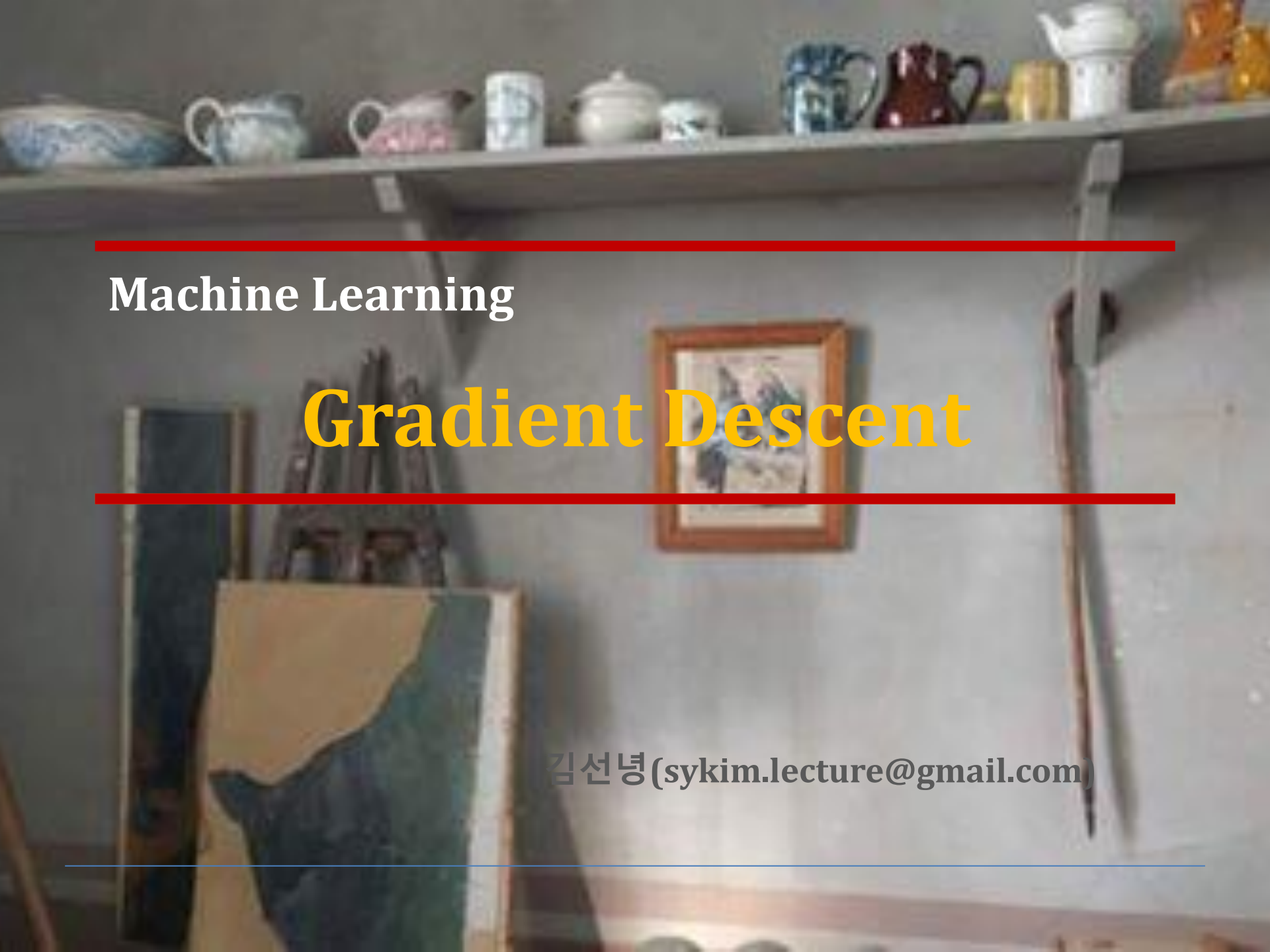


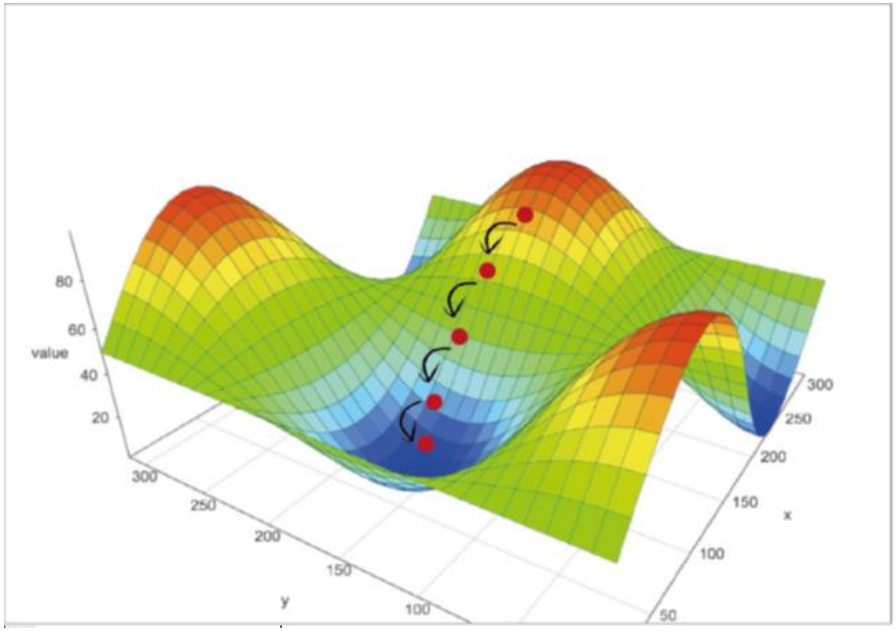
Machine Learning

Gradient Descent

김선녕(sykim.lecture@gmail.com)

개요

- 최적화(optimization)
  - x의 값을 바꾸어 가면서 어떤 함수 $f(x)$의 값을 최대화 또는 최소화 하는 것
- 목적함수$(objective\ function)$ 또는 판정기준$(criterion)$
  - 최대화 : 이익$(profit)$, 점수$(score)$
  - 최소화 : 비용함수$(cost\ function)$, 손실함수$(loss\ function)$, 오차함수$(error\ function)$
- 경사 하강법(Gradient descent)
  - 최적의 해법을 찾을 수 있는 최적화 알고리즘
  - 비용 함수를 최소화하기 위해 반복해서 파라미터를 조정해가는 것
  - 배치$(batch)$ 경사하강법
  - 확률적$(stochastic)$경사하강법
  - 미니배치$(mini-batch)$ 경사하강법



Ref : Make Your Own Neural Network by Tariq Rashid

Best Fit

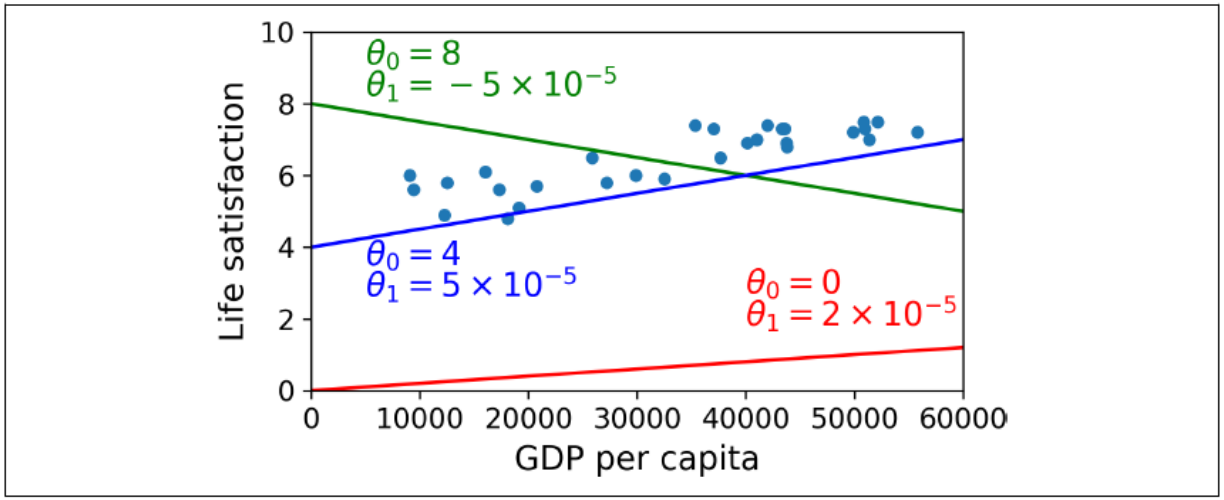


Figure 1-18. A few possible linear models

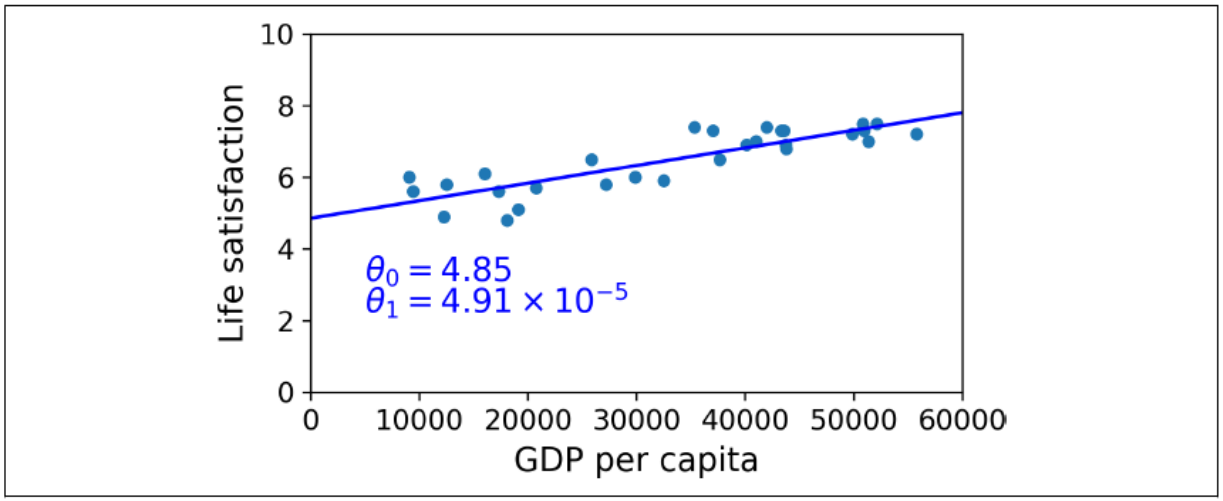


Figure 1-19. The linear model that fits the training data best

Ref : hands on machine learning 2nd - oreily

비용의 최소화

$$\hat{y}(x) = wx + b$$

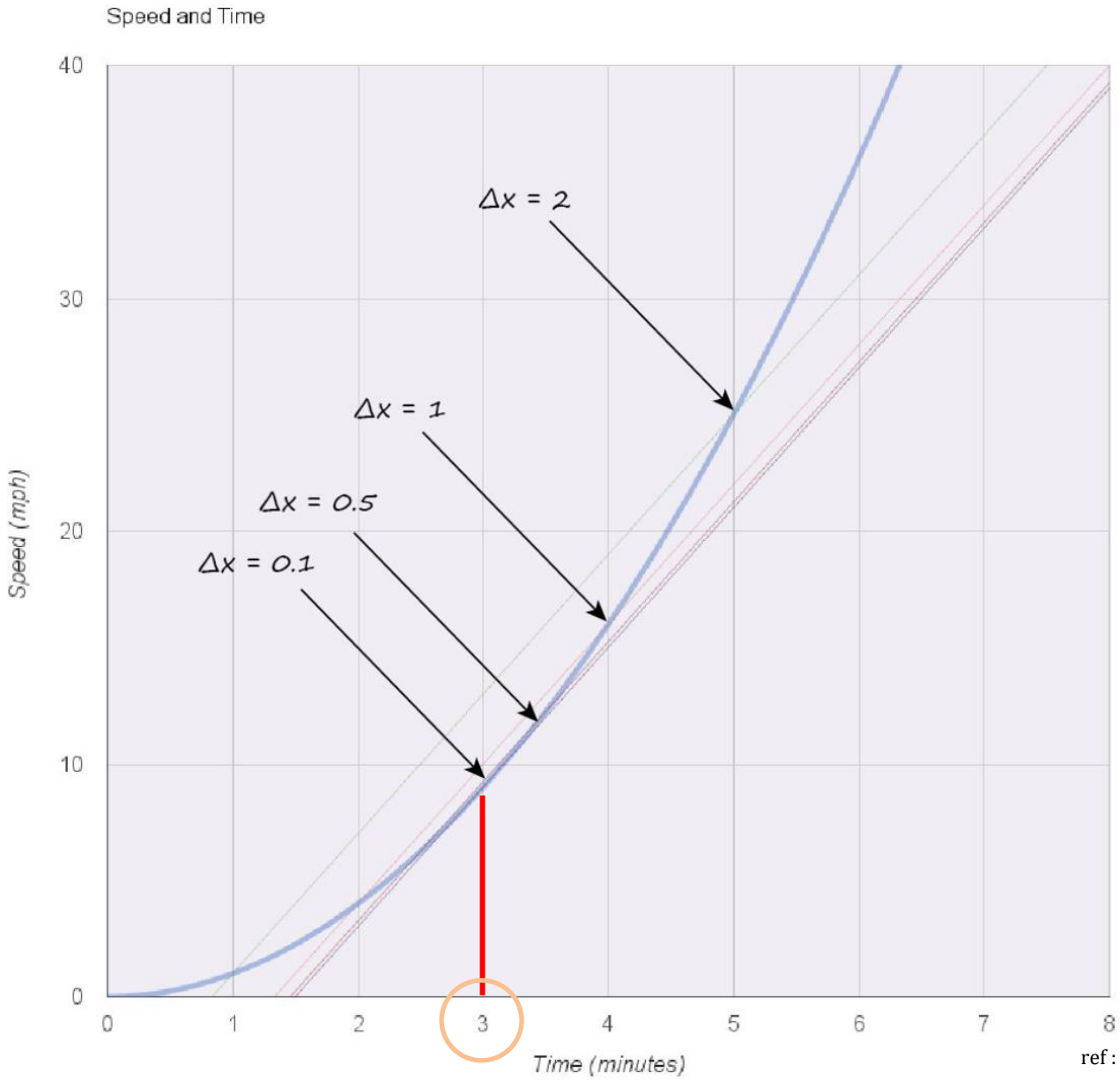
$$cost(w,b) = \frac{1}{n}\sum_{i=1}^{n}(\hat{y}(x_i) - y_i)^2 = \frac{1}{n}\sum_{i=1}^{n}(wx_i + b - y_i)^2$$

비용을 최소화하는 w, b를 구하라 : $\underset{w,b}{minimize}\, cost(w,b)$

$$\frac{\delta}{\delta w} cost(w) = \frac{2}{n}\sum_{i=1}^{n}(wx_i - y_i)\cdot x_i$$

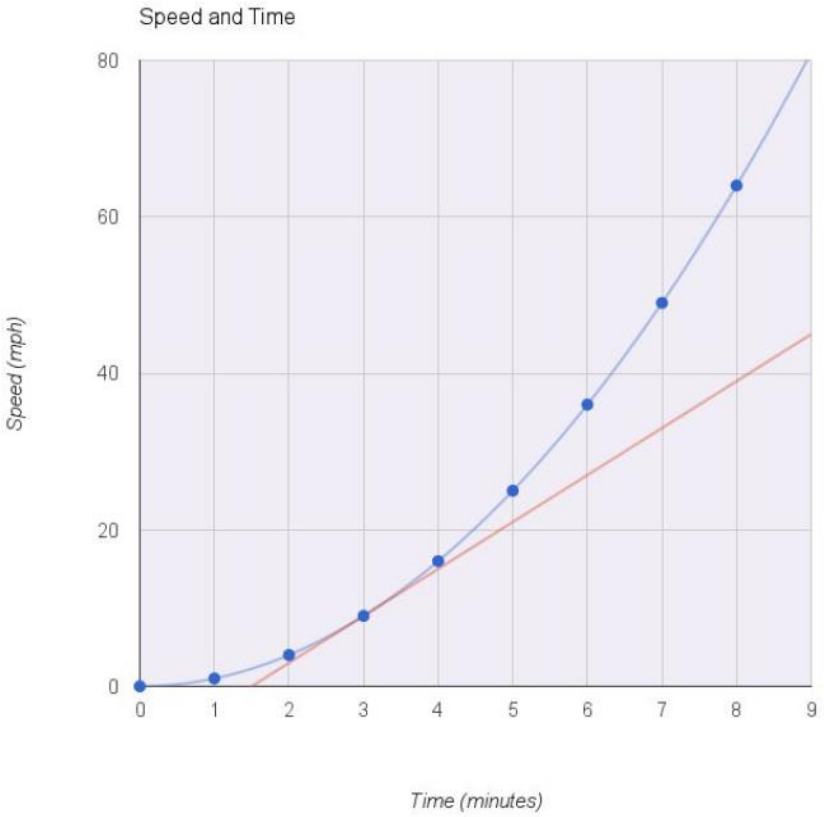
$$w := w - \alpha \sum_{i=1}^{n}(wx_i - y_i)\cdot x_i$$

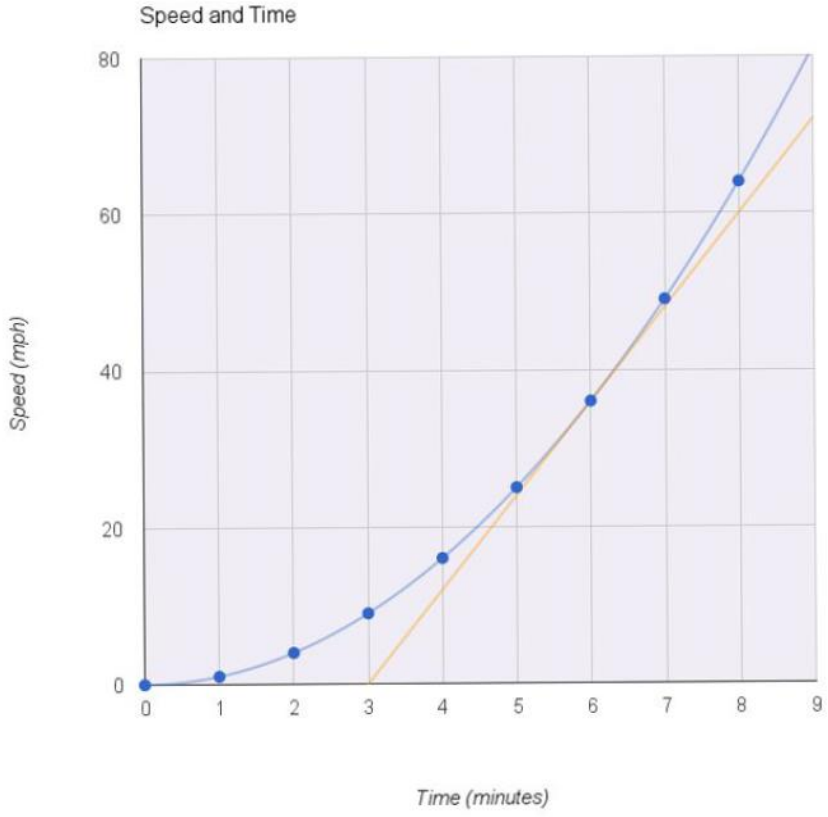
※ α : ***learning rate***



ref : Make Your Own Neural Network, Tariq Rashid

기울기 변화

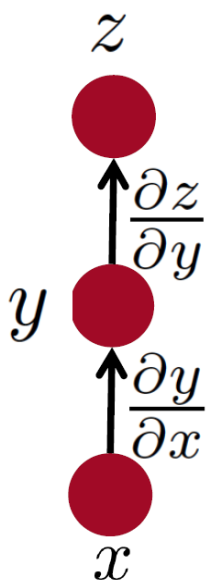




$$y' = f'(x) = \frac{dy}{dx} = \frac{d}{dx}y = \frac{df(x)}{dx} = \frac{d}{dx}f(x) = \frac{\partial f}{\partial x} = \frac{\delta f}{\delta x}$$

합성함수(Chain Rule)의 미분

Simple chain rule

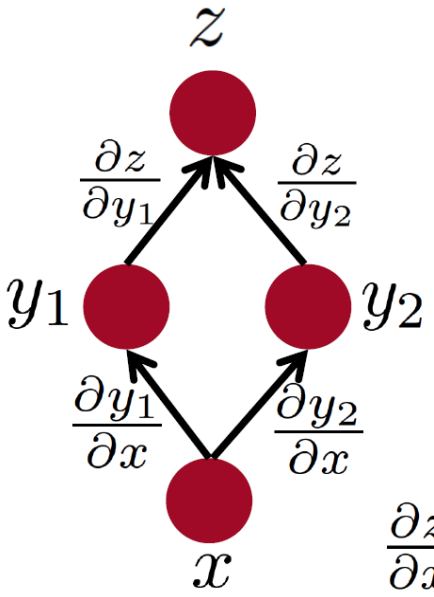


$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y}\frac{\partial y}{\partial x}$$

$$y = f(u),\ u = g(v),\ v = h(x)$$

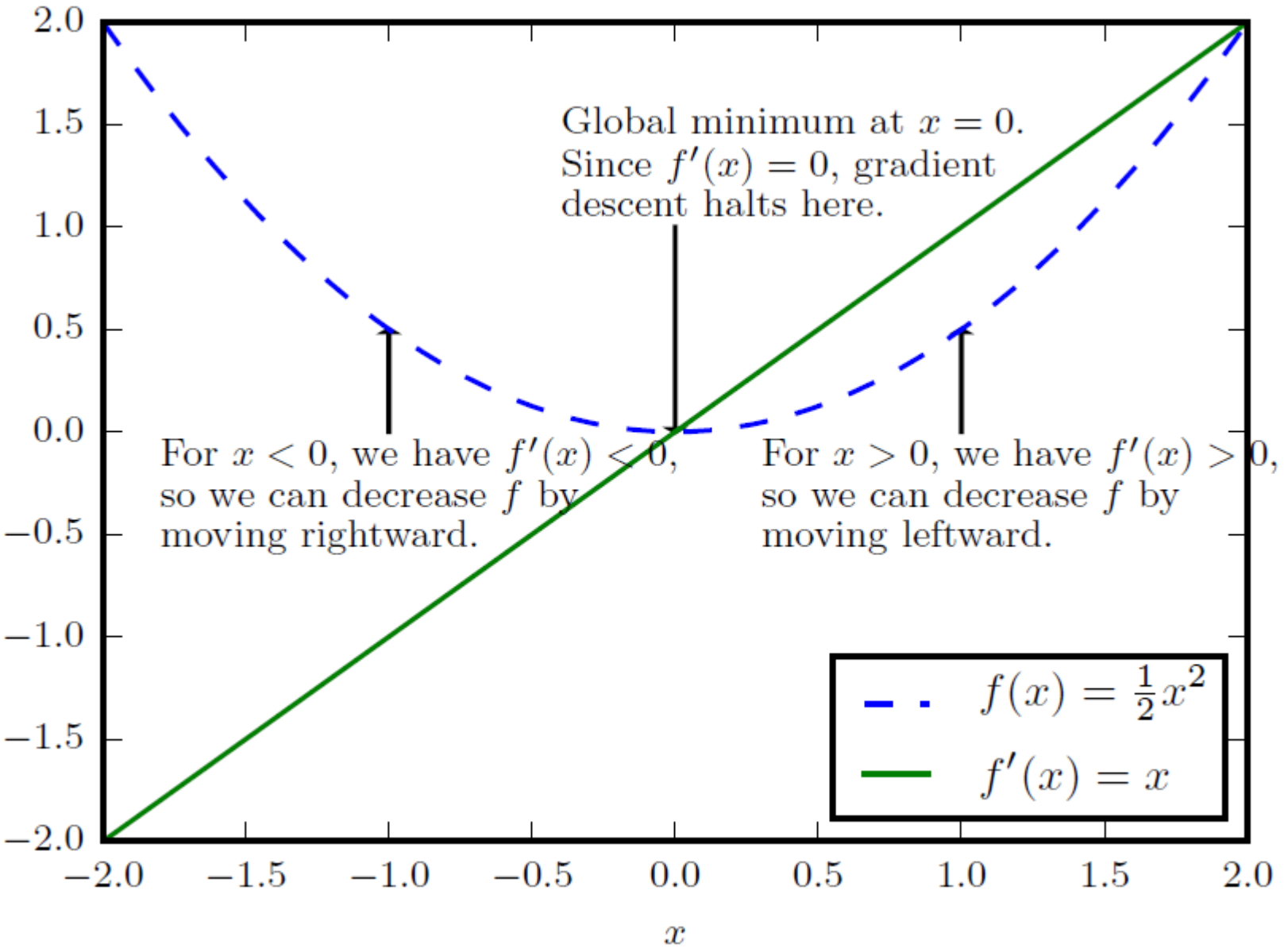
$$\frac{dy}{dx} = \frac{dy}{du} \cdot \frac{du}{dv} \cdot \frac{dv}{dx}$$

Multiple path chain rule

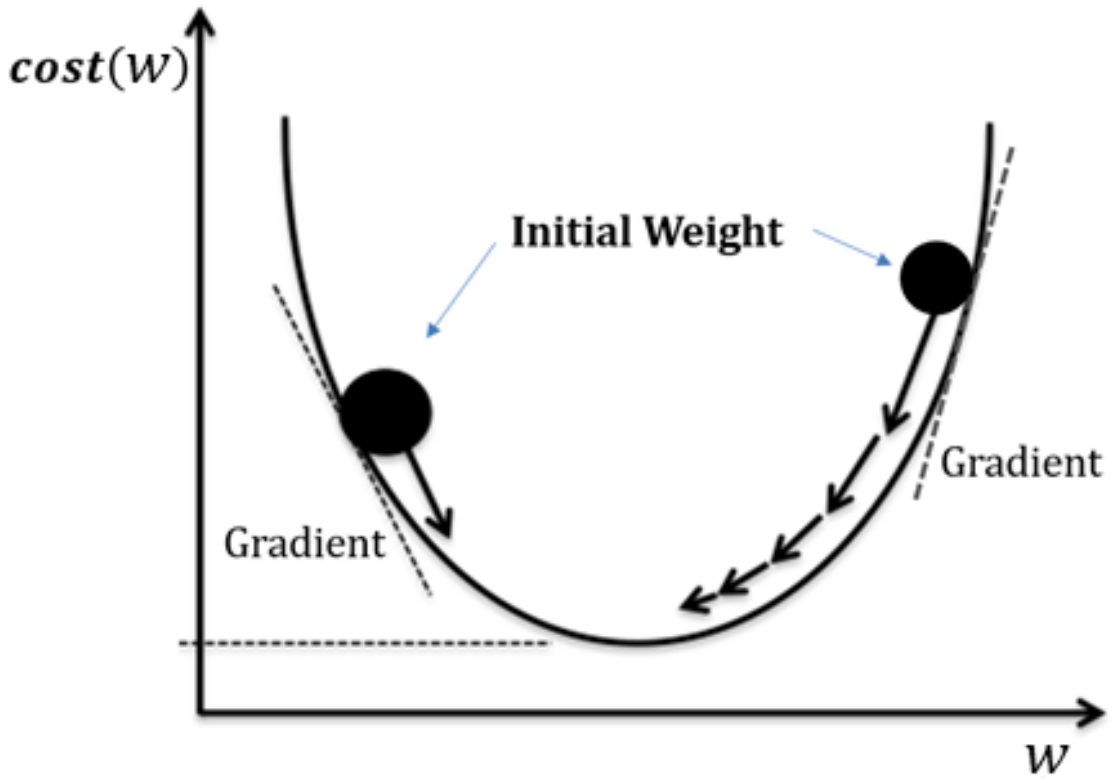


$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y_1}\frac{\partial y_1}{\partial x} + \frac{\partial z}{\partial y_2}\frac{\partial y_2}{\partial x}$$

http://cs224d.stanford.edu/syllabus.html

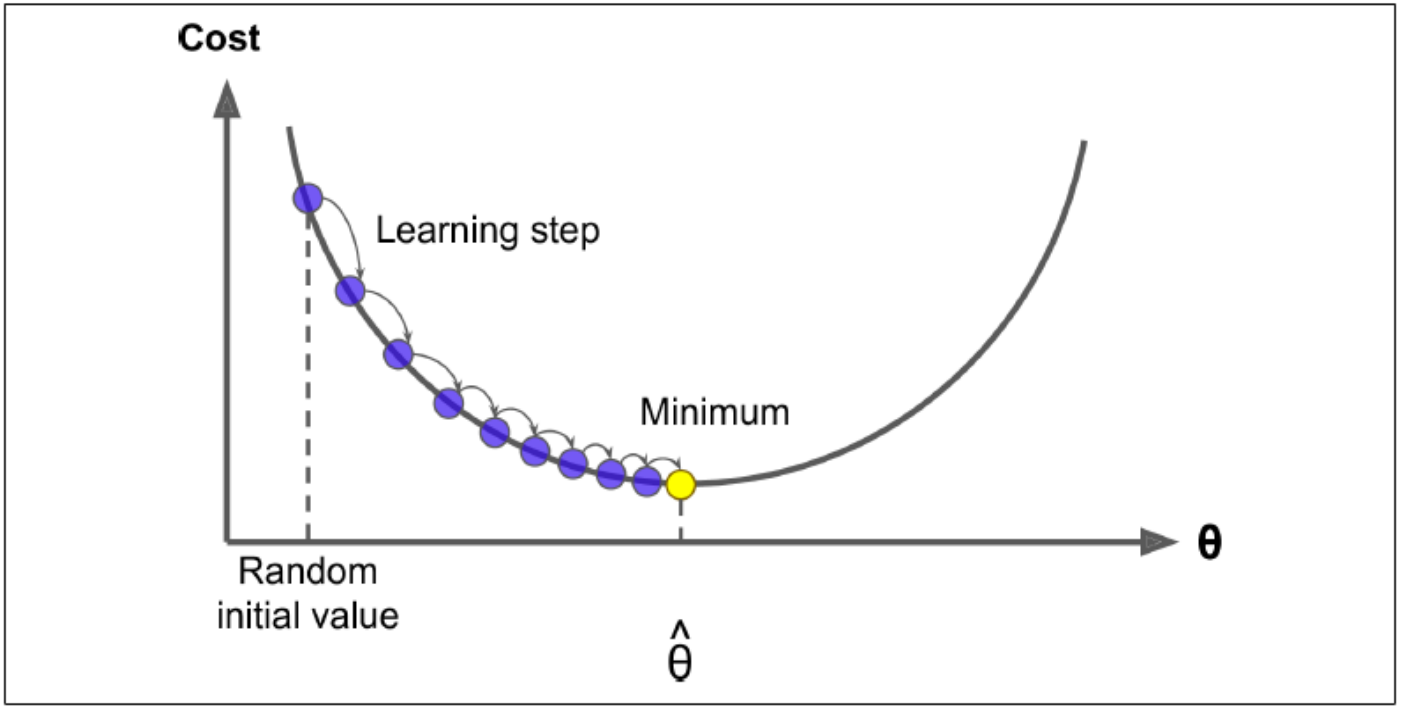

Global minimum at $x = 0$.
Since $f'(x) = 0$, gradient
descent halts here.
For $x < 0$, we have $f'(x) < 0$,
so we can decrease f by
moving rightward.
For $x > 0$, we have $f'(x) > 0$,
so we can decrease f by
moving leftward.
$f(x) = \frac{1}{2}x^2$
$f'(x) = x$
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
x

$$w := w - \alpha \sum_{i=1}^{n} (wx_i - y_i) \cdot x_i$$

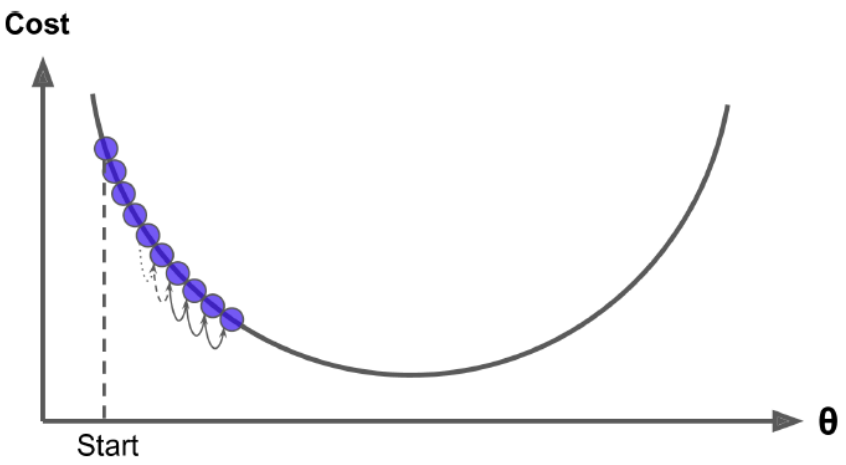


학습률($learning\ rate : \alpha$)

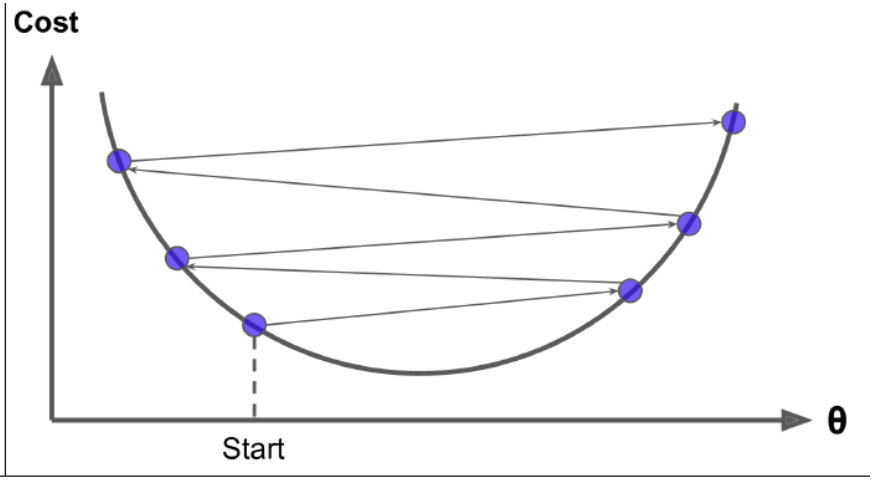
- θ : 임의의 값으로 시작. 즉, 무작위 초기화($random\ initialization$)
- 학습률($learning\ rate$) : 경사 하강법 단계($step$) 크기



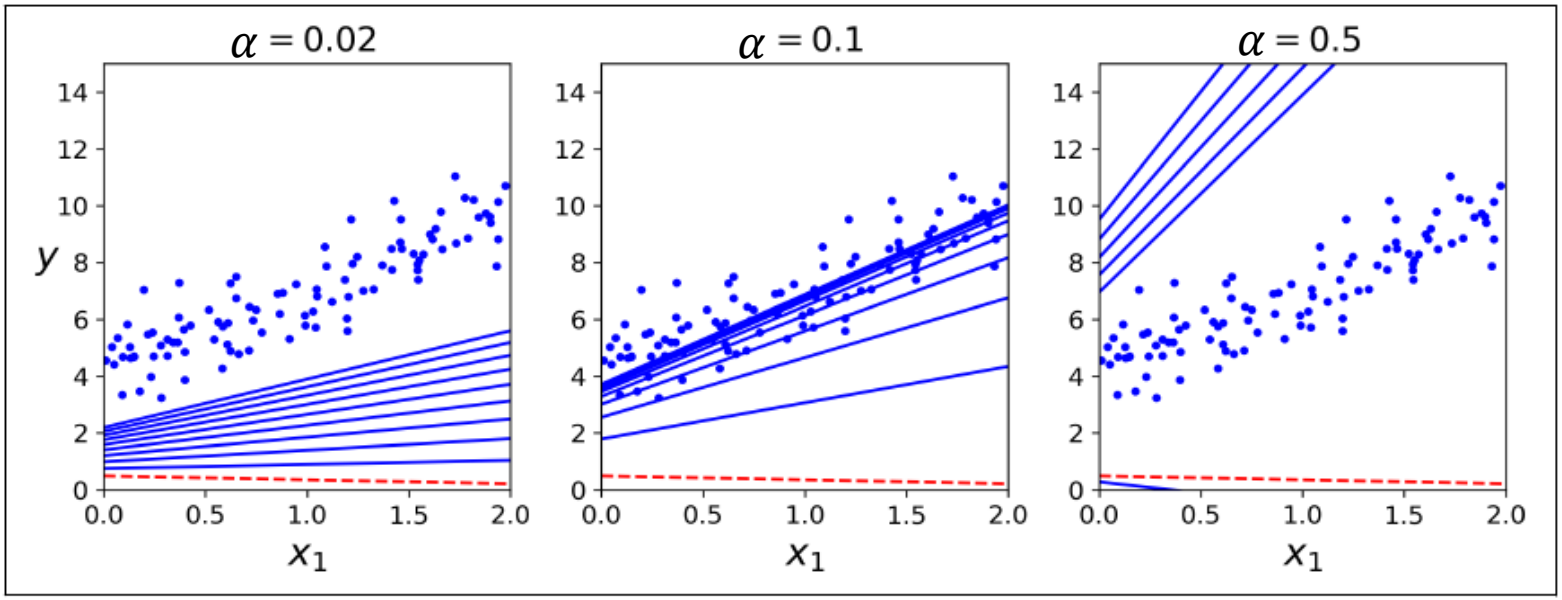
Learning rate



Learning rate too small

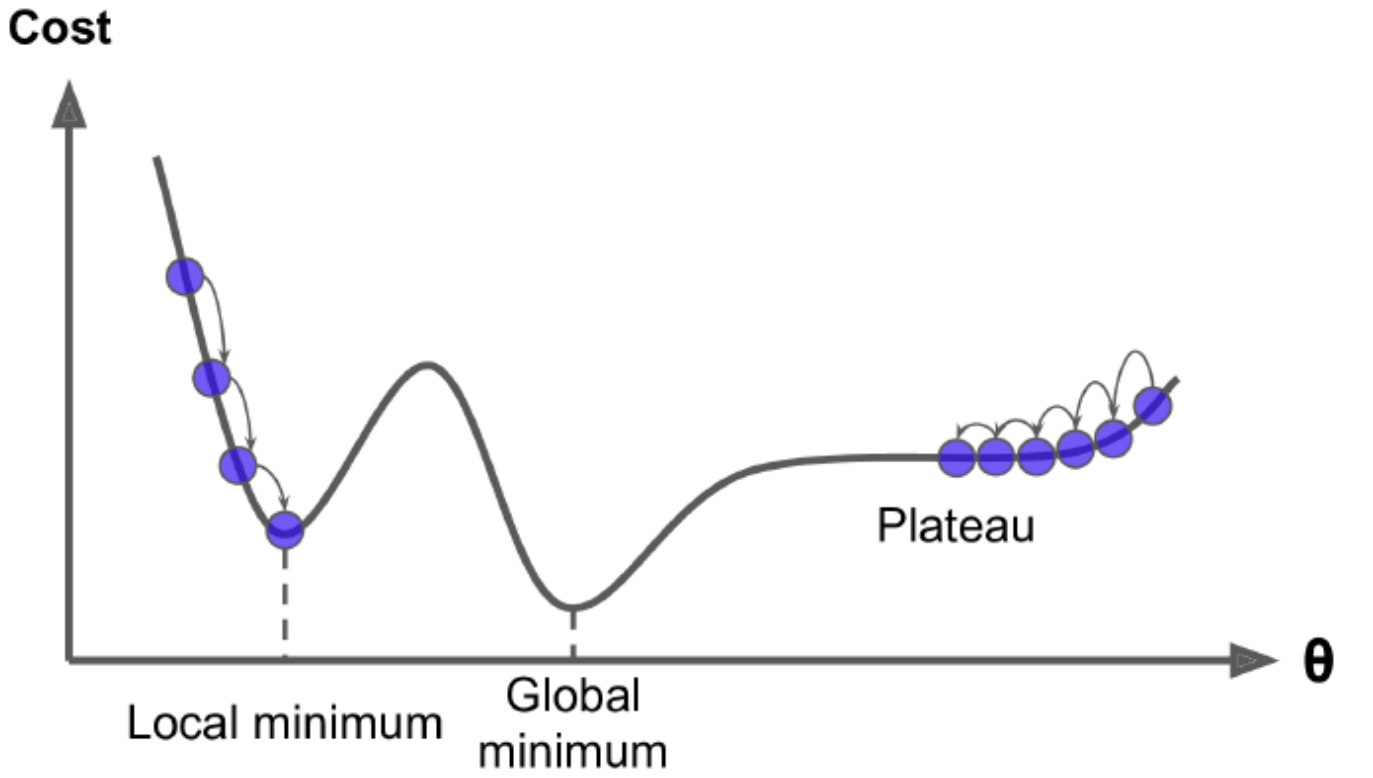


Learning rate too large



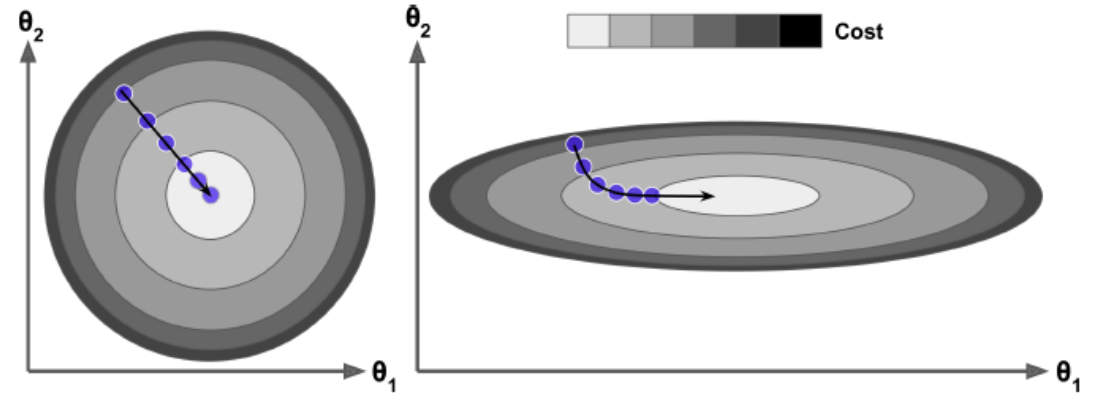
Ref : Hands-on Machine Learning with Scikit-Learn, Keras & TensorFlow - O'REILLY

Local minimum vs Global minimum



Gradient Descent pitfalls

- 특성1과 특성 2의 스케일의 크기의 차이
  - 최소값에 도달하는 시간
- 경사 하강법을 사용할 때는 데이터의 모든 특성이 같은 스케일을 갖도록 처리
  - (예) 사이킷런의 StandardScaler를 사용



Gradient Descent with and without feature scaling

Epoch/Batch

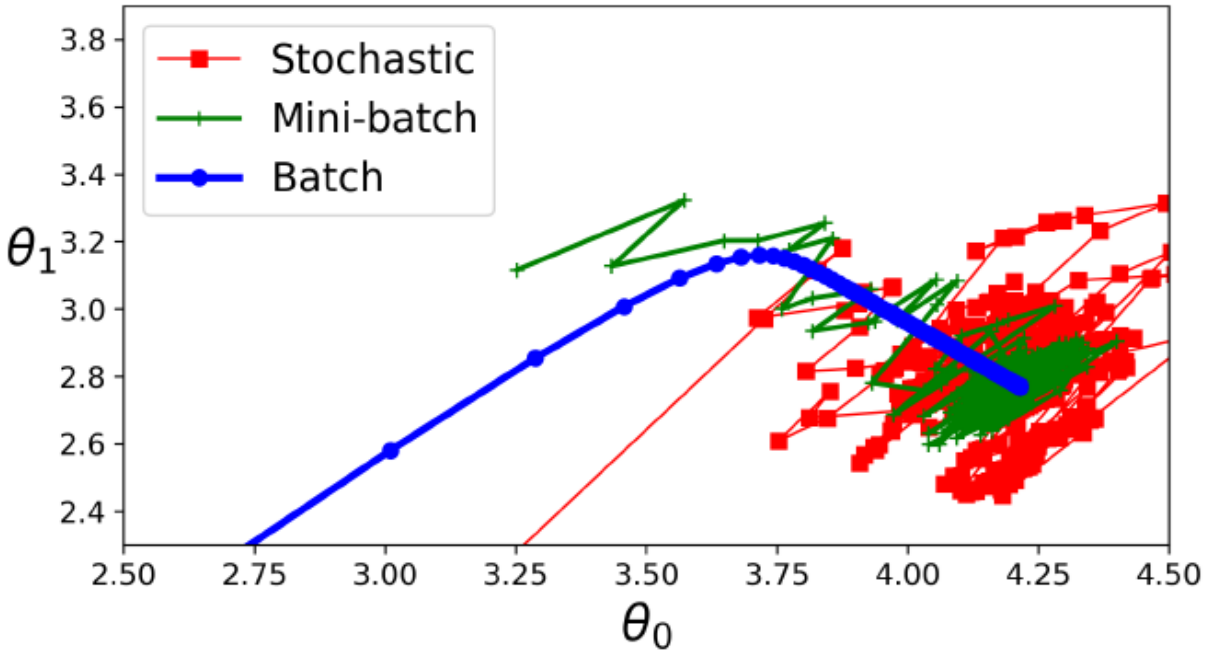
- one **epoch** : one forward pass and one backward pass of all the training examples
- **batch size** : the number of training examples in one forward/backward pass. The higher the batch size, the more memory space you'll need.
- number of **iterations** : number of passes, each pass using [batch size]number of examples.

  To be clear, one pass = one forward pass + one backward pass
  - we do not count the forward pass and backward pass as two different passes.
- Example
  - if you have 1000 training examples, and your batch size is 500, then it will take 2 iterations to complete 1 epoch

경사 하강법의 종류

- 배치 경사하강법$(batch\ gradient\ descent)$
  - 전체 훈련 데이터셋을 사용해 매 스텝에서 사용
  - 큰 훈련 데이터 셋에서 속도가 느림(비용이 많이 든다)
- 확률적 경사하강법$(stochastic\ gradient\ descent, SGD)$
  - 일정량의 훈련 데이터셋을 무작위로 선택하여 매 스텝에서 사용
  - 데이터량이 적기 때문에 속도가 빠름
  - 새로운 데이터가 도착하는 대로 훈련(온라인 학습으로 사용)
  - 최소값에 다다를 때까지 불규칙하여 Local minimum을 건너뛰도록 도와주게 되어 $Global\ minimum$을 찾을 가능성이 높다
- 미니배치 경사하강법$(mini-batch\ gradient\ descent)$
  - 배치 경사하강법과 확률적 경사하강법의 절충
  - 임의의 작은 훈련데이터셋을 선택하여 매 스텝에서 사용
  - 확률적보다 덜 불규칙하지만 $Local\ minimum$에서 빠져나오기는 더 힘들 수 있다.

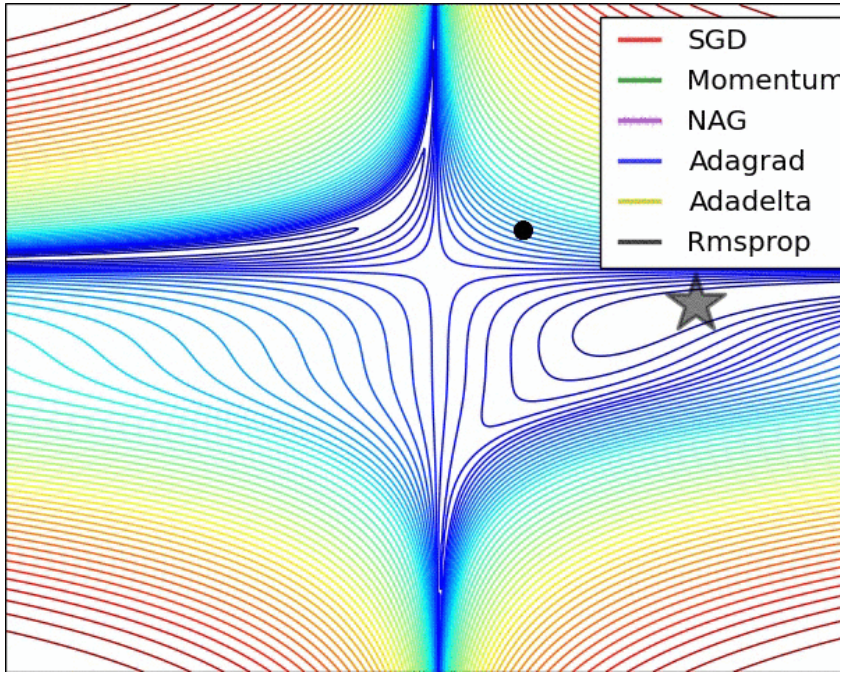
- 전부 최소값 근처에 도달
- 배치 경사하강법의 경로가 실제로 최솟값에 멈춘 반면(많은 시간 소요)
- 확률적/미니배치 경사하강법은 근처에서 맴돌고 있다



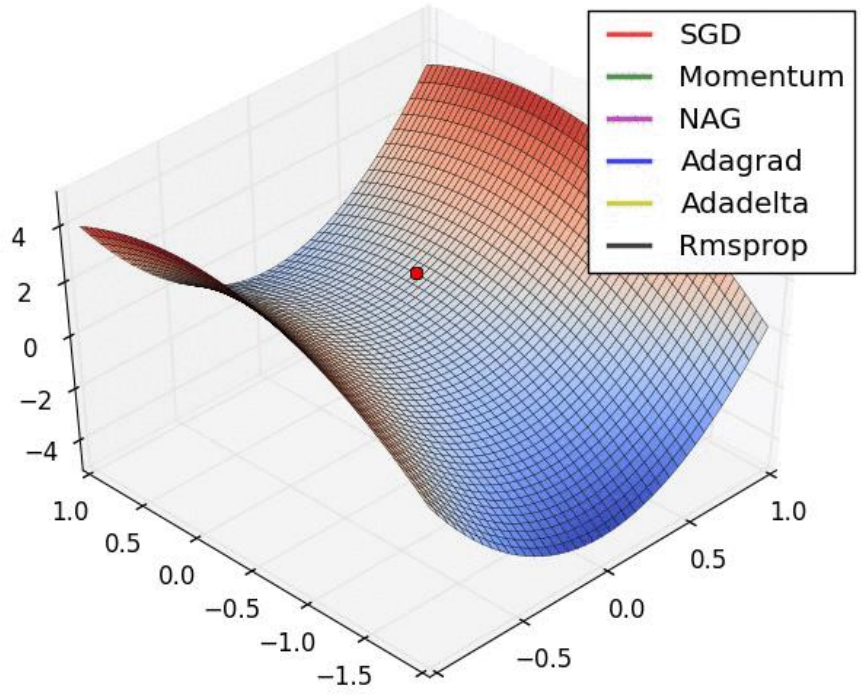
기타 알고리즘

- Momentum
  - Gradient Descent를 통해 이동하는 과정에서 일종의 관성(momentum)값을 더해 주는 것
- NAG(Nesterov Accelerated Gradient)
  - Momentum 값이 적용된 지점에서 gradient값이 계산
  - 한 단계를 미리 예측함으로써 불필요한 이동을 줄인다.
- Adagrad(Adaptive Gradient)
  - SGD를 개선한 형태
  - 변수의 업데이트 횟수에 따라 학습률(Learning rate)를 조절하는 옵션이 추가된 방법
- RMSProp
  - AdaGrad를 개선한 형태
- AdaDelta(Adaptive Delta)
  - RMSProp과 유사하게 AdaGrad의 단점을 보완하기 위해 제안된 방법
- Adam(Adaptive Moment Estimation)
  - Momentum/AdaGrad/RMS prop의 장점만을 모아 하나로 결합한 형태

https://ruder.io/optimizing-gradient-descent/



SGD optimization on loss surface contours



SGD optimization on saddle point