



CNU 데이터 분석 교육



9th lecture
"Linear Analysis-3"

2021 - 11 - 14

지난시간?

1. Loss function

- The key to determining the performance of a model.
- SMNP, OD, log cosh

오늘은 무엇을?

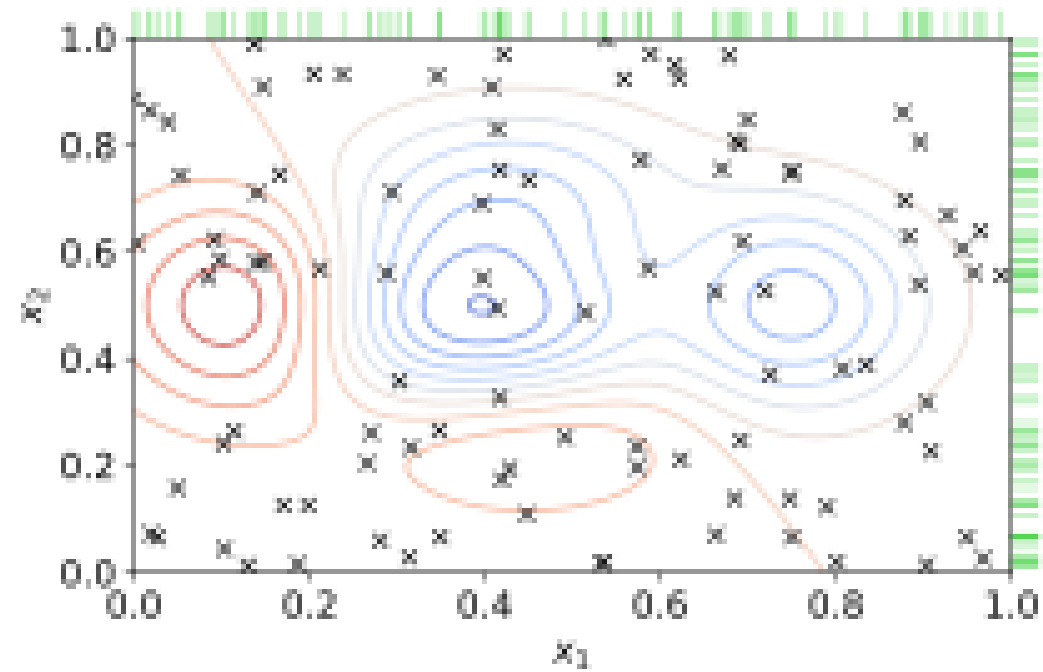
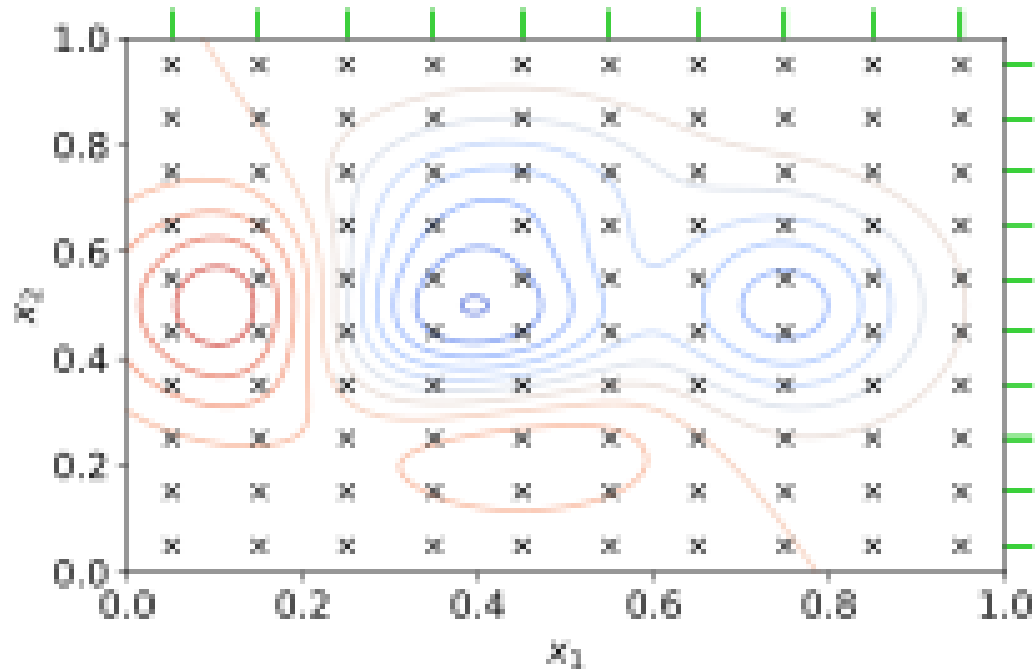
1. Loss function을 최소화 하는 parameter를 찾는 방법?

- Gradient descent method
- Calculus analysis

2. Linear regression model의 성능을 평가할 수 있는 방법?

Grid search

꼭 격자여야 하는가?

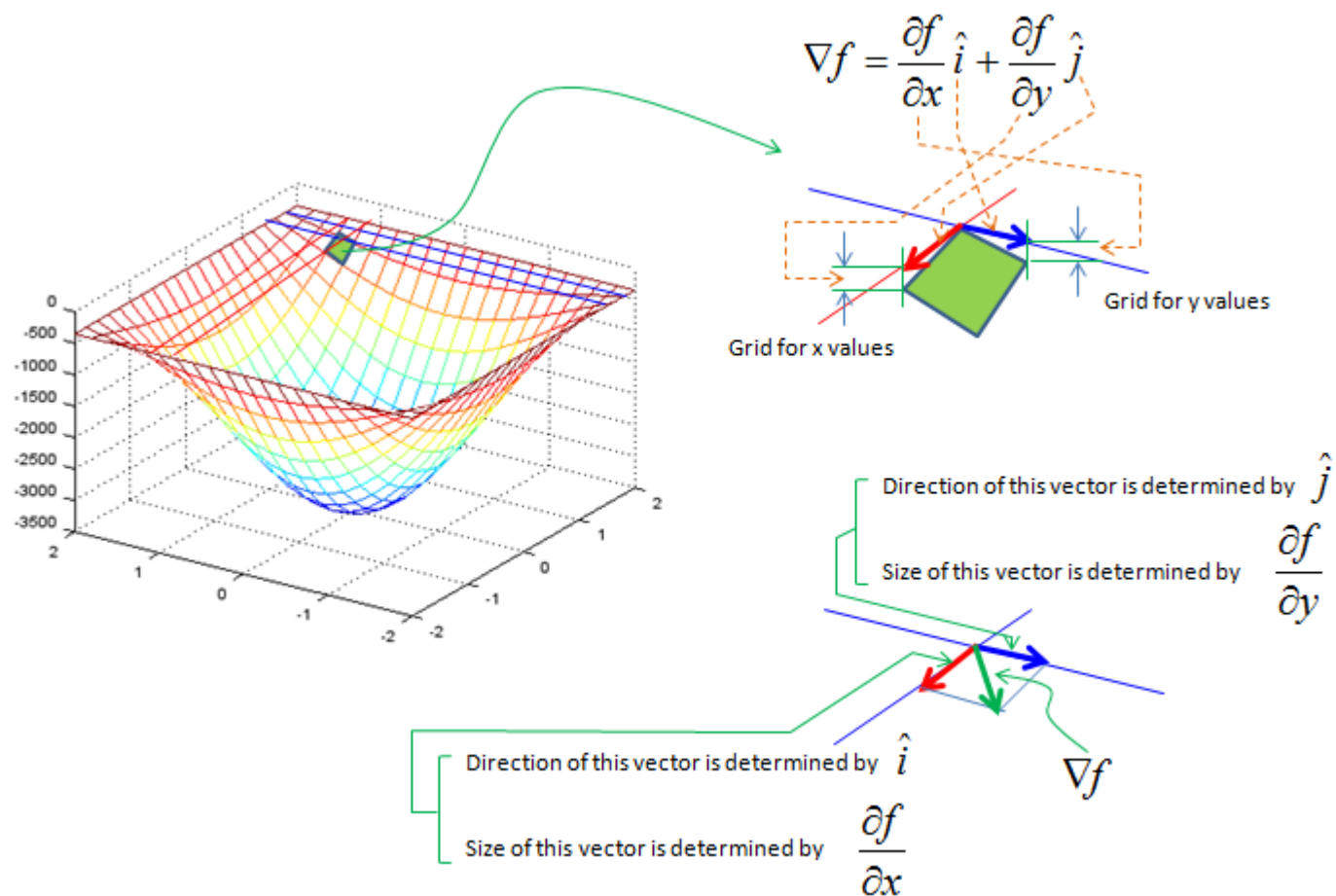


https://en.wikipedia.org/wiki/Hyperparameter_optimization

Gradient descent

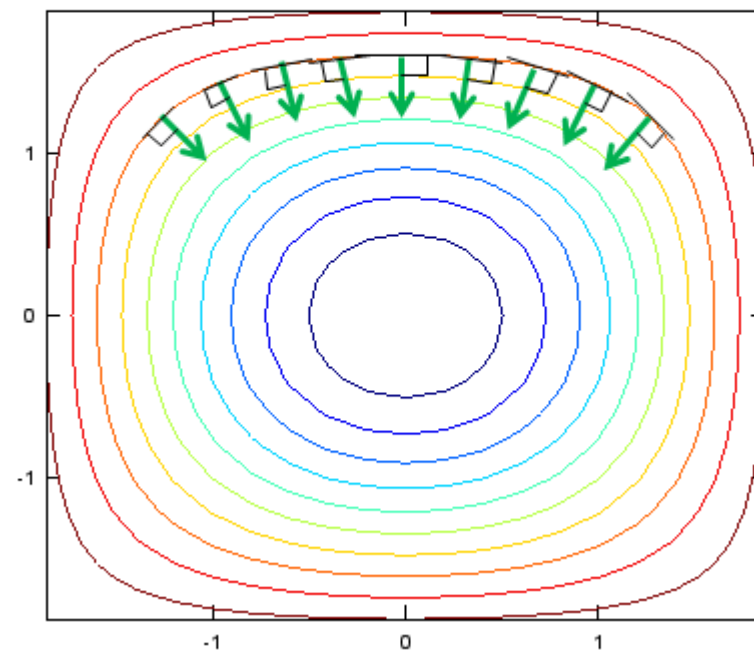
★Gradient : 해당 점에서 함숫값이 가장 크게 증가하는 방향

$$\nabla f = \left(\frac{\partial f}{\partial x_1}, \dots, \frac{\partial f}{\partial x_n} \right)$$



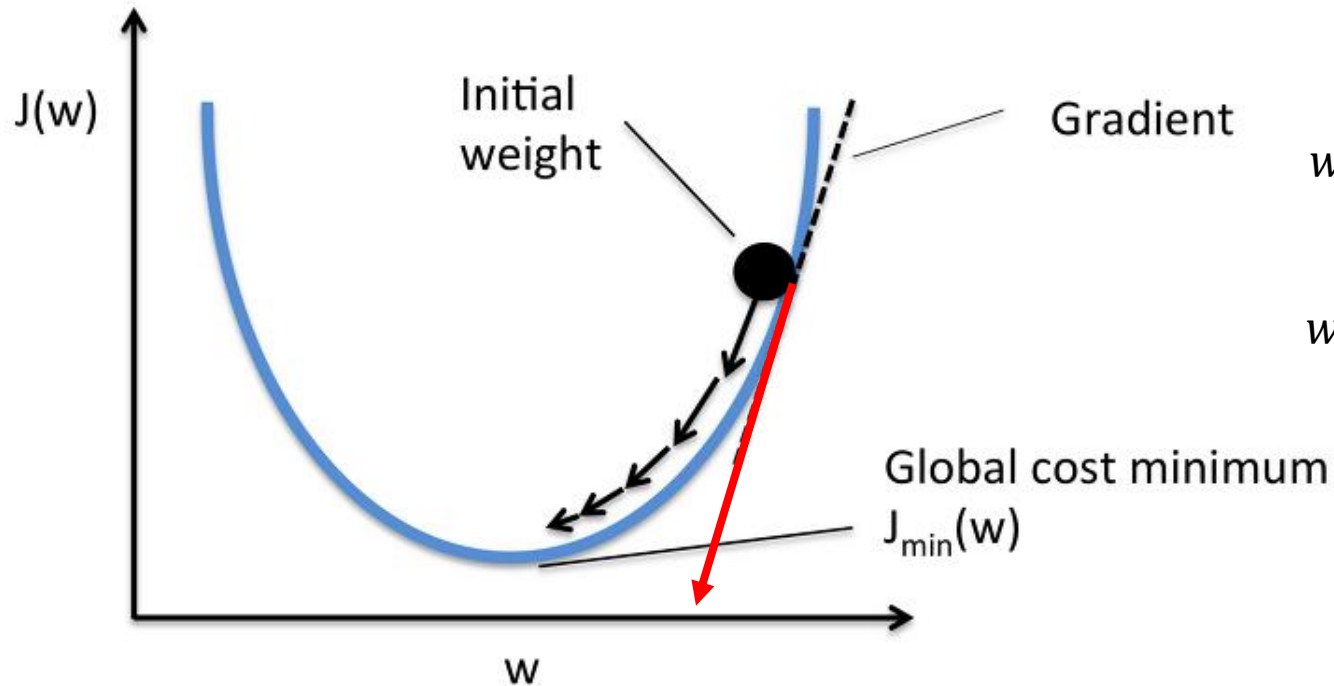
Gradient Vectors

- Perpendicular to Contour Line
- Steepest slope



http://www.sharetechnote.com/html/Calculus_Gradient.html

Gradient descent



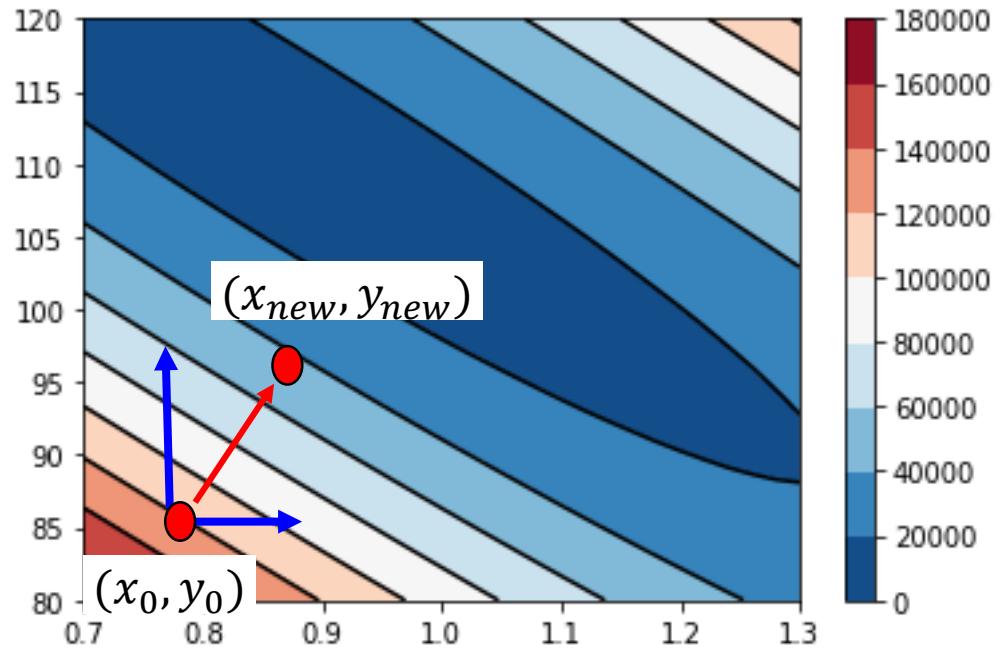
https://en.wikipedia.org/wiki/Gradient_descent

$$w_{new} = w_0 - J'(w_0)$$

$$w_{new} = w_0 - \alpha J'(w_0) \text{ 이동하는 정도를 조절해준다!}$$

이 α 를 "learning rate"라 한다.

Gradient descent



$$x_{new} = x_0 - \alpha \frac{\partial}{\partial x} J(x_0, y_0)$$
$$y_{new} = y_0 - \alpha \frac{\partial}{\partial y} J(x_0, y_0)$$

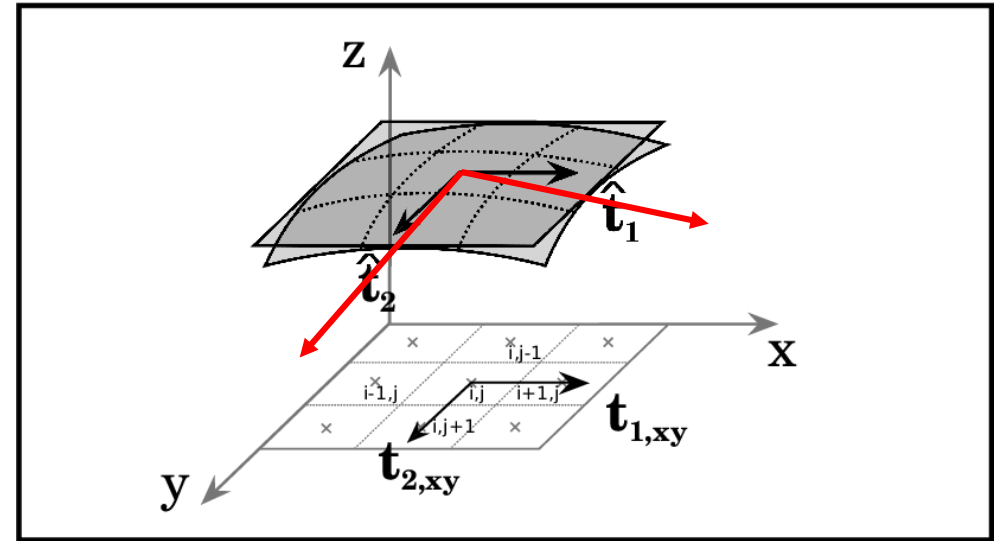
Gradient descent

For n-th parameter $(\theta_1, \theta_2, \dots, \theta_n)$, update by

$$\theta_i = \theta_i - \alpha \frac{\partial}{\partial \theta_i} J(\theta_1, \theta_2, \dots, \theta_n)$$

Where α is "learning rate",

$J(\theta_1, \theta_2, \dots, \theta_n)$ is "loss function"
(or "object function")



https://www.researchgate.net/figure/A-stencil-used-for-computing-surface-gradient-in-the-column-containing-the-cell-C-i-j_fig1_314152762

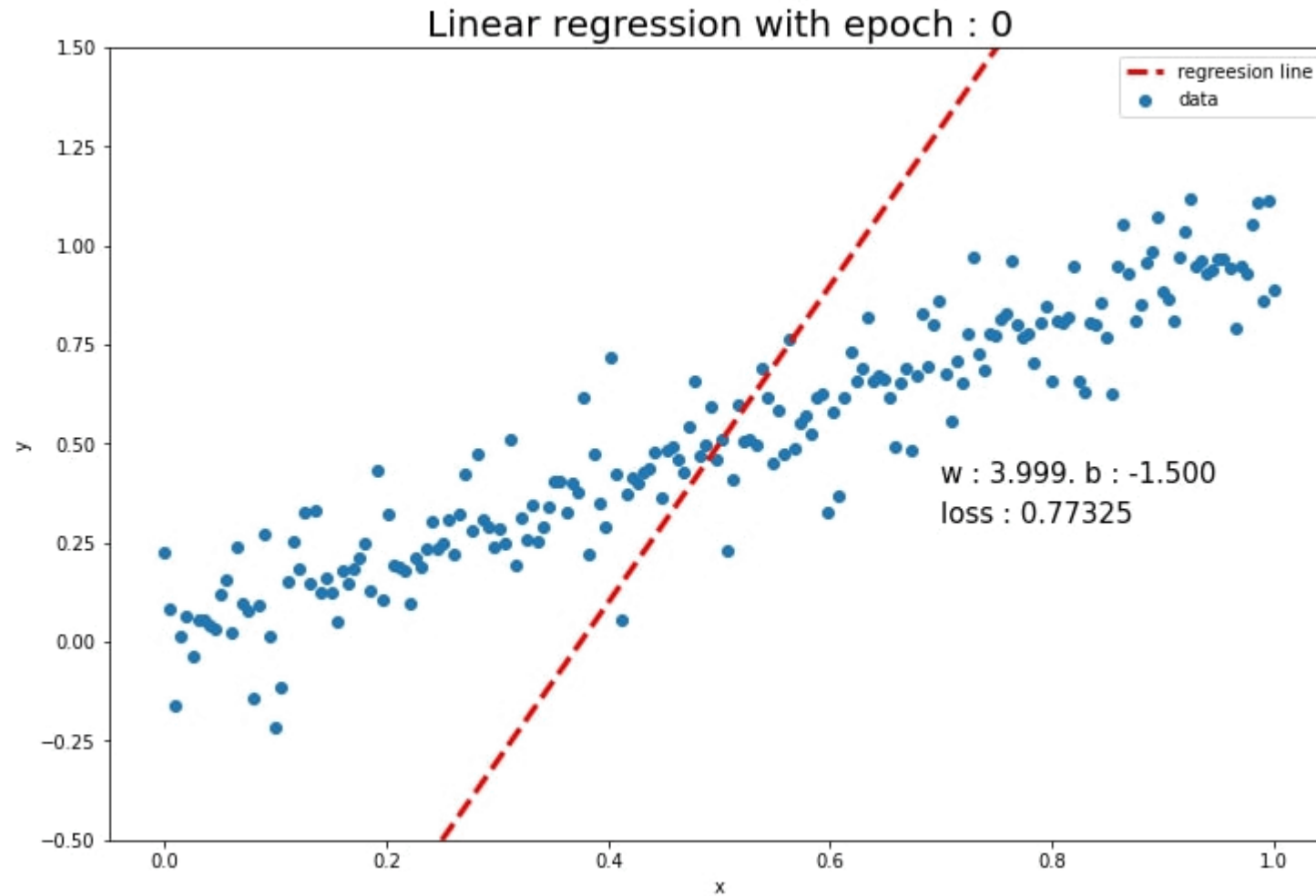
Gradient descent

Our loss function is $J(w, b) = \sum (wx + b - y)^2$

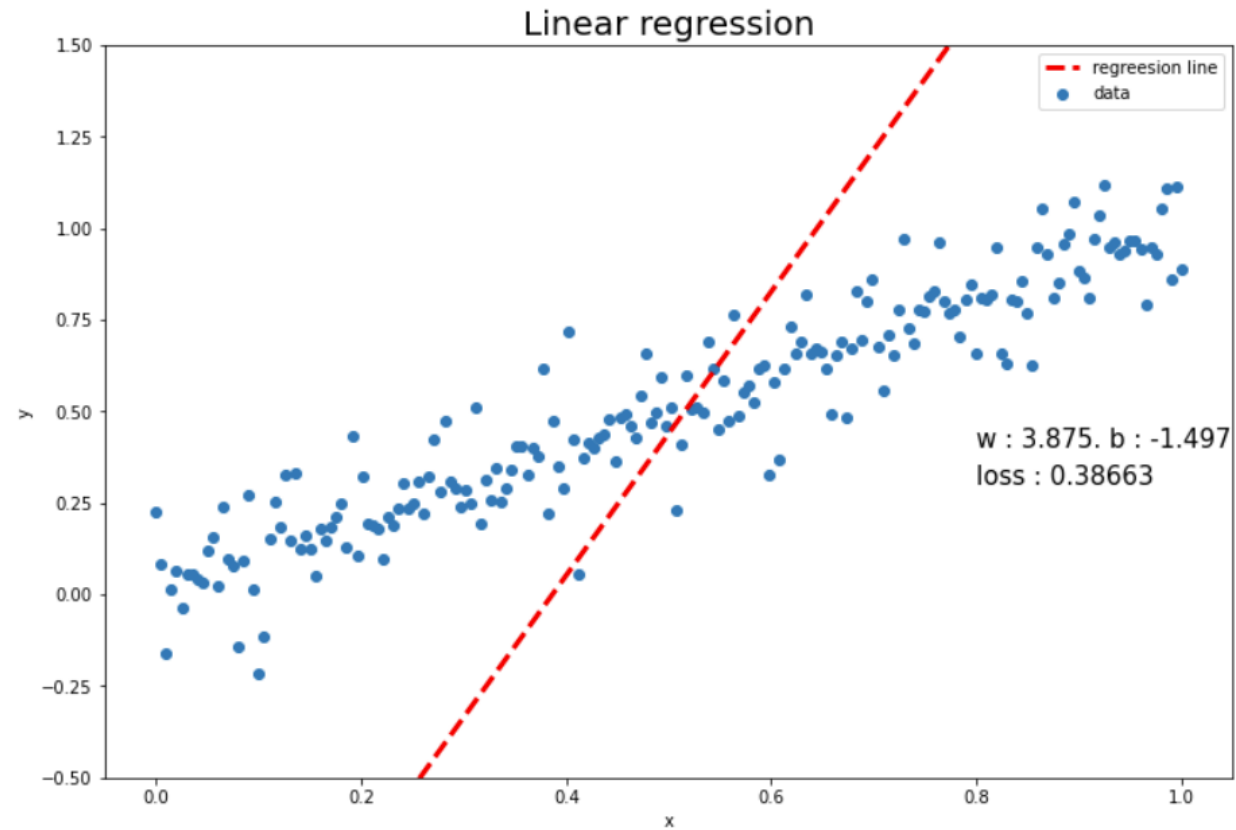
For gradient descent, $w = w - \alpha \frac{\partial}{\partial w} J(w, b) = w - \alpha \sum 2(wx + b - y)x$

$$b = b - \alpha \frac{\partial}{\partial b} J(w, b) = b - \alpha \sum 2(wx + b - y)$$

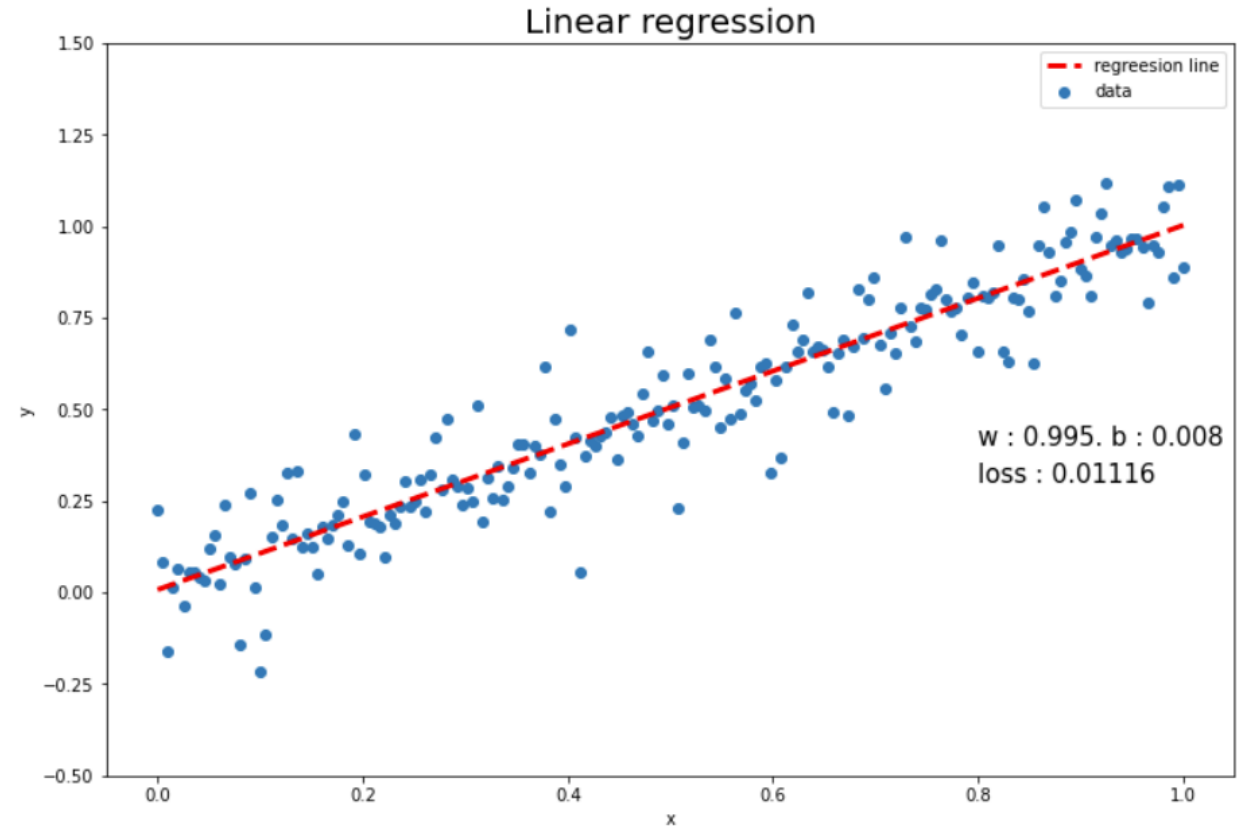
Gradient descent



Gradient descent

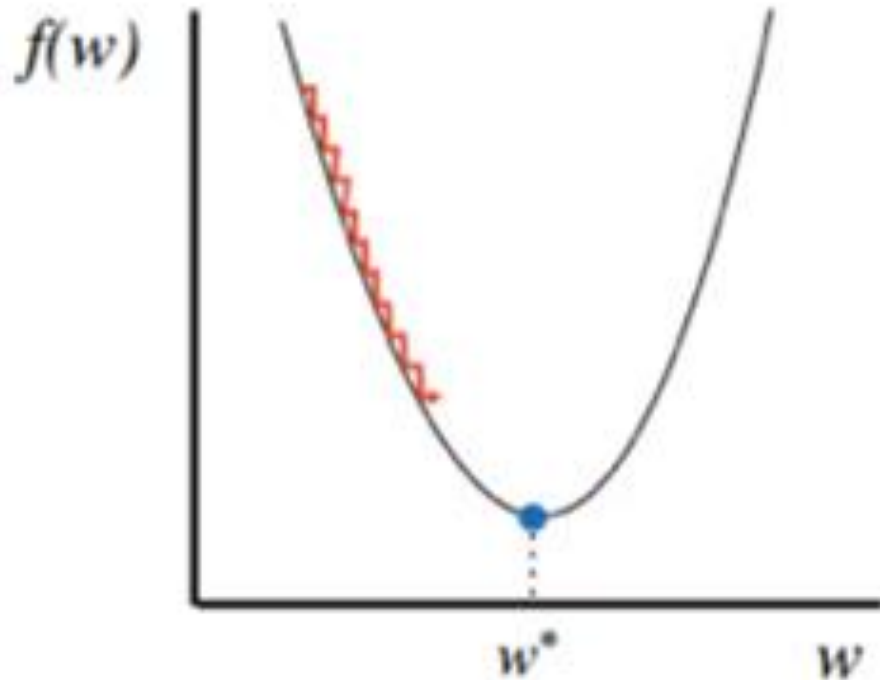


Epoch = 20000 이후

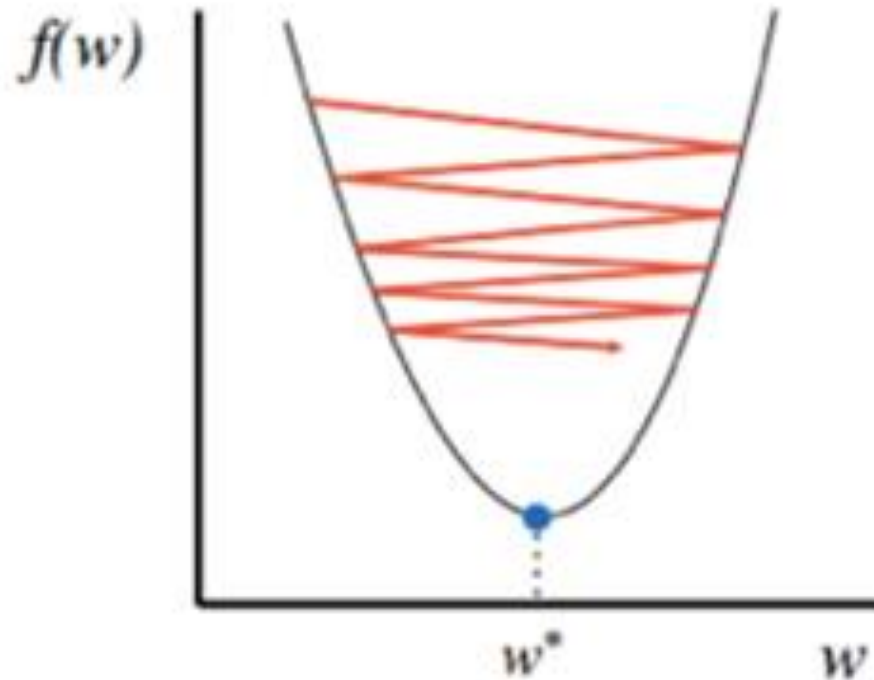


Gradient descent 단점

Learning rate를 잘 조절해야 한다.



Too small: converge
very slowly

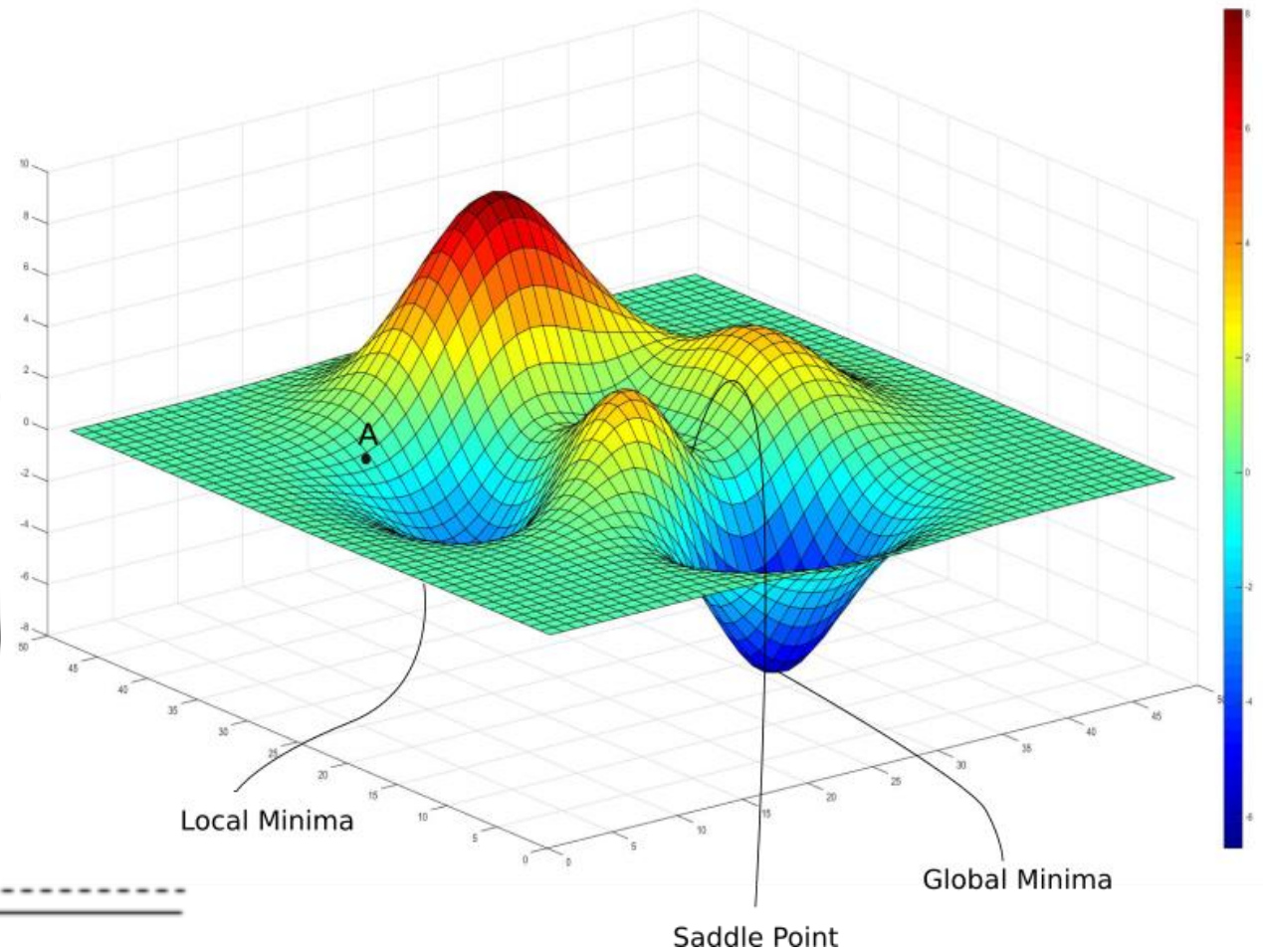
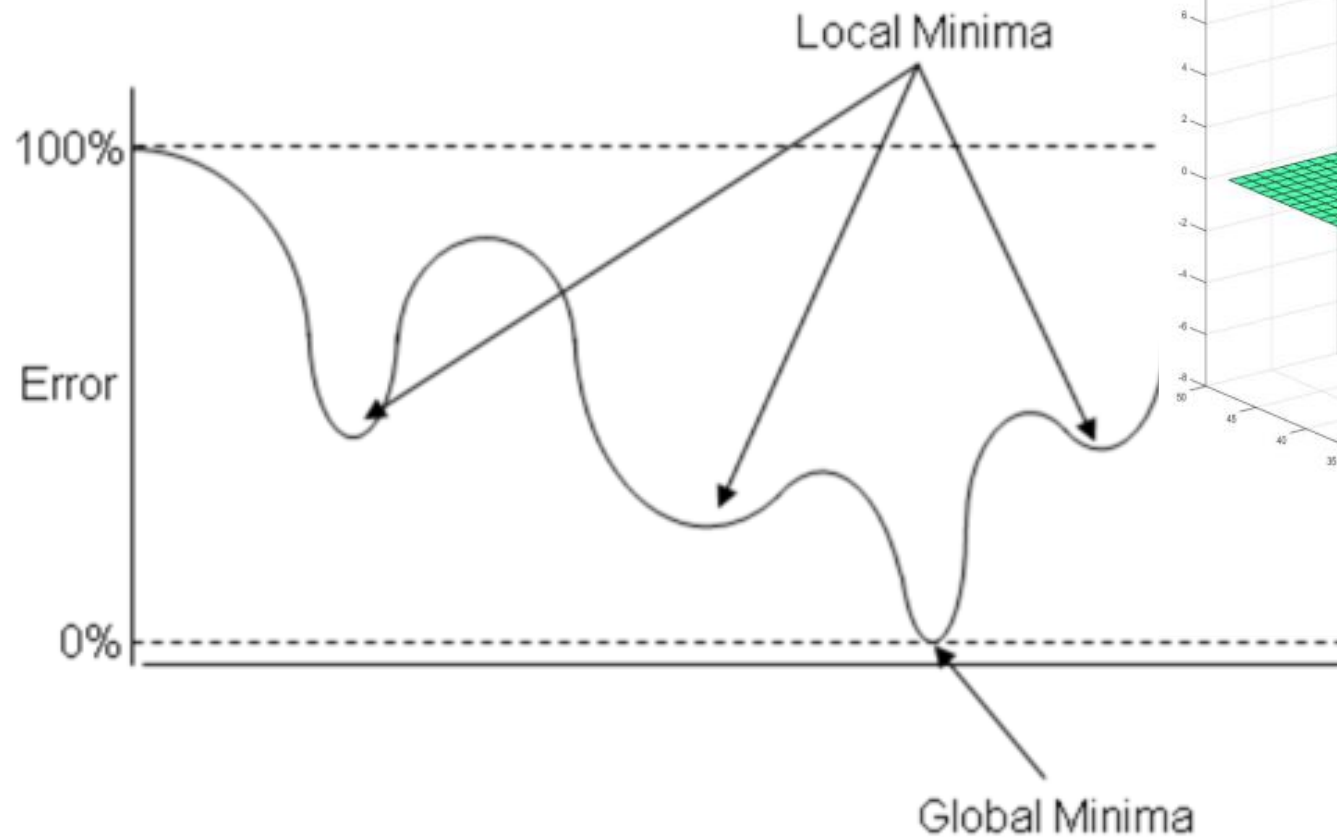


Too big: overshoot and
even diverge

<https://m.blog.naver.com/jevida/221855713144>

Gradient descent 단점

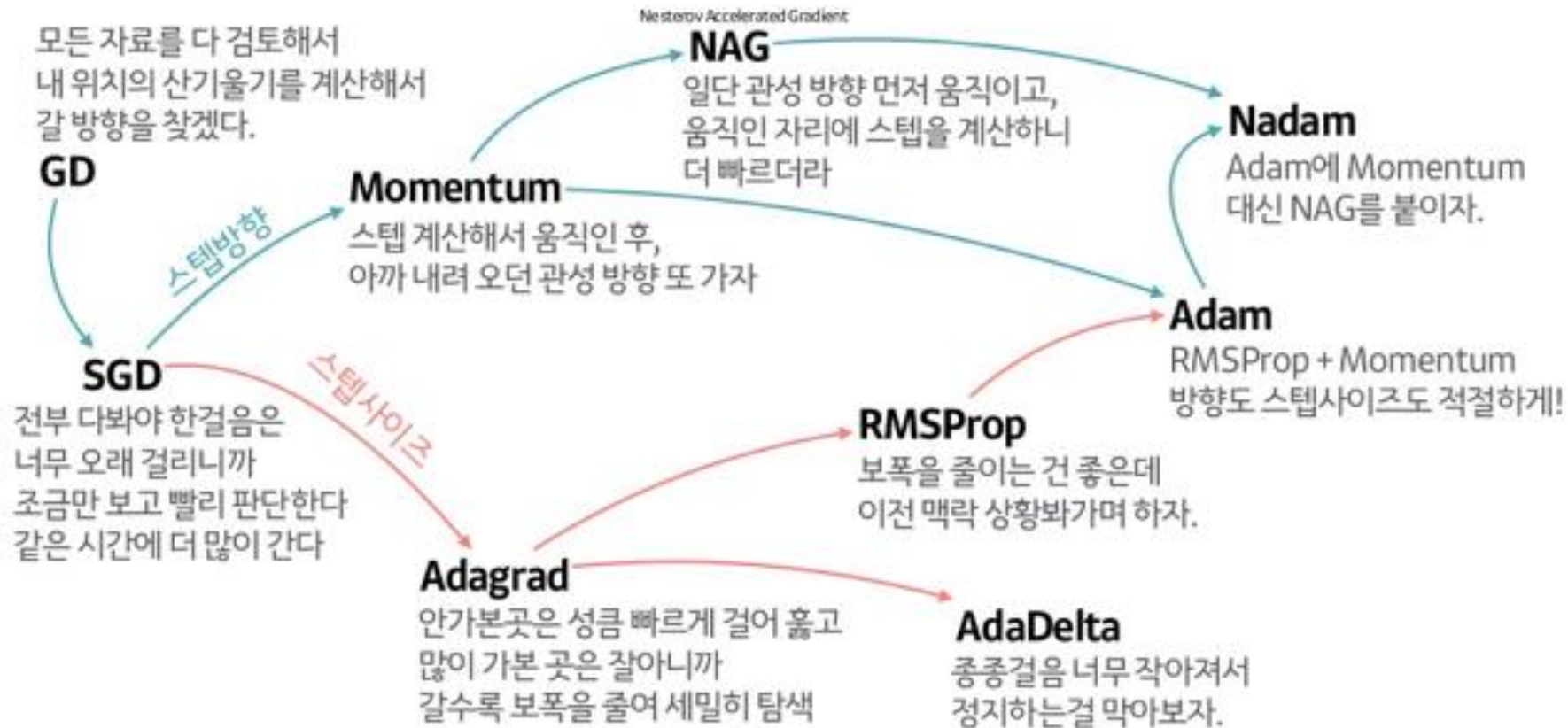
지역최솟값(Local Minima)에 빠지면 억까당함



<https://m.blog.naver.com/jevida/221855713144>

Gradient descent 단점

지역최솟값(Local Minima)를 벗어나게 하는 다양한 알고리즘이 존재.



<https://truman.tistory.com/164>

Linear Regression coefficient

수학적인 관점에서 $\text{loss} = (y_{\text{pred}} - y)^2 = (wx + b - y)^2$ 인데,
각각 w, b 에 대한 편미분이 0인점을 계산해보면 되지 않을까?

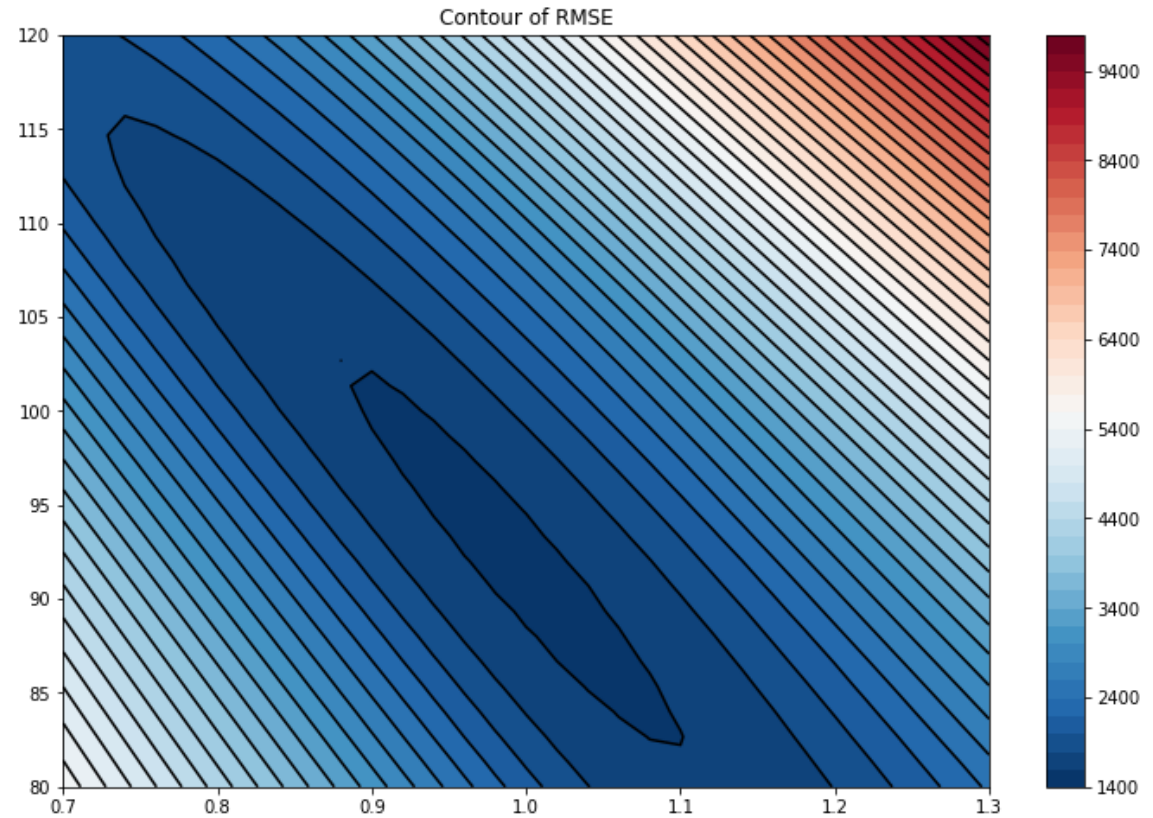
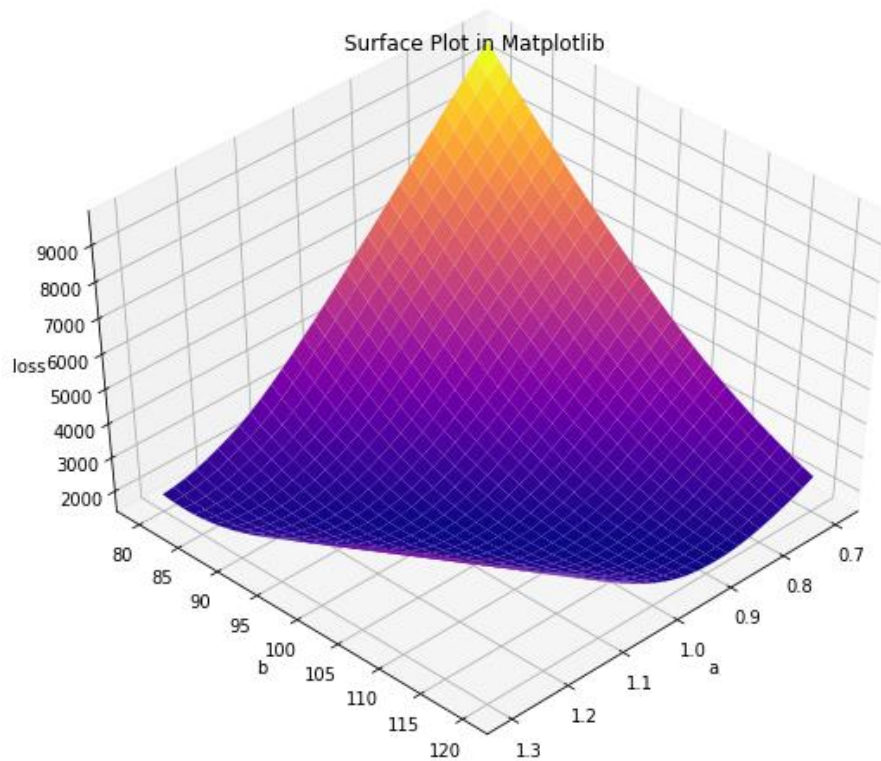
1학년 미분적분학...

$$\nabla_p f = (y, x) = (0, 0) \quad H_f = \begin{vmatrix} f_{xx} & f_{xy} \\ f_{yx} & f_{yy} \end{vmatrix} = f_{xx}f_{yy} - f_{xy}f_{yx}$$

- 1) P is Local Maximum, when $H_f(P) > 0, f_{xx}(P) > 0$
- 2) P is Local Minimum, when $H_f(P) > 0, f_{xx}(P) < 0$
- 3) P is Saddle Point, when $H_f(P) < 0$
- 4) Impossible, when $H_f(P) = 0$

Linear Regression coefficient

$z = (x - y)^2$ 꼴의 함수는 볼록(convex) 함수이고, 연속이기에 전역최솟값(Global minimizer)가 존재한다.



Linear Regression coefficient

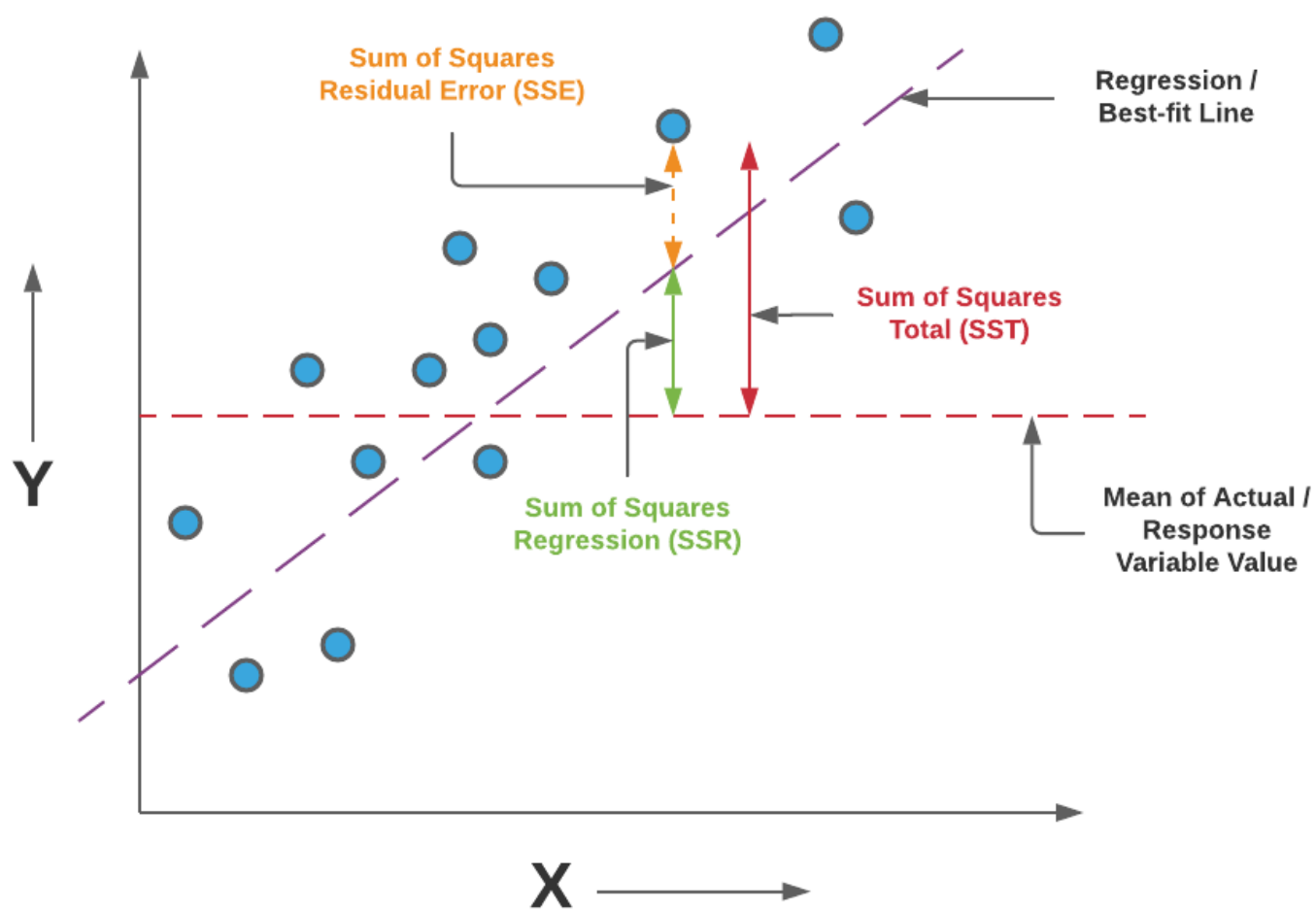
$$y = wx + b$$

각각 편미분해서 0이 되는 점을 계산한 것!

$$w = \frac{Cov(X, Y)}{Var(X)}$$

$$b = E(Y) - wE(X)$$

R2 Score



$$SST = \sum_{i=1}^n (y_i - \bar{y})^2$$

$$SSR = \sum_{i=1}^n (\hat{y}_i - \bar{y})^2$$

$$SSE = \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

<https://vitalflux.com/mean-square-error-r-squared-which-one-to-use/>

R2 Score

Property 1.

$$SST = SSE + SSR$$

$$SST = \sum_{i=1}^n (y_i - \bar{y})^2$$

$$SSR = \sum_{i=1}^n (\hat{y}_i - \bar{y})^2$$

$$SSE = \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

$(a - b)^2 = (a - c)^2 + (c - b)^2$??????? 이게 된다고?

$$1 = \frac{SSR + SSE}{SST} \Rightarrow \frac{SSR}{SST} = 1 - \frac{SSE}{SST}$$

R² Score

$$R^2 = \frac{SSR}{SST} = 1 - \frac{SSE}{SST}$$

Linear Regression을 평가할 수 있는 척도!
너의 의미는??

전체중에 설명가능한 아이가 얼마나 있니???

$0 \leq R^2 \leq 1$ 즉, 데이터의 개수와 상관없이 Linear Regression 모델의 성능 평가 가능!

문제 1

Loss function이 RMSE이고, optimizer가 Gradient descent method인 Linear Regression 함수를 아래 조건에 따라 만들어라.

1. 함수이름 : LR_GD($X, Y, w, b, num_epoch, learning_rate$)
2. Output : $w, b, loss, loss_list$
3. Loss가 0.00005 보다 작으면 정지 후 몇 번째 epoch에서 정지했는지 출력.
4. Epoch가 500의 배수일때마다 epoch, $w, b, loss$ 를 print 하게 설정.

문제 1

정답

```
def LR_GD(X, Y, w, b, num_epoch, learning_rate):  
    # w_list = []  
    # b_list = []  
    loss_list = []  
  
    for epoch in range(num_epoch):  
        Y_hat = w*X + b  
  
        loss = ((Y_hat - Y) ** 2).mean()  
  
        if loss < 0.0005:  
            break  
  
        w = w - learning_rate * ((Y_hat - Y)*X).mean()  
        b = b - learning_rate * (Y_hat - Y).mean()  
  
        loss_list.append(loss)  
  
        if epoch % 500 == 0:  
            print("{} epoch  w = {:.3f}, b = {:.3f}, loss = {:.5f}".format(epoch, w, b, loss))  
  
    print("stop at :{}".format(epoch))  
  
    return w, b, loss, loss_list
```

정리 요약

1. Gradient descent method
 - learning rate를 잘 정하는 것이 중요하다.
 - local minima에 빠지면 노답이다.
2. RMSE를 이용한 loss function은 Global minimizer가 존재한다.
 - 따라서 수학적 계산을 통해 가장 좋은 parameter를 해석적으로 찾을 수 있다.
3. 그런데 대부분의 모델들의 Global minimizer를 해석적으로 찾을 수 없으니 Gradient descent method 같은 수치해석방법을 이용하여 접근한다.

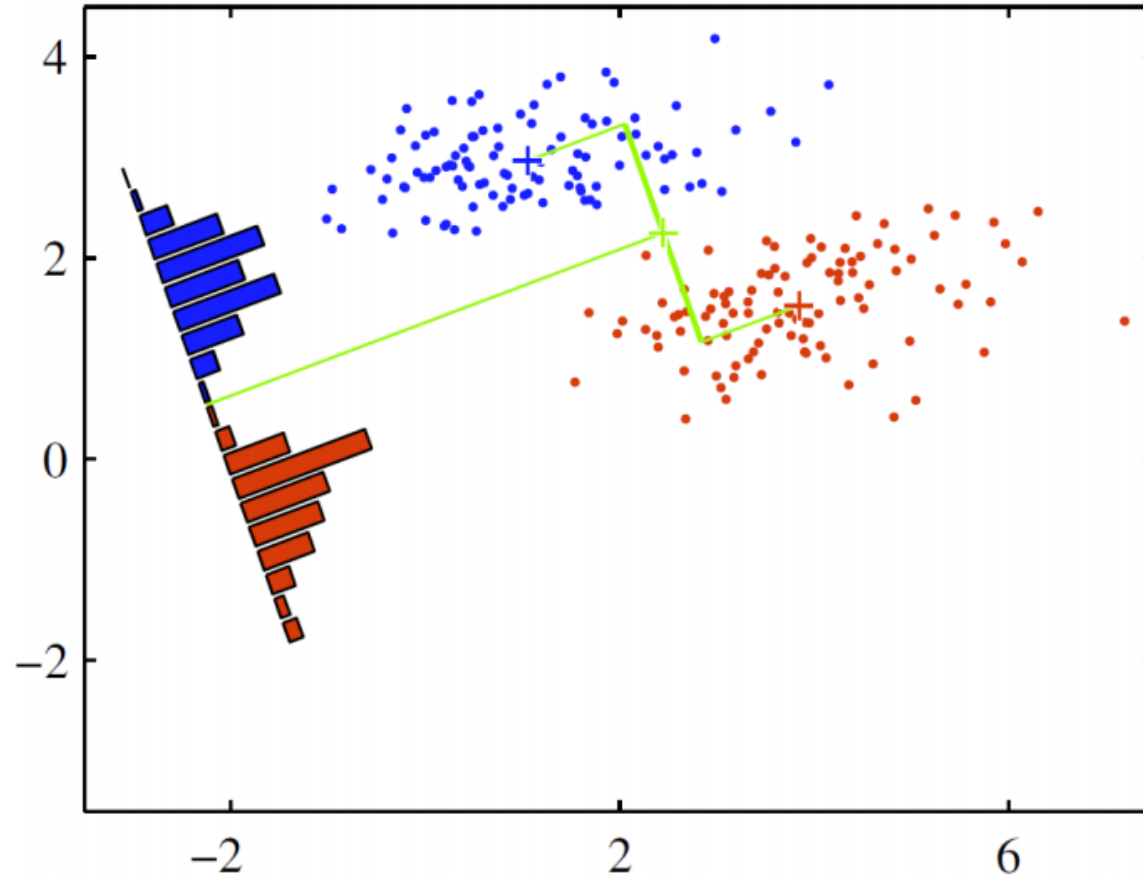
정리 요약

4. R^2 Score는 RMSE를 이용한 Linear regression 모델에서만 설명 가능.
(아무 regression에서 막 사용하면 안됨!)

(근데 현업에서는 그냥 무시하고 쓰는 경우도 있더라...)

공지

1. 다음시간에는 선형판별분석(Linear Discriminant Analysis)에 대해 배울 것



끼 트



담에뵈시당