Optimization Algorithms

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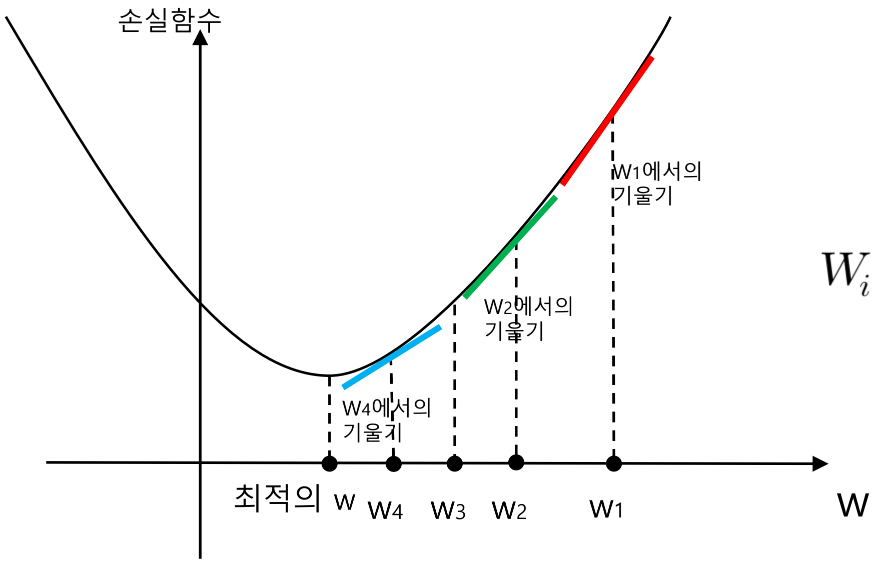
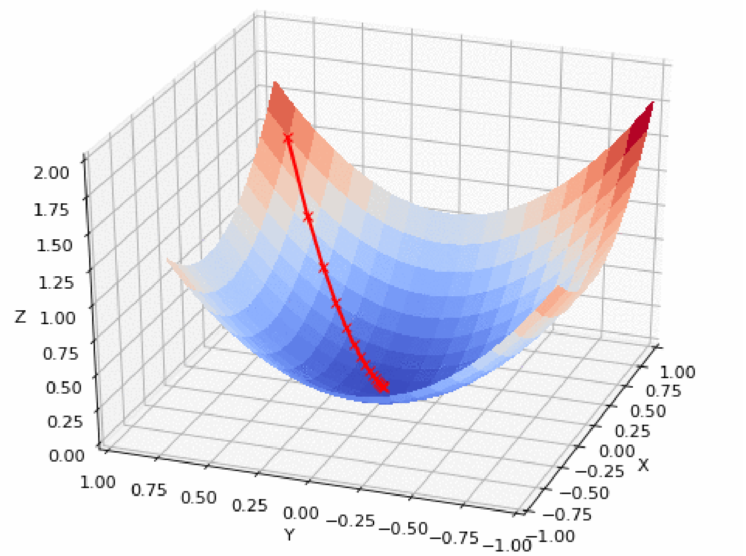
[참고] 본 자료에는 인터넷에서 다운받아 사용한 그림이나 수식들이 들어
있으니 다른 용도로 사용하거나 외부로 유출을 금해 주시기 바랍니다.

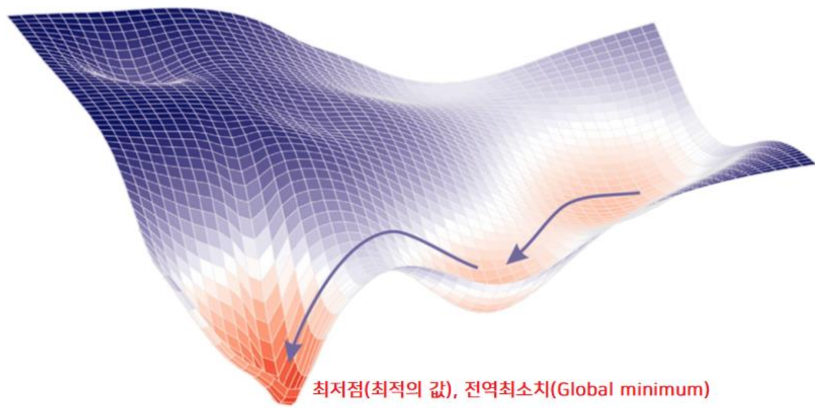
Optimization algorithms

- **Gradient Descent (경사하강법)**
  - General optimization algorithm
  - take repeated steps in the opposite direction of the **gradient** (or approximate **gradient**) of the function at the current point



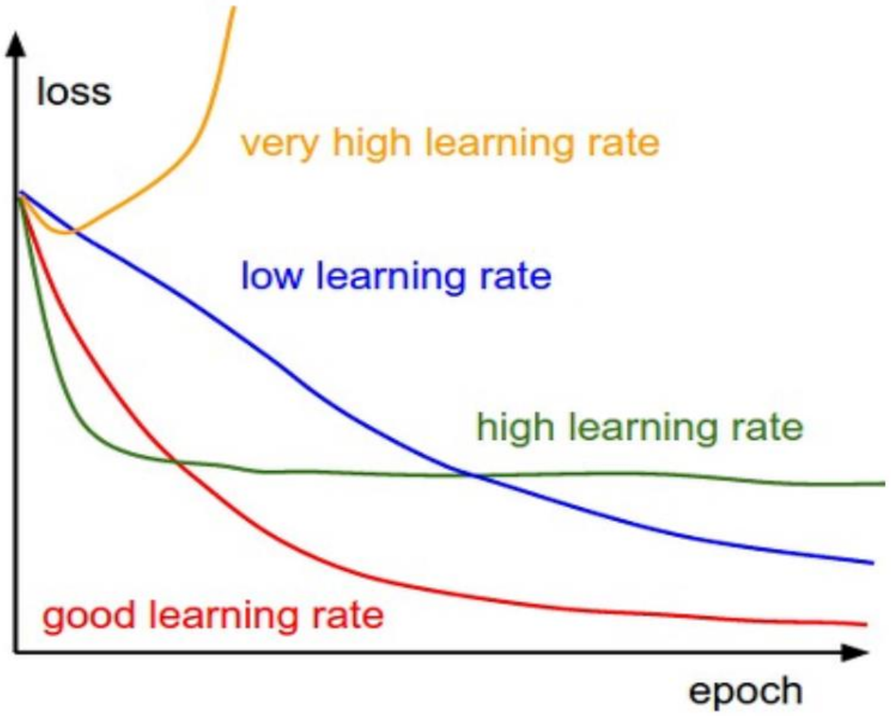
$$W_i = W_{i-1} - \eta Grad(i)$$





Optimization algorithms

- **Learning rate: η (eta)**
  - low: takes time to converge, and may get stuck in an undesirable local minimum
  - high: may jump over minima
  - too high: may diverge
  - Need adaptive adjustment

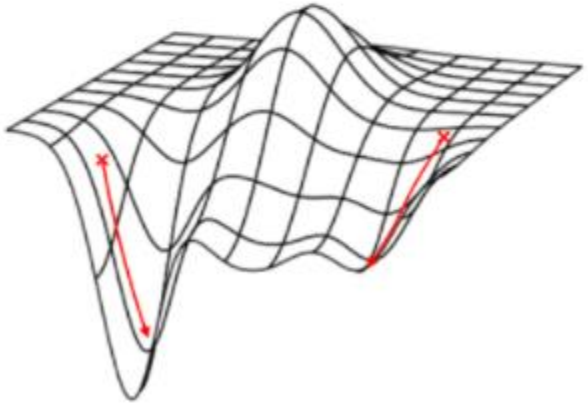


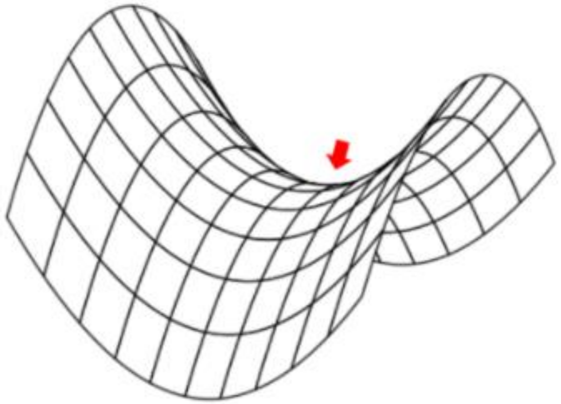
Optimization algorithms

- **Gradient descent**
  - computes the gradient of the cost function w.r.t. to the parameters θ for the entire training dataset for each update (too much computation)

$$\theta = \theta - \eta \cdot \nabla_\theta J(\theta)$$

  - Local minimum
  - Saddle Point

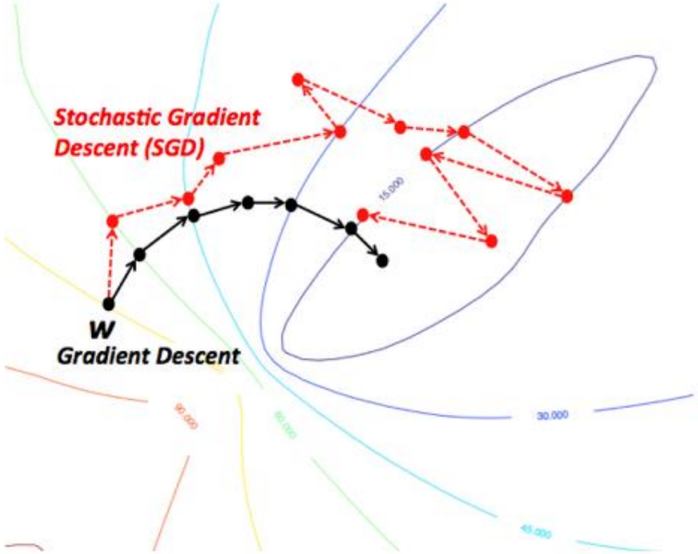




Optimization algorithms

- **Stochastic gradient descent (SGD)**
  - performs a parameter update for each training example $x^{(i)}$ and label $y^{(i)}$
  - usually much faster and can also be used to learn online
  - It performs frequent updates with a high variance that cause the objective function to fluctuate heavily.
  - higher probability not to fall in local minima

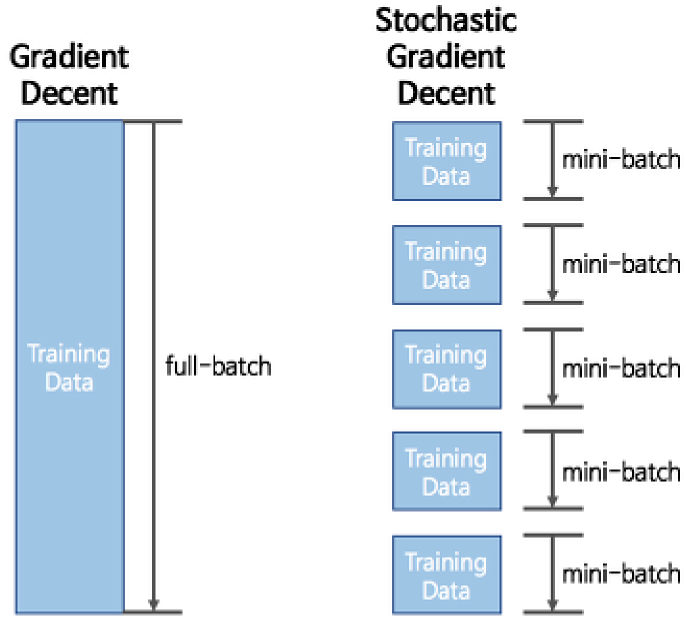
$$\theta = \theta - \eta \cdot \nabla_\theta J(\theta; x^{(i)}; y^{(i)})$$



Optimization algorithms

- **Mini-batch gradient descent**
  - performs an update for every **mini-batch** of *n* training examples
  - common mini-batch sizes range between 50 and 256, but can vary for different applications

$$\theta = \theta - \eta \cdot \nabla_\theta J(\theta; x^{(i:i+n)}; y^{(i:i+n)})$$



- **Challenges**
  - GD does **not guarantee good convergence**, but offers few challenges.
  - How to find optimal learning rates? -> decaying (step size)
  - How often should the parameters be updated? -> batch size
  - How to escape from local minima? -> momentum (step direction)

Optimization algorithms

- **Momentum (batch GD with Momentum)**
  - movement(update) vector (v) introduced
  - Also use the results from previous batch (momentum term ***m*** is close to 0.9)
  - Converge faster, reduced vibration, and helps to escape from local minimums.

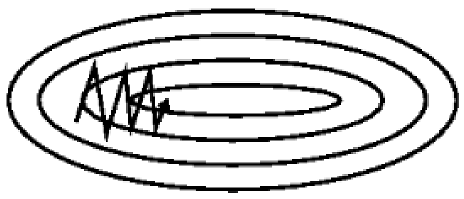


Image 2: SGD without momentum

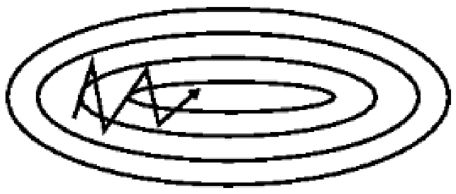
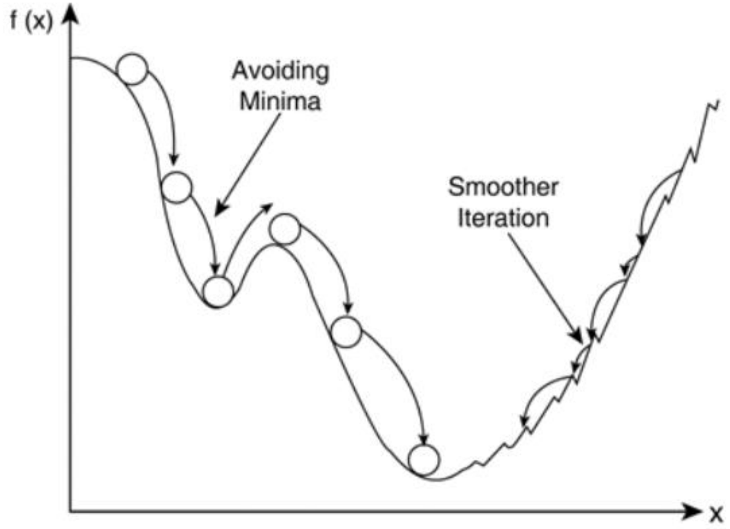


Image 3: SGD with momentum

$$V_t = m \times V_{t-1} - \eta \nabla_\omega J(\omega_t)$$

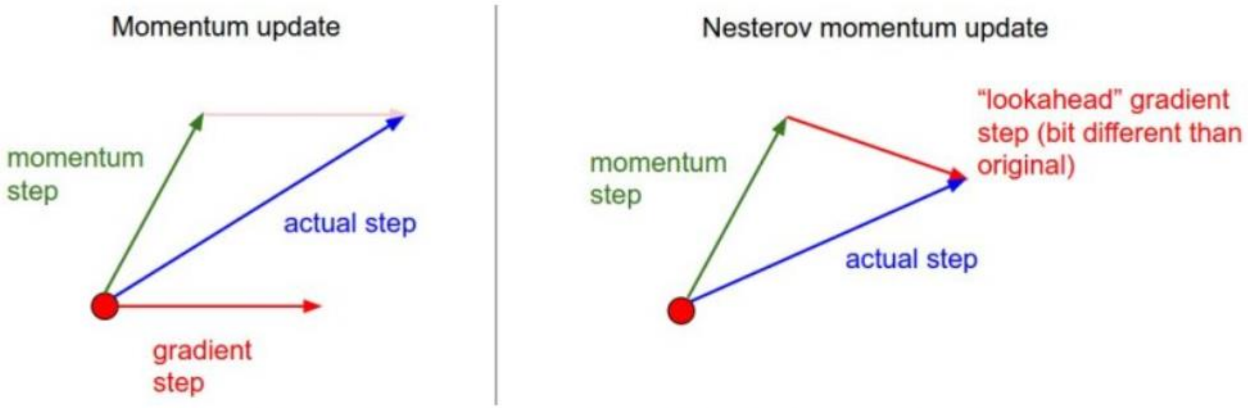
$$\omega_{t+1} = \omega_t + V_t$$



Avoiding Local Minima. Picture from http://www.yaldex.com.

Optimization algorithms

- Improved Momentum (**Nesterov accelerated gradient (NAG)**)
  - Momentum 방법과 동일하지만 Gradient 계산이 약간 다름
  - Momentum 에서는 현재 위치의 기울기와 모멘텀을 따로 계산하고 나중에 더하지만, 여기서는 먼저 모멘텀을 계산 후 기울기 를 계산



Difference between Momentum and NAG. Picture from CS231.

$$V_t = m \times V_{t-1} - \eta \nabla_\omega \boxed{J(\omega_t - m \times V_{t-1})}$$

$$\omega_{t+1} = \omega_t + V_t$$

Optimization algorithms

- Separate adaptive learning rates: 학습률을 Weight 에 따라 다르게 함.
- **Adagrad** (Adaptive gradient)
  - 파라미터 별 update (different learning rates for ωi's)
  - 과거에 많이 변경되지 않은 매개 변수에 더 큰 learning rate 적용 -> step-size 감소
  - 아래 식에서 squaring 과 dot(.) 연산은 element-wise 연산

$$G_t = G_{t-1} + (\nabla_\omega J(\omega_t))^2 = \sum_{i=1}^{k} (\nabla_{\omega_i} J(\omega_i))^2$$

$$\omega_{t+1} = \omega_t - \frac{\eta}{\sqrt{G_t + \epsilon}} \cdot \nabla_\omega J(\omega_t)$$

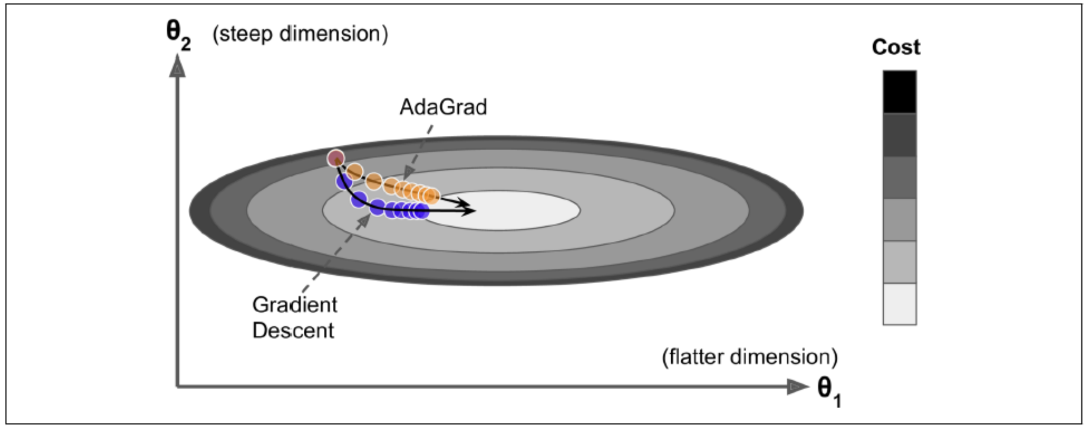


Figure 11-7. AdaGrad versus Gradient Descent

파이썬 소스 코드

```
g += gradient**2
weight[i] += - learning_rate ( gradient / (np.sqrt(g) + e)
```

Tensorflow 소스 코드

```
optimizer = tf.train.AdagradOptimizer(learning_rate=0.01).minimize(loss)
```

Keras 소스 코드

```
keras.optimizers.Adagrad(lr=0.01, epsilon=1e-6)
```

Ref: Hands-on-Machine Learning (2nd)

Optimization algorithms

- **RMSProp** (root mean square propagation)
  - Adagrad 알고리즘은 너무 급격히 감소하여 global optimum 에 도달하지 못하는 경우 발생
  - 처음부터 모든 gradient Gt를 합산하는 대신 지수 평균 (exponential moving average) 사용하여 최근 것 사용 (more weights on the recent gradient): typical decay rate γ = 0.9~0.999
  - **Always performs much better than Adagrad, and most preferred until Adam came around.**

$$G_t = \gamma G_{t-1} + (1-\gamma)(\nabla_\omega J(\omega_t))^2$$

$$\omega_{t+1} = \omega_t - \frac{\eta}{\sqrt{G_t + \epsilon}} \cdot \nabla_\omega J(\omega_t)$$

```
optimizer = keras.optimizers.RMSprop(lr=0.001, rho=0.9)
```

gamma

Optimization algorithms

- **Adam** (Adaptive Moment Estimation)
  - RMSProp + Momentum
  - Momentum 과 유사하게 기울기의 지수 평균 반영 (과거 기울기 (past gradient) 의 지수적으로 감소하는 평균을 유지)
  - RMSProp 과 유사하게 기울기 제곱 값의 지수 평균 반영 (각 매개 변수에 대한 적응형 학습률 (adaptive learning rate))
  - Recommended values: $\varepsilon=10^{-8}$, $\beta_1=0.9$, $\beta_2=0.999$

$$m_t = \beta_1 m_{t-1} + (1-\beta_1)\nabla_\omega J(\omega_t)$$

first moment

$$v_t = \beta_2 v_{t-1} + (1-\beta_2)(\nabla_\omega J(\omega_t))^2$$

second moment

$$\omega_{t+1} = \omega_t - m_t \frac{\eta}{\sqrt{v_t + \epsilon}}$$

$$\mathrm{M(t)} = \beta_1 M(t-1) + (1-\beta_1)\frac{\partial}{\partial w(t)} Cost(w(t))$$

$$\mathrm{V(t)} = \beta_2 V(t-1) + (1-\beta_2)\left(\frac{\partial}{\partial w(i)} Cost(w(i))\right)^2$$

$$\widehat{M}(t) = \frac{M(t)}{1-\beta_1{}^t} \qquad \widehat{V}(t) = \frac{V(t)}{1-\beta_2{}^t}$$

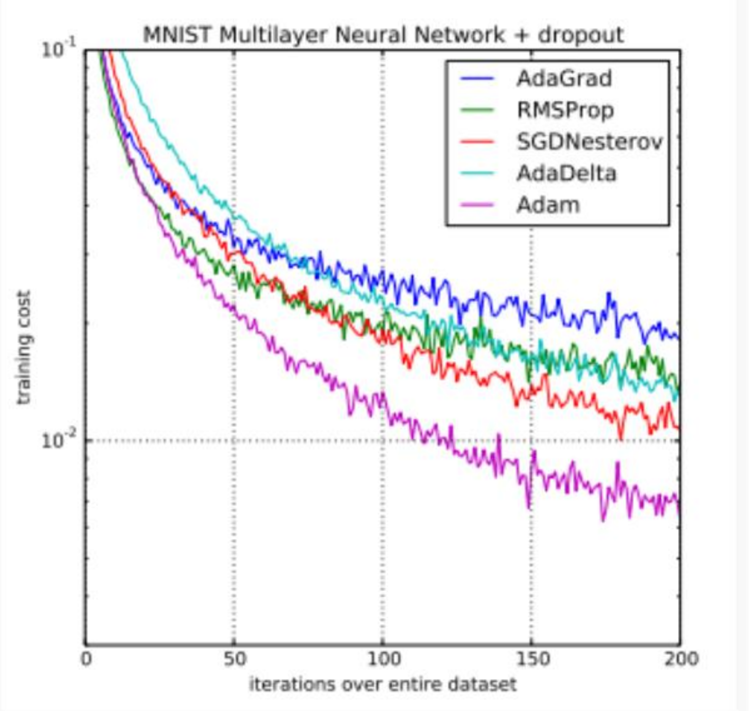
$$\mathrm{W(t+1)} = W(t) - \alpha * \frac{\widehat{M}(t)}{\sqrt{\widehat{V}(t) + \epsilon}}$$

bias correction
(due to scale difference between β_1 and β_2)

Optimization algorithms

- **Adam** (Adaptive Moment Estimation)

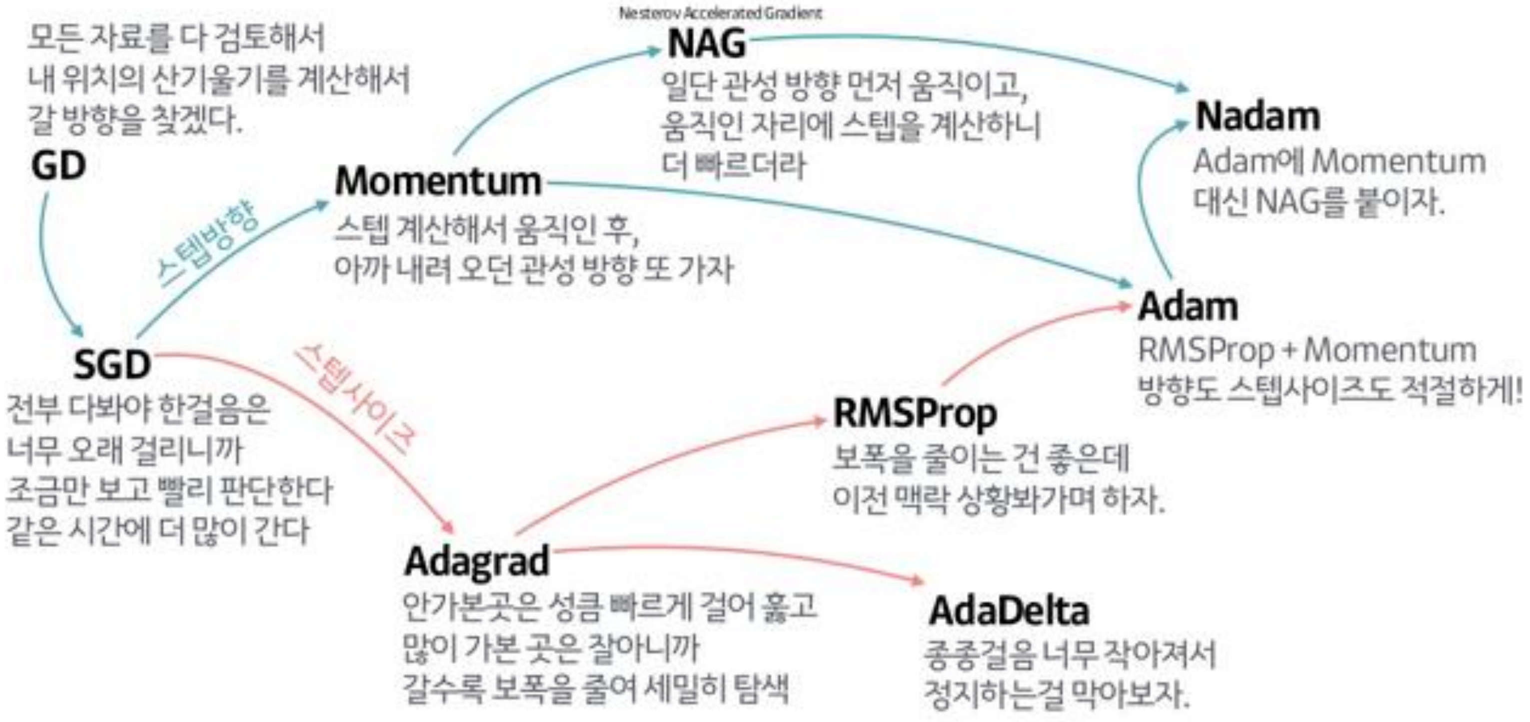
Require: α: Stepsize
Require: $\beta_1, \beta_2 \in [0, 1)$: Exponential decay rates for the moment estimates
Require: $f(\theta)$: Stochastic objective function with parameters θ
Require: θ_0: Initial parameter vector
  $m_0 \leftarrow 0$ (Initialize 1st moment vector)
  $v_0 \leftarrow 0$ (Initialize 2nd moment vector)
  $t \leftarrow 0$ (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)



Comparison of Adam to Other Optimization Algorithms Training a Multilayer Perceptron
Taken from Adam: A Method for Stochastic Optimization, 2015.

Optimization algorithms

- **Summary**



- **More:**
  - Adamax
  - Nadam
  - AMSGrad
  - more …
- **Good animation**
  - https://wiserloner.tistory.com/1032