

Design Matrix

$$A = \begin{bmatrix} 1 & x_1 & x_1^2 & \dots & x_1^{m-1} \\ \vdots & x_2 & x_2^2 & \dots & x_2^{m-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_1 & x_n & x_n^2 & \dots & x_n^{m-1} \end{bmatrix}_{n \times m}$$

Weight Vector

$$W = \begin{bmatrix} W_0 \\ W_1 \\ \vdots \\ W_{m-1} \end{bmatrix}_{m \times 1}$$

Target Vector

$$b = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}_{n \times 1}$$

① LSE is we hope

Find a W to make

$$AW = b$$

But A is not

invertible (perhaps not)

→ We only find \vec{W}

such $AW = b$ to $\min \|AW - b\|^2$

$$\begin{aligned} \|Aw - b\|^2 &= (Aw - b)^T (Aw - b) \\ &= W^T A^T A W - \underline{2W^T A^T b} + b^T b \end{aligned}$$

★ $W^T A^T b$ is "Scalar" not a Vector

$$\text{So, } (W^T A^T b)^T = b^T A W = W^T A^T b$$

$$\begin{aligned} \min_{W_{LSE}} \|Aw - b\|^2 &\Rightarrow \frac{\partial}{\partial W} (W^T A^T A W) - \frac{\partial}{\partial W} (2W^T A^T b) + \frac{\partial}{\partial W} (b^T b) \\ &\Rightarrow 2A^T A W - 2A^T b + 0 \\ &\Rightarrow A^T A W = A^T b \\ &\Rightarrow W_{LSE} = (A^T A)^{-1} A^T b \neq \end{aligned}$$

But $W = (A^T A)^{-1} A^T b \Rightarrow$ We only know $\det(A^T A)^{-1} \geq 0$

Can't 100% make sure full rank (invertible)

We must add regularized term "L1 norm" or "L2 norm"

To 100% make sure full rank (invertible)

We usually call rLSE,

We choose L_2 norm $= \lambda \|W\|^2 \Rightarrow \frac{\partial}{\partial W} L_2 = 2\lambda W$

$$\min_W \|AW - b\|^2 \Rightarrow 2A^T A W - 2A^T b + 2\lambda W = 0$$

$$\Rightarrow (A^T A + \lambda I) W = A^T b \Rightarrow W_{\text{rLSE}} = (A^T A + \lambda I)^{-1} A^T b \#$$

While $\lambda > 0$, $A^T A + \lambda I$ 100% det > 0 , invertible #

Both LSE / rLSE We all need to calculate

Inverse Matrix, I will choose LU

Because only we ① solve I each row e_i

To solve $LUx_i = e_i$ ② Assemble together we

Let A^{-1} For example: $A = LU \Rightarrow A^{-1} = U^{-1} L^{-1}$

$A^{-1} = [x_1, x_2, \dots, x_n]$, x_i is a column vector

By $AA^{-1} = I \Rightarrow Ax_i = e_i$, $i = 1 \dots n$ ① \Rightarrow solve y_i

$\Rightarrow Ax_i = e_i \Rightarrow LUx_i = e_i$, let $Ux_i = y_i$ ② solve x_i

Summary

- ① Forward substitution $Ly_i = e_i$, solve y_i
- ② Backward substitution $Ux_i = y_i$, solve x_i

$A^{-1} = [X_1, X_2 \dots X_n] \rightarrow$ We can get A^{-1} #

⑥ Steepest decent

The update formula of steepest decent

$$W_{t+1} = W_t - \eta \nabla f(W_t)$$

W_t is parameter of t steps

η is learning rate (Steps size)

$\nabla f(W_t)$ is W_t 's gradient

Lipschitz continuous with $L > 0$ (L is Lipschitz constant)
This make sure the change will not so fierce

From $f(W_t)$ we expansion of f (f is Loss function)

by Taylor

$$\begin{aligned} f(W_{t+1}) &\leq f(W_t) + \nabla f(W_t)^T (W_{t+1} - W_t) + \frac{L}{2} \|W_{t+1} - W_t\|^2 \\ &= f(W_t) - \eta \|\nabla f(W_t)\|^2 + \frac{L\eta^2}{2} \|\nabla f(W_t)\|^2 \\ &= f(W_t) - \eta \left(1 - \frac{L\eta}{2}\right) \|\nabla f(W_t)\|^2 \end{aligned}$$

$\|W_{t+1} - W_t\|$ must be small enough, which implies η also must be small enough

While $\eta \leq \frac{2}{L}$, this is monotonically increasing (unless $\nabla f(W_t) = 0$)

\Rightarrow Best learning rate: $\eta = \frac{1}{L}$

$\Rightarrow f(W_{t+1}) \leq f(W_t) - \frac{1}{2L} \|\nabla f(W_t)\|^2$ this is description of convergence properties

Regularized term in L_1 norm

the gradient of it can be written

as sign function $\text{Sign}(W_i) = \begin{cases} 1, & \text{if } W_i > 0 \\ -1, & \text{if } W_i < 0 \\ 0, & \text{if } W_i = 0 \end{cases}$

The gradient in total is $2A^T(A\vec{W} - b) + \lambda \cdot \text{Sign}(\vec{W})$

⑨ Newton's method

Basic type:

Based Taylor's expression

$$f(x) \approx f(x_0) + \nabla f(x_0)^T (x - x_0) + \frac{1}{2} (x - x_0)^T H(x_0) (x - x_0)$$

$H(x_0) = \nabla^2 f(x_0)$ is Hessian Matrix

Newton's method optimization problem :

Same We wanna solve $\min_w f(w)$

We must find $\nabla f(w) = 0$

$$\nabla f(w_t) + \underline{H(t)} (w - w_t) = 0$$

Solve step : $w - w_t = -H(t)^{-1} \nabla f(w_t)$

Update formula : $w_{t+1} = w_t - H(t)^{-1} \nabla f(w_t)$

For LSE problem

We already knew $f(w) = \|Aw - b\|^2$

$$\nabla f(w) = 2A^T(Aw - b)$$

$$\nabla^2 f(w) \hat{=} H(w) = \underline{2A^T A} \quad \left(\begin{array}{l} \text{it not related} \\ \text{with } w! \end{array} \right)$$

Apply Update formula $w_{t+1} = w_t - (2A^T A)^{-1} \cdot 2A^T(Aw_t - b)$

$$\Rightarrow w_{t+1} = w_t - (A^T A)^{-1} A^T (Aw_t - b)$$

Special properties of Newton's method

For any quadratic func (ie. LSE)

One step is enough!

$$\begin{aligned}W_1 &= W_0 - (A^T A)^{-1} A^T (A W_0 - b) \\&= W_0 - (A^T A)^{-1} A^T A W_0 + (A^T A)^{-1} A^T b \\&= W_0 - W_0 + (A^T A)^{-1} A^T b \\&= (A^T A)^{-1} A^T b\end{aligned}$$

Does it look familer ~

Because this is optimal solution
of LSE, as shown in previous

We calauted #