

4. Neural networks 설계 고려사항



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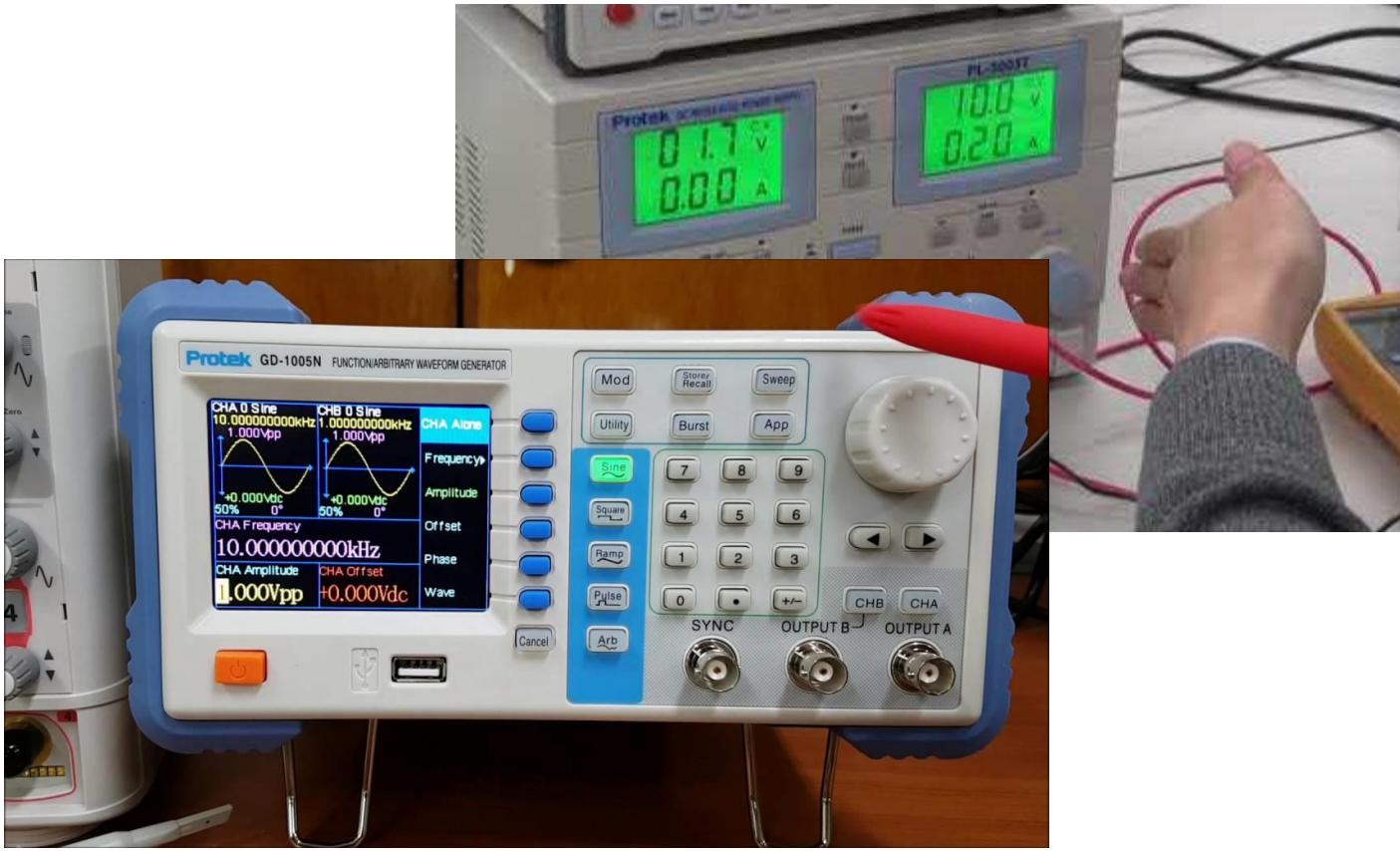
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학습목표

- Deep neural networks를 설계하고 학습하기 위하여 tool을 사용할 때 고려해야 할 다양한 조건들을 알아본다.



참고 자료

- <https://www.deeplearningbook.org/>
 - Chapter 8 Optimization for Training Deep Models
- <http://cs231n.stanford.edu/syllabus.html>
 - Lecture 8 April 25 Training Neural Networks, part II
- Youtube: Lecture Collection | Convolutional Neural Networks for Visual Recognition (Spring 2017) Stanford University School of Engineering
 - Lecture 7 | Training Neural Networks II



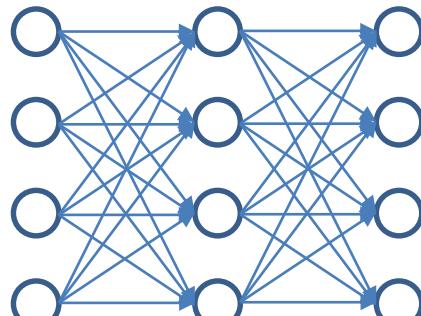
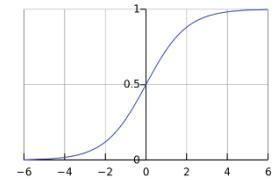
목차

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- Deep Belief Networks
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- Regularization
- Initialization
- Output Units
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- Summary : Neural networks 설계 고려사항



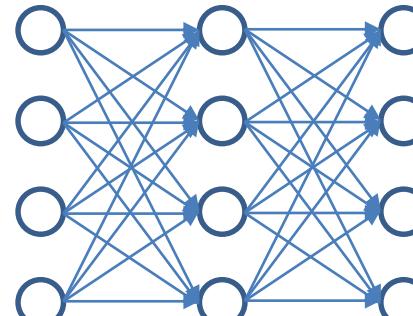
기울기 소실 문제 (vanishing gradient problem)

- Deep neural network 에서 문제
 - Back propagation 중 작은 기울기가 계속 곱해져서 0에 수렴
- 해결방법
 - Bottom-up layerwise unsupervised pre-training
 - ReLU
 - Gradient Flow



w_1

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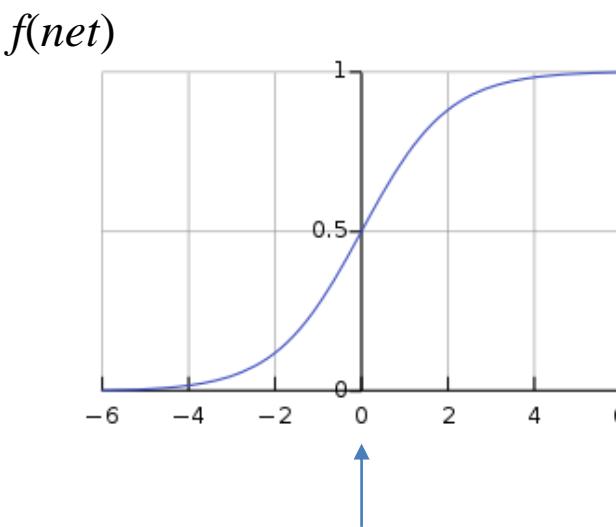
w_{10}

E

Vanishing gradient problem



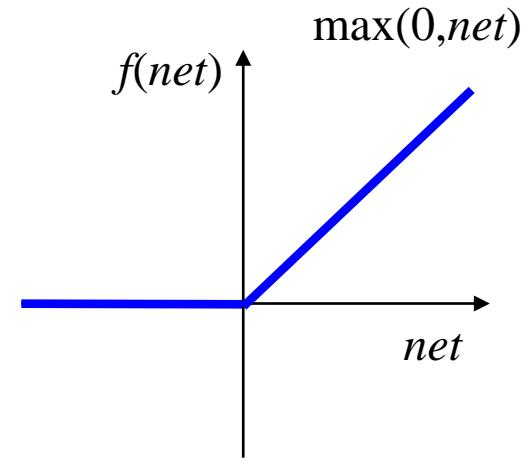
$$\Delta w_{ij} = c f'(net_j) x_i \sum_k \delta_k w_{jk} = c \delta_j x_i$$



$$f'(net_j) \rightarrow 0$$

$$\Delta w_{ij} \rightarrow 0$$

$$\text{Update} \rightarrow 0$$



Rectified linear unit
(ReLU)

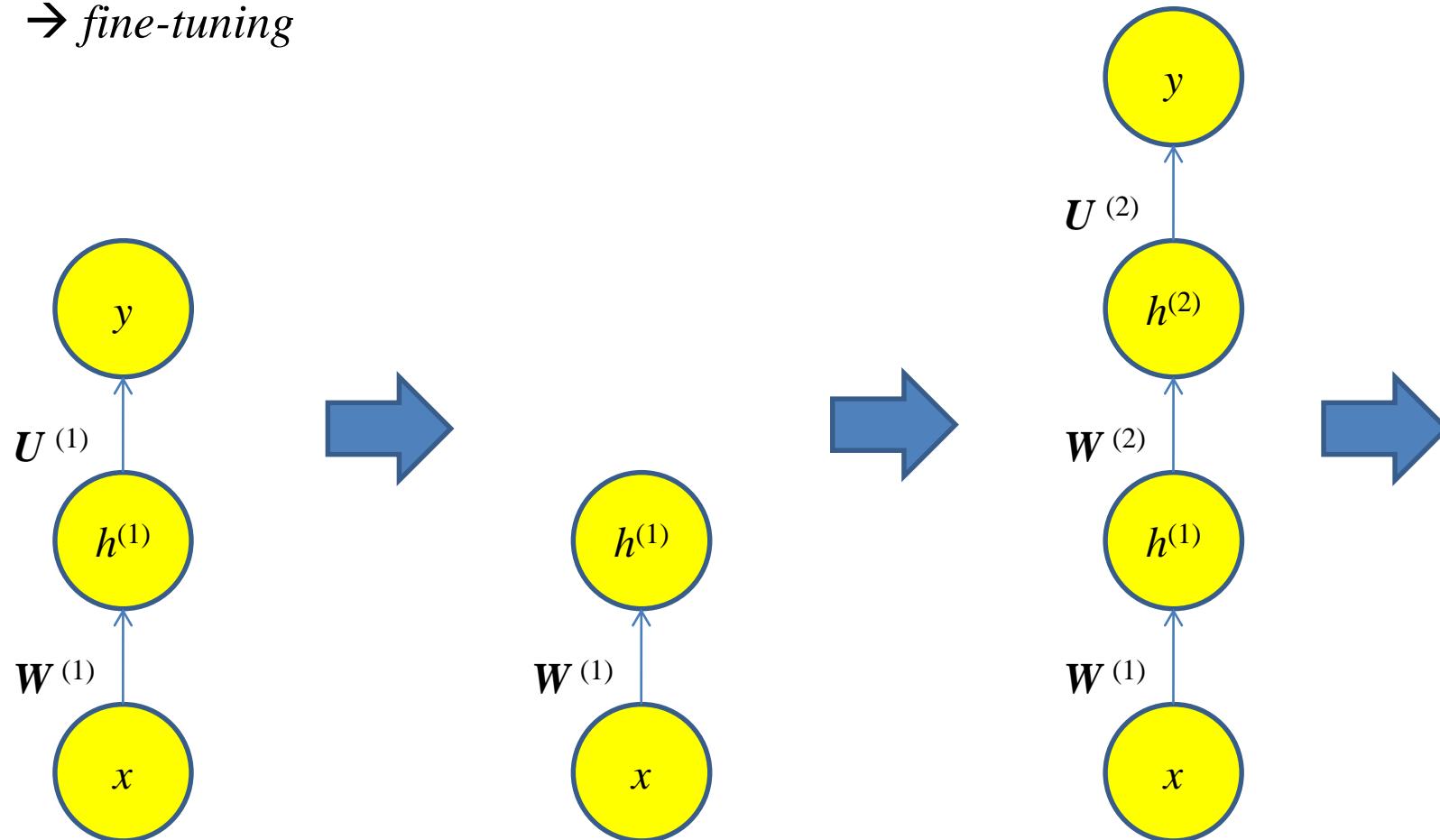
$$\begin{aligned} f'(net) &= 1 & \text{if } net > 0 \\ f'(0) &= 0.5 \end{aligned}$$

- $f'(net) = 0$ 에 가까운 값이 층마다 계속 곱해짐.



Greedy layerwise supervised pretraining

- 작은 부분을 차례로 학습
→ *fine-tuning*



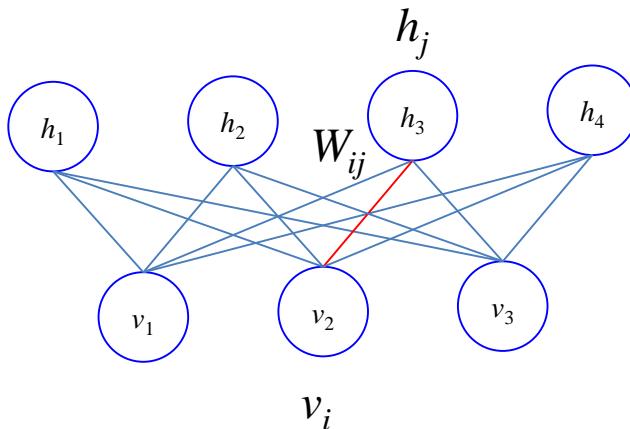
Restricted Boltzmann Machine(RBM)

- Stochastic : data distribution 학습 가능
- Generative : 데이터 생성 가능

- Energy:

$$E(\mathbf{v}, \mathbf{h}) = -\mathbf{b}^T \mathbf{v} - \mathbf{c}^T \mathbf{h} - \mathbf{v}^T \mathbf{W} \mathbf{h}$$

Hidden
units \mathbf{h}



Visible
units \mathbf{v}

$$p(\mathbf{h} \mid \mathbf{v}) = \prod_i p(h_i \mid \mathbf{v})$$

$$p(\mathbf{v} \mid \mathbf{h}) = \prod_i p(v_i \mid \mathbf{h}).$$

- 생성 확률:

$$P(\mathbf{v}, \mathbf{h}) = \frac{1}{Z} \exp(-E(\mathbf{v}, \mathbf{h}))$$

$$E(\mathbf{v}, \mathbf{h}) = -\sum_j b_j v_j - \sum_i h_i c_i - \sum_{i,j} v_i W_{ij} h_j$$

$$P(h_i = 1 \mid \mathbf{v}) = \sigma \left(\mathbf{v}^\top \mathbf{W}_{:,i} + b_i \right),$$

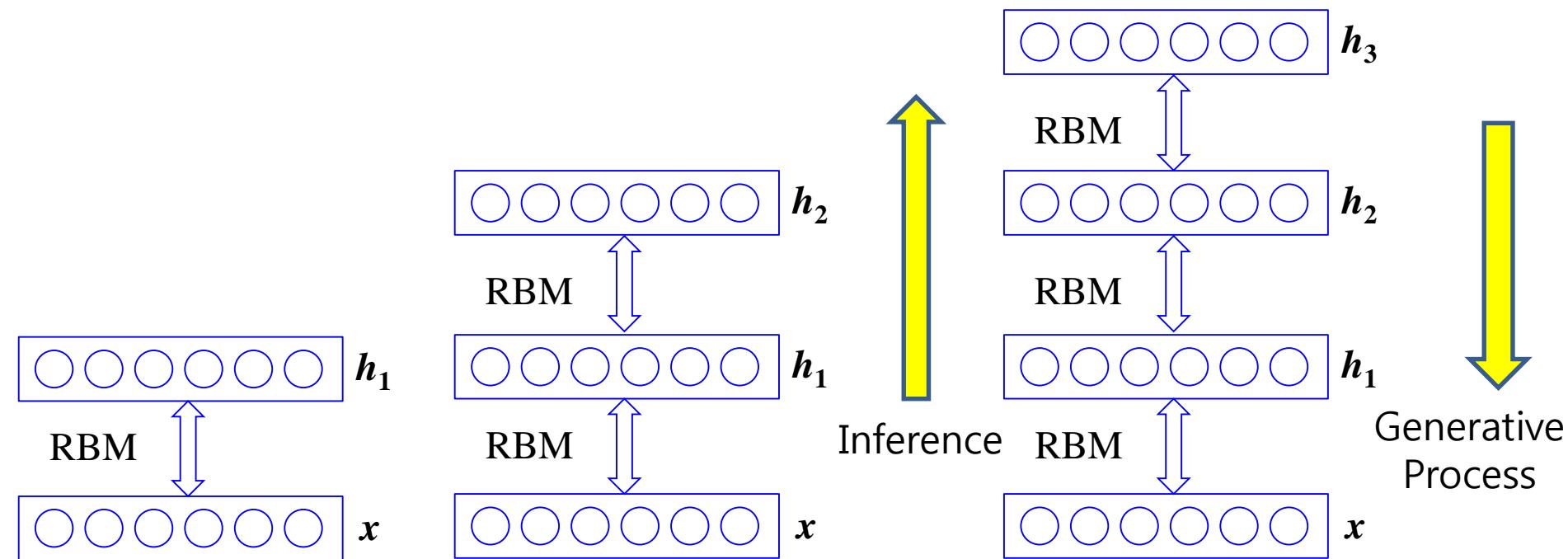
$$P(h_i = 0 \mid \mathbf{v}) = 1 - \sigma \left(\mathbf{v}^\top \mathbf{W}_{:,i} + b_i \right)$$

$$\frac{\partial}{\partial W_{i,j}} E(\mathbf{v}, \mathbf{h}) = -v_i h_j.$$

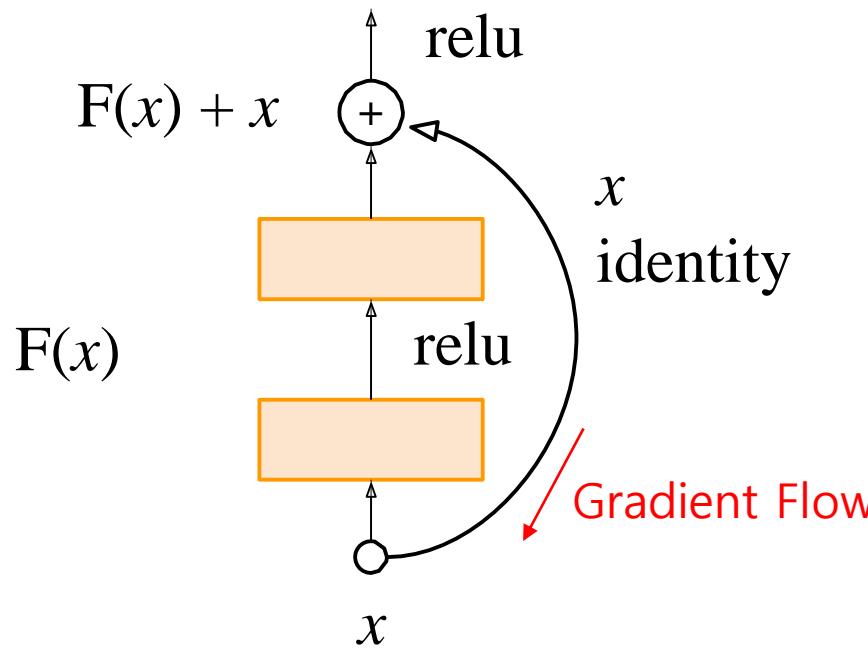


Deep Belief Networks (Hinton et al., 2006)

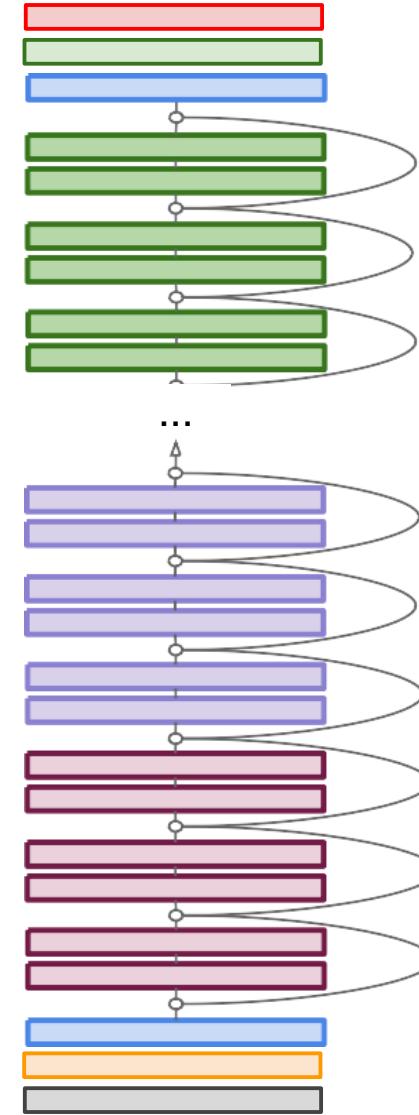
- Greedy layer-wise training
- 나중에 Supervised fine-tuning
- Deep learning의 시작 → 지금은 많이 사용되지 않음



Residual Net

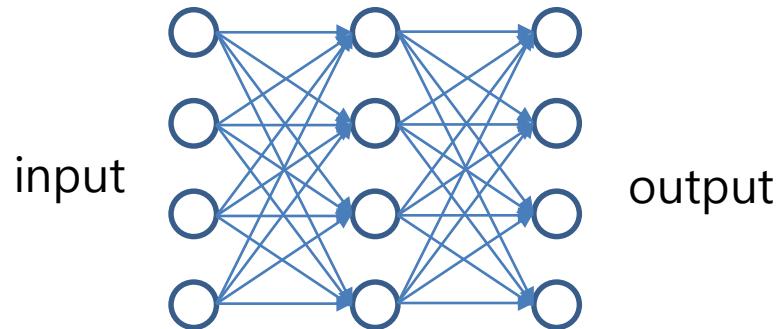


- Gradient Flow 를 위한 통로를 만들어 깊은 층 구현 가능



Summary : Neural networks 설계 고려사항

- Network topology : 어떤 모양?
- Activation function : 출력의 형태?
 - linear or non-linear?
- Objectives : 훈련의 목적?
 - Classification or regression ?
= Loss function, Error
- Optimizers : 훈련의 방법?
 - Weights update
- Regularization
 - overfitting 을 어떻게 방지할까?



Output 형태

- **One-hot vector**

$$\mathbf{d}_n = [0\ 0\ 1\ 0\ 0\ 0\ 0\ 0\ 0]^\top$$



...



Objective functions



Objectives (목적함수)

- Mean squared error

$$MSE = \frac{1}{2} (t - f(x))^2$$

- Cross entropy = negative log likelihood

$$E(\mathbf{w}) = - \sum_{n=1}^N \sum_{k=1}^K d_{nk} \log y_k(\mathbf{x}_n; \mathbf{w})$$

- Binary cross entropy:

$$C = -\frac{1}{n} \sum_x [y \ln f(x) + (1-y) \ln(1-f(x))]$$

- Categorical cross entropy:

$$C = -\frac{1}{n} \sum_x \sum_y [y \ln f(x) + (1-y) \ln(1-f(x))]$$



문제의 유형에 따라 사용되는 활성화 함수 및 오차함수의 종류

문제의 유형	Output Activation function	Objectives
Regression	Linear	Mean squared error
Binary classification	Logistic function (sigmoid)	Binary cross entropy
Multi class classification	Softmax	Categorical cross entropy

참고도서: 딥 러닝 제대로 시작하기



회기 (regression)

- 출력이 연속값을 갖는 함수를 대상으로 훈련 data 를 잘 재현하는 함수를 찾는 것.
- Squared error

$$\| \mathbf{d} - \mathbf{y}(\mathbf{x}, \mathbf{w}) \|^2$$

\mathbf{d} : desired output (target)

$\mathbf{y}(\mathbf{x}, \mathbf{w})$: 신경망의 output

N : number of training samples

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^N \| \mathbf{d}_n - \mathbf{y}(\mathbf{x}_n, \mathbf{w}) \|^2$$

- 응용 분야: 매출액 추정, 생산 속도에 따른 불량률 추정, ..., ∞



Binary Classification

- Two classes : $d = 0, d = 1$ if $d = 1$ then output $p(1|x)$
- 훈련 데이터 $\{(\mathbf{x}_n, \mathbf{d}_n)\}, n=1, \dots, N$ if $d = 0$ then output $p(0|x)$

$$p(d=1|\mathbf{x}) \approx y(\mathbf{x}, \mathbf{w})$$

$$p(d|\mathbf{x}) = p(d=1|\mathbf{x})^d p(d=0|\mathbf{x})^{1-d}$$

- Maximum likelihood estimation

likelihood 를 가장 크게 하는 \mathbf{w} 를 구한다.

$$f(u) = \frac{1}{1 + e^{-u}}$$

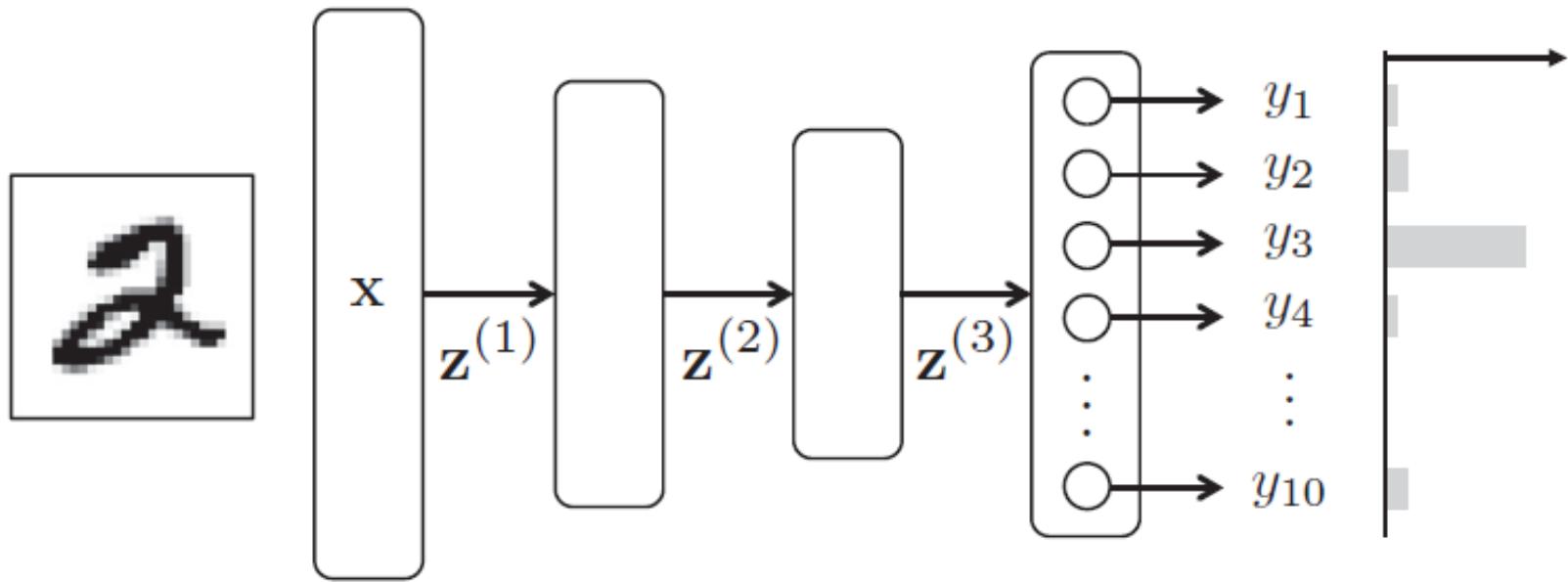
$$L(\mathbf{w}) \equiv \prod_{n=1}^N p(d_n|\mathbf{x}_n; \mathbf{w}) = \prod_{n=1}^N \{y(\mathbf{x}_n; \mathbf{w})\}^{d_n} \{1 - y(\mathbf{x}_n; \mathbf{w})\}^{1-d_n}$$

- 곱셈을 반복하면 underflow 가 생기므로 log 로 변환

$$E(\mathbf{w}) = - \sum_{n=1}^N [d_n \log y(\mathbf{x}_n, \mathbf{w}) + (1 - d_n) \log \{1 - y(\mathbf{x}_n, \mathbf{w})\}]$$



Multi-class Classification



- Classification 문제의 예. 숫자 필기 인식.
- 입력 이미지 x 가 0에서 9까지의 숫자 중 어느 것인지를 판별한다.
- Softmax 층은 0에서 9까지의 숫자 중 입력 이미지가 어느 것에 가까운지를 나타내는 p_1, \dots, p_{10} 의 수치로 출력한다.

출처: 딥 러닝 제대로 시작하기

다클래스 분류의 오차 함수

- Classes: C_1, \dots, C_K
- 목표 출력 (binary): $\mathbf{d}_n = [d_{n1}, \dots, d_{nK}]^T$ ex) $\mathbf{d}_n = [0 0 1 0 0 0 0 0 0]^T$
- 사후 확률: **One-hot vector**

$$p(\mathbf{d}|\mathbf{x}) = \prod_{k=1}^K p(C_k|\mathbf{x})^{d_k}$$

- 훈련 데이터 $\{(\mathbf{x}_n, \mathbf{d}_n)\}, n=1, \dots, N$ 에 대한 likelihood

$$L(\mathbf{w}) = \prod_{n=1}^N p(\mathbf{d}_n | \mathbf{x}_n; \mathbf{w}) = \prod_{n=1}^N \prod_{k=1}^K p(C_k | \mathbf{x}_n)^{d_{nk}} = \prod_{n=1}^N \prod_{k=1}^K (y_k(\mathbf{x}; \mathbf{w}))^{d_{nk}}$$

- Cross entropy, negative log likelihood

$$E(\mathbf{w}) = - \sum_{n=1}^N \sum_{k=1}^K d_{nk} \log y_k(\mathbf{x}_n; \mathbf{w})$$



기타 Objectives (목적함수)

- Mean absolute error / mae
- Mean absolute percentage error / mape
- Mean squared logarithmic error / msle
- Hinge = $\max(0, 1 - t \cdot f(x))$
- Squared hinge
- Sparse categorical cross entropy
- Kullback leibler divergence / kld
- Poisson: mean of (predictions - targets * log(predictions))
- Cosine proximity: the opposite (negative) of the mean cosine proximity between predictions and targets.

t : desired output



Optimizers



Optimizers – weight update 방법

- Stochastic gradient descent
- Momentum
- Learning rate decay
- Rmsprop
- Adagrad
- Adadelta
- Adam
- Adamax
- Nadam
- Nesterov



Batch and Minibatch Algorithms

1. **Oneline** : Sample 하나마다 update

2. **batch** or **deterministic gradient methods** :

- 모든 training sample에 대하여 계산되는 error function 사용
- 모든 input에 대하여 Δw 를 계산하여 평균 이용 → 많은 시간 소요

$$E(\mathbf{w}) = \sum_{n=1}^N E_n(\mathbf{w})$$



3. **minibatch** or **minibatch stochastic** methods

- sample의 일부만을 사용하여 파라미터 update

$$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \epsilon \nabla E_n$$



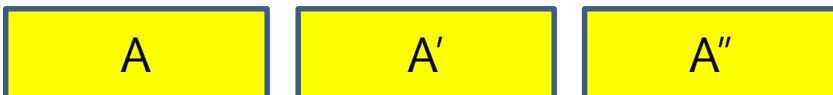
minibatch

Stochastic gradient descent의 장점

- 훈련 데이터에 중복성이 있을 때 효율이 향상되고 학습이 빨리 진행된다



전체 데이터



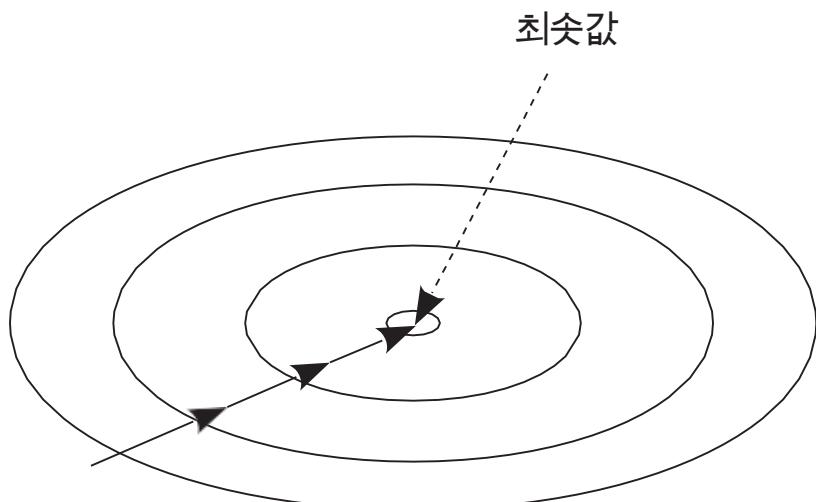
Stochastic gradient descent (sgd)

- Local minimum에 빠질 위험이 줄어든다
 - 반복할 때마다 random sample selection
- Update의 크기가 작은 상태로 학습이 진행
 - 학습의 경과 관찰이 용이
- Online 학습
 - 데이터의 수집과 최적화가 동시에 진행

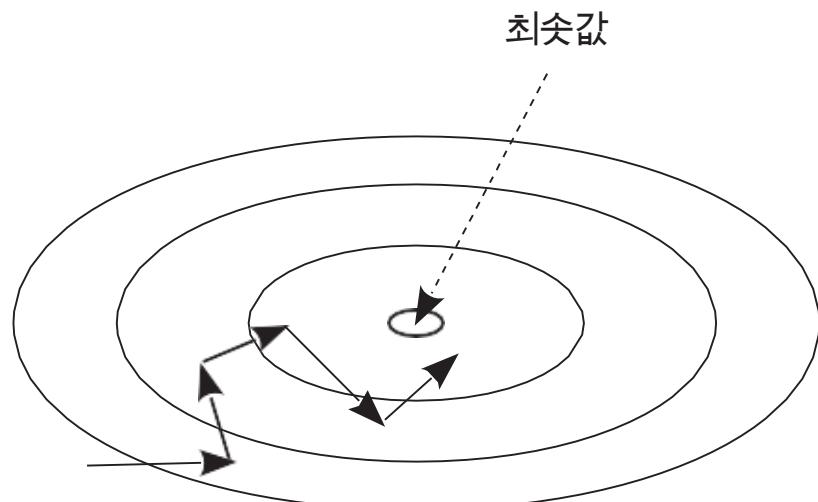


Stochastic gradient descent

- 기울기 벡터가 정확하게 계산되지 않음
- Avoid local minimum



모든 데이터를 사용한 경사 하강법



미니 배치에 의한 확률적 경사 하강법

그림 2-24 Stochastic gradient descent 방법으로 최솟값으로 향하는 모습

Algorithm 8.1 Stochastic gradient descent (SGD) update at training iteration k

Require: Learning rate ε .

Require: Initial parameter θ

while stopping criterion not met do

 Sample a minibatch of m examples from the training set $\{\mathbf{x}(1), \dots, \mathbf{x}(m)\}$ with corresponding targets $y^{(i)}$.

 Compute gradient estimate: $\mathbf{g} \leftarrow 1/m \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)} ; \theta), y^{(i)})$

 Apply update: $\theta \leftarrow \theta - \varepsilon \mathbf{g}$

end while

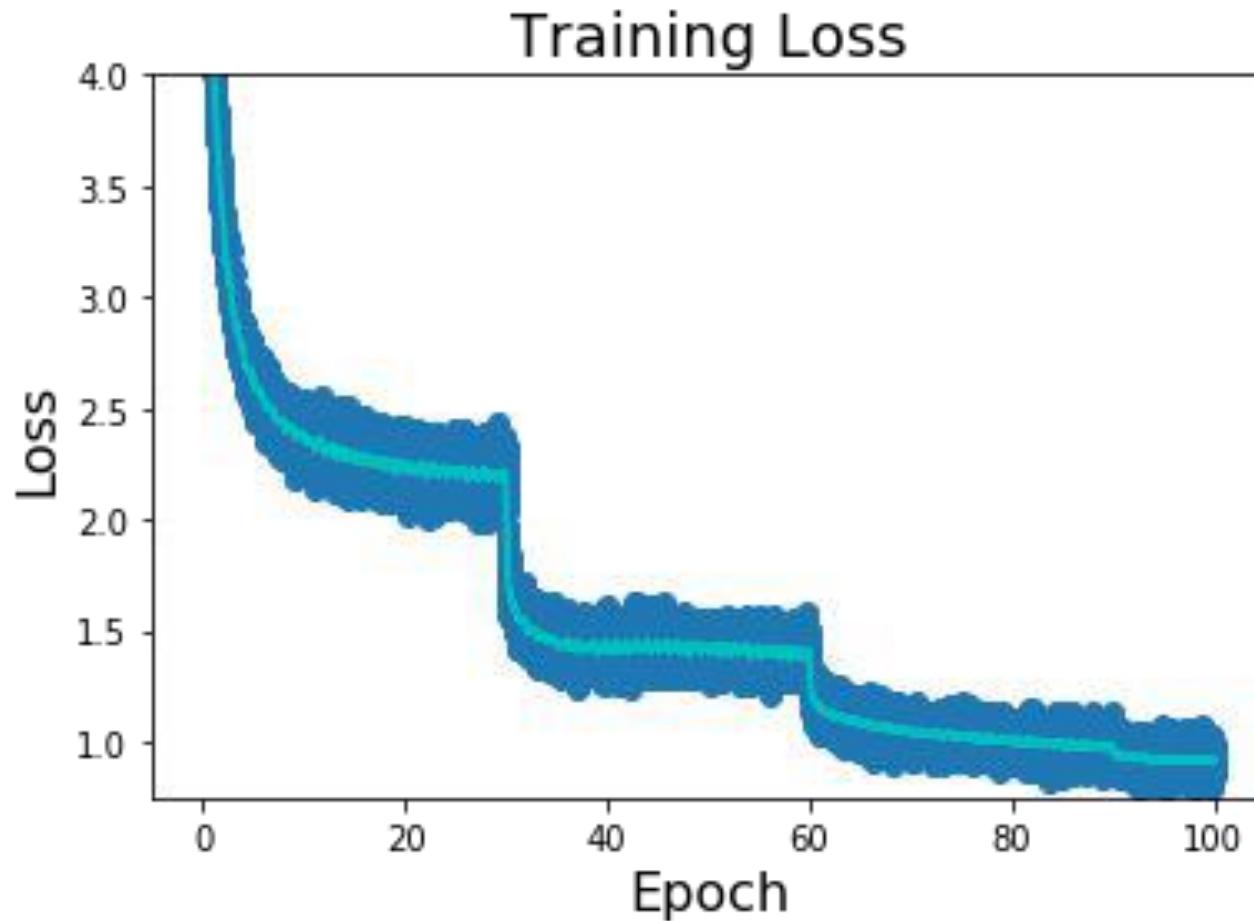
기울기
↑

학습률(ϵ)의 결정 방법

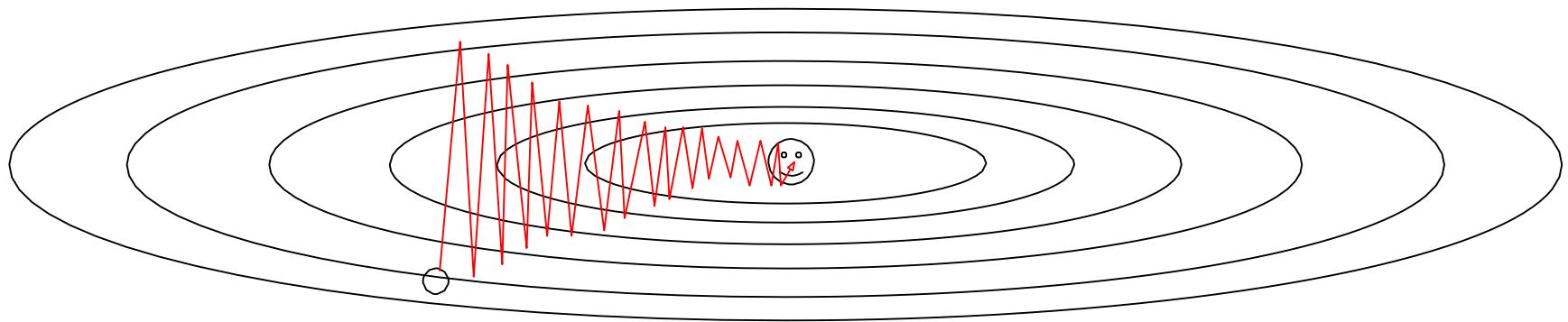
- Learning Rate Decay : 학습 초기에 값을 크게 설정했다가 학습의 진행과 함께 학습률을 점점 줄여가는 방법
 - 학습률을 파라미터 업데이트 회수에 비례해서 작아지도록
$$\epsilon = \epsilon_0 / (at)$$
 - 처음에 상수 $\epsilon = \epsilon_0$ 을 설정하고 어느 정도 학습이 진행되면 그 값을 1/10로 줄여
- 다른 예: 각 층마다 서로 다른 값을 사용
 - 각 층의 weight 업데이트 속도가 비슷하게 되도록
 - 예)
 - 출력에 가까운 층 : 작게
 - 입력에 가까운 층 : 크게



Learning Rate Decay



Problems with SGD



Momentum

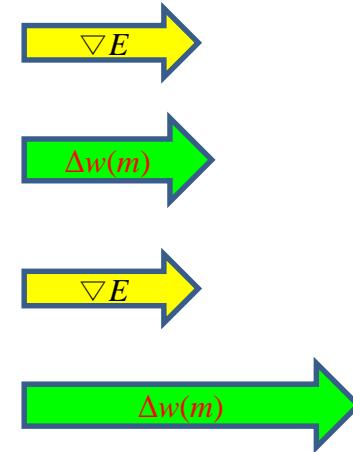
- 가속도 (gradient 가 속도를 조절하는 역할)
- 이전 weight 변화를 어느정도 유지

$$\Delta w^{(t)} = \mu \Delta w^{(t-1)} - \epsilon \nabla E_t$$

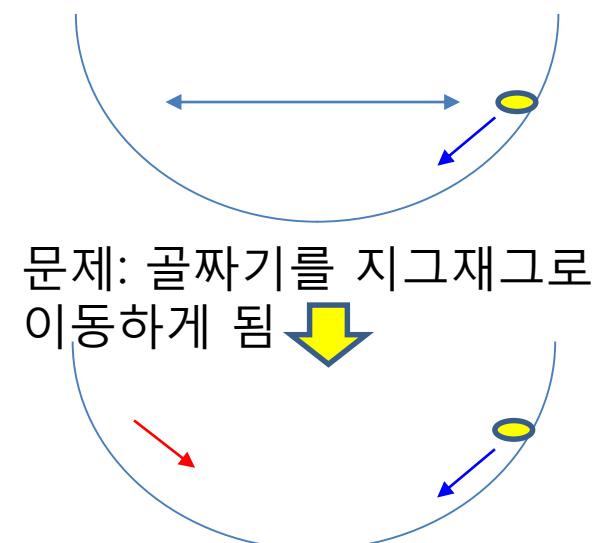
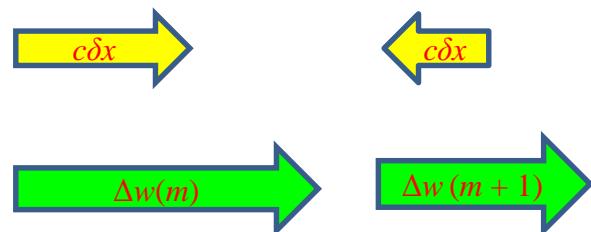
이전 변화량 (속도 v) 현재 기울기

Momentum constant

Learning rate

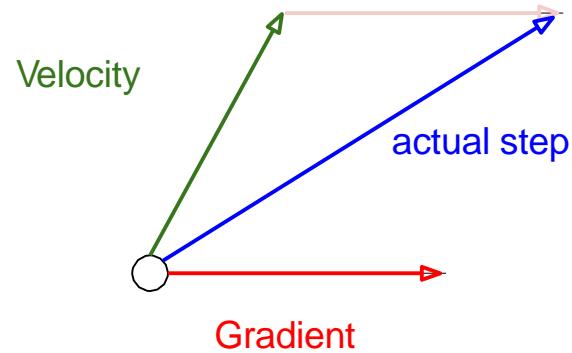
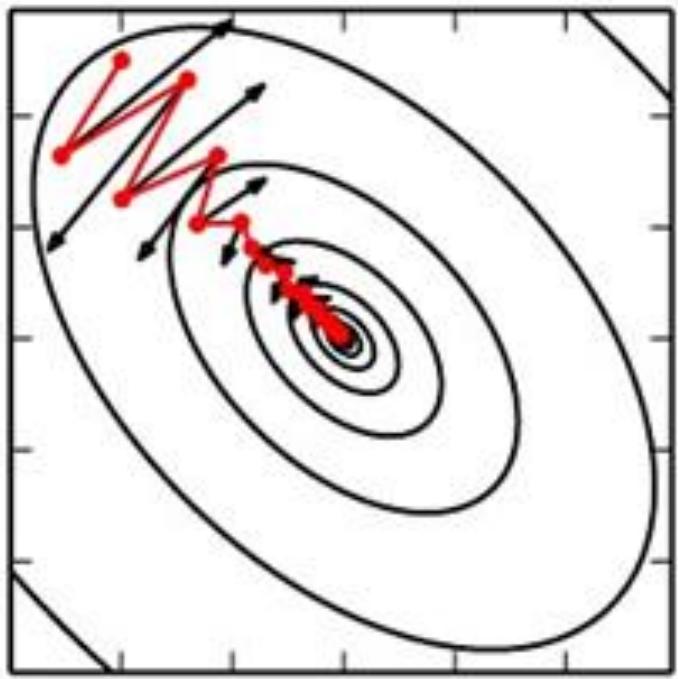


- weight의 업데이트 값에 이전 업데이트 값의 일정 비율을 더함.
- $\mu = 0.5 \sim 0.9$
- ϵ : learning rate
- Weight 변화가 oscillating 하는 것 방지



문제: 골짜기를 지그재그로
이동하게 됨

The effect of momentum



Nesterov Momentum (Sutskever *et al.* 2013)

- a variant of the momentum algorithm
- inspired by Nesterov's accelerated gradient method (Nesterov, 1983, 2004).
- The update rules :

$$\begin{aligned} \mathbf{v} &\leftarrow \alpha \mathbf{v} - \epsilon \nabla_{\theta} \left[\frac{1}{m} \sum_{i=1}^m L\left(f(\mathbf{x}^{(i)}; \theta + \alpha \mathbf{v}), \mathbf{y}^{(i)}\right) \right] \\ \theta &\leftarrow \theta + \mathbf{v}, \end{aligned}$$


- The difference between Nesterov momentum and standard momentum is
 - where the **gradient** is evaluated.
- With Nesterov momentum the gradient is evaluated
 - after the current **velocity** is applied.
- Thus one can interpret Nesterov momentum as attempting to add a **correction factor** to the standard method of momentum.
- The complete Nesterov momentum algorithm is presented in Algorithm 8.3.

Nesterov momentum

Require: Learning rate ϵ , momentum parameter α .

Require: Initial parameter θ , initial velocity v .

while stopping criterion not met **do**

 Sample a minibatch of m examples from the training set $\{x^{(1)}, \dots, x^{(m)}\}$ with corresponding labels $y^{(i)}$.

Apply interim update: $\tilde{\theta} \leftarrow \theta + \alpha v$

 Compute gradient (at interim point): $g \leftarrow \frac{1}{m} \nabla_{\tilde{\theta}} \sum_i L(f(\mathbf{x}^{(i)}; \tilde{\theta}), \mathbf{y}^{(i)})$

 Compute velocity update: $v \leftarrow \alpha v - \epsilon g$

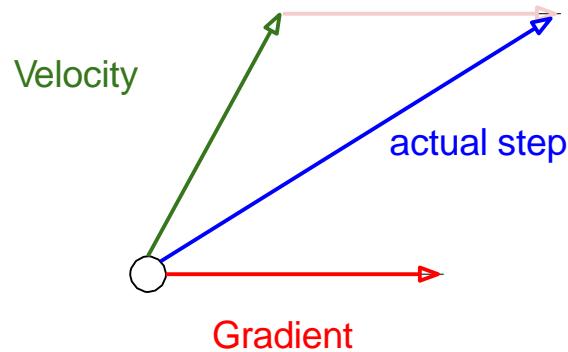
Apply update: $\theta \leftarrow \theta + v$

end while

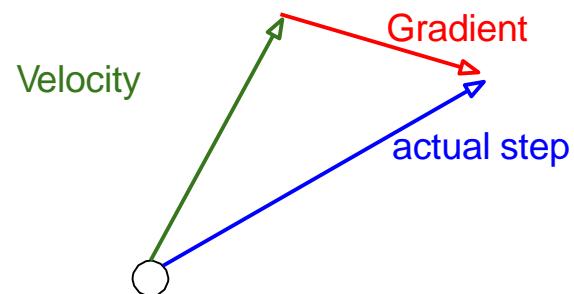


Nesterov momentum

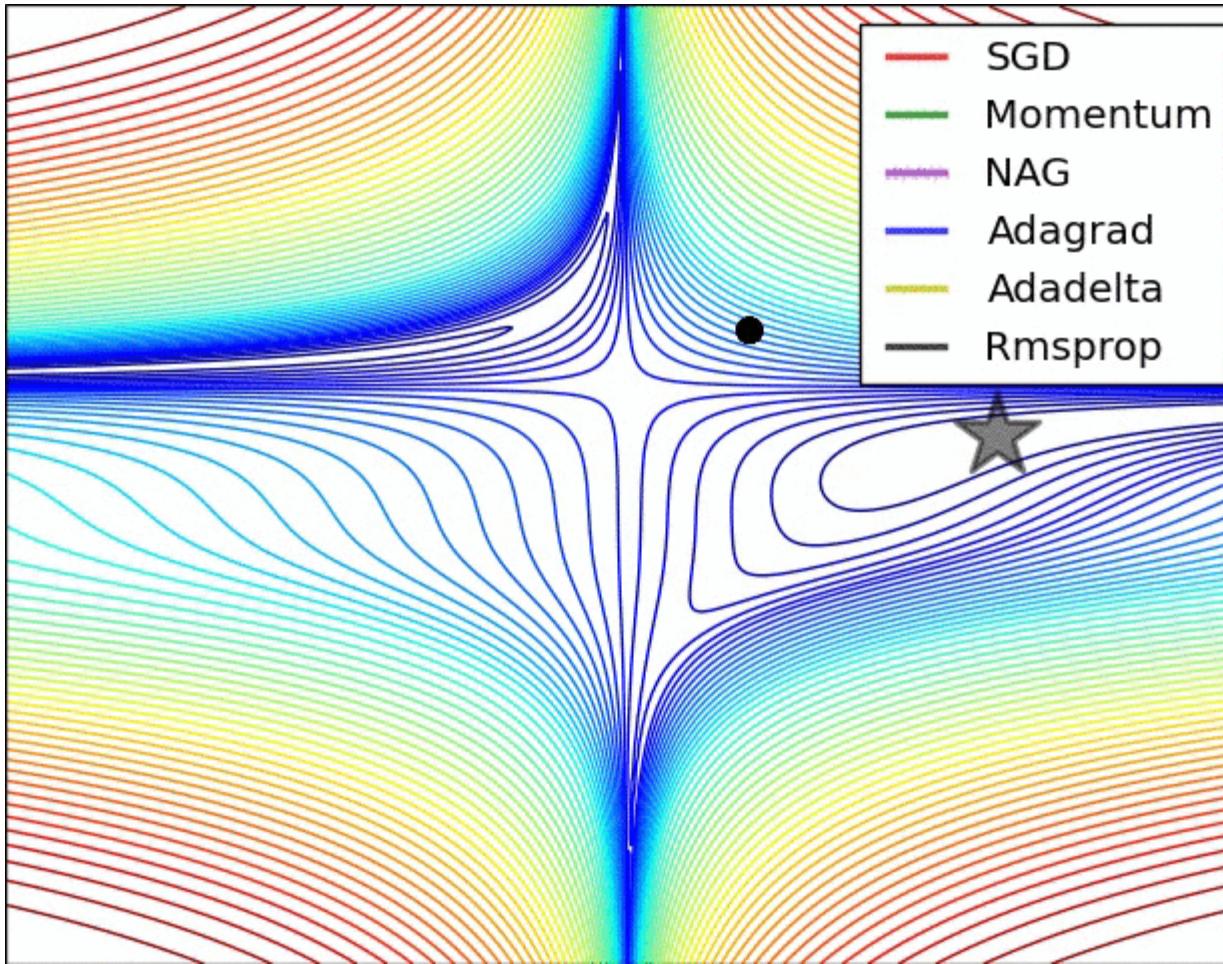
Momentum update:



Nesterov Momentum



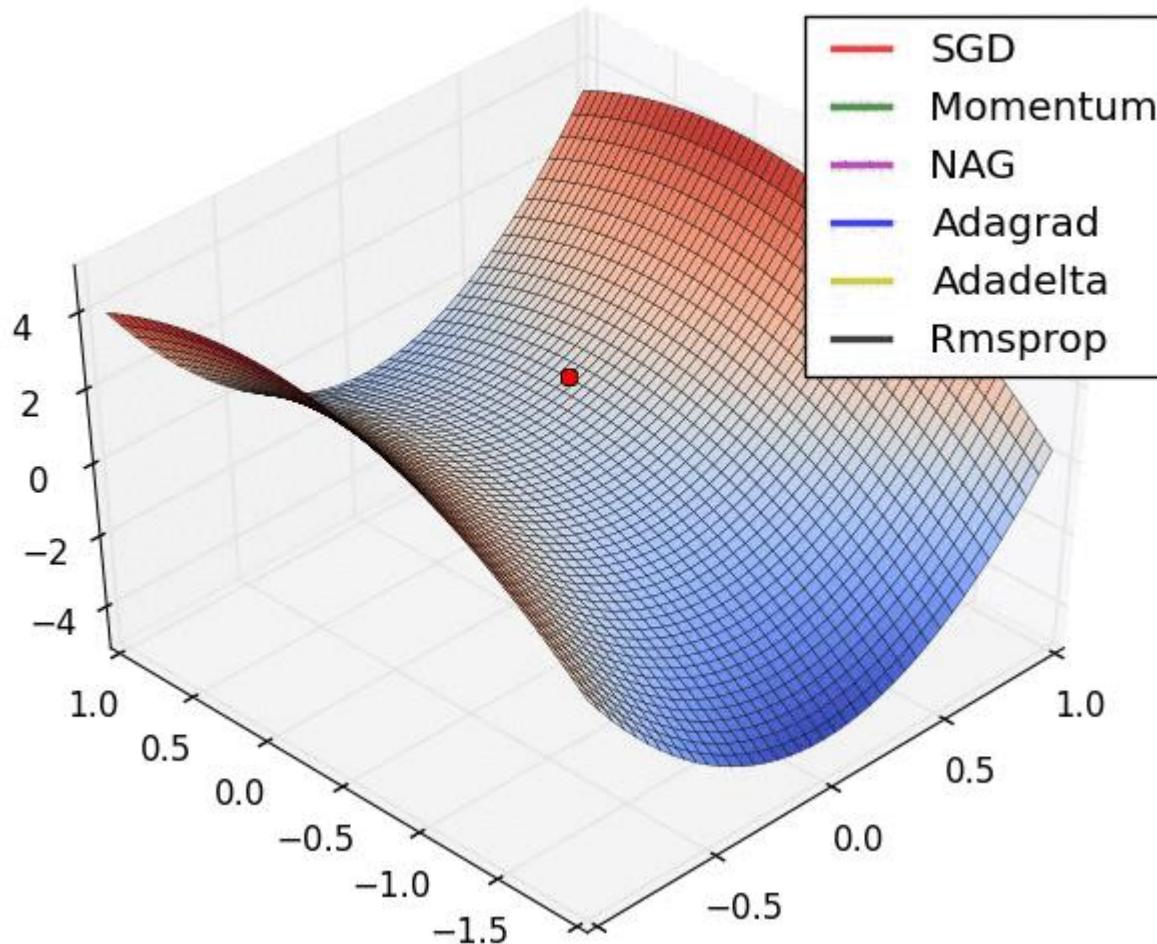
SGD optimization on loss surface contours



<http://ruder.io/optimizing-gradient-descent/>



SGD optimization on saddle point



<http://ruder.io/optimizing-gradient-descent/>



AdaGrad

- 자주 나타나는 기울기의 성분보다 드물게 나타나는 기울기 성분을 더 중시해서 파라미터를 업데이트
- 자주 나오는 파라미터 → learning rate 적게
 - 드물게 나오는 파라미터로는 크게
- 오차함수의 기울기: $\mathbf{g}_t \equiv \nabla E_t$
- $g_{t,i}$: 기울기 함수의 벡터 성분
- 업데이트 양의 성분:

$$-\frac{\epsilon}{\sqrt{\sum_{t'=1}^t g_{t',i}^2}} g_{t,i}$$

ϵ : learning rate



The AdaGrad algorithm

Global learning rate ε

Initial parameter θ

Small constant δ , (10^{-7})

$$\theta = [w_0, w_1, \dots, w_N]$$

$$x^{(i)} = [x_0, x_1, \dots, x_N]$$

$$\Delta\theta = [\Delta w_0, \Delta w_1, \dots, \Delta w_N]$$

Initialize gradient accumulation variable $r = 0$

while stopping criterion not met **do**

 Sample a **minibatch** of m examples from the training set
 $\{x^{(1)}, x^{(2)}, \dots, x^{(m)}\}$ with corresponding targets $y^{(i)}$.

 Compute gradient: $g \leftarrow 1/m \nabla_{\theta_i} L(f(x^{(i)}; \theta), y^{(i)})$

 Accumulate squared gradient: $r \leftarrow r + g \odot g$

 Compute update: $\Delta\theta \leftarrow -\frac{\epsilon}{\delta + \sqrt{r}} \odot g$

 Apply update: $\theta \leftarrow \theta + \Delta\theta$

end while

(Division and square root applied element-wise)

$$r = [r_0, r_1, \dots, r_N]$$

$$g \leftarrow 1/m \nabla_{\theta} L = [\partial L / \partial w_0, \dots, \partial L / \partial w_N]$$

$f(x^{(i)}; \theta)$ = network output

$L(f(x^{(i)}; \theta), y^{(i)})$: Loss

$$\text{Ex)} L = \frac{1}{2} \sum_i (t_i - O_i)^2$$

\odot : 벡터의 성분별 곱

$$r \leftarrow \rho r + (1 - \rho)g \odot g$$

rmsprop

Adam (adaptive moments)



Rmsprop (Root Mean Square Propagation)

Require: Global learning rate ϵ , decay rate ρ , momentum coefficient α .

Require: Initial parameter θ , initial velocity v .

Initialize accumulation variable $r = 0$

while stopping criterion not met **do**

 Sample a minibatch of m examples from the training set $\{x^{(1)}, \dots, x^{(m)}\}$ with corresponding targets $y^{(i)}$.

 Compute interim update: $\tilde{\theta} \leftarrow \theta + \alpha v$

 Compute gradient: $g \leftarrow \frac{1}{m} \nabla_{\tilde{\theta}} \sum_i L(f(x^{(i)}; \tilde{\theta}), y^{(i)})$

 Accumulate gradient: $r \leftarrow \rho r + (1 - \rho)g \odot g$

 Compute velocity update: $v \leftarrow \alpha v - \frac{\epsilon}{\sqrt{r}} \odot g$. ($\frac{1}{\sqrt{r}}$ applied element-wise)

 Apply update: $\theta \leftarrow \theta + v$

end while

- AdaGrad 의 문제: 시간이 흐를수록 update 양이 작아짐.
→ exponentially decaying average to discard history from the extreme past

The Adam algorithm

Require: Step size ϵ (Suggested default: 0.001)

Require: Exponential decay rates for moment estimates, ρ_1 and ρ_2 in $[0, 1]$.
(Suggested defaults: 0.9 and 0.999 respectively)

Require: Small constant δ used for numerical stabilization. (Suggested default: 10^{-8})

Require: Initial parameters θ

Initialize 1st and 2nd moment variables $s = \mathbf{0}$, $r = \mathbf{0}$

Initialize time step $t = 0$

while stopping criterion not met **do**

 Sample a minibatch of m examples from the training set $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$ with corresponding targets $\mathbf{y}^{(i)}$.

 Compute gradient: $\mathbf{g} \leftarrow \frac{1}{m} \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$

$t \leftarrow t + 1$

 Update biased first moment estimate: $\mathbf{s} \leftarrow \rho_1 \mathbf{s} + (1 - \rho_1) \mathbf{g}$

 Update biased second moment estimate: $\mathbf{r} \leftarrow \rho_2 \mathbf{r} + (1 - \rho_2) \mathbf{g} \odot \mathbf{g}$

 Correct bias in first moment: $\hat{\mathbf{s}} \leftarrow \frac{\mathbf{s}}{1 - \rho_1^t}$

 Correct bias in second moment: $\hat{\mathbf{r}} \leftarrow \frac{\mathbf{r}}{1 - \rho_2^t}$

 Compute update: $\Delta\theta = -\epsilon \frac{\hat{\mathbf{s}}}{\sqrt{\hat{\mathbf{r}}} + \delta}$ (operations applied element-wise)

 Apply update: $\theta \leftarrow \theta + \Delta\theta$

end while



The Adam algorithm

- adaptive moments.
- a variant on the combination of RMSProp and momentum.
- Bias correction for the fact that first and second moment estimates start at zero
- Adam is generally regarded as being fairly robust to the choice of hyperparameters.

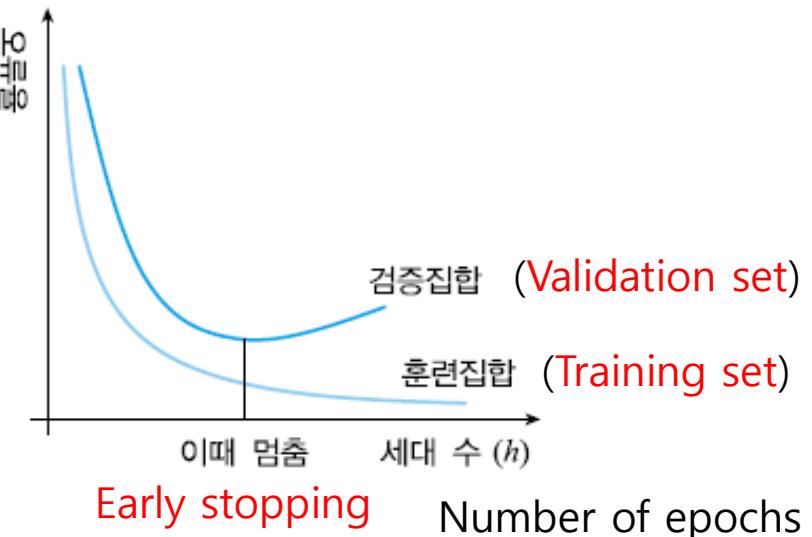
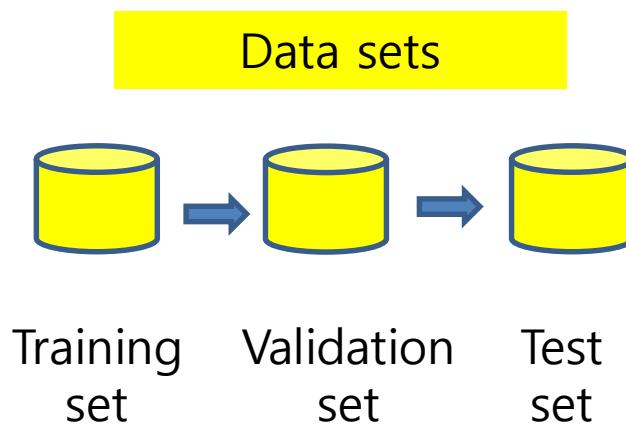


Generalization



Generalization

- **Generalization** : training 에 사용되지 않은 data 에 대한 성능
- **Overfitting (과적합)**:
training error 에 비하여 generalization error 가 커지는 경우
← 모델 파라미터에 비하여 학습 데이터가 너무 적은 경우



Regularization

- Regularization :
Overfitting 을 방지하도록 loss function에 complexity penalty 추가
- Weight decay
 - L2 Regularization
 - 목적 함수 $J(\mathbf{w}) = \text{MSE} + \lambda \mathbf{w}^\top \mathbf{w}$ ← *regularizer*
 - λ : controls the strength of our preference for smaller weights.
 - L1 regularization (LASSO)
 - 목적 함수 $J(\mathbf{w}) = \text{MSE} + \lambda \|\mathbf{w}\|_1$

$$\|\mathbf{w}\|_1 = \sum_{j=1}^D w_j$$



Initialization

- **he_normal:** initialization scaled by fan_in (He et al., 2014)

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

- W = the initialization distribution for the neuron in question
- n_{in} = the number of neurons feeding into it.
- Gaussian or uniform.

- Glorot & Bengio's paper

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



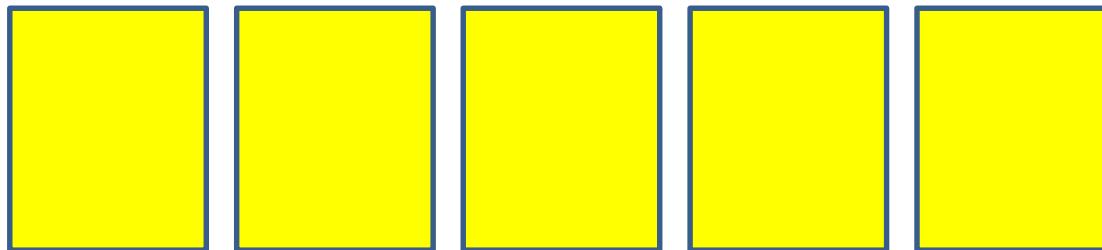
Model Ensembles

1. Train multiple independent models

2. At test time average their results

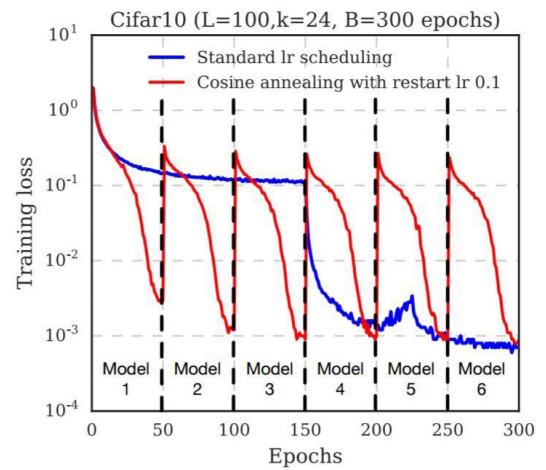
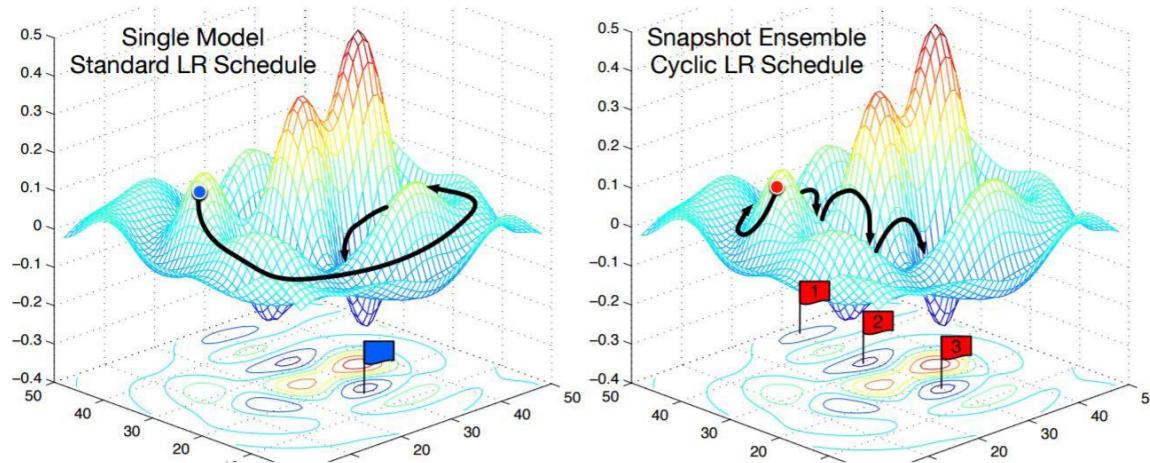
(다양한 방법으로 조합)

→ 큰 성능 향상은 없지만 거의 대부분 조금씩 (2%) 향상됨.



Model Ensembles: new idea (2017)

- Instead of training independent models, use multiple snapshots of a single model during training!

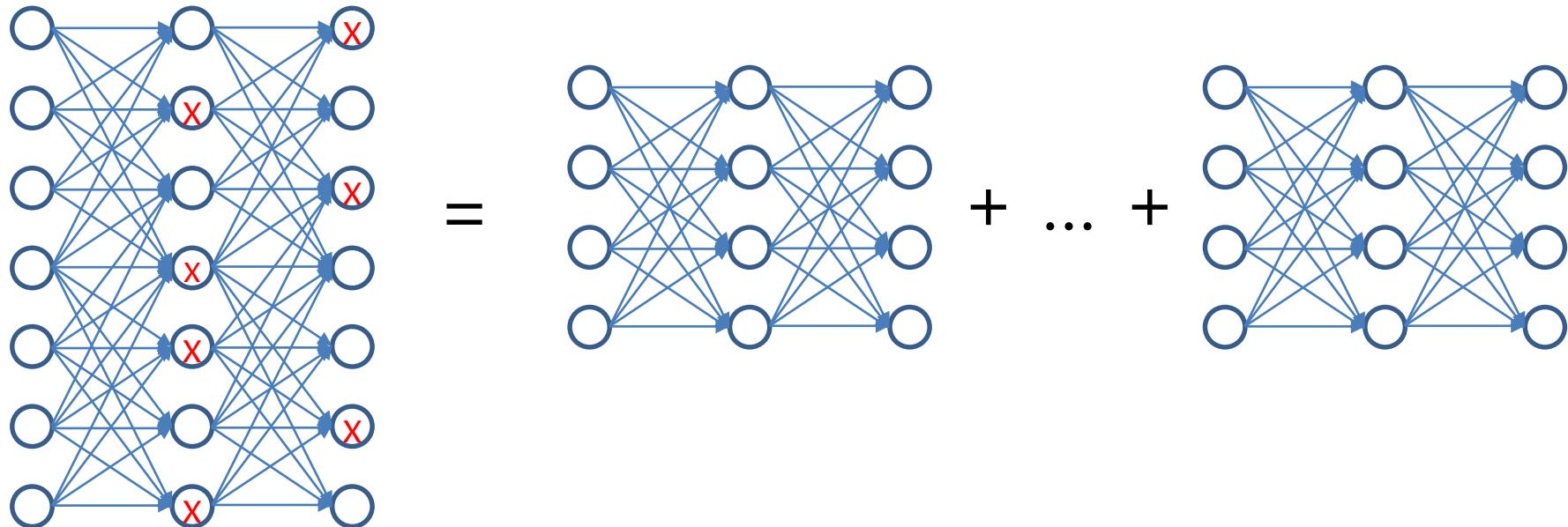


- Learning rate을 크게했다 작게했다 반복.



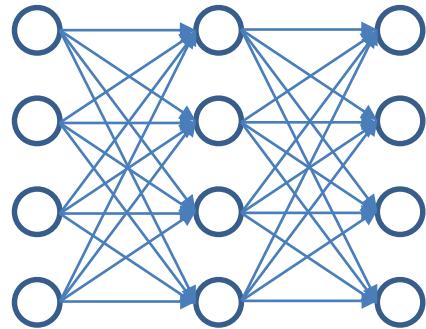
Dropout

- 문제: Overfitting 해결
- Dropout : Training example마다 일부 hidden unit 을 없는 것으로 계산
- 다층 신경망의 유닛 중 일부를 확률적으로 선택하여 학습
- Randomly, 확률 $p = 0.5$ 적용
- 결국 2^n 개의 서로 다른 모델을 사용하는 효과

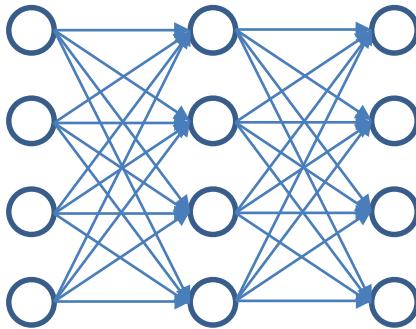


Ensemble Learning (예: adaboost)

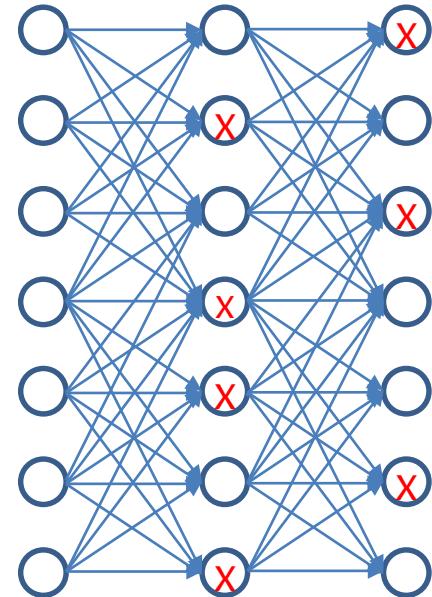
- 작은 model을 많이 만들어서 각 output의 조합을 사용하면 성능이 높다



+ ... +



=



ReLU 도 비슷한 효과



데이터 확장 (data augmentation)

- 훈련 데이터의 부족 → overfitting 의 원인
- Data augmentation :
이미 확보한 샘플 데이터를 일정하게 가공하여 양을 늘임
- 예
 - 이미지의 평행이동, 대칭이동, 회전 등의 기하학적 변환
 - 픽셀의 명암값, 색에 변동을 가한 결과 이미지
 - 가우스 분포를 따르는 랜덤 노이즈 추가



Summary : Neural networks 설계 고려사항

- Network topology : 어떤 모양?
 - Feed forward, feed backward
- Activation function : 출력의 형태?
 - linear or non-linear?
- Objectives : 훈련의 목적?
 - Classification or regression ?
= Loss function, Error
- Optimizers : 훈련의 방법?
 - Weights update
- Regularization : overfitting 을 어떻게 방지할까?

