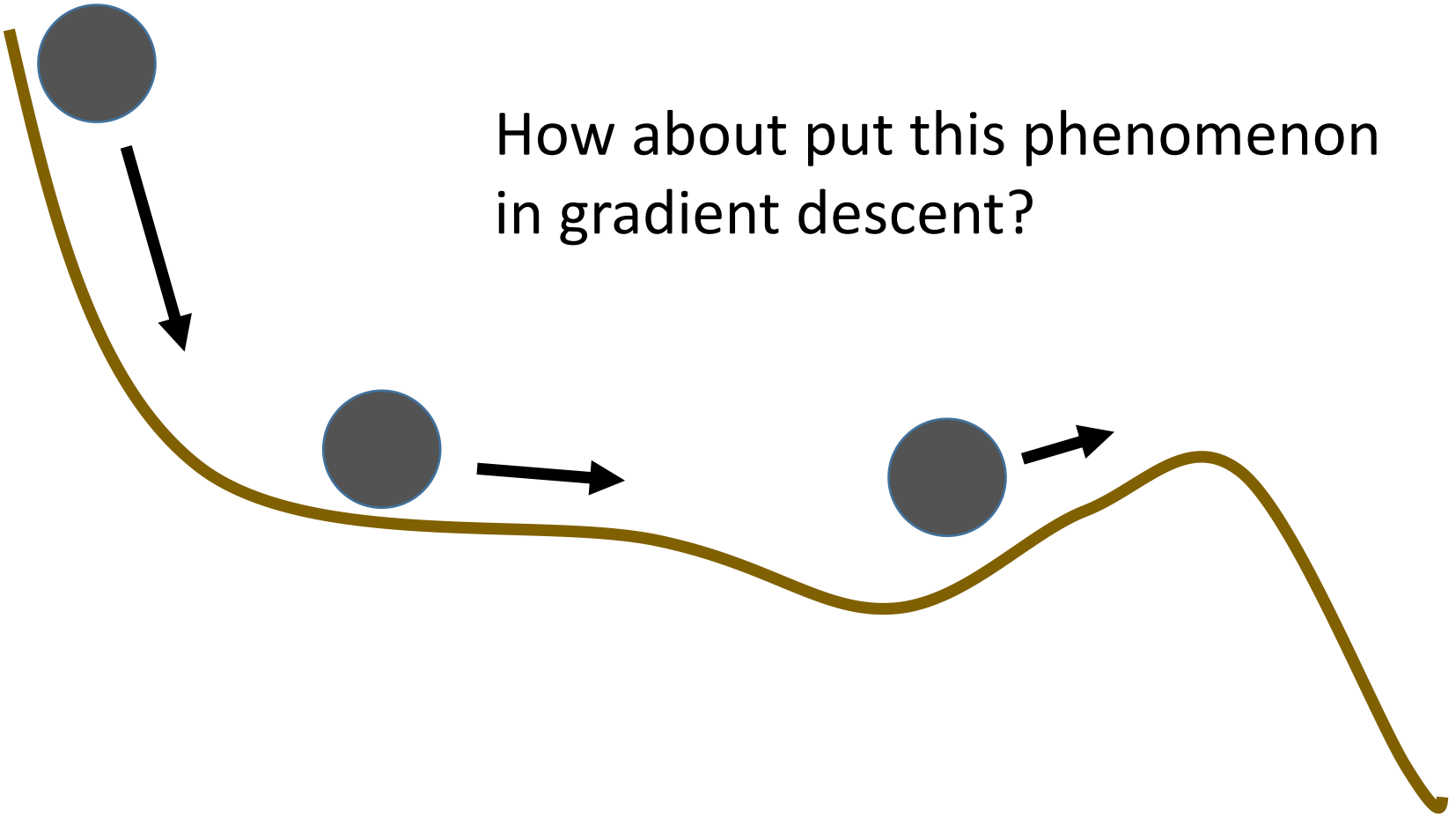
Root Mean Square of the gradients with previous gradients being decayed

Hard to find optimal network parameters



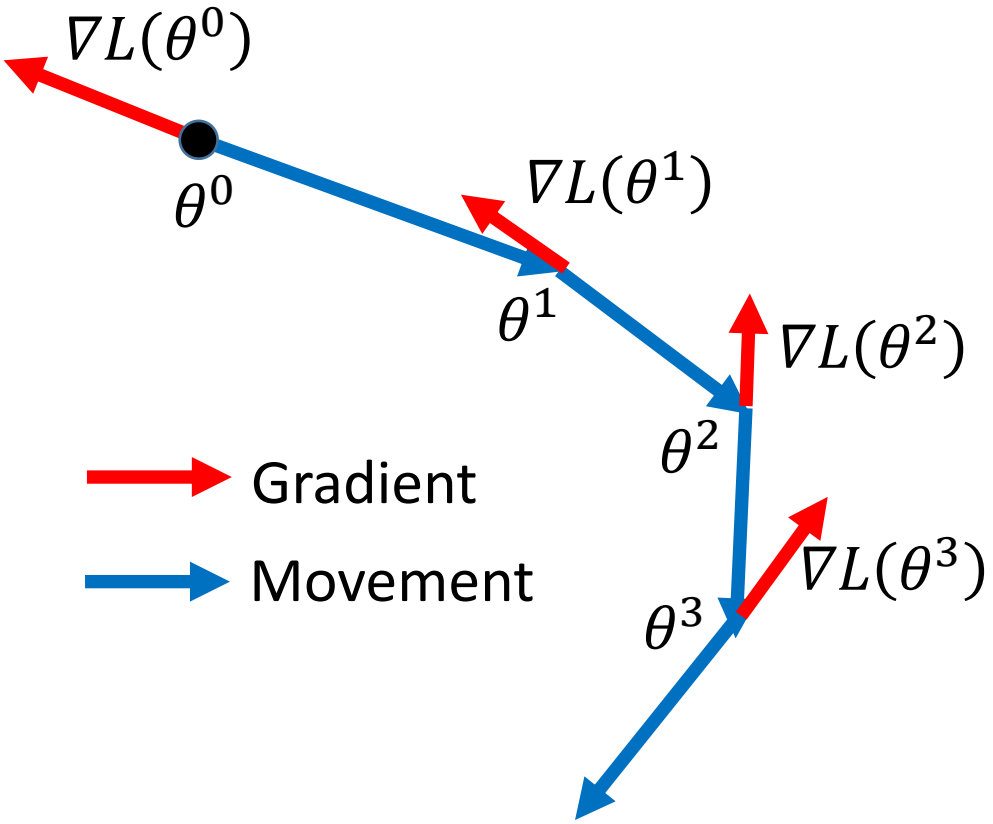
In physical world ……

- Momentum



How about put this phenomenon in gradient descent?

Review: Vanilla Gradient Descent



Start at position θ^0

Compute gradient at θ^0

Move to $\theta^1 = \theta^0 - \eta\nabla L(\theta^0)$

Compute gradient at θ^1

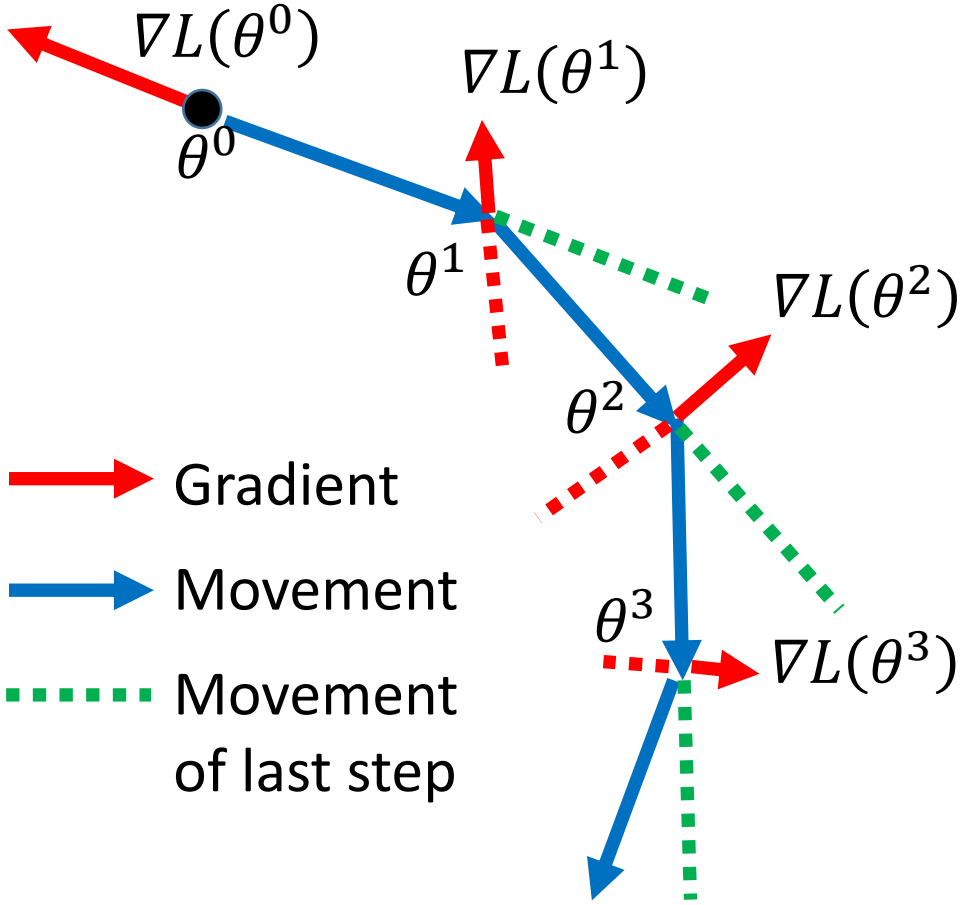
Move to $\theta^2 = \theta^1 - \eta\nabla L(\theta^1)$

⋮

Stop until $\nabla L(\theta^t) \approx 0$

Momentum

Movement: movement of last step minus gradient at present



Start at point θ^0

Movement $v^0=0$

Compute gradient at θ^0

Movement $v^1 = \lambda v^0 - \eta \nabla L(\theta^0)$

Move to $\theta^1 = \theta^0 + v^1$

Compute gradient at θ^1

Movement $v^2 = \lambda v^1 - \eta \nabla L(\theta^1)$

Move to $\theta^2 = \theta^1 + v^2$

Movement not just based on gradient, but previous movement.

Momentum

Movement: movement of last step minus gradient at present

v^i is actually the weighted sum of all the previous gradient: $\nabla L(\theta^0), \nabla L(\theta^1), \ldots \nabla L(\theta^{i-1})$

$v^0 = 0$

$v^1 = -\eta \nabla L(\theta^0)$

$v^2 = -\lambda \eta \nabla L(\theta^0) - \eta \nabla L(\theta^1)$

⋮

Start at point θ^0

Movement $v^0=0$

Compute gradient at θ^0

Movement $v^1 = \lambda v^0 - \eta \nabla L(\theta^0)$

Move to $\theta^1 = \theta^0 + v^1$

Compute gradient at θ^1

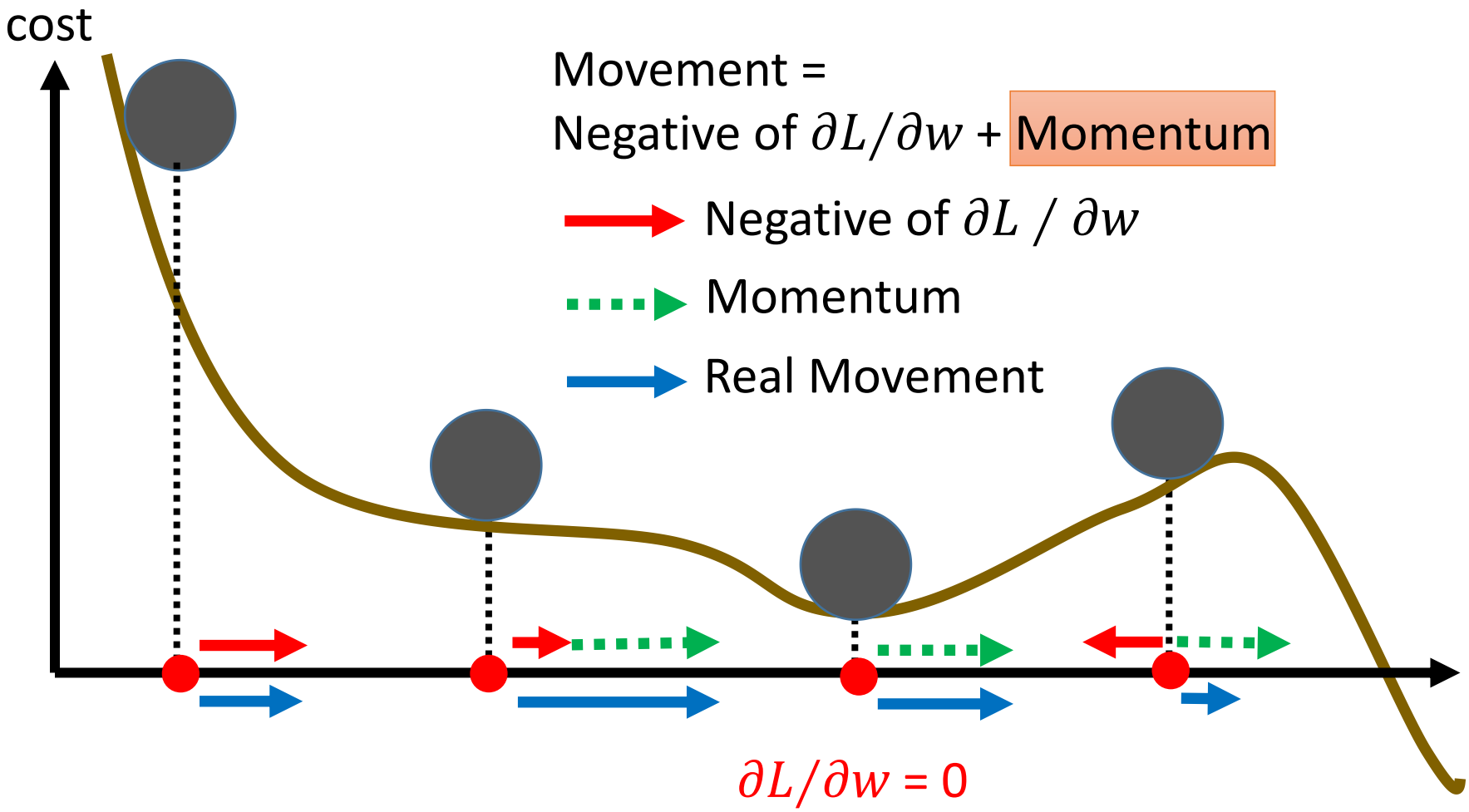
Movement $v^2 = \lambda v^1 - \eta \nabla L(\theta^1)$

Move to $\theta^2 = \theta^1 + v^2$

Movement not just based on gradient, but previous movement

Momentum

Still not guarantee reaching global minima, but give some hope ……



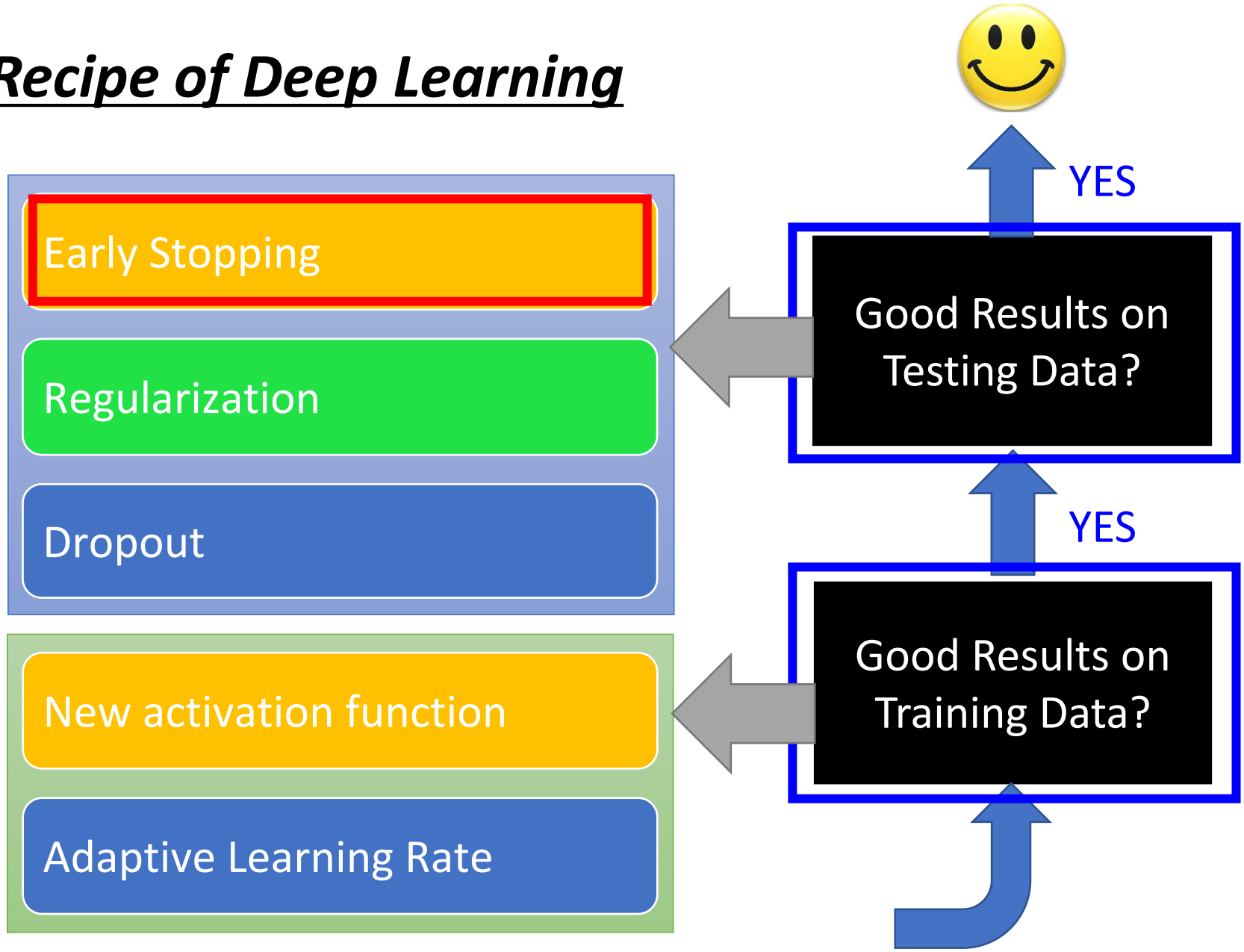
Adam

RMSProp + Momentum

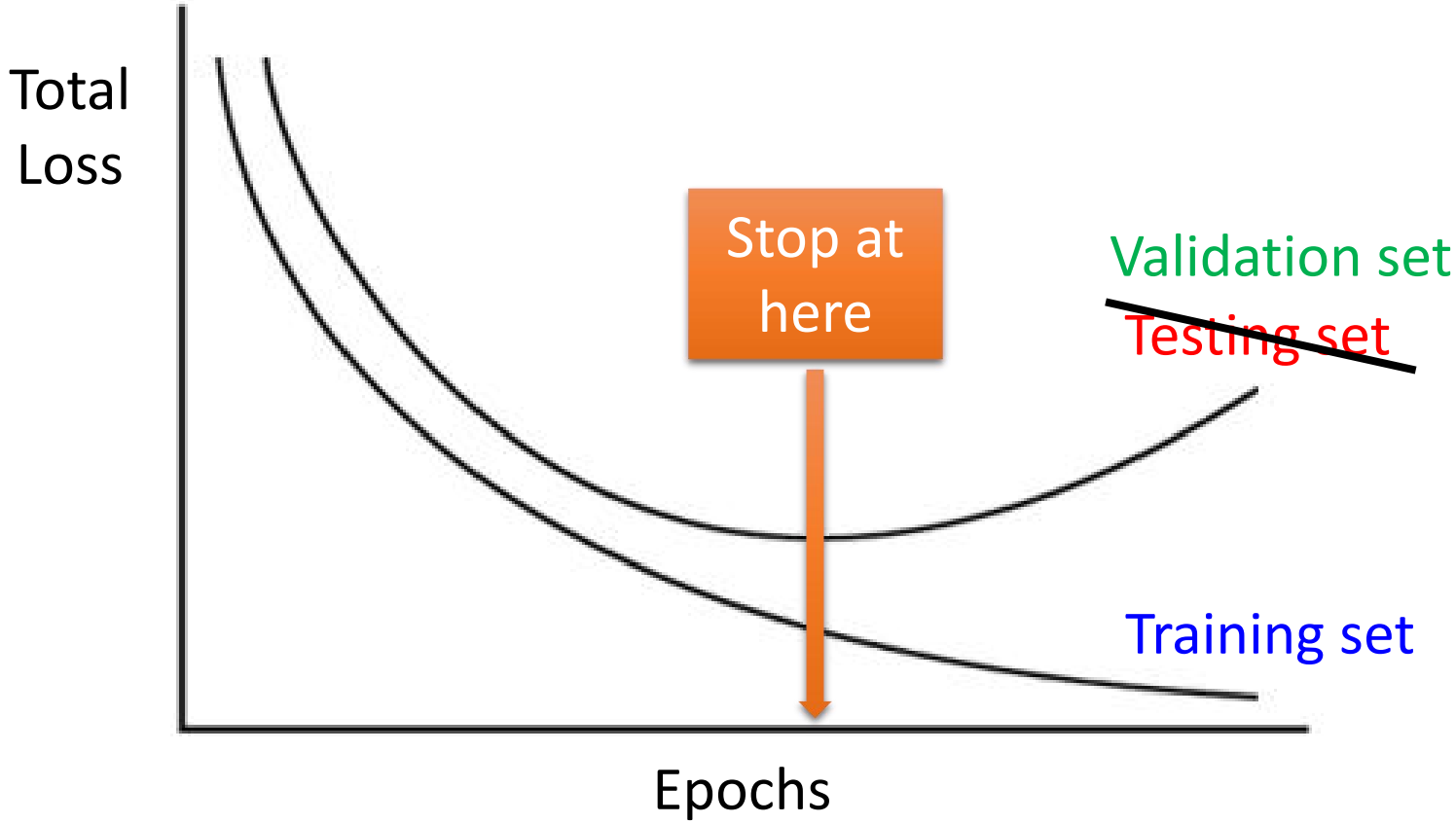
Algorithm 1: *Adam*, our proposed algorithm for stochastic optimization. See section 2 for details, and for a slightly more efficient (but less clear) order of computation. g_t^2 indicates the elementwise square $g_t \odot g_t$. Good default settings for the tested machine learning problems are $\alpha = 0.001$, $\beta_1 = 0.9$, $\beta_2 = 0.999$ and $\epsilon = 10^{-8}$. All operations on vectors are element-wise. With β_1^t and β_2^t we denote β_1 and β_2 to the power t.

Require: α: Stepsize
Require: $\beta_1, \beta_2 \in [0, 1)$: Exponential decay rates for the moment estimates
Require: $f(\theta)$: Stochastic objective function with parameters θ
Require: θ_0: Initial parameter vector
$m_0 \leftarrow 0$ (Initialize 1st moment vector) → for momentum
$v_0 \leftarrow 0$ (Initialize 2nd moment vector) → for RMSprop
$t \leftarrow 0$ (Initialize timestep)
while θ_t not converged **do**
$t \leftarrow t + 1$
$g_t \leftarrow \nabla_\theta f_t(\theta_{t-1})$ (Get gradients w.r.t. stochastic objective at timestep t)
$m_t \leftarrow \beta_1 \cdot m_{t-1} + (1 - \beta_1) \cdot g_t$ (Update biased first moment estimate)
$v_t \leftarrow \beta_2 \cdot v_{t-1} + (1 - \beta_2) \cdot g_t^2$ (Update biased second raw moment estimate)
$\widehat{m}_t \leftarrow m_t / (1 - \beta_1^t)$ (Compute bias-corrected first moment estimate)
$\widehat{v}_t \leftarrow v_t / (1 - \beta_2^t)$ (Compute bias-corrected second raw moment estimate)
$\theta_t \leftarrow \theta_{t-1} - \alpha \cdot \widehat{m}_t / (\sqrt{\widehat{v}_t} + \epsilon)$ (Update parameters)
end while
return θ_t (Resulting parameters)

Recipe of Deep Learning

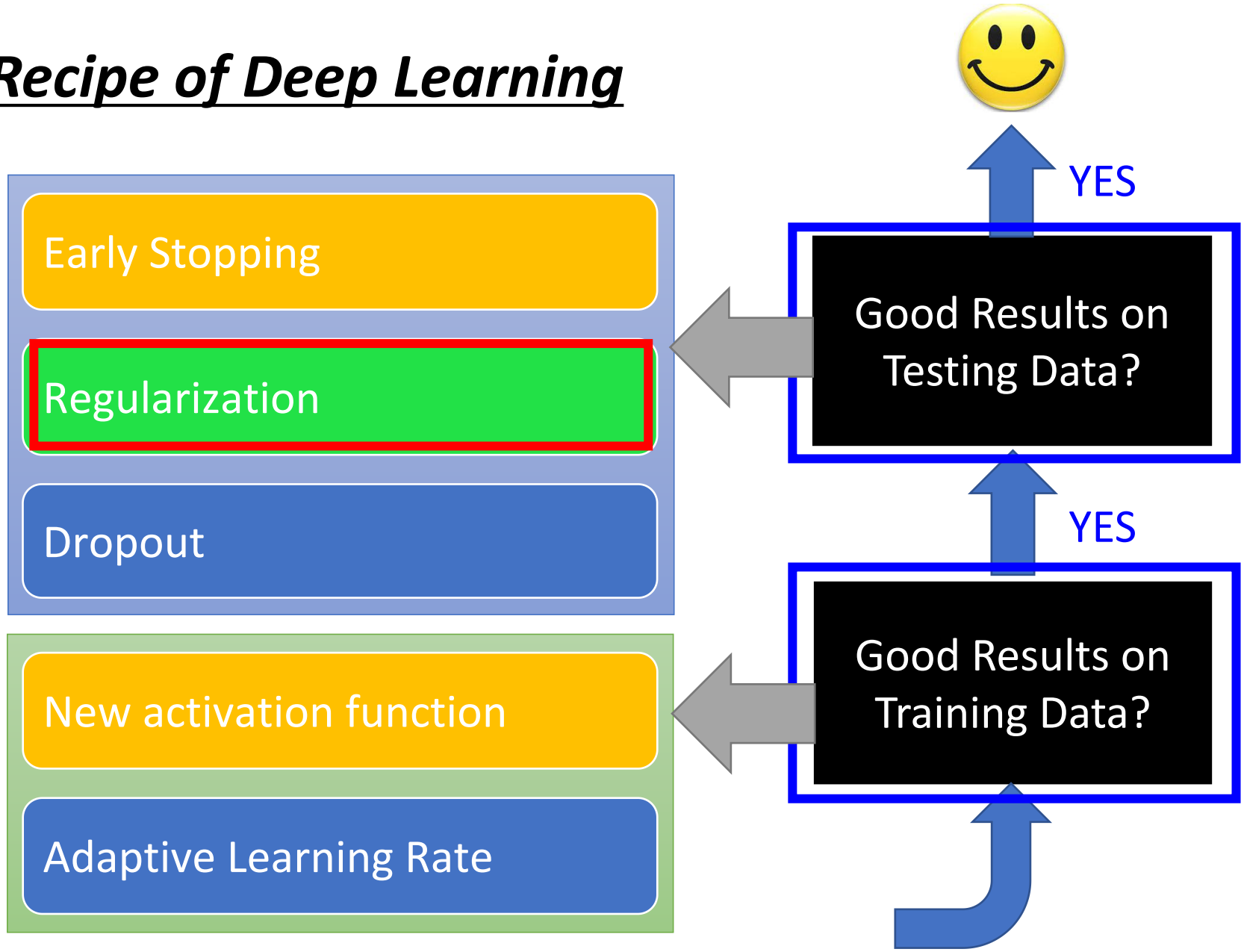


Early Stopping



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

Recipe of Deep Learning



Regularization

- New loss function to be minimized
  - 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)

Regularization

L2 regularization:

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

- New loss function to be minimized

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

Gradient: $\frac{\partial L'}{\partial w} = \frac{\partial L}{\partial w} + \lambda w$

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

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

Weight Decay

Closer to zero

Regularization

L1 regularization:

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

- New loss function to be minimized

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

Update:

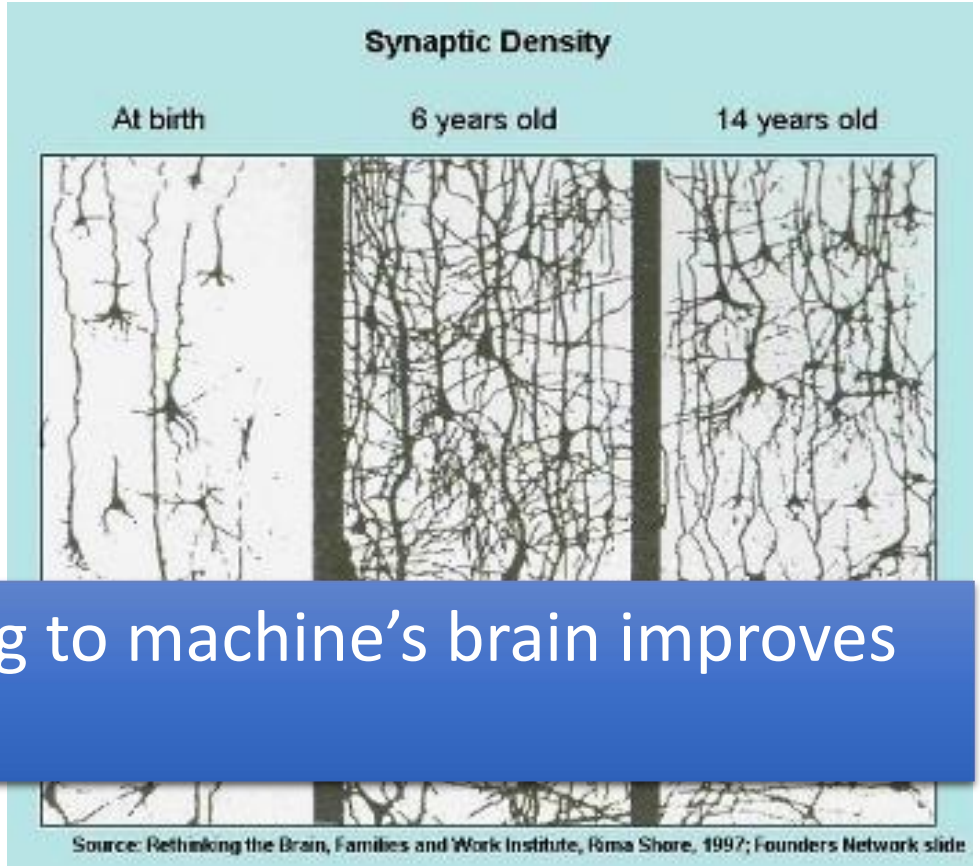
$$w^{t+1} \rightarrow w^t - \eta \frac{\partial L'}{\partial w} = w^t - \eta \left(\frac{\partial L}{\partial w} + \lambda \, \mathrm{sgn}(w^t) \right)$$

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

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

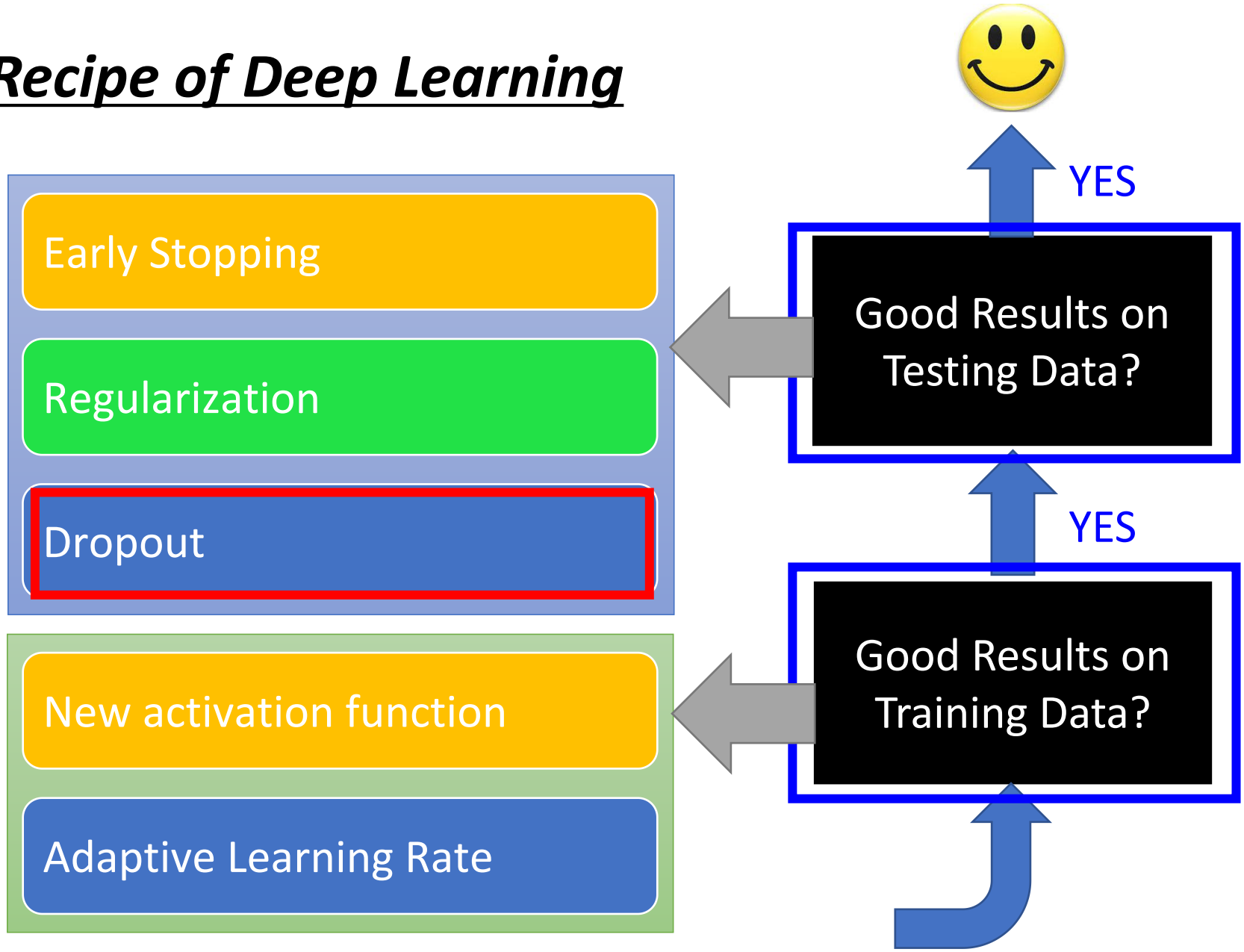
Regularization - Weight Decay

- Our brain prunes out the useless link between neurons.



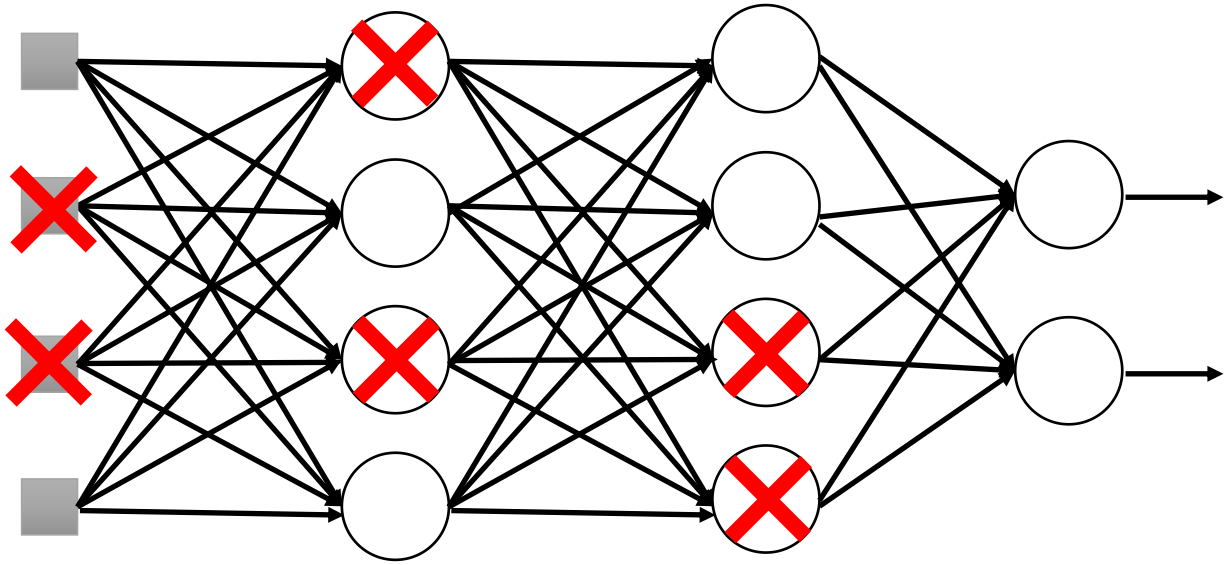
Doing the same thing to machine's brain improves the performance.

Recipe of Deep Learning



Dropout

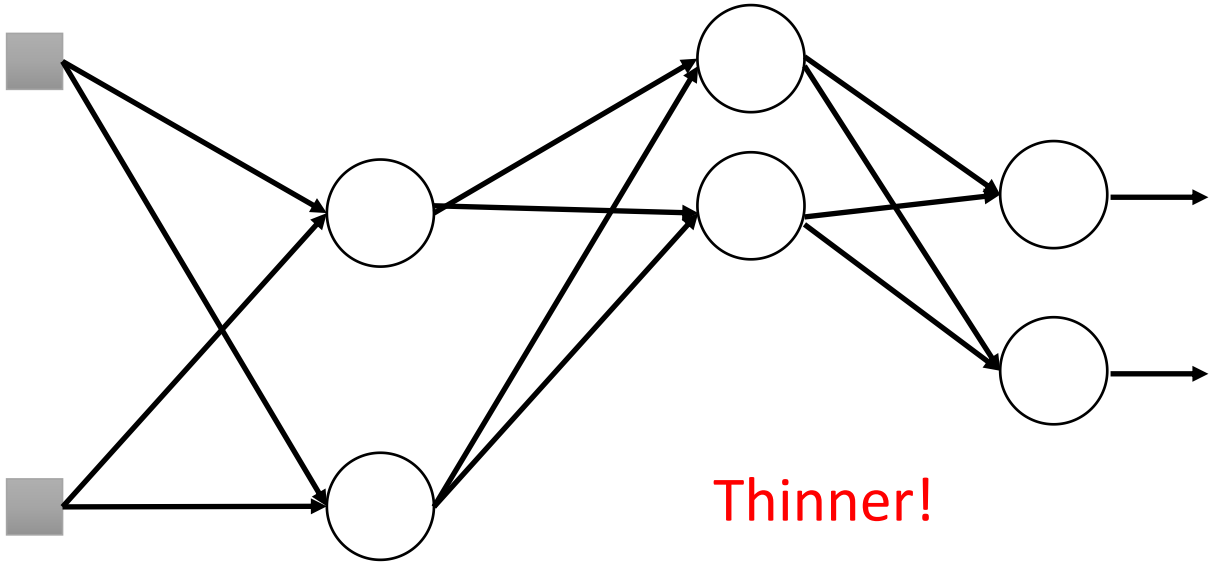
Training:



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

Dropout

Training:



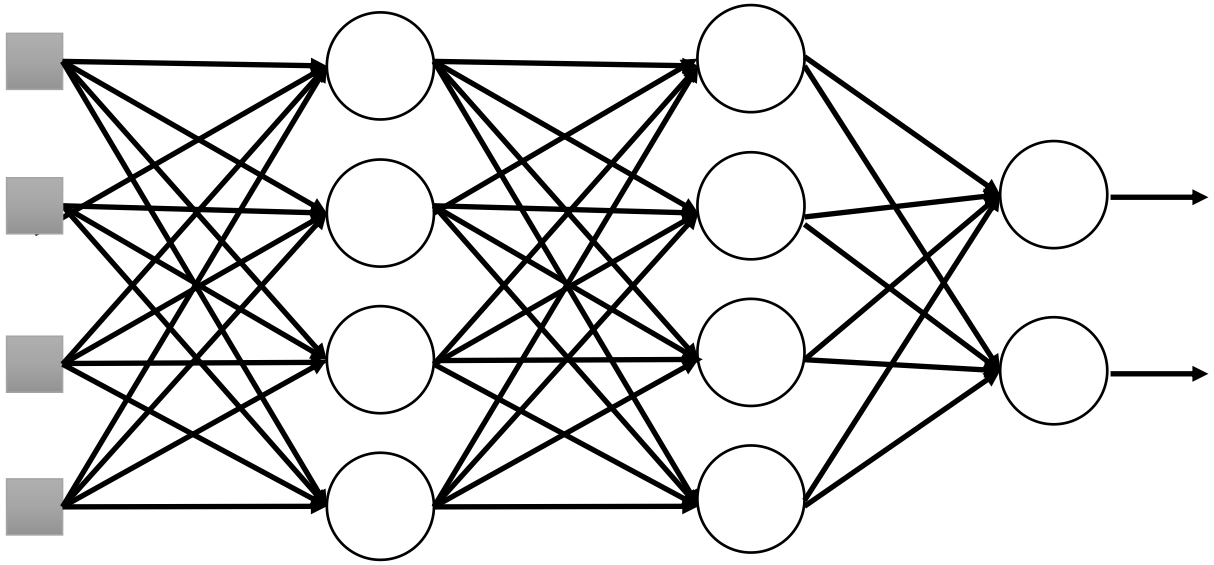
- **Each time before updating the parameters**
  - Each neuron has p% to dropout

    The structure of the network is changed.
  - Using the new network for training

For each mini-batch, we resample the dropout neurons

Dropout

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.

Dropout
- Intuitive Reason

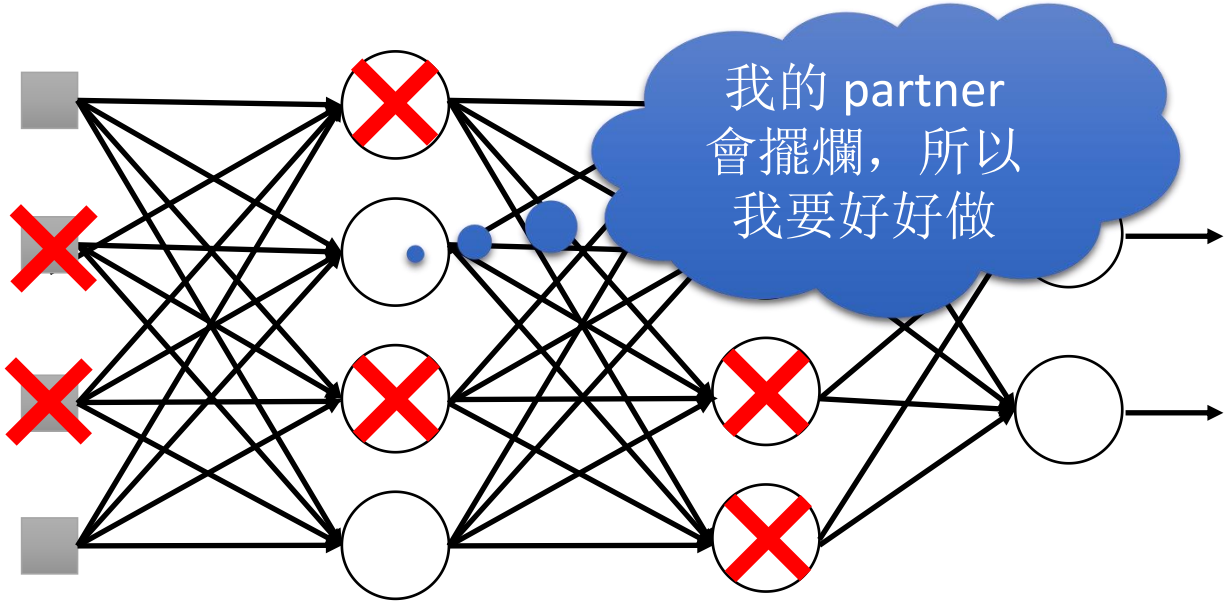
Testing

No dropout
(拿下重物後就變很強)

Training

Dropout (腳上綁重物)

Dropout - Intuitive Reason



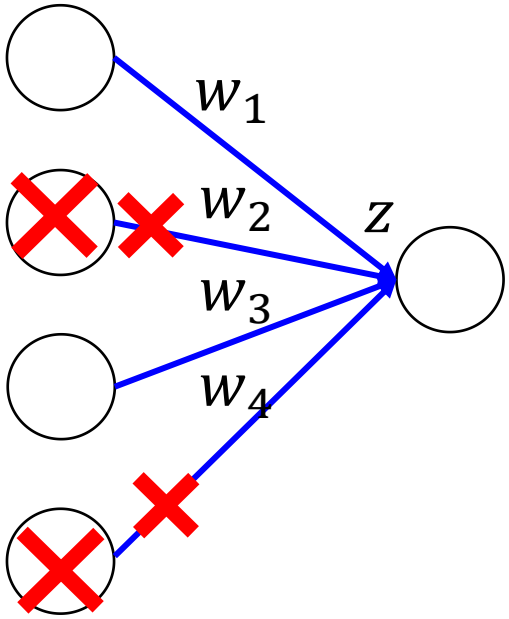
- When teams up, if everyone expect the partner will do the work, nothing will be done finally.
- However, if you know your partner will dropout, you will do better.
- When testing, no one dropout actually, so obtaining good results eventually.

Dropout - Intuitive Reason

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

Training of Dropout

Assume dropout rate is 50%

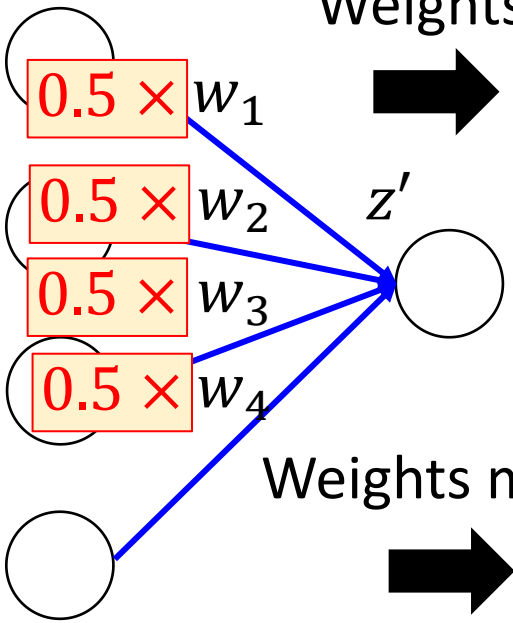


Testing of Dropout

No dropout

Weights from training

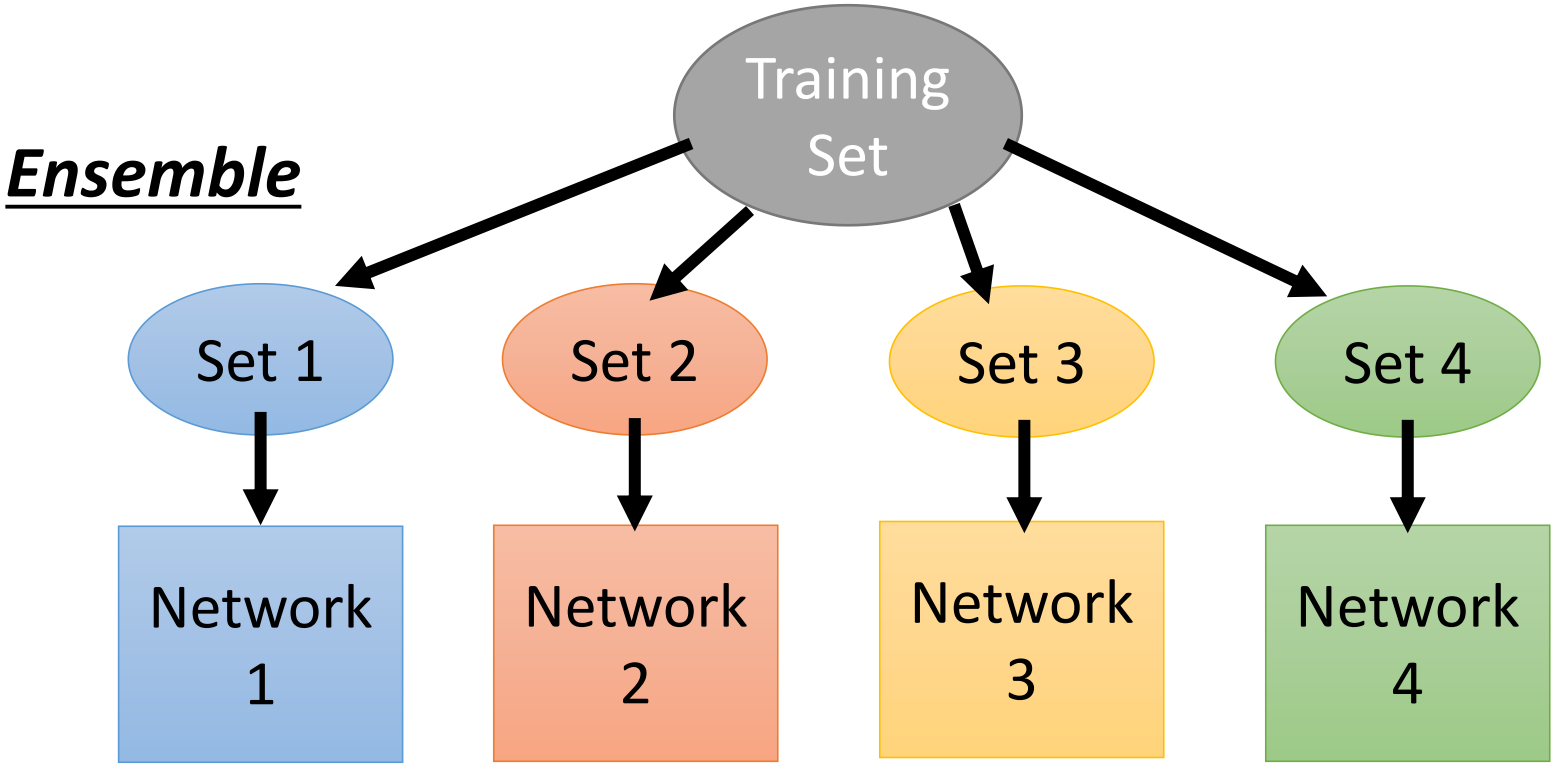
$z' \approx 2z$



Weights multiply 1-p%

$z' \approx z$

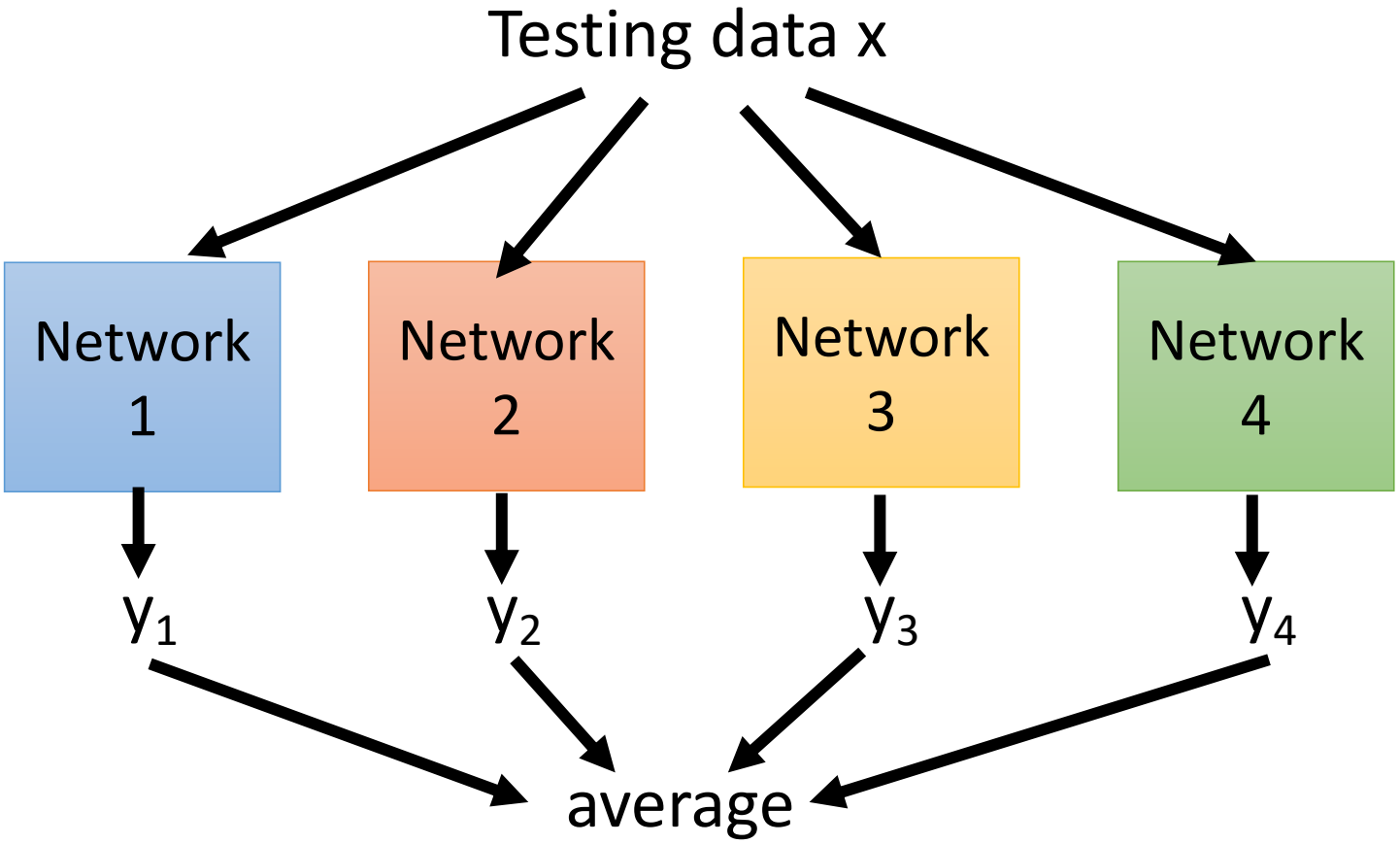
Dropout is a kind of ensemble.



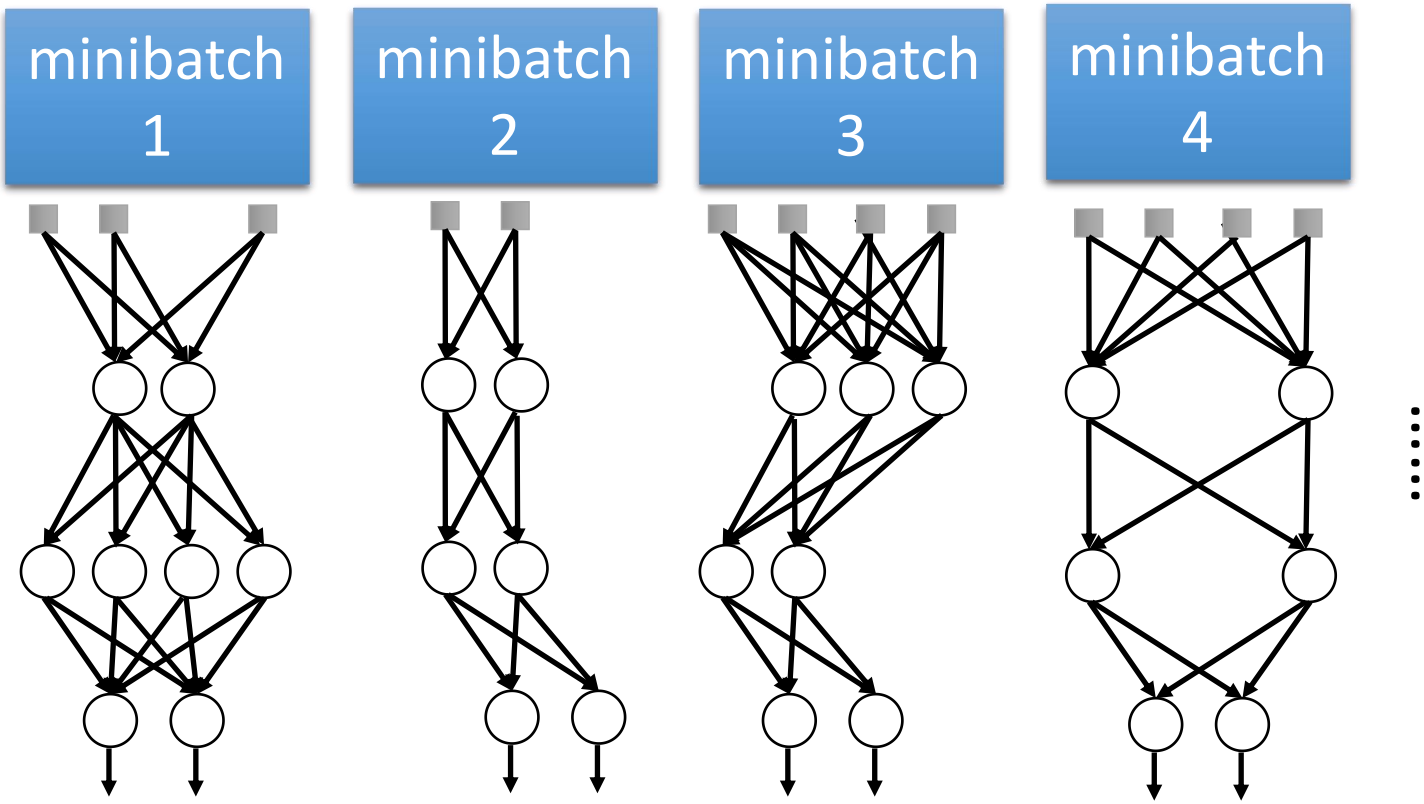
Train a bunch of networks with different structures

Dropout is a kind of ensemble.

Ensemble



Dropout is a kind of ensemble.



Training of Dropout

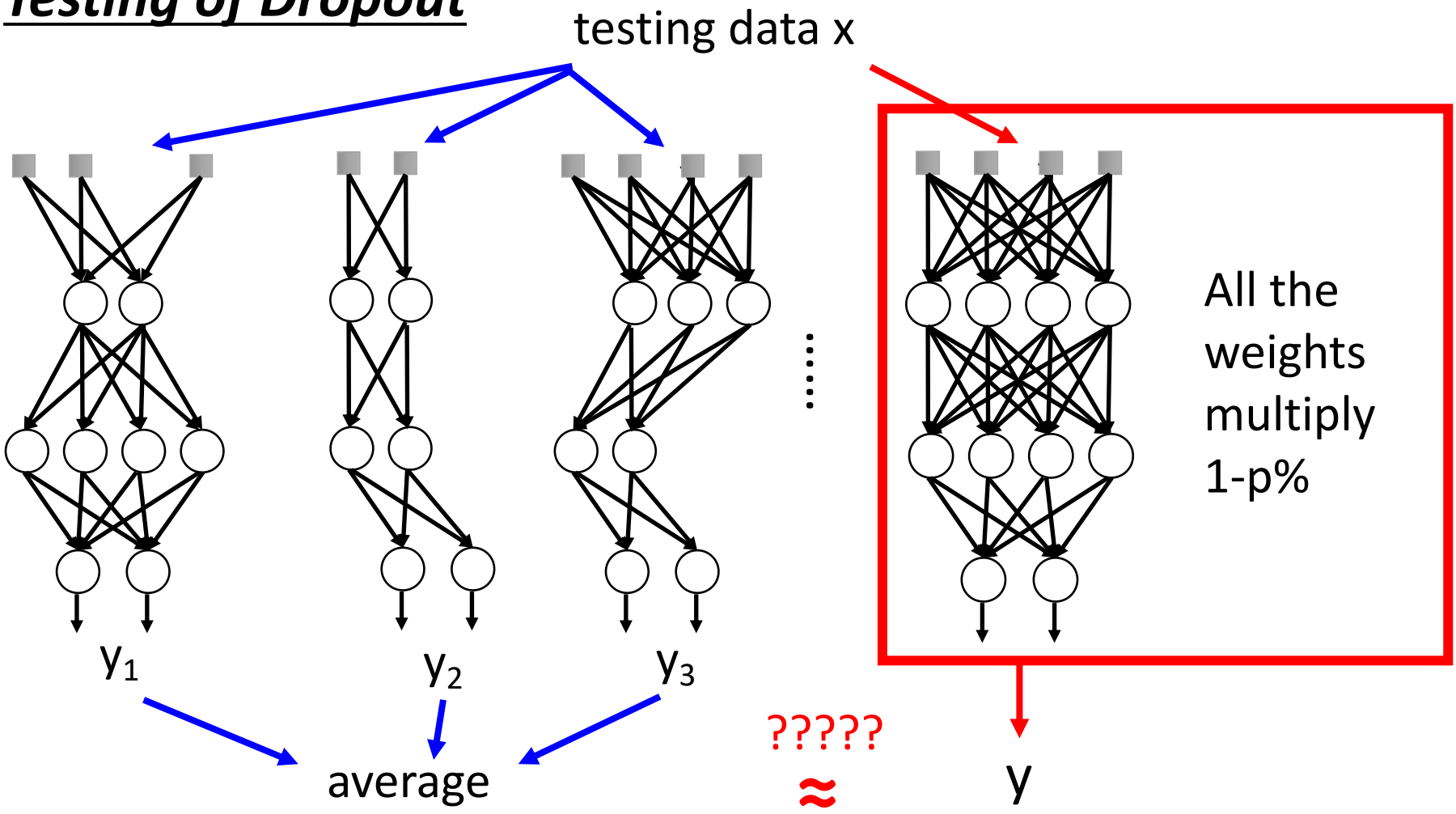
M neurons

2^M possible networks

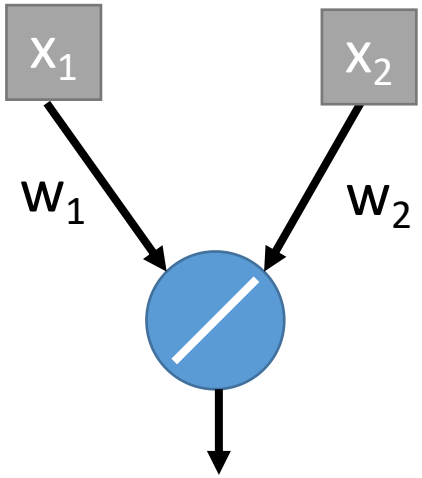
- Using one mini-batch to train one network
- Some parameters in the network are shared

Dropout is a kind of ensemble.

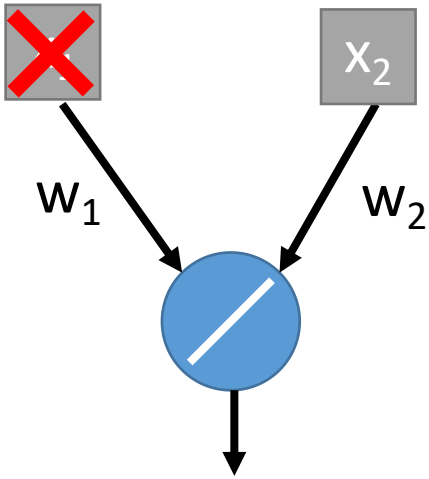
Testing of Dropout



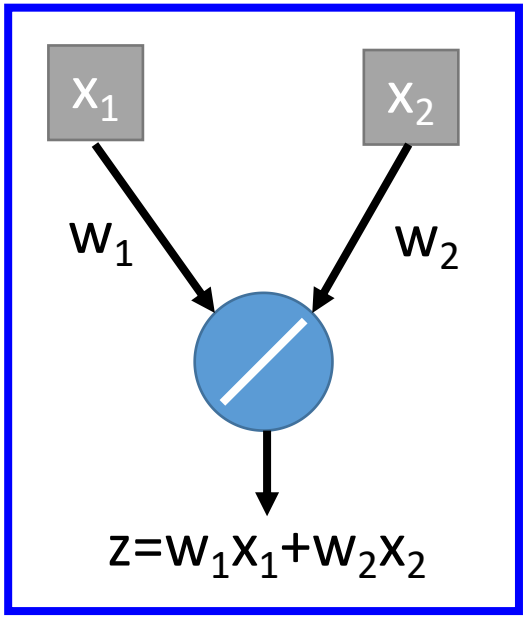
Testing of Dropout

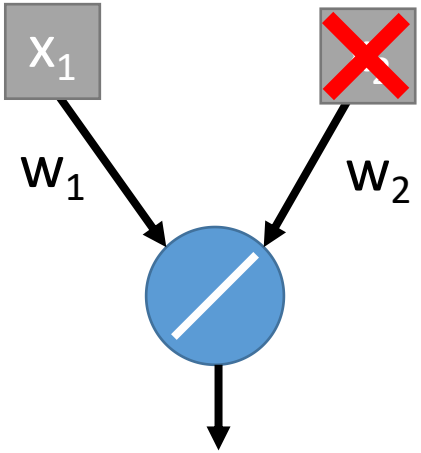


$z=w_1x_1+w_2x_2$

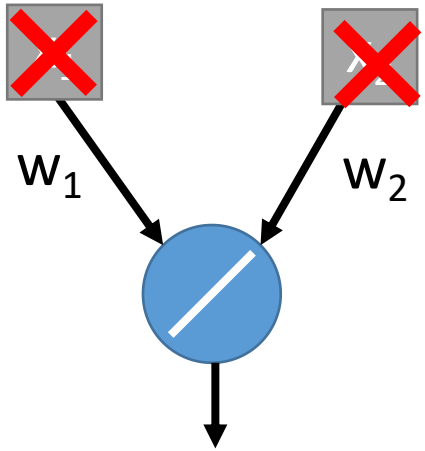


$z=w_2x_2$

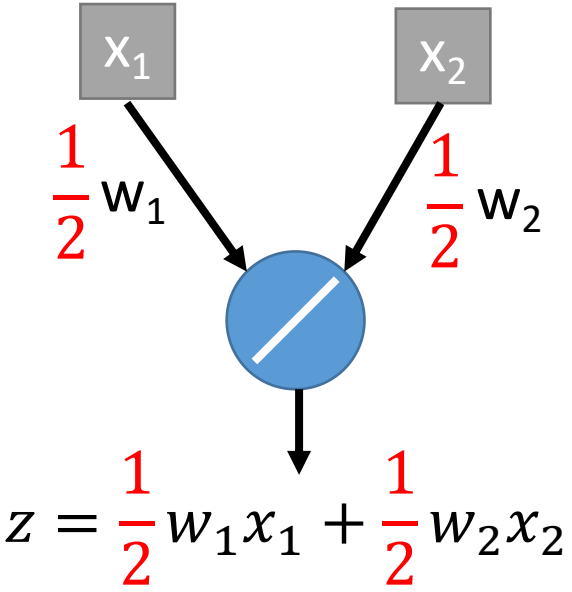




$z=w_1x_1$

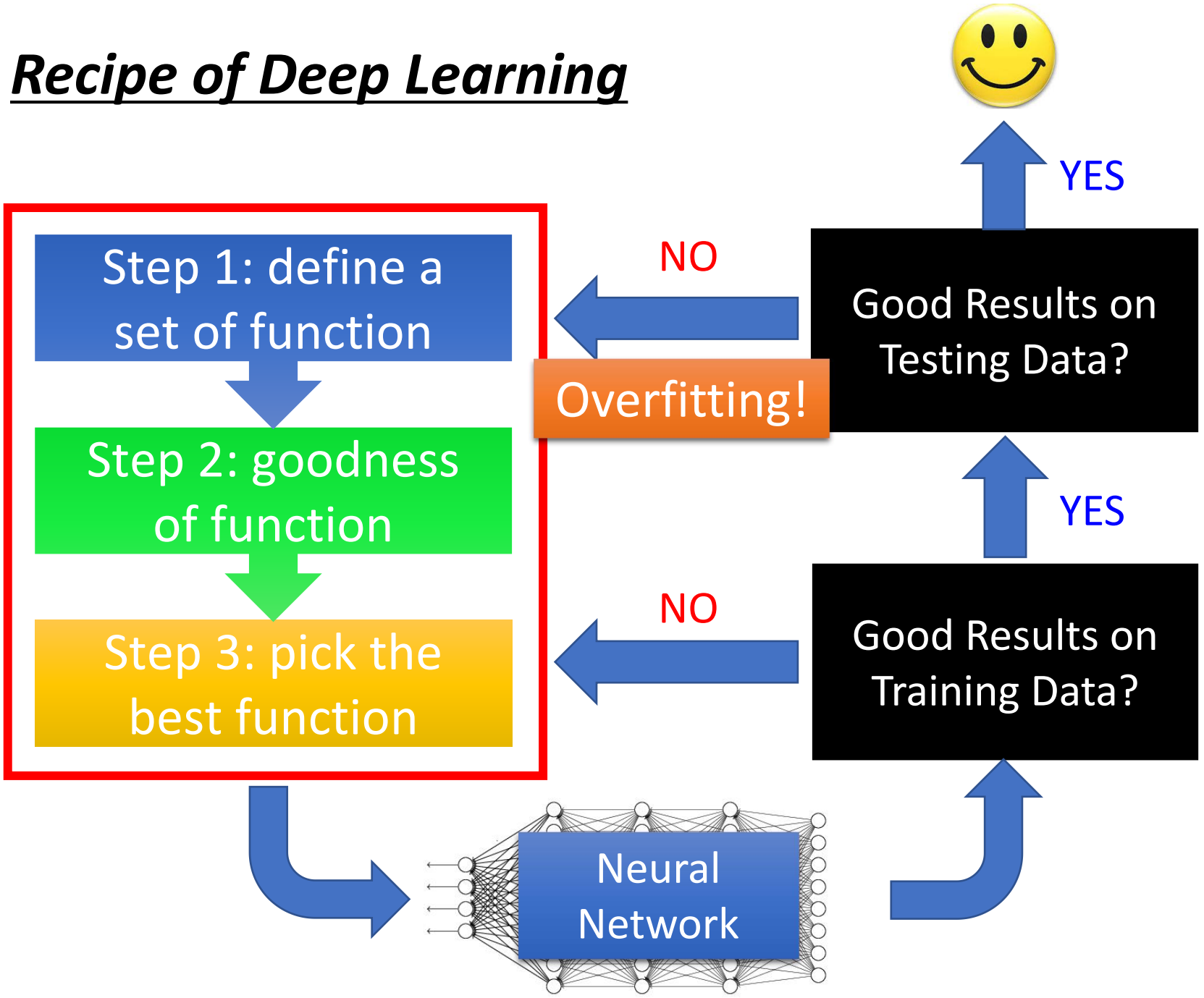


$z=0$

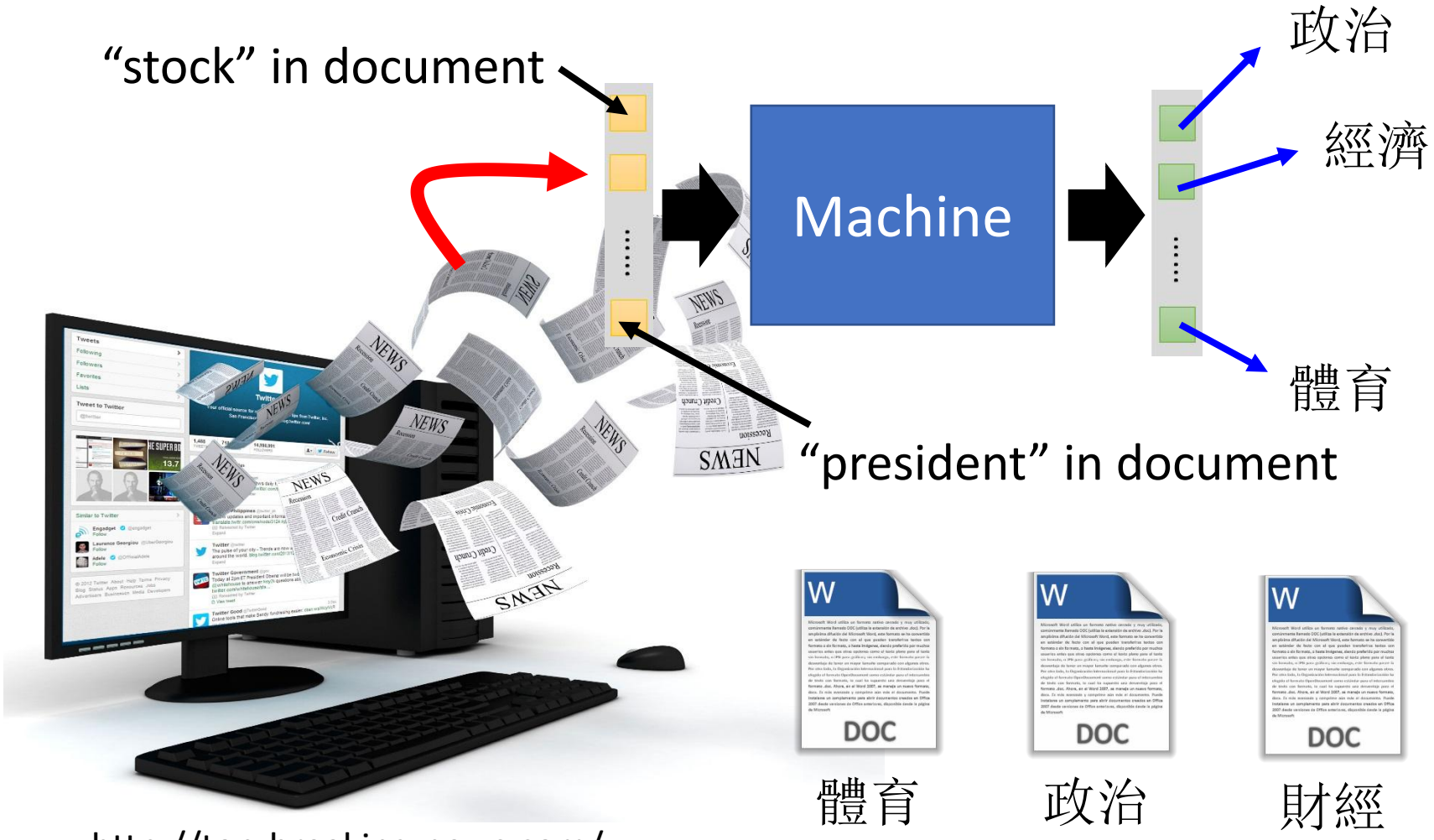


$$z = \frac{1}{2}w_1x_1 + \frac{1}{2}w_2x_2$$

Recipe of Deep Learning



Try another task



Try another task

```
In [8]: x_train.shape
Out[8]: (8982, 1000)

In [9]: y_train.shape
Out[9]: (8982, 46)

In [10]: x_test.shape
Out[10]: (2246, 1000)

In [11]: y_test.shape
Out[11]: (2246, 46)
```

```
In [12]: x_train[0]
Out[12]:
array([ 0.,  1.,  1.,  0.,  1.,  1.,  1.,  1.,  1.,
        0.,  0.,  1.,  1.,  1.,  0.,  1.,  0.,  0.,
        1.,  0.,  0.,  1.,  1.,  0.,  1.,  0.,  0.,
        1.,  0.,  0.,  0.,  1.,  1.,  0.,  0.,  0.,
        1.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
        0.,  0.,  1.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
        0.,  0.,  0.,  0.,  0.,  1.,  1.,  0.,  0.,  0.,  0.,  1.,  1.,
        0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  1.,  0.,
        0.,  0.,  0.,  0.,  0.,  1.,  0.,  1.,  0.,  0.,  0.,  0.,  0.,
        0.,  0.,  0.,  0.,  0.,  0.,  0.,  1.,  0.,  0.,  0.,  0.,  0.,
        0.,  0.,  1.,  0.,  1.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
        0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  1.,  0.,  0.,  1.,  1.,
        0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
        0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
        0.,  0.,  0.,  0.,  1.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
        0.,  0.,  1.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  1.,
        0.,  1.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
        0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
```

```
In [13]: y_train[0]
Out[13]:
array([ 0.,  0.,  0.,  1.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
        0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
        0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,
        0.,  0.,  0.,  0.,  0.,  0.,  0.])
```

Live Demo