Tips for Training Deep Learning

Recap: Stochastic Gradient Descent



$$l^{(i)} = -\log\left(\exp\left(z_k^{(i)}\right) / \sum_{j} \exp(z_j^{(i)})\right)$$

$$L = \frac{1}{N} \sum_{i=1}^{N} l^{(i)}$$

Loss is the summation over all training examples

$$\theta^{(i+1)} \leftarrow \theta^{(i)} - \eta \nabla L(\theta^{(i)})$$

Stochastic Gradient Descent (SGD)

Faster!

Randomly pick one example $x^{(i)}$ to update parameters

$$l^{(i)} = -\log\left(\exp\left(z_k^{(i)}\right) / \sum_{j} \exp(z_j^{(i)})\right) \quad \theta^{(i+1)} \leftarrow \theta^{(i)} - \eta \nabla l(\theta^{(i)})$$

Loss for only one example, i.e. ith sample

Minibatch SGD

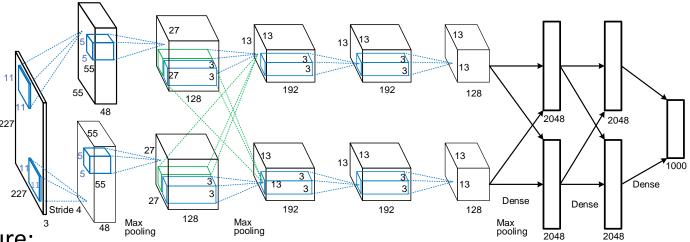


Loop:

- 1. Sample a batch of data
- 2. **Forward** prop it through the graph (network), get loss
- 3. **Backprop** to calculate the gradients
- 4. Update the parameters using the gradient

Case Study: AlexNet

[Krizhevsky et al. 2012]



Full (simplified) AlexNet architecture:

[227x227x3] INPUT

[55x55x96] CONV1: 96 11x11 filters at stride 4, pad 0

[27x27x96] MAX POOL1: 3x3 filters at stride 2

[27x27x96] NORM1: Normalization layer

[27x27x256] CONV2: 256 5x5 filters at stride 1, pad 2

[13x13x256] MAX POOL2: 3x3 filters at stride 2

[13x13x256] NORM2: Normalization layer

[13x13x384] CONV3: 384 3x3 filters at stride 1, pad 1

[13x13x384] CONV4: 384 3x3 filters at stride 1, pad 1

[13x13x256] CONV5: 256 3x3 filters at stride 1, pad 1

[6x6x256] MAX POOL3: 3x3 filters at stride 2

[4096] FC6: 4096 neurons [4096] FC7: 4096 neurons

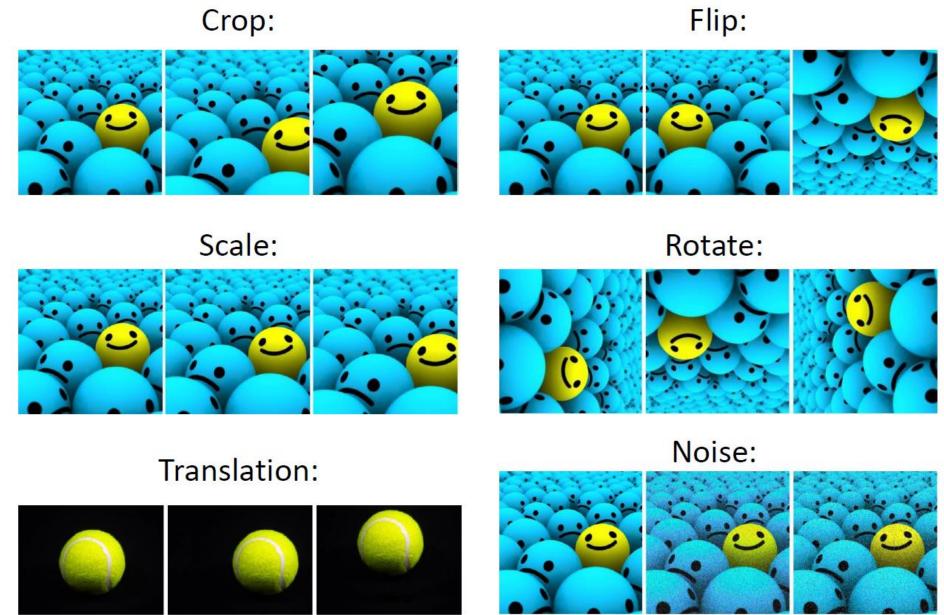
[1000] FC8: 1000 neurons (class scores)

Details:

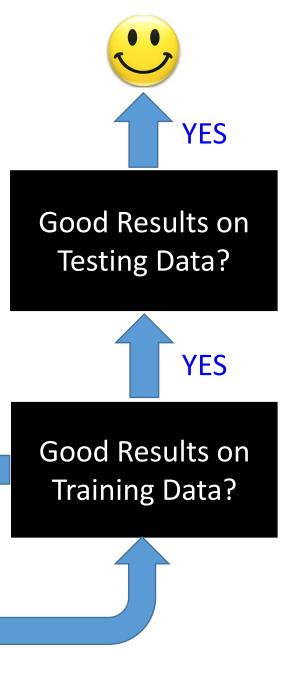
- heavy data augmentation
- first use of ReLU
- used Norm layers (not common anymore)
- dropout 0.5
- batch size 128
- SGD Momentum 0.9
- Learning rate 0.01, reduced by 10 manually when val accuracy plateaus
- L2 weight decay 0.0005

7 CNN ensemble: 18.2%→ 15.4%

Data Augmentation



Recipe of Deep Learning



Step 1: Define a Set of Function

Step 2: Goodness of Function

Step 3: Pick the Best Function

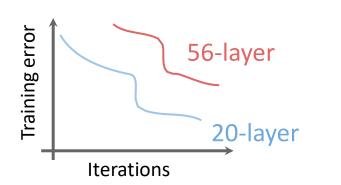
Neural Network

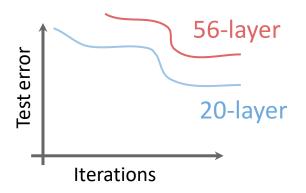
NO

Overfitting!

NO

Do not always blame Overfitting





Please refer to:

Kaiming He, Xiangyu Zhang, Shaoqing Ren, Jian Sun, Deep Residual Learning for Image Recognition, CVPR, 2016.

Recipe of Deep Learning



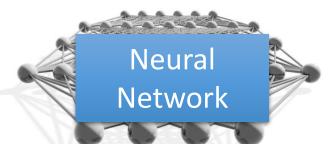
Different approaches for different problems.

e.g. dropout for good results on testing data

Good Results on Testing Data?

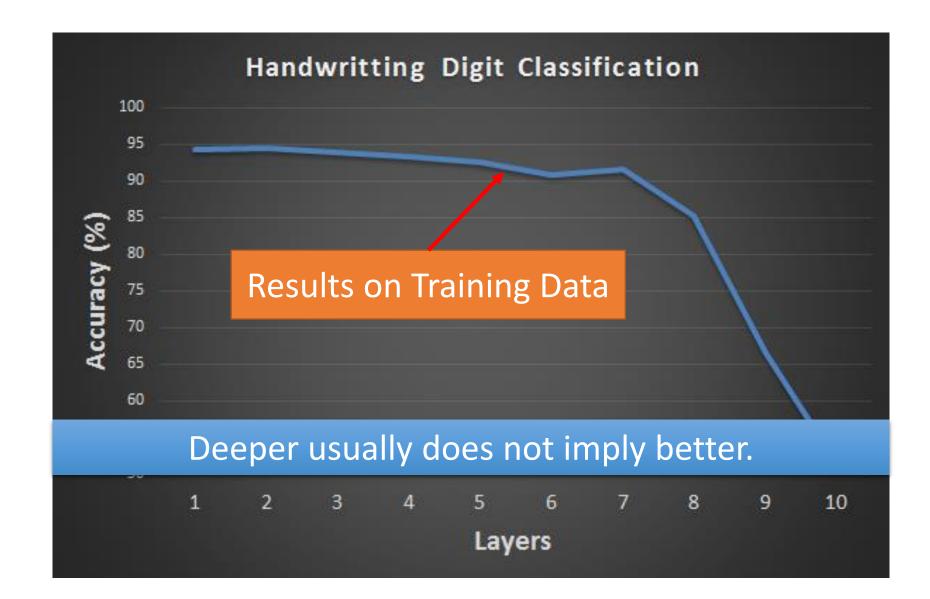


Good Results on Training Data?



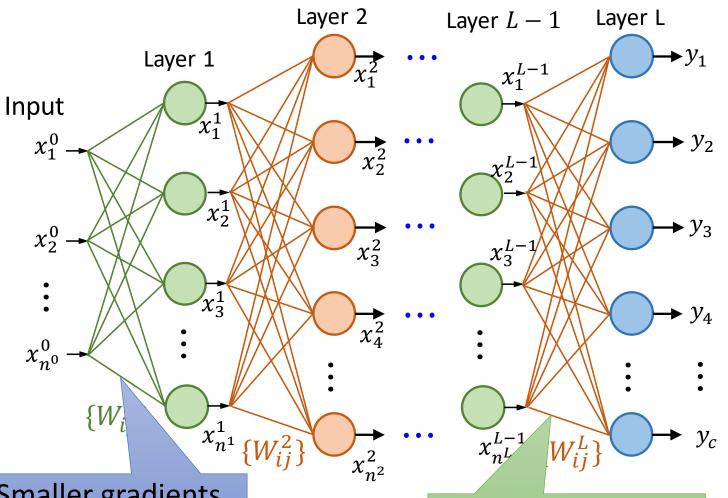
Recipe of Deep Learning YES **Early Stopping** Good Results on Testing Data? Regularization YES Dropout Good Results on New activation function **Training Data?** Adaptive Learning Rate

Hard to get the power of Deep ...



Vanishing Gradient Problem

See Gradient flow in recurrent nets: the difficulty of learning long term dependencies, by Sepp Hochreiter, Yoshua Bengio, Paolo Frasconi, and Jürgen Schmidhuber (2001).



converge based on random!?

Smaller gradients

Learn very slow

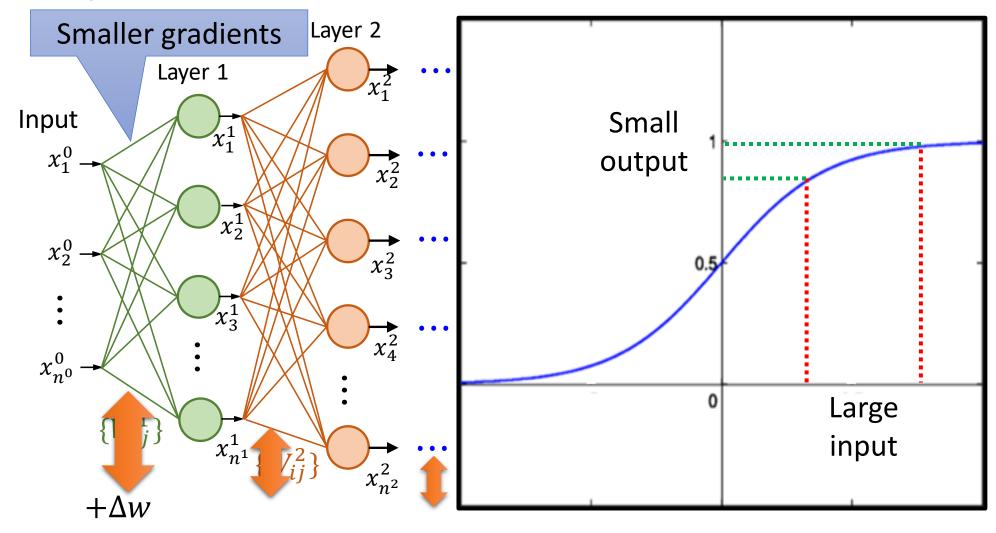
Almost random

Larger gradients

Learn very fast

Already converge

Vanishing Gradient Problem

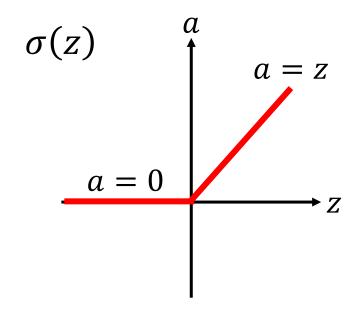


Intuitive way to compute the derivatives ...

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

ReLU

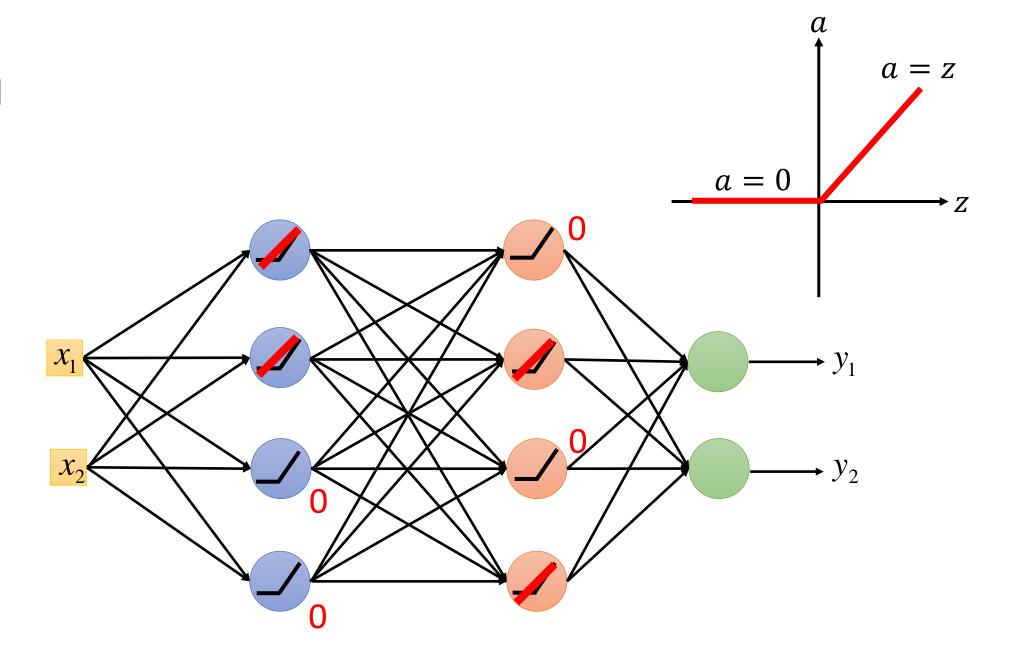
Rectified Linear Unit (ReLU)



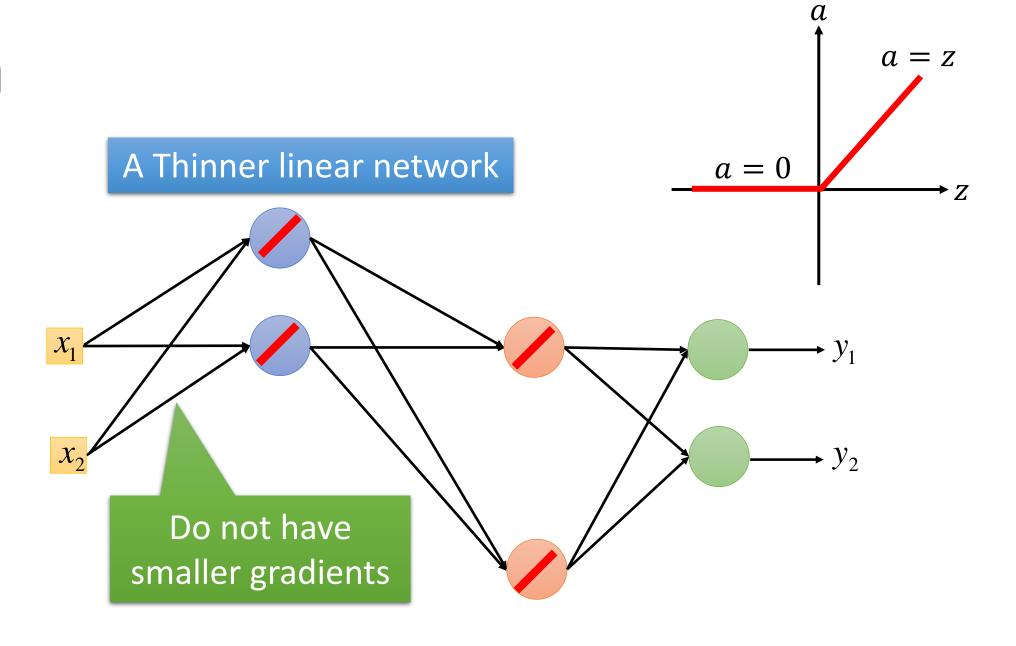
Reason:

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

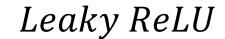
ReLU

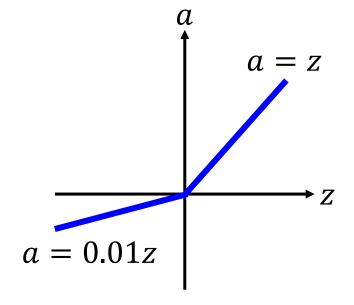


ReLU

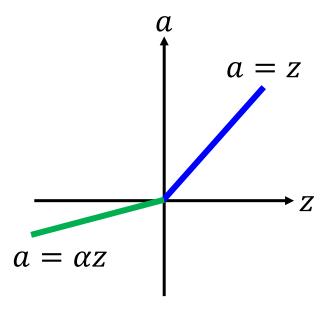


Variants of ReLU





Parametric ReLU



α also learned by gradient descent

Maxout

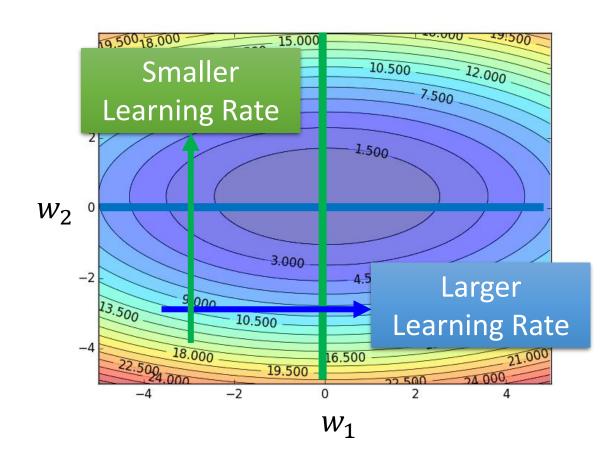
ReLU is a special case of Maxout

• Learnable activation function [lan J. Goodfellow, ICML'13]

Recipe of Deep Learning YES **Early Stopping** Good Results on Testing Data? Regularization YES Dropout Good Results on New activation function **Training Data?** Adaptive Learning Rate

Review

AdaGrad

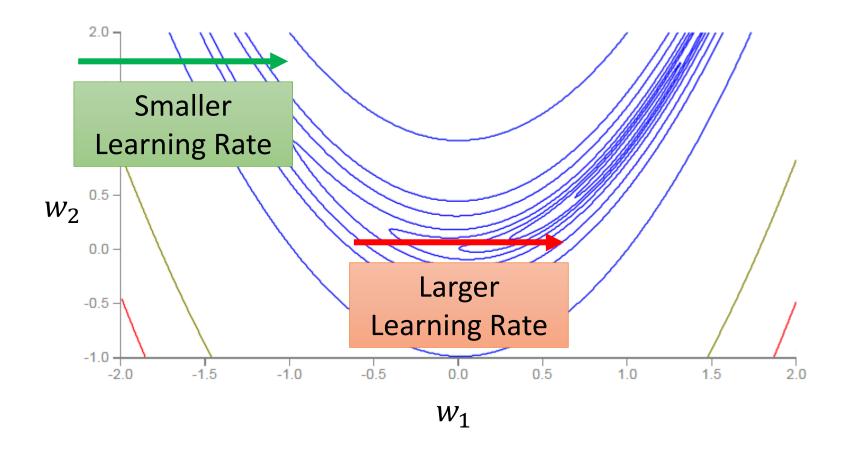


$$w^{(t+1)} \leftarrow w^{(t)} - \frac{\eta}{\sqrt{\sum_{i=0}^{t} (g^{(i)})^2}} g^{(t)}$$

Use first derivative to estimate second derivative

RMSProp

Error Surface can be very complex when training NN.



RMSProp

$$w^{(1)} \leftarrow w^{(0)} - \frac{\eta}{\sigma^{(0)}} g^{(0)}$$

$$w^{(2)} \leftarrow w^{(1)} - \frac{\eta}{\sigma^{(1)}} g^{(1)}$$

$$w^{(3)} \leftarrow w^{(2)} - \frac{\eta}{\sigma^{(2)}} g^{(2)}$$
 \vdots

$$w^{(t+1)} \leftarrow w^{(t)} - \frac{\eta}{\sigma^{(t)}} g^{(t)}$$

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

$$AdaGrad$$

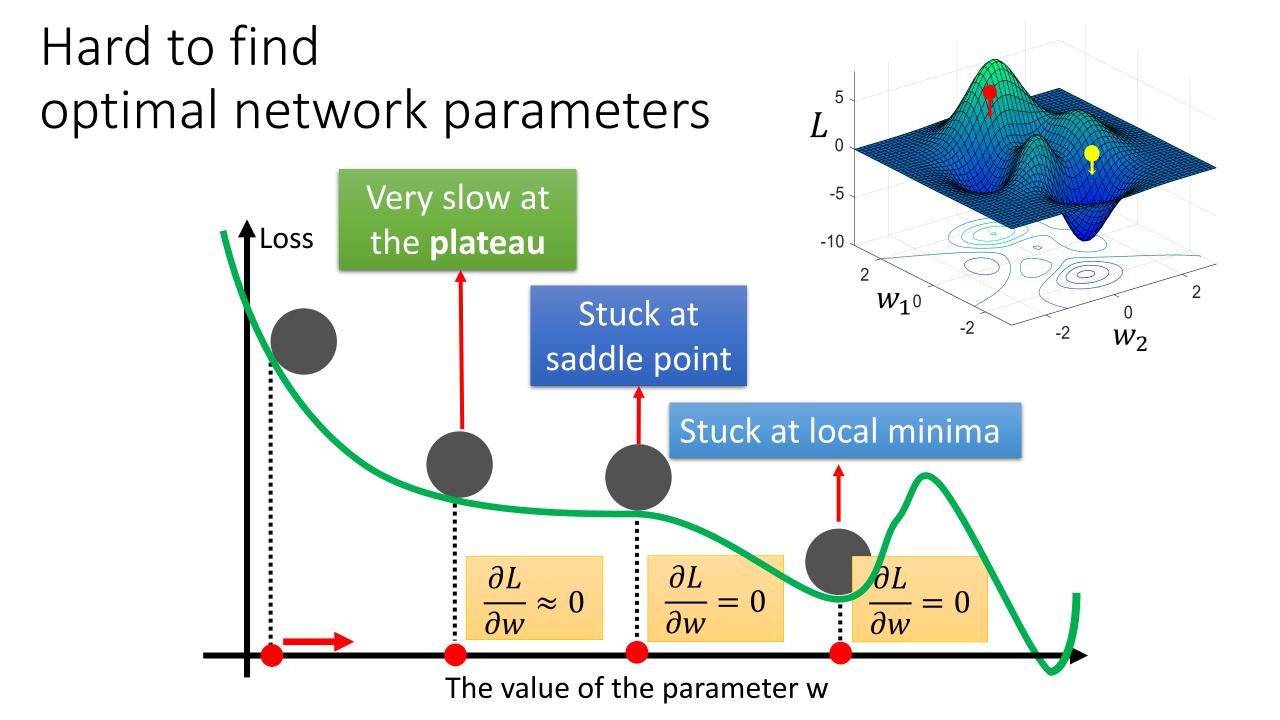
$$\sigma^{(0)}=g^{(0)}$$

$$\sigma^{(1)} = \sqrt{\alpha(\sigma^{(0)})^2 + (1 - \alpha)(g^{(1)})^2}$$

$$\sigma^{(2)} = \sqrt{\alpha(\sigma^{(1)})^2 + (1 - \alpha)(g^{(2)})^2}$$
:

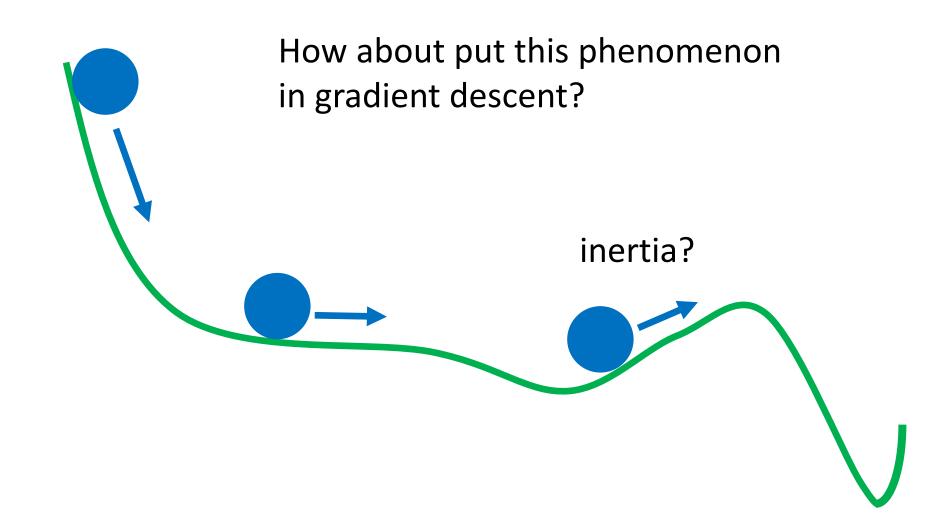
$$\sigma^{(t)} = \sqrt{\alpha(\sigma^{(t-1)})^2 + (1-\alpha)(g^{(t)})^2}$$

Root Mean Square of the gradients with previous gradients being decayed

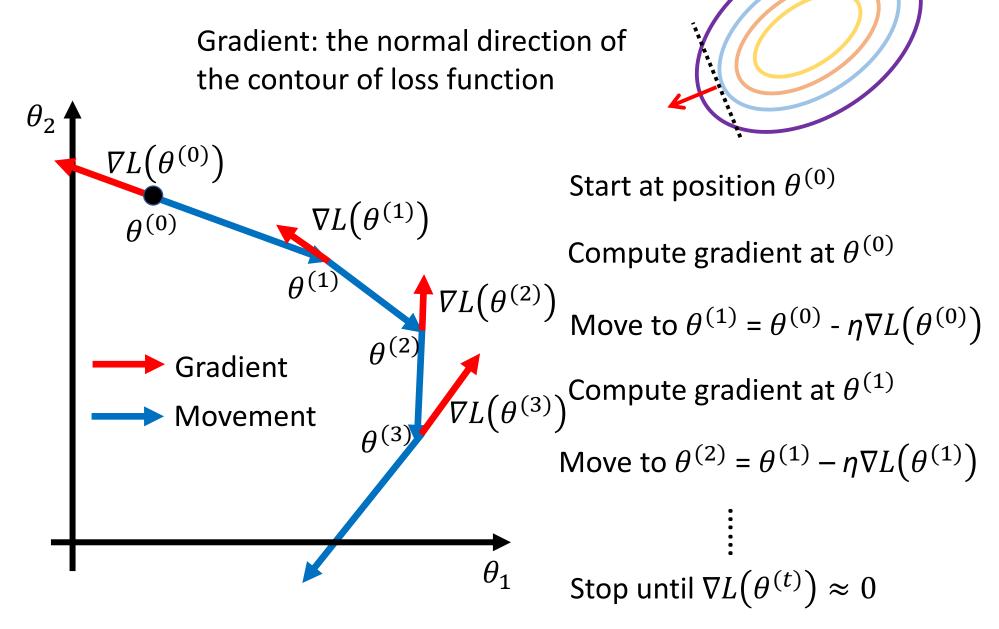


In physical world

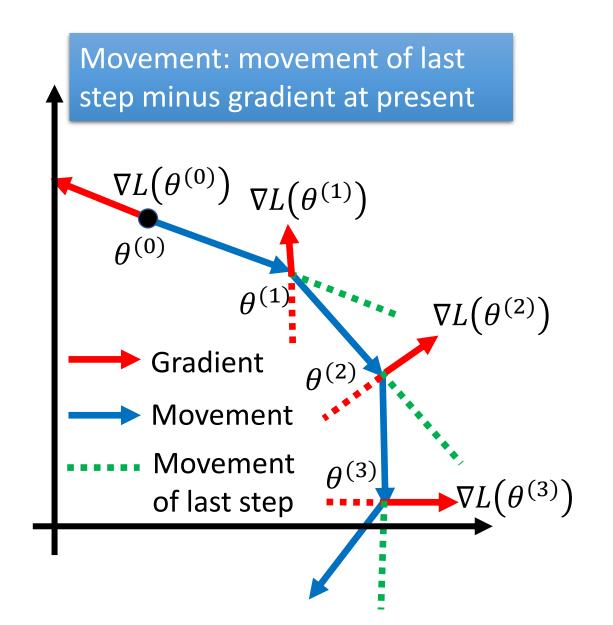
Momentum



Review: Vanilla Gradient Descent



Momentum



Start at point $\theta^{(0)}$

Movement $v^{(0)} = 0$

Compute gradient at $\theta^{(0)}$

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

Move to $\theta^{(1)} = \theta^{(0)} + v^{(1)}$

Compute gradient at $\theta^{(1)}$

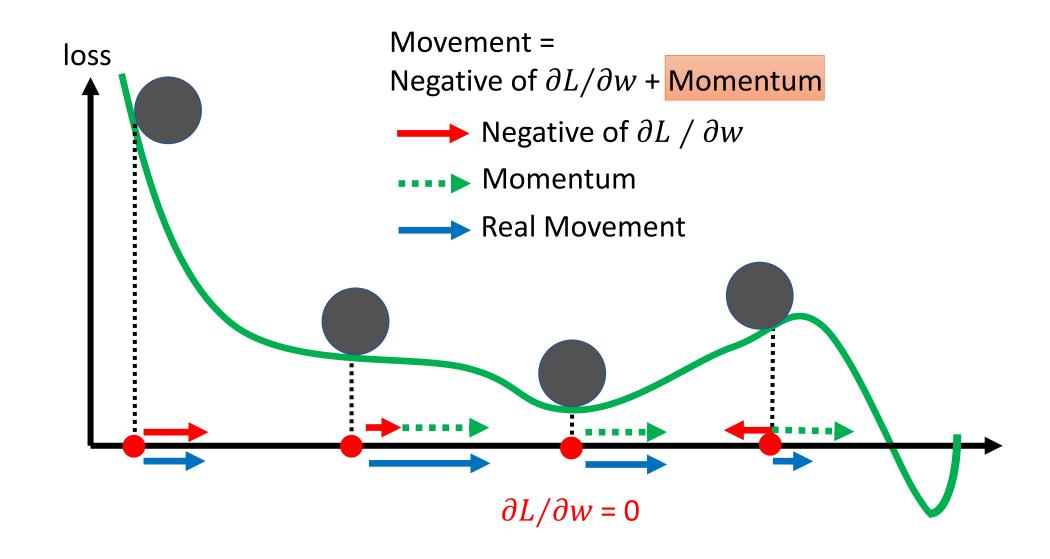
Movement $v^{(2)} = \lambda v^{(1)} - \eta \nabla L(\theta^{(1)})$

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

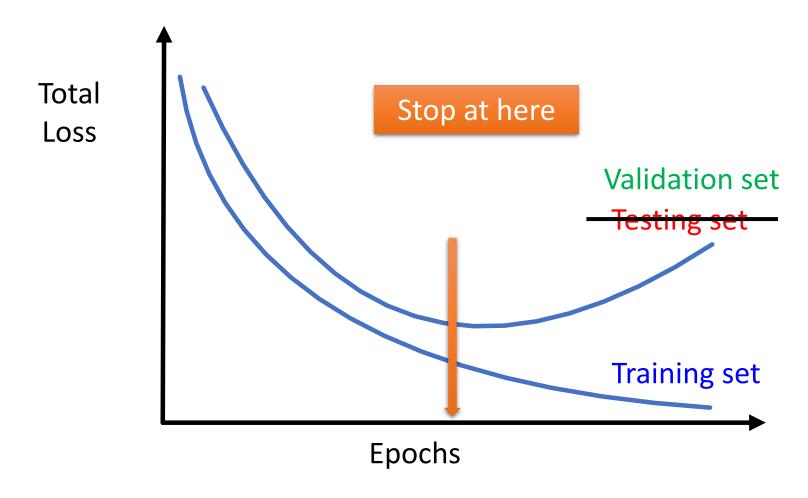
Algorithm 1: Adam, our proposed algorithm for stochastic optimization. See section 2 for details, and for a slightly more efficient (but less clear) order of computation. g_t^2 indicates the elementwise square $g_t \odot g_t$. Good default settings for the tested machine learning problems are $\alpha = 0.001$, $\beta_1 = 0.9$, $\beta_2 = 0.999$ 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: \alpha: Stepsize
Require: \beta_1, \beta_2 \in [0, 1): Exponential decay rates for the moment estimates
Require: f(\theta): Stochastic objective function with parameters \theta
Require: \theta_0: Initial parameter vector
   m_0 \leftarrow 0 (Initialize 1st moment vector) \longrightarrow for momentum
   v_0 \leftarrow 0 (Initialize 2<sup>nd</sup> moment vector) \longrightarrow for RMSprop
   t \leftarrow 0 (Initialize timestep)
   while \theta_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)
      \hat{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)
                                                                                    RMSProp + Momentum
   end while
```

return θ_t (Resulting parameters)

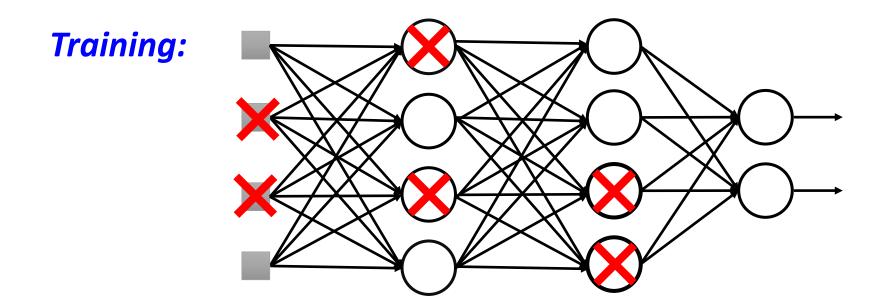
Recipe of Deep Learning YES Early Stopping Good Results on Testing Data? Regularization YES Dropout Good Results on New activation function **Training Data?** Adaptive Learning Rate

Early Stopping



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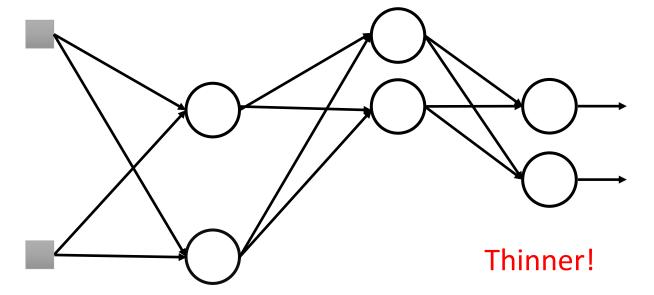
Dropout



- Each time before updating the parameters
- Each neuron has p% to be preserved, i.e. 1 p% to dropout

Dropout

Training:

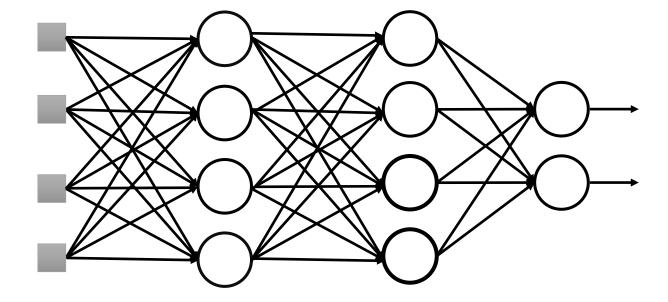


- Each time before updating the parameters
 - Each neuron has p% to be preserved
 - The structure of the network is changed.
 - Using the new network for training

For each minibatch, we resample the dropout neurons

Dropout

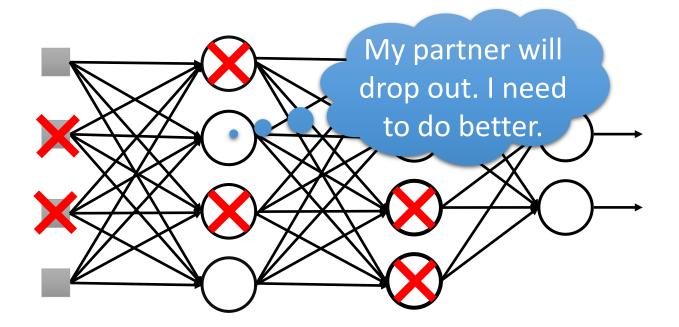
Testing:



No dropout

- If the keep rate at training is p%, all the weights at testing times p%
- Assume that the keep rate is 50%.
- If a weight w = 1 by training, set w = 0.5 for testing.

Dropout: Intuitive Reason



Dropout: A Simple Way to Prevent Neural Networks from Overfitting

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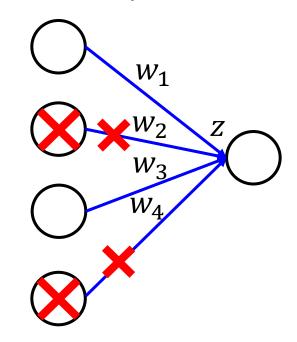
- When teams up, if everyone expect the partner will do the work, nothing will be done finally.
- However, if you know your partner will dropout, you will do better.
- When testing, no one dropout actually, so obtaining good results eventually.

Dropout: Intuitive Reason

• Why the weights should multiply p% (p% is the keep rate) when testing?

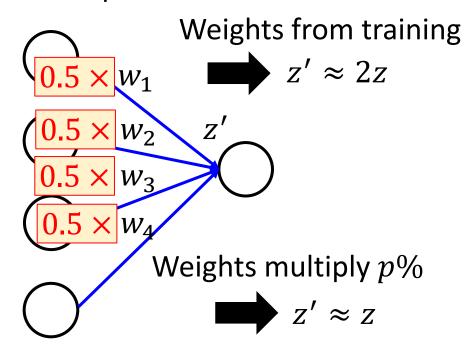
Training of Dropout

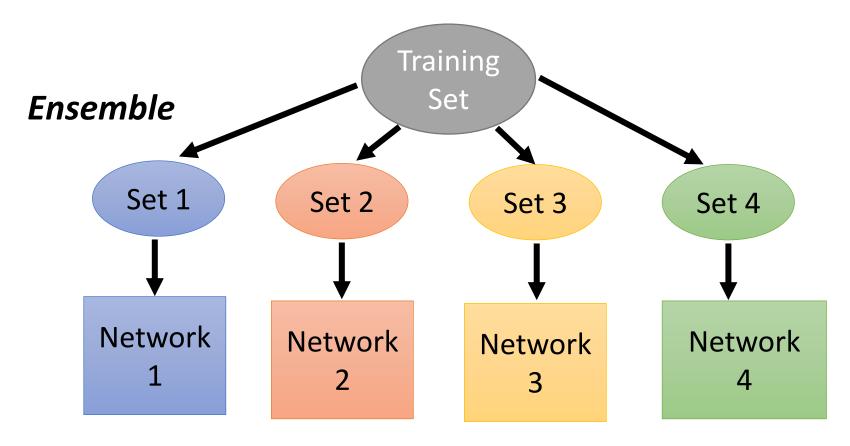
Assume keep rate is 50%



Testing of Dropout

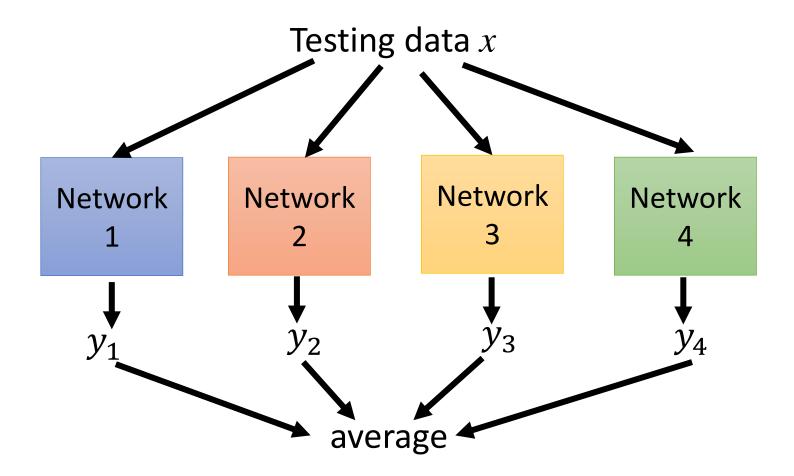
No dropout

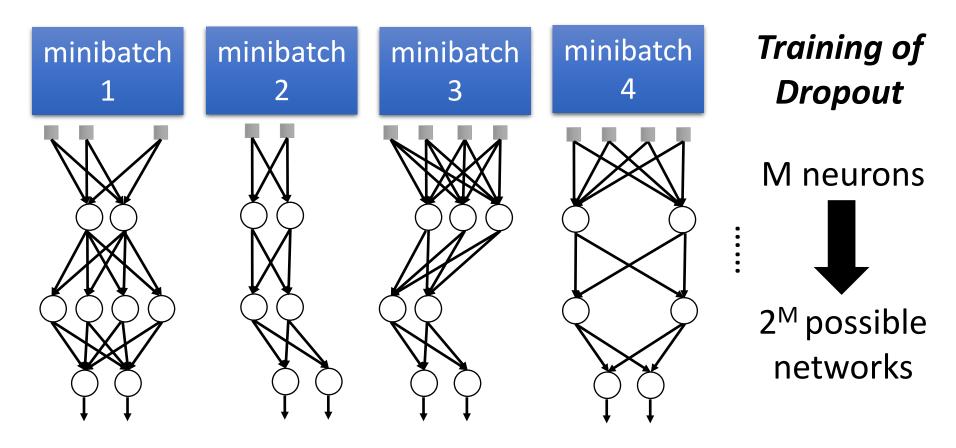




Train a bunch of networks with different structures

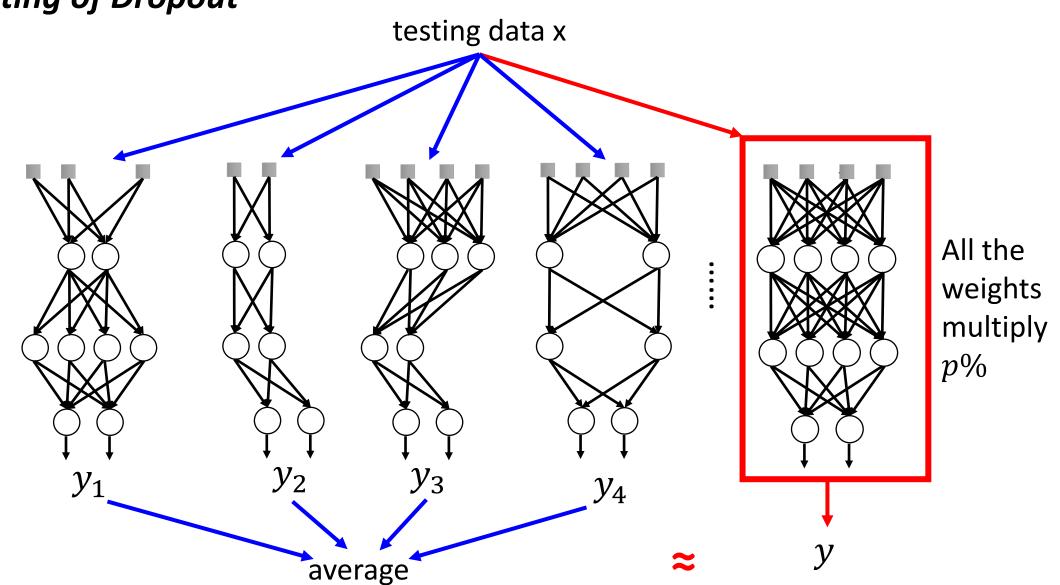
Ensemble



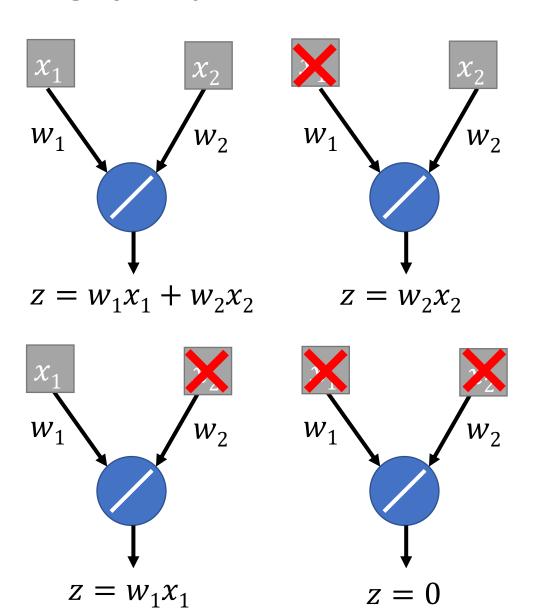


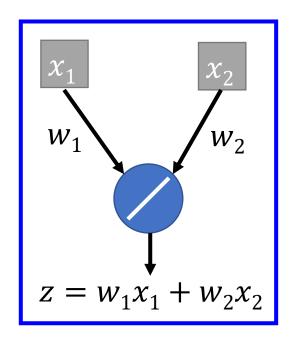
- Using one minibatch to train one network
- Some parameters in the network are shared

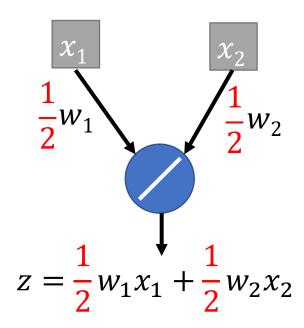
Testing of Dropout



Testing of Dropout







Recipe of Deep Learning YES **Early Stopping** Good Results on Testing Data? Regularization YES Dropout Good Results on New activation function **Training Data?** Adaptive Learning Rate

Regularization

- New loss function to be minimized
 - Find a set of weight not only minimizing original cost but also close to zero

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

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

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

L2 regularization:

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

(usually not consider biases)

Regularization

L2 regularization: $\|\theta\|_2 = (w_1)^2 + (w_2)^2 + \cdots$

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

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

Regularization

L1 regularization:

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

New loss function to be minimized

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

Update:

$$w^{(t+1)} \to w^{(t)} - \eta \frac{\partial L'}{\partial w} = w^{(t)} - \eta \left(\frac{\partial L}{\partial w} + \lambda \operatorname{sgn}(w^t) \right)$$
$$= w^{(t)} - \eta \frac{\partial L}{\partial w} - \underline{\eta} \lambda \operatorname{sgn}(w^{(t)}) \text{ Always delete}$$

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

Regularization: L1 vs. L2

L1 regularization: $\|\theta\|_1 = |w_1| + |w_2| + \cdots$

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

L2 regularization: $\|\theta\|_2 = (w_1)^2 + (w_2)^2 + \cdots$

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

