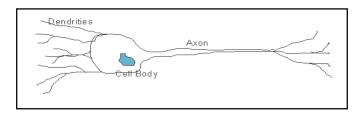
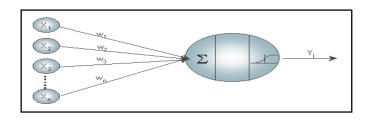
Neural Networks



- 머신러닝 알고리즘 중 가장 많이 알려진 것이 신경망 분석이며, 보통 머신러닝에서
 "신경망 분석 = 패턴을 찾아내는 것"이라고 연상할 만큼 잘 알려진 분석
- 인간 두뇌의 신경망(860억 개의 뉴런과 5000조 개의 시냅스로 구성)을 흉내 내어 데이터로부터의 반복적인 학습 과정을 거쳐 데이터에 숨어 있는 패턴을 찾아내는 모델링 기법



신경세포(neuron)

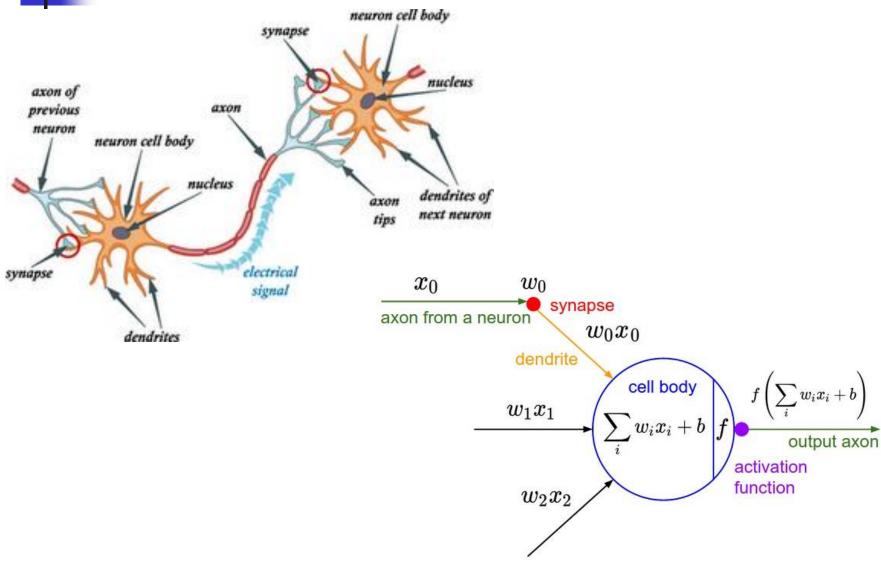


신경망(neural networks)

- 계층 구조를 갖는 수많은 프로세싱 요소로 이루어진 수학모형
 - 신경망 이론의 다양한 아키텍처를 기반으로 데이터로부터 패턴을 학습하여 최적해를 도출
- 장단점
 - 비선형 자료, 범주/연속형 혼합 자료 처리가 탁월하고 통계적 가정이 불필요
 - 설명변수들이 목표변수에 구체적으로 어떠한 영향을 주는지 해석하기 어렵고, Over-Fitting 가능성 높음



Biological vs. Artificial neural network





How neural networks work

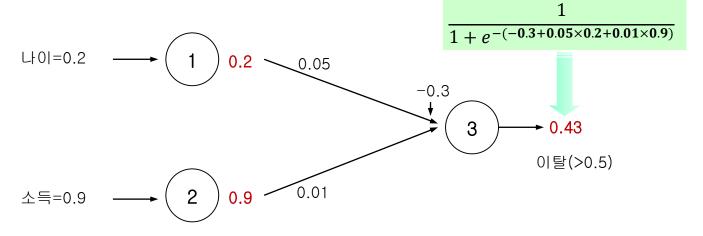
Single layer neural network

	φ(z) =	$\frac{1}{1 + e^{-}}$	-2	١,		
€ 0.5				/		

나이	소득	이탈
0.2	0.9	1
0.3	0.5	0
0.7	0.9	1



0.6	0.2	0
		_

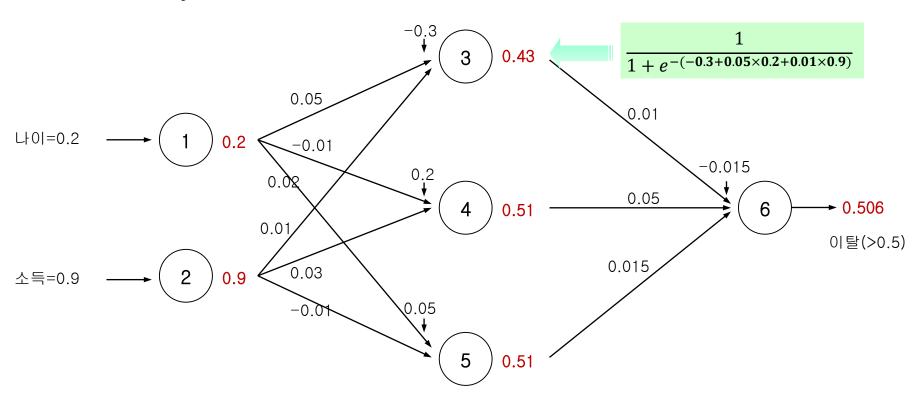


입력계층 (input layer) 출력계층 (output layer)



How neural networks work

Multi-layer neural network



입력계층 (input layer) 은닉계층 (hidden layer) 출력계층 (output layer)



Mathematical notation

Single layer neural network

• Neuron pre-activation (or input activation):

$$a(\mathbf{x}) = b + \sum_{i} w_i x_i = b + \mathbf{w}^{\mathsf{T}} \mathbf{x}$$

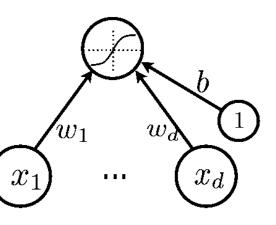
Neuron (output) activation

$$h(\mathbf{x}) = g(a(\mathbf{x})) = g(b + \sum_{i} w_i x_i)$$

w are the connection weights

b is the neuron bias

 $g(\cdot)$ is called the activation function





Mathematical notation

Multi-layer neural network

- Could have L hidden layers:
 - layer pre-activation for k>0 $(\mathbf{h}^{(0)}(\mathbf{x})=\mathbf{x})$

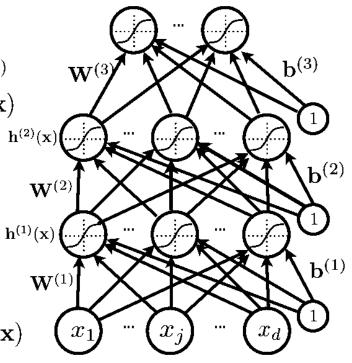
$$\mathbf{a}^{(k)}(\mathbf{x}) = \mathbf{b}^{(k)} + \mathbf{W}^{(k)}\mathbf{h}^{(k-1)}(\mathbf{x})$$

• hidden layer activation (k from 1 to L):

$$\mathbf{h}^{(k)}(\mathbf{x}) = \mathbf{g}(\mathbf{a}^{(k)}(\mathbf{x}))$$

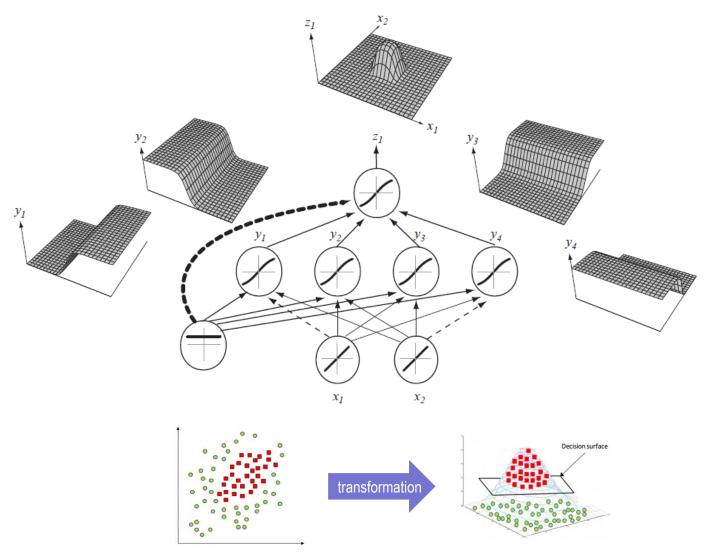
• output layer activation (k=L+1):

$$\mathbf{h}^{(L+1)}(\mathbf{x}) = \mathbf{o}(\mathbf{a}^{(L+1)}(\mathbf{x})) = \mathbf{f}(\mathbf{x})$$





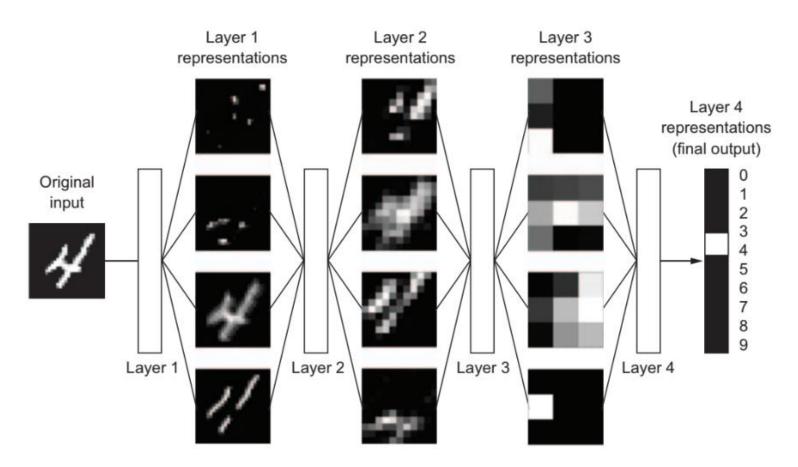
Capacity of neural network



Source: Neural Networks by Hugo Larochelle

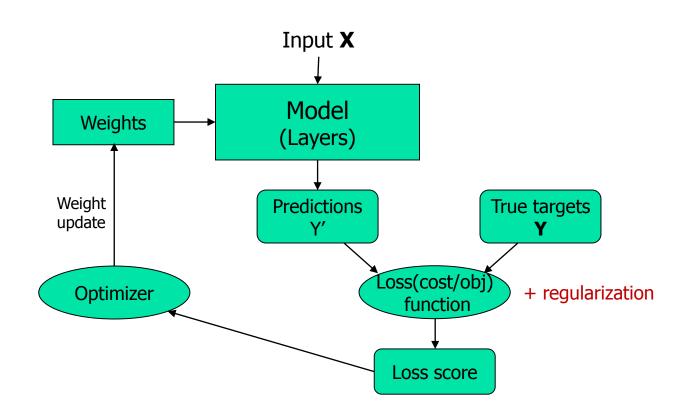
Capacity of neural network

 Neural networks do input-to-target mapping via a deep sequence of simple data transformations





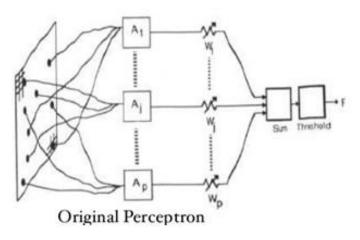
Training loop in NN



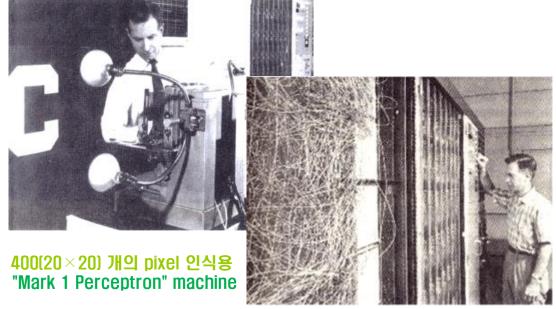


Perceptron: the simplest NN architecture

- 1943년, McCulloch와 Pitts는 인간의 두뇌를 수많은 신경세포들로 구성된 컴퓨터라 생각하고 최초로 신경망의 모델을 제안
- 1951년, Edmonds와 Minsky는 학습 기능을 갖는 최초의 신경망을 구축
- 1957년, <u>Frank Rosenblatt는 Perceptron이라는 신경망모델을 제안</u>하였는데, 이것은 패턴을 인식하기 위하여 학습 기능을 이용

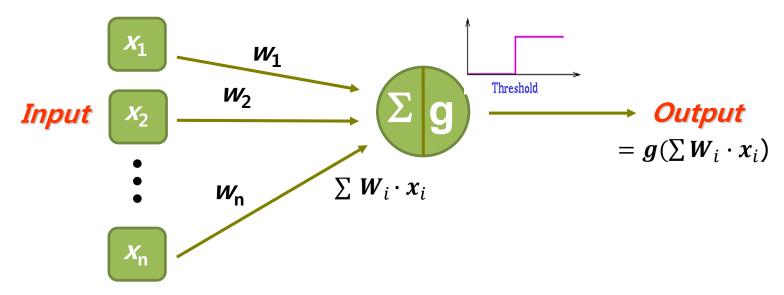


Source: https://www.slideshare.net/roelofp/220115dlmeetup



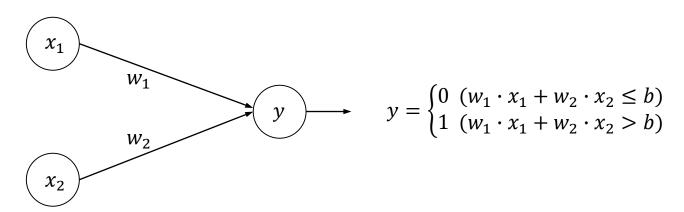
Source: http://www.aistudy.com/neural/model_kim.htm

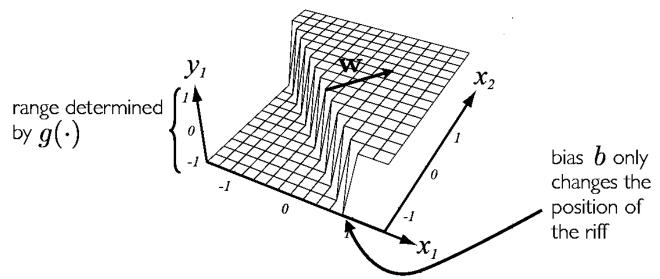
- 가중치(weight)
 - 입력신호의 강도를 표현: W_1, W_2, \dots, W_n
- 입력신호의 총합(total net input)
 - 각 입력신호에 해당 가중치를 곱하여 합한 값
 - $W_1 \cdot x_1 + W_2 \cdot x_2 + \cdots + W_n \cdot x_n = \sum W_i \cdot x_i$
- 활성화 함수(activation/transfer function)
 - 입력신호의 총합이 활성화되는지(출력 값)를 결정하는 함수
 - 임계 값 θ를 갖는 Step Function 사용



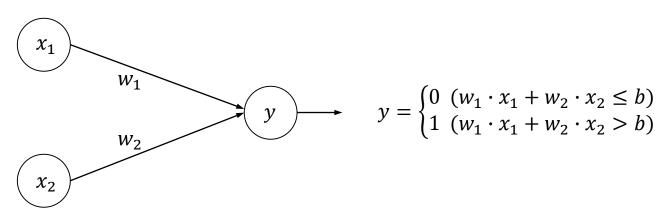


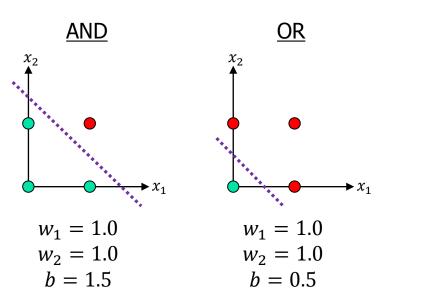
How a perceptron works

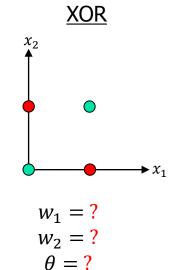




Limitation of (single layer) perceptron

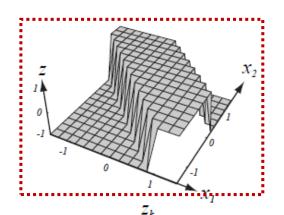


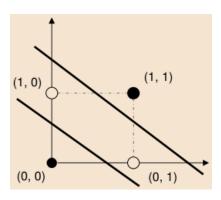


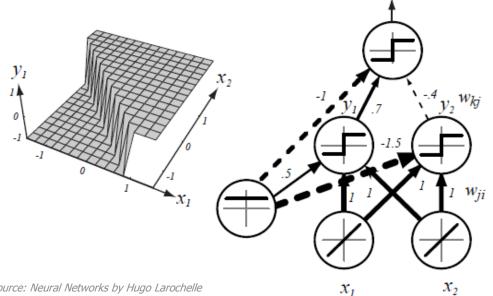


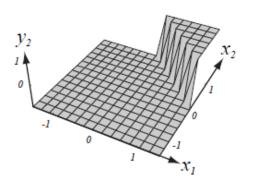


Capacity of multi-layer perceptron

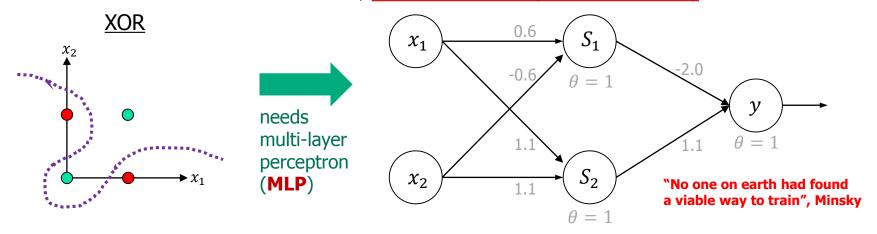




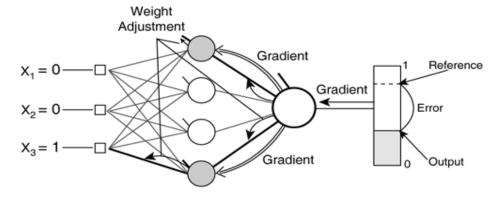




1969년, Minsky와 Papert가 그들의 저서 "Perceptrons"에서 퍼셉트론이 비선형 분리 문제를 풀 수 없음을 증명하여, 침체기에 들어감 (1st Al winter)

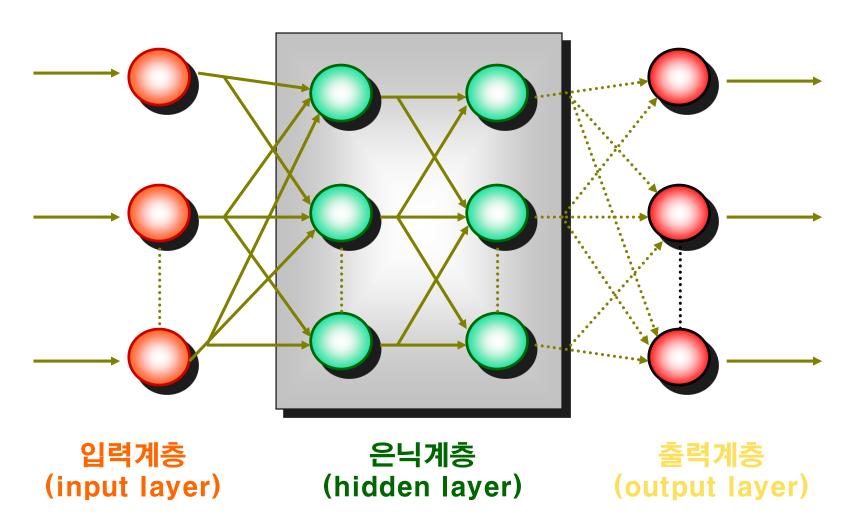


■ 1986년, PDP그룹에 의해 <u>Back-Propagation 알고리즘을 사용하는 MLP가 탄생</u>되 어 신경망의 다양한 분야에 대한 연구와 응용이 이루어짐.





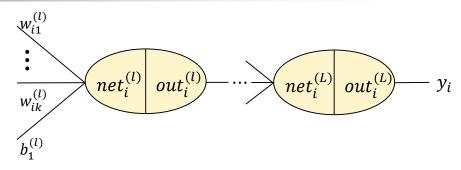
MLP: multi-layer perceptron



MLP

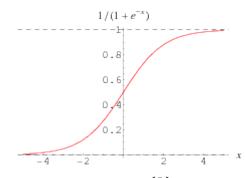


$$net_i^{(l)} = \sum_{j=1}^k w_{ij}^{(l)} \cdot out_j^{(l-1)} + b_1^{(l)}$$



- Activation 함수
 - Hidden Node: 주로 시그모이드(sigmoid / logistic) 함수 사용

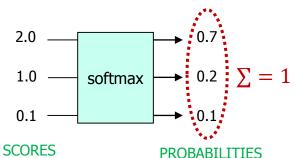
$$out_i^{(l)} = \frac{1}{1 + \exp(-net_i^{(l)})}$$



- Output Node
 - 추정(y가 연속형) 문제에는 항등(identity) 함수 사용. 즉, $\mathbf{y} = net^{(L)}$
 - 분류 문제에는 소프트맥스(softmax) 함수 사용

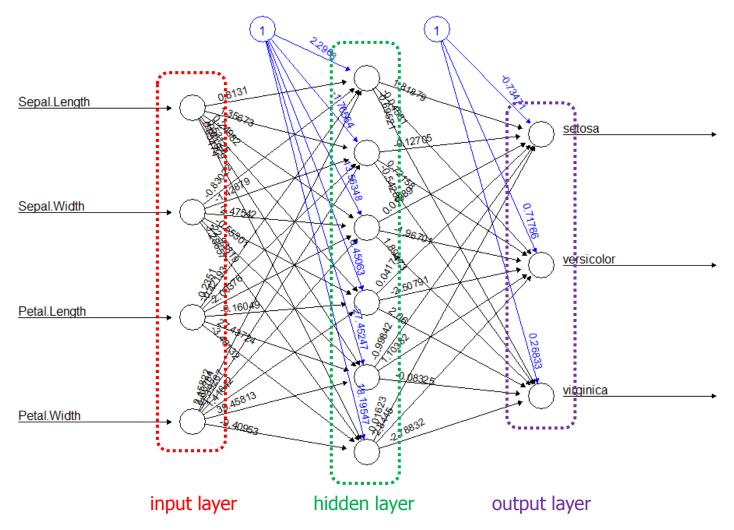
$$y_n = \frac{\exp(net_n^{(L)})}{\sum_{i=1}^N \exp(net_i^{(L)})}$$

N: 출력층의 뉴런 수, $0 \le y_n \le 1$



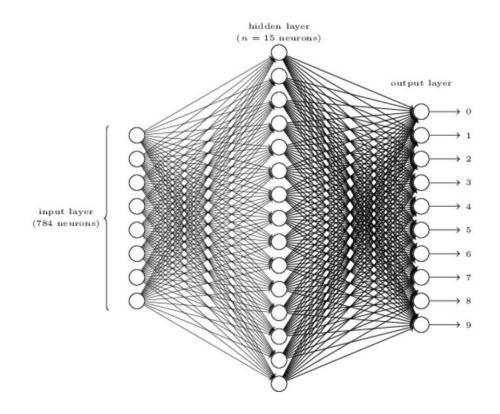
MLP

Classification Example for IRIS data by MLP



MLP

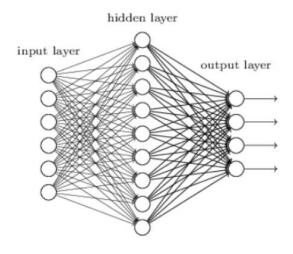
- A simple network to classify handwritten digits
 - Training data: 28X28(784) pixel, greyscale(0.0~1.0)





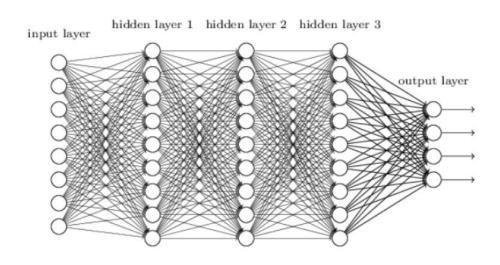
Shallow NN vs. Deep NN

"Non-deep" feedforward neural network



- Input layer: 6개의 input neuron으로 구성 (dimension = 6)
- Hidden layer: 1개 layer, 9개 neuron(unit)
- Output layer: 4개 unit

Deep neural network



- Input layer: 8개의 input neuron으로 구성 (dimension = 8)
- Hidden layer: 3개 layer, 각 9개 unit
- Output layer: 4개 unit

4

Learning algorithm

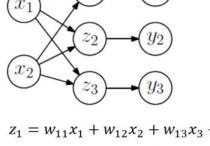
Error(cost) function

- Mean squared error: $E(\mathbf{W}) = \frac{1}{2} \sum_{i=1}^{N} (y_i \hat{y}_i)^2$
- Cross entropy error: $E(\mathbf{W}) = -\sum_{i=1}^{N} y_i \log(\hat{y}_i)$

Learning network

- adjusting weights to minimize error (E)
- Iterative numerical procedure

$$\boldsymbol{W}^{(t+1)} = \boldsymbol{W}^{(t)} + \nabla \boldsymbol{W}^{(t)}$$



$$z_{1} = w_{11}x_{1} + w_{12}x_{2} + w_{13}x_{3} + b_{1}$$

$$z_{2} = w_{21}x_{1} + w_{22}x_{2} + w_{23}x_{3} + b_{2}$$

$$z_{3} = w_{31}x_{1} + w_{32}x_{2} + w_{33}x_{3} + b_{3}$$

$$\mathbf{Z=Wb}$$

$$y_{i} = \sigma(z_{i})$$

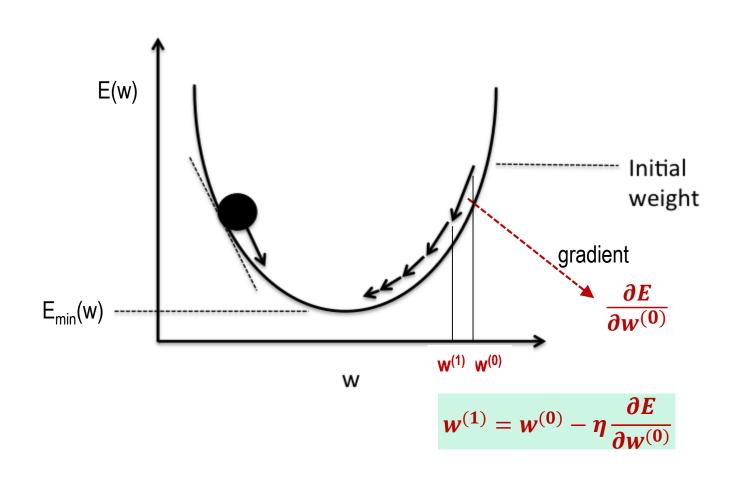
Gradient descent optimization

$$\mathbf{W}^{(t+1)} = \mathbf{W}^{(t)} - \eta \frac{\partial E(\mathbf{W}^{(t)})}{\partial \mathbf{W}^{(t)}}$$
 η : learning rate $(0 \sim 1)$

- Mini-batch stochastic gradient descent (mini-batch SGD)
 - Instead of the entire training data, work with mini-batch of m examples in each iteration (note: epoch)



Schematics of gradient descent



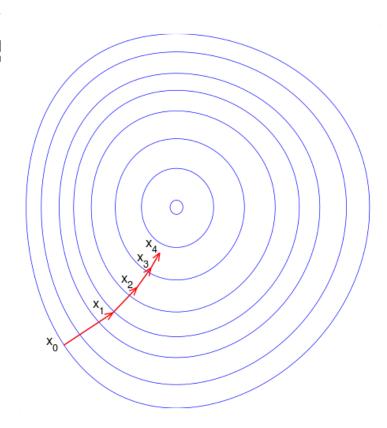


Schematics of gradient descent

- $x \in \mathbb{R}^n$
- 현재값 $x^{(k)}$ 에서 가장 빠르게 f(x)를 감소시키는 방향 $-\nabla f(x^{(k)})$ 으로 α 만큼씩이동

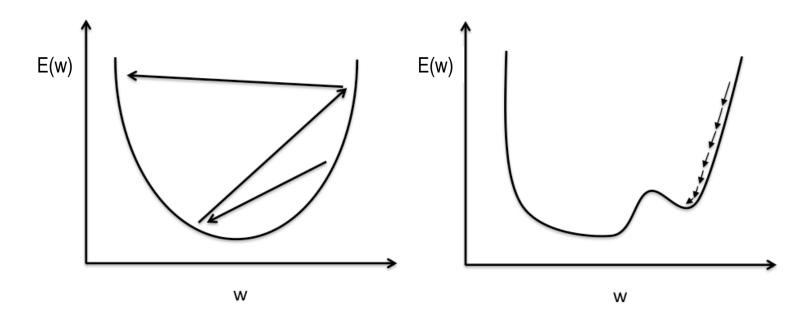
$$\begin{bmatrix} x_1^{(k+1)} \\ x_2^{(k+1)} \\ \vdots \\ x_n^{(k+1)} \end{bmatrix} = \begin{bmatrix} x_1^{(k)} \\ x_2^{(k)} \\ \vdots \\ x_n^{(k)} \end{bmatrix} - \alpha \begin{bmatrix} \frac{\partial}{\partial x_1} f(x_1^{(k)}) \\ \frac{\partial}{\partial x_2} f(x_2^{(k)}) \\ \vdots \\ \frac{\partial}{\partial x_n} f(x_n^{(k)}) \end{bmatrix}$$

$$\boldsymbol{x}^{(k+1)} = \boldsymbol{x}^{(k)} - \alpha \left\{ \nabla f\left(\boldsymbol{x}^{(k)}\right) \right\}^{T}$$





Learning rate

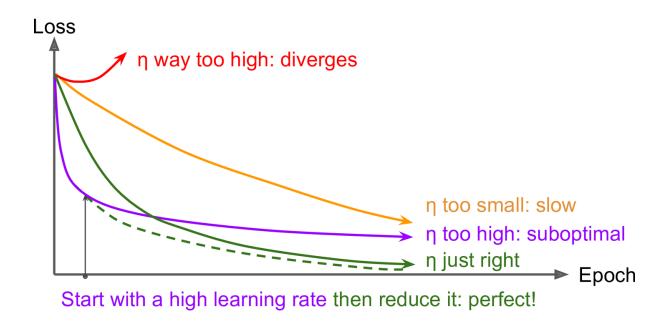


Large learning rate: Overshooting.

Small learning rate: Many iterations until convergence and trapping in local minima.



Learning rate Scheduling



- 미리 정의된 개별적인 고정 학습률
- 성능 기반 스케줄링
- 지수 기반 스케줄링 (Exponential Scheduling) *
- 거듭제곱 기반 스케줄링 (Power Scheduling)



Computing the gradient

Numerical gradient

 computes the partial derivative of each weight using the finite difference approximation

$$\frac{\partial \mathbf{E}}{\partial w_{ji}} = \frac{\mathbf{E}(w_{ji} + \epsilon) - \mathbf{E}(w_{ji})}{\epsilon} + O(\epsilon)$$

• is very simple, but approximate and very computationally expensive; $O(W^2)$

Back-propagation

- enables us to compute the gradients very efficiently; O(W)
- uses the chain rule for gradient decent
- consists of a two-pass procedure:
 - forward pass: fix weights, evaluate y from x
 - backward pass: compute the error E and back propagate it

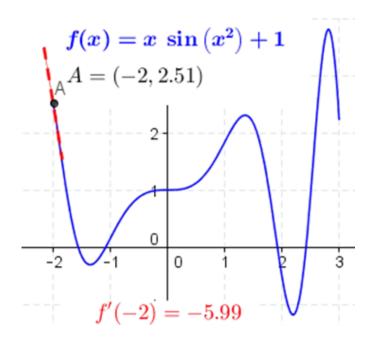


[Ref] Scalar Differentiation

- 미분의 정의
 - 함수 y = f(x)의 정의역에서 임의의 x에서 미분은 다음과 같이 정의된다.

$$f'(x) = \frac{df}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

점 x에서 f가 변하는 <u>순간 변화율</u>





[Ref] Scalar Differentiation: Formulas

많이 사용되는 미분 공식

$$\frac{d}{dx}(x^n) = nx^{n-1} \qquad \frac{d}{dx}(\ln x) = \frac{1}{x}$$

$$\frac{d}{dx}(e^x) = e^x \qquad \qquad \frac{d}{dx}(\sin x) = \cos x$$

$$\frac{d}{dx}(\cos x) = -\sin x$$
 $\frac{d}{dx}(\tanh x) = 1 - \tanh^2 x$

$$\frac{d}{dx}\left(\frac{1}{1+\exp(-x)}\right) = \left(\frac{1}{1+\exp(-x)}\right)\left(1-\frac{1}{1+\exp(-x)}\right)$$



[Ref] Scalar Differentiation: Rules

Sum rule

$$(f(x) + g(x))' = f'(x) + g'(x) = \frac{df}{dx} + \frac{dg}{dx}$$

Product rule

$$(f(x)g(x))' = f'(x)g(x) + f(x)g'(x) = \frac{df}{dx}g(x) + f(x)\frac{dg}{dx}$$

Chain rule

$$(g \circ f)'(x) = (g(f(x)))' = g'(f(x))f'(x) = \frac{dg}{df}\frac{df}{dx}$$



[Ref] Scalar Differentiation: Chain Rule

Example

$$g(z) = \tanh(z)$$

$$z = f(x) = x^{n}$$

$$(g \circ f)'(x) = \underbrace{(1 - \tanh^{2}(x^{n})) \underbrace{nx^{n-1}}_{df/dx}}_{dg/df}$$

Backpropagation (an easy case)

$$y = g(h \cdot w_2) = g(g(x \cdot w_1) \cdot w_2)$$

$$x$$
 y y y

$$E(\mathbf{w}) = \frac{1}{2}(y - y_i)^2$$
, where y_i is a real value.
 $g' = g(1 - g)$, when g is a sigmod ft .

$$\frac{\partial E(w)}{\partial w_2} = (y - y_i) \cdot \frac{\partial y}{\partial w_2}
= (y - y_i) \cdot \frac{\partial g(h \cdot w_2)}{\partial w_2}
= (y - y_i) \cdot g(h \cdot w_2) \cdot (1 - g(h \cdot w_2)) \times \frac{\partial (h \cdot w_2)}{\partial w_2}
= (y - y_i) \cdot y \cdot (1 - y) \cdot h = E_y \cdot h$$

$$\frac{\partial E(w)}{\partial w_1} = (y - y_i) \cdot \frac{\partial y}{\partial w_1}$$

$$= (y - y_i) \cdot y \cdot (1 - y) \cdot \frac{\partial (h \cdot w_2)}{\partial w_1}$$

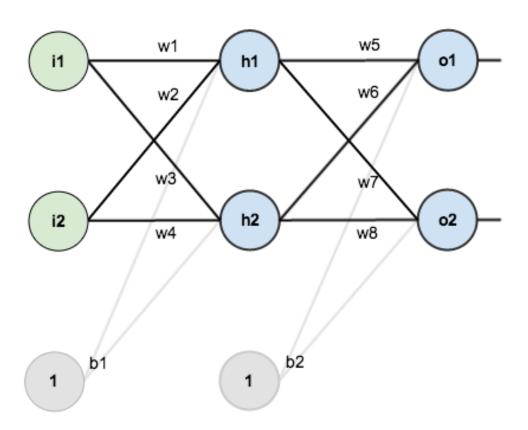
$$= (y - y_i) \cdot y \cdot (1 - y) \cdot w_2 \cdot \frac{\partial h}{\partial w_1}$$

$$= (y - y_i) \cdot y \cdot (1 - y) \cdot w_2 \cdot h \cdot (1 - h) \cdot \frac{\partial (x \cdot w_1)}{\partial w_1}$$

$$= (y - y_i) \cdot y \cdot (1 - y) \cdot w_2 \cdot h \cdot (1 - h) \cdot x = E_h \cdot x$$



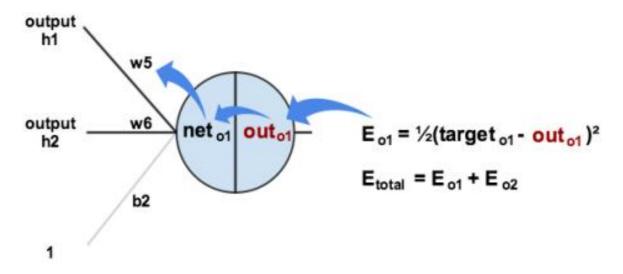
Backpropagation



Assume the hidden and output neurons use the sigmoid function for activation

Backpropagation

Output layer



$$\frac{\partial E_{total}}{\partial w_5} = \frac{\partial E_{01}}{\partial out_{01}} \times \frac{\partial out_{01}}{\partial net_{01}} \times \frac{\partial net_{01}}{\partial w_5}$$

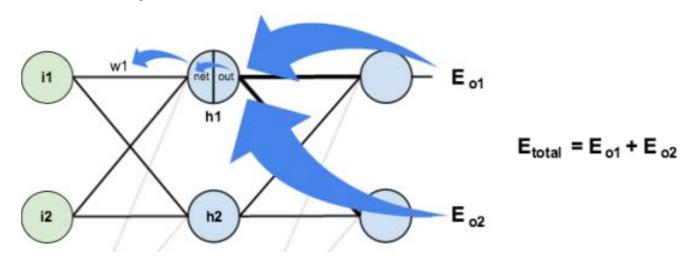
$$= -(target_{01} - out_{01}) \times out_{01}(1 - out_{01}) \times out_{h1}$$

$$= \delta_{01} \times out_{h1}$$



Backpropagation

Hidden layer



$$\frac{\partial E_{total}}{\partial w_1} = \frac{\partial E_{total}}{\partial out_{h1}} \times \frac{\partial out_{h1}}{\partial net_{h1}} \times \frac{\partial net_{h1}}{\partial w_1} \qquad \frac{\partial E_{total}}{\partial out_{h1}} = \frac{\partial E_{01}}{\partial out_{h1}} + \frac{\partial E_{02}}{\partial out_{h1}} \qquad \frac{\partial E_{01}}{\partial out_{h1}} = \frac{\partial E_{01}}{\partial net_{01}} \times \frac{\partial net_{01}}{\partial out_{h1}} \times \frac{\partial net_{01}}{\partial out_{h1}} = \frac{\partial E_{01}}{\partial out_{h1}} \times \frac{\partial e_{01}}{\partial out_{h1}} = \frac{\partial e_{01}}{\partial out_{h1}} \times \frac{\partial e_{01$$

$$\frac{\partial E_{total}}{\partial out_{h1}} = \frac{\partial E_{01}}{\partial out_{h1}} + \frac{\partial E_{02}}{\partial out_{h1}}$$

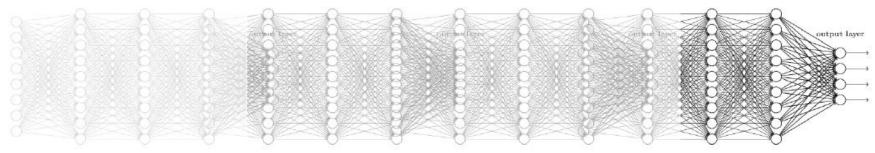
$$\frac{\partial E_{01}}{\partial out_{h1}} = \frac{\partial E_{01}}{\partial net_{01}} \times \frac{\partial net_{01}}{\partial out_{h1}}$$

$$= \left(\sum_{o} \frac{\partial E_{o}}{\partial out_{o}} \times \frac{\partial out_{o}}{\partial net_{o}} \times \frac{\partial net_{o}}{\partial out_{h1}}\right) \times \frac{\partial out_{h1}}{\partial net_{h1}} \times \frac{\partial net_{h1}}{\partial w_{1}}$$

$$= \left(\sum_{o} \delta_{o} \times w_{ho}\right) \times out_{h1}(1 - out_{h1}) \times i_{1}$$

$$\frac{\partial E_{01}}{\partial net_{01}} = \frac{\partial E_{01}}{\partial out_{01}} \times \frac{\partial out_{01}}{\partial net_{01}}$$

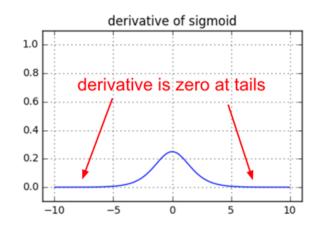


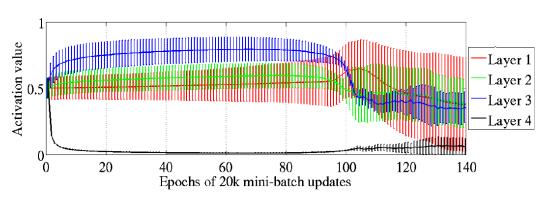


Source: http://hunkim.github.io/ml/

- meaning that the gradient (error signal) decreases
 exponentially with n and the front layers train very slowly.
- why?
 - Initializing the weights in a stupid way
 - Using wrong type of non-linearity





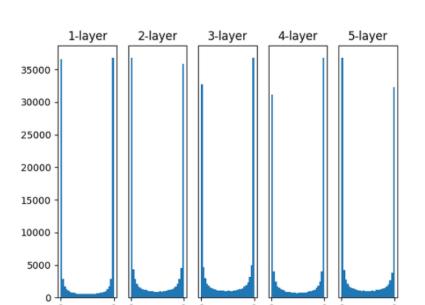


Source: Understanding the difficulty of training deep feedforward neural networks

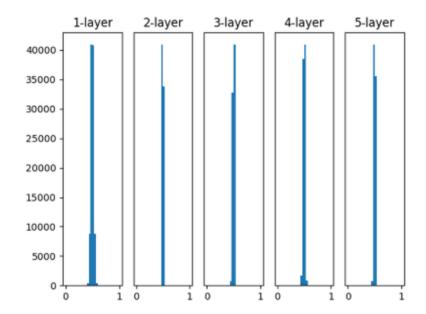


초기 가중치에 따른 활성화 값 분포

Activation function = sigmoid, init. W ~ N(0, 1)



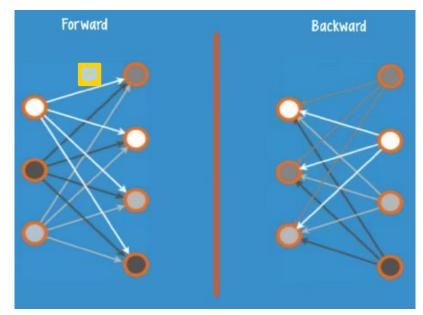
 Activation function = sigmoid, init. W ~ N(0, 0.01)



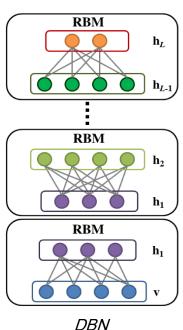
Source: "밑바닥부터 시작하는 딥러닝", 사이토 고키

Deep learning begins

- 2006년, <u>Geoffrey Hinton</u>에 의해 RBM 기반의 pre-training으로 Deep Neural Network의 학습이 가능해 지면서 <u>"Deep Learning"이라는 새로운 이름으로 다시 주</u> 목을 받기 시작함.
- Deep Belief Networks
 - Hinton et al. (2006) "A Fast Learning Algorithm for Deep Belief Nets"
 - Apply the RBM idea on adjacent two layers as a pre-training step, and continue the first process to all layers => This will initialize good weight values!



RBM(Restricted Boatman Machine) structure





Modern weight value initialization

Makes sure the weights are 'just right', not too small, not too big

Xavier initialization

- Glorot & Bengio (2010) "Understanding the difficulty of training deep feedforward neural networks"
- initializes the weights by drawing them from a distribution with zero mean and a specific variance,

$$Var(\mathbf{W}) = \frac{1}{n_{in}}$$

where W is the initialization distribution for the neuron in question, and n_{in} is the number of neurons feeding into it. The distribution used is typically Gaussian or uniform.

He's initialization

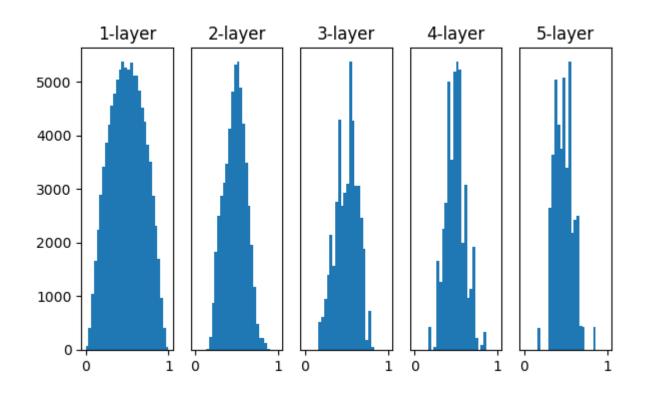
- He et al. (2015) "Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification"
- For ReLU, it is recommended using

$$Var(\mathbf{W}) = \frac{2}{n_{in}}$$



Modern weight value initialization

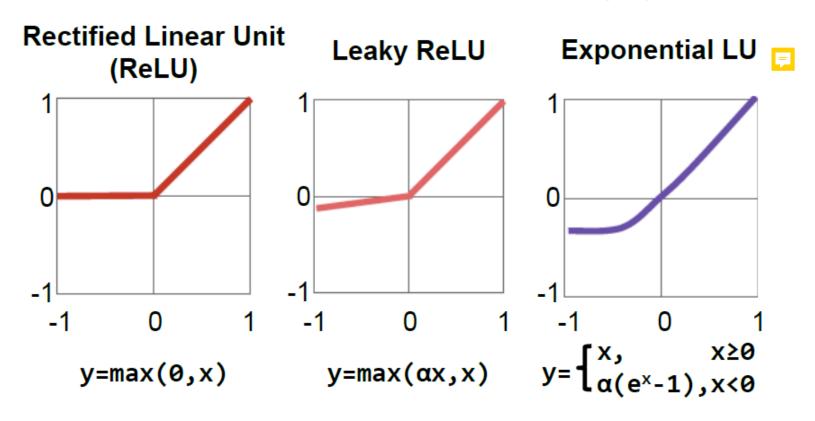
■ Xavier initialization 적용 시의 활성화 값 분포





Modern activation functions

Source: Efficient Processing of Deep Neural Networks: A Tutorial and Survey

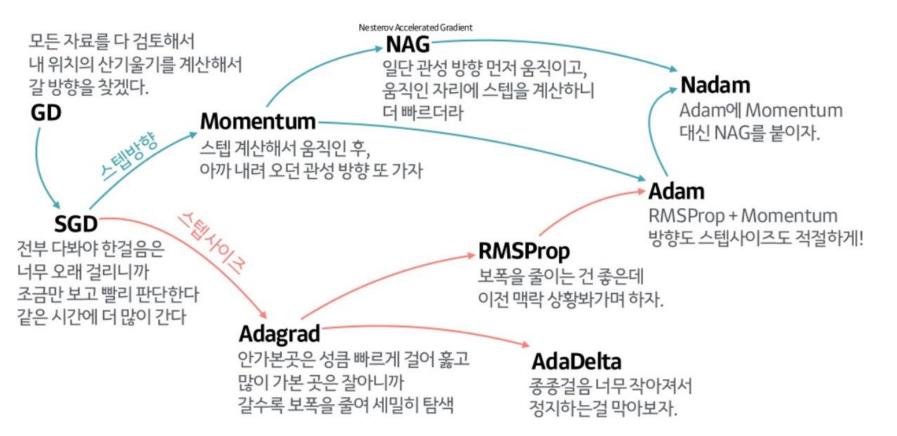


scikit-learn에서는 relu(기본값), logistic, tanh, identity를 지원



Optimization techniques

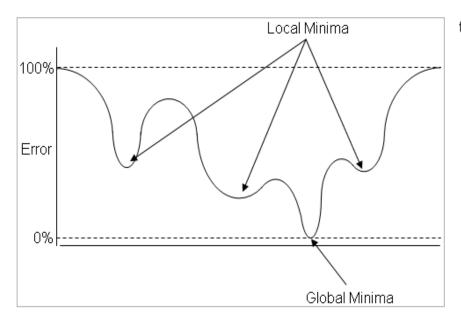
Source: https://www.slideshare.net/yongho/ss-79607172



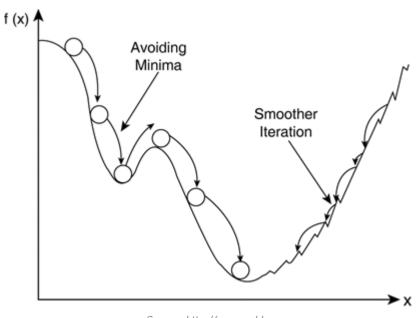
scikit-learn에서는 adam(기본값), sgd, lbfgs를 지원



Momentum







Source: http://www.yaldex.com

기존 업데이트에 사용했던 기울기의 일정 비율을 남겨서 현재의 기울기와 더하여 업데이트함.

$$v^{(t+1)} = \alpha v^{(t)} + \eta \frac{\partial E}{\partial W^{(t)}}$$
$$W^{(t+1)} = W^{(t)} - v^{(t+1)}$$

recommended $\alpha \approx 0.9$



Modern optimizers

Adagrad
 (Adaptive Gradient)

$$G_t = G_{t-1} + (\nabla_{\theta}J(\theta_t))^2$$

$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{G_t + \epsilon}} \cdot \nabla_{\theta}J(\theta_t)$$

RMSProp



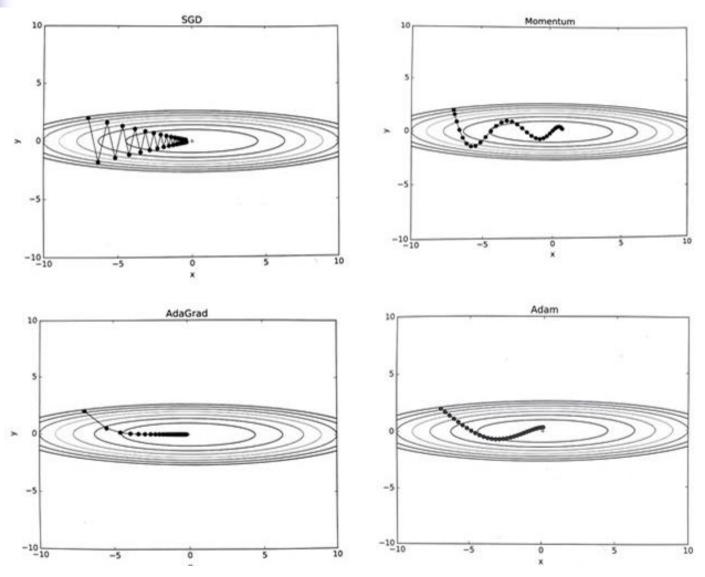
$$G = \gamma G + (1 - \gamma)(\nabla_{\theta} J(\theta_t))^2$$
$$\theta = \theta - \frac{\eta}{\sqrt{G + \epsilon}} \cdot \nabla_{\theta} J(\theta_t)$$

Adam (Adaptive Moment Estimation)

$$m_t = \beta_1 m_{t-1} + (1 - \beta_1) \nabla_{\theta} J(\theta)$$
 \longleftarrow Momentum $v_t = \beta_2 v_{t-1} + (1 - \beta_2) (\nabla_{\theta} J(\theta))^2$ \longleftarrow RMSProp

$$\begin{split} \hat{m_t} &= \frac{m_t}{1 - \beta_1^t} \\ \hat{v_t} &= \frac{v_t}{1 - \beta_2^t} \\ \theta &= \theta - \frac{\eta}{\sqrt{\hat{v_t} + \epsilon}} \hat{m_t} \end{split}$$







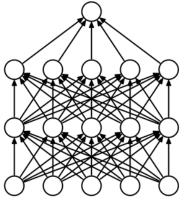
Solutions for overfitting

- Regularization (L2 penalty)
 - Let's not have too big numbers in the weight

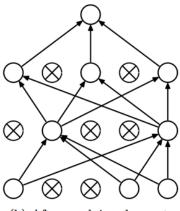
$$E(W) + \frac{1}{2}\lambda W^2$$

Dropout

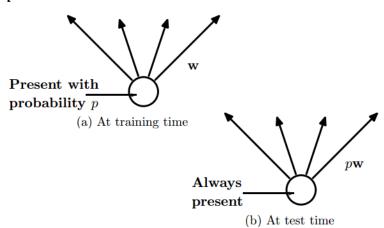
- Srivastava et al. (2014) "Dropout: A Simple Way to Prevent Neural Networks from Overfitting"
- randomly selected neurons are ignored during training
- If a unit is retained with probability p during training, the outgoing weights of that unit are multiplied by p at test time



(a) Standard Neural Net



(b) After applying dropout.



1

How to tune hyperparameter

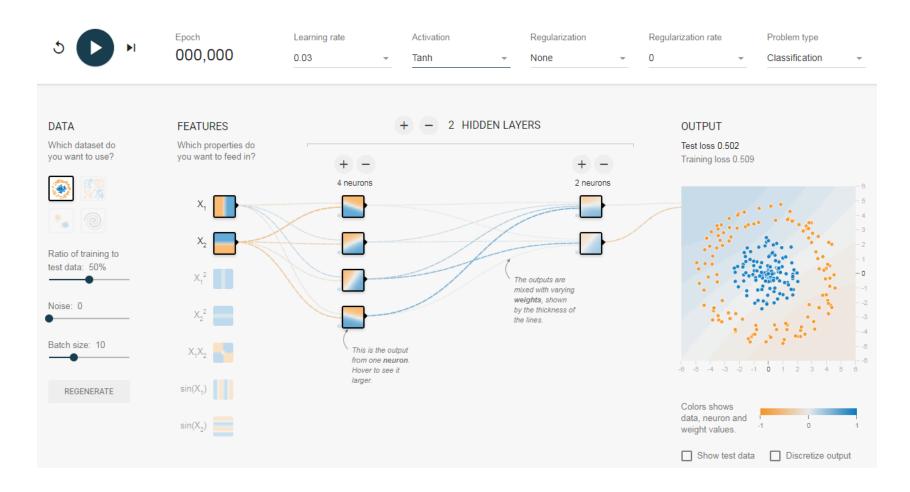
• 주요 파라미터

- 은익층과 은익노드의 개수
- 활성화함수
- Regularization
- 최적화 기법
- 가중치 초기화 방식
- learning rate와 mini-batch size

■ 일반적인 방법

- 'Stretch pants' 접근법
 - ▶ 충분히 과적합되어 원하는 성능이 나올만한 복잡한 모델을 만든 후 신경망 구조를 줄이거나 regularization을 강화하여 일반화 성능을 향상
 - ▶ Deep network이 shallow network 보다 파라미터 효율성이 좋음 훨씬 적은 수의 뉴런 사용
 - ▶ 최근에는 고려할 hyperparameter의 수를 줄이기 위해 모든 은익층에서 같은 수의 은익노드를 갖는 추세
- Random Search 활용
 - CV를 통해 적절한 hyperparameter를 찾고자 할 때 grid search 보다 random search가 더 효율적

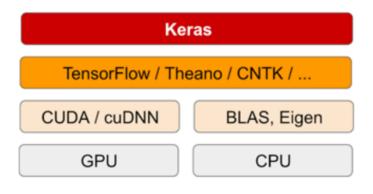
Neural Network Playground: An interactive tool for learning neural networks



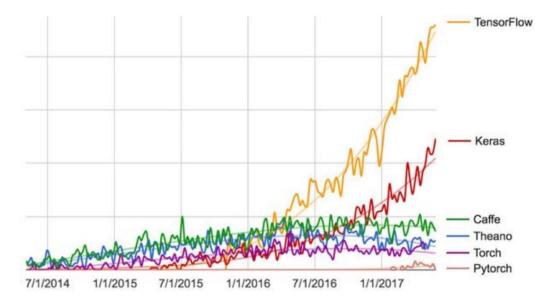


Keras Framework

- What is Keras
 - Tensorflow, CNTK, Theano를 사용하기 편하게 만들어 놓은 high-level API
 - Documentation: http://keras.io/



Source: Deep Learning with Python by François Chollet



Model building steps (Sequential API)

- Specify Architecture
 - model = Sequential(): 모형 생성
 - model.add(): 레이어 추가
- Compile
 - model.compile(): 목적함수 및 최적화 방법 지정
- Fit
 - model.fit(): 입력, 출력 데이터를 사용하여 가중치 계산
- Predict
 - model.predict()

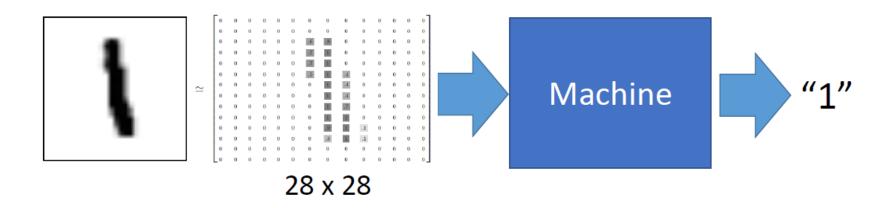
Core layers

- Dense()
- Activation()
 - softmax(): multi-category output
 - sigmoid(): binary output
- Dropout()



Training DNN with keras

Application - Handwriting Digit Recognition



Source: Deep Learning Toolkit: Keras 50

Training

Training DNN with keras

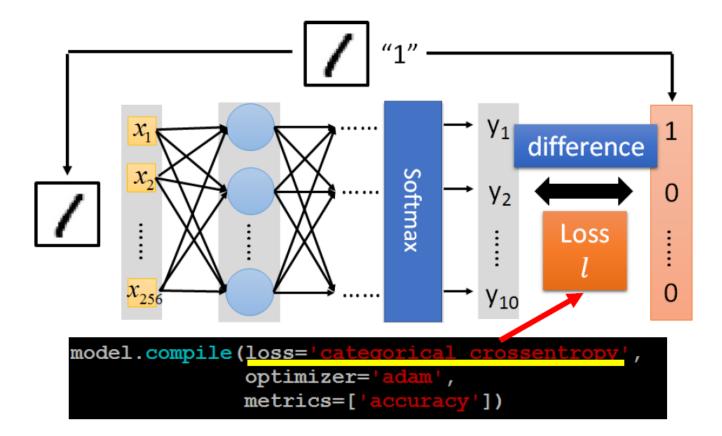
Step 1. define a model

```
28x28
                                        model = Sequential()
                                 model.add( Dense( input dim=
   500
                                 model.add( Activation('sigmoi
                                             softplus, softsign, relu, tanh,
                                             hard sigmoid, linear
   500
                                 model.add( Dense( output dim=500
model.add( Activation('sigmoid')
               Softmax
                                 model.add( Dense(output dim=
                                 model.add( Activation('softr
                 y_{2}..... y_{10}
```

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Training DNN with keras

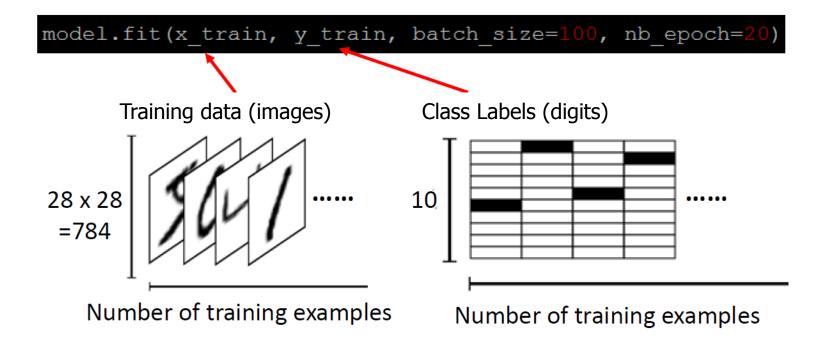
Step 2. configure the learning process



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Step 3. iterate on the training data



Source: Deep Learning Toolkit: Keras 53

Training DNN with keras

Step 4. evaluate & use the model

```
score = model.evaluate(x_test,y_test)
print('Total loss on Testing Set:', score[0])
print('Accuracy of Testing Set:', score[1])

result = model.predict(x_test)
```