벡터미분 / 매트릭스 미분.

① 정의1 : 벡터로 미분.

$$\frac{\partial}{\partial y} := \begin{bmatrix} \frac{\partial}{\partial y_1} \\ \vdots \\ \frac{\partial}{\partial y_n} \end{bmatrix}, \quad y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$$

② 정의2 : 매트릭스로 미분.

$$\frac{\partial}{\partial X} := \begin{bmatrix} \frac{\partial}{\partial x_{11}} & \cdots & \frac{\partial}{\partial x_{1p}} \\ \vdots & & \vdots \\ \frac{\partial}{\partial x_{n1}} & \cdots & \frac{\partial}{x_{np}} \end{bmatrix}, \quad X = \begin{bmatrix} x_{11} & \cdots & x_{1p} \\ \vdots & & \vdots \\ x_{n1} & \cdots & x_{np} \end{bmatrix}$$

---

① $\frac{\partial}{\partial x}(x^T y) = y.$, $x = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$, $y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$

pf. $x^T y = [x_1 \cdots x_n] \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = x_1 y_1 + x_2 y_2 + \cdots + x_n y_n.$

- $\frac{\partial}{\partial x} = \begin{bmatrix} \frac{\partial}{\partial x_1} \\ \vdots \\ \frac{\partial}{\partial x_n} \end{bmatrix}$ 이므로.

$$\left(\frac{\partial}{\partial x}\right) x^T y = \begin{bmatrix} \frac{\partial}{\partial x_1} \\ \vdots \\ \frac{\partial}{\partial x_n} \end{bmatrix} (x_1 y_1 + x_2 y_2 + \cdots + x_n y_n)$$

$$= \begin{bmatrix} \frac{\partial}{\partial x_1}(x_1 y_1 + \cdots + x_n y_n) \\ \vdots \\ \frac{\partial}{\partial x_n}(x_1 y_1 + \cdots + x_n y_n) \end{bmatrix}$$

$$= \begin{bmatrix} \frac{\partial}{\partial x_1} x_1 y_1 + \frac{\partial}{\partial x_1} x_2 y_2 + \cdots + \frac{\partial}{\partial x_1} x_n y_n \\ \\ \frac{\partial}{\partial x_n} x_1 y_1 + \frac{\partial}{\partial x_n} x_2 y_2 + \cdots + \frac{\partial}{\partial x_n} x_n y_n \end{bmatrix}$$

$$= \begin{bmatrix} y_1 + 0 + \cdots + 0 \\ \vdots \\ 0 + 0 + \cdots + y_n \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = y.$$

$\frac{\partial}{\partial x}(x^T y) = y$ 임을 보이는 다른풀이

pf. $\frac{\partial}{\partial x}(x^T y) = \left(\frac{\partial}{\partial x} x^T\right) y = I y = y.$

$$\frac{\partial}{\partial x} x^T = \begin{bmatrix} \frac{\partial}{\partial x_1} \\ \vdots \\ \frac{\partial}{\partial x_n} \end{bmatrix} [x_1 \cdots x_n] = \begin{bmatrix} \frac{\partial}{\partial x_1} x_1 & \cdots & \frac{\partial}{\partial x_1} x_n \\ \vdots & & \\ \frac{\partial}{\partial x_n} x_1 & \cdots & \frac{\partial}{\partial x_n} x_n \end{bmatrix} = I$$

② $\frac{\partial}{\partial x}(y^T x) = y.$

pf. $\frac{\partial}{\partial x}(y^T x) = \frac{\partial}{\partial x}(x^T y) = y.$

③ $\frac{\partial}{\partial \beta}(y^T X \beta) = X^T y.$ 단, $\beta :=$ $p\times 1$ vector
$X :=$ $n \times p$ matrix
$y :=$ $n \times 1$ vector.

pf. $y^T X \beta$ 는 스칼라이므로.

$$y^T X \beta = (y^T X \beta)^T = \beta^T X^T y.$$

$$\frac{\partial}{\partial \beta}(y^T X \beta) = \frac{\partial}{\partial \beta}(\beta^T X^T y) = \left(\frac{\partial}{\partial \beta}\beta^T\right) X^T y = X^T y.$$

(다른풀이) $\frac{\partial}{\partial \beta}(y^T X \beta) = X^T y.$ 임을 보이는 다른풀이.

$$\cdot\ X\beta = \begin{bmatrix} x_{11} & \cdots & x_{1p} \\ \vdots & & \\ x_{n1} & \cdots & x_{np} \end{bmatrix} \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_p \end{bmatrix} = \begin{bmatrix} x_{11}\beta_1 + \cdots + x_{1p}\beta_p \\ x_{21}\beta_1 + \cdots + x_{2p}\beta_p \\ \vdots \\ x_{n1}\beta_1 + \cdots + x_{np}\beta_p \end{bmatrix}$$

$$\cdot\ y^T X \beta = [y_1 \cdots y_n] \begin{bmatrix} x_{11}\beta_1 + \cdots + x_{1p}\beta_p \\ x_{21}\beta_1 + \cdots + x_{2p}\beta_p \\ \vdots \\ x_{n1}\beta_1 + \cdots + x_{np}\beta_p \end{bmatrix}$$

$= y_1(x_{11}\beta_1 + \cdots + x_{1p}\beta_p) + y_2(x_{21}\beta_1 + \cdots + x_{2p}\beta_p) + \cdots$

$+ y_n(x_{n1}\beta_1 + \cdots + x_{np}\beta_p) = A_1 + A_2 + \cdots + A_n.$

* note : $A_1, A_2, \cdots, A_n$은 모두 스칼라.

· $\left(\frac{\partial}{\partial \beta}\right)(y^T X \beta) = \begin{bmatrix} \frac{\partial}{\partial \beta_1} \\ \vdots \\ \frac{\partial}{\partial \beta_p} \end{bmatrix} (A_1 + A_2 + \cdots + A_n)$

$$= \begin{bmatrix} \frac{\partial}{\partial \beta_1} A_1 \\ \vdots \\ \frac{\partial}{\partial \beta_p} A_1 \end{bmatrix} + \begin{bmatrix} \frac{\partial}{\partial \beta_1} A_2 \\ \vdots \\ \frac{\partial}{\partial \beta_p} A_2 \end{bmatrix} + \cdots + \begin{bmatrix} \frac{\partial}{\partial \beta_1} A_n \\ \vdots \\ \frac{\partial}{\partial \beta_p} A_n \end{bmatrix}$$

· $\frac{\partial}{\partial \beta_1} A_1 = \frac{\partial}{\partial \beta_1} y_1(x_{11}\beta_1 + \cdots + x_{1p}\beta_p) = y_1 x_{11} + 0 + \cdots + 0.$

· $\frac{\partial}{\partial \beta_2} A_1 = \frac{\partial}{\partial \beta_2} y_1(x_{11}\beta_1 + \cdots + x_{1p}\beta_p) = 0 + y_1 x_{12} + 0 + \cdots + 0$

$$= \begin{bmatrix} y_1 x_{11} \\ y_1 x_{12} \\ \vdots \\ y_1 x_{1p} \end{bmatrix} + \begin{bmatrix} y_2 x_{21} \\ y_2 x_{22} \\ \vdots \\ y_2 x_{2p} \end{bmatrix} + \cdots + \begin{bmatrix} y_n x_{n1} \\ y_n x_{n2} \\ \vdots \\ y_n x_{np} \end{bmatrix}$$

$$= \begin{bmatrix} y_1 x_{11} + y_2 x_{21} + \cdots + y_n x_{n1} \\ y_1 x_{12} + y_2 x_{22} + \cdots + y_n x_{n2} \\ \vdots \\ y_n x_{1p} + y_2 x_{2p} + \cdots + y_n x_{np} \end{bmatrix} = \begin{bmatrix} x_{11} & x_{21} & \cdots & x_{n1} \\ x_{12} & x_{22} & \cdots & x_{n2} \\ \vdots & \vdots & & \\ x_{1p} & x_{2p} & \cdots & x_{np} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

$$= X^T y.$$

④ $\frac{\partial}{\partial y} y^T y = 2y.$

pf. $y^T y = [y_1 \cdots y_n] \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = y_1^2 + \cdots + y_n^2.$

$$\therefore \frac{\partial}{\partial y}(y^T y) = \frac{\partial}{\partial y}(y_1^2 + \cdots + y_n^2) = \begin{bmatrix} \frac{\partial}{\partial y_1} \\ \vdots \\ \frac{\partial}{\partial y_n} \end{bmatrix} (y_1^2 + \cdots + y_n^2)$$

$$= \begin{bmatrix} \frac{\partial}{\partial y_1}(y_1^2 + \cdots + y_n^2) \\ \vdots \\ \frac{\partial}{\partial y_n}(y_1^2 + \cdots + y_n^2) \end{bmatrix}$$

$$= \begin{bmatrix} 2y_1 + 0 + \cdots + 0 \\ 0 + 2y_2 + \cdots + 0 \\ \vdots \\ 0 + 0 + \cdots + 2y_n \end{bmatrix} = 2 \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = 2y.$$

(틀린풀이) $\frac{\partial}{\partial y}(y^T y) = \left(\frac{\partial}{\partial y} y^T\right) y$

그런데 $\left(\frac{\partial}{\partial y} y^T\right) = I$. 이므로, $\frac{\partial}{\partial y}(y^T y) = Iy = y$.

(틀린풀이의 스칼라 버전) $\frac{d}{dy}y^2 = \left(\frac{d}{dy}y\right)\cdot y = 1\cdot y = y.$

(올바른 풀이) : $\frac{d}{dy}y^2 = \left(\frac{d}{dy}\right)\underbrace{y}_{f(y)}\cdot\underbrace{y}_{g(y)} = \left(\frac{d}{dy}\underbrace{y}_{f'(y)}\right)\cdot\underbrace{y}_{g(y)} + \underbrace{y}_{f(y)}\left(\frac{d}{dy}\underbrace{y}_{g'(y)}\right)$

Note: 곱의 미분 : 함수 $f(x), g(x)$ 가 x에 대하여 미분가능하면

$$\{f(x)\cdot g(x)\}' = f'(x)\,g(x) + f(x)\cdot g'(x)$$

다시 벡터로 돌아오자.

(올바른 풀이) $\left(\frac{\partial}{\partial y}\right)(y^T y) = A + B. = Iy + Iy = 2y.$

$A :=$ 빨간 y만 변수로 보고 미분

$B :=$ 파란 y 만 변수로보고 미분

$A = \left(\frac{\partial}{\partial y}y^T\right)y = Iy$

$B = \left(\frac{\partial}{\partial y}\right)(y^T y) = \left(\frac{\partial}{\partial y}\right)(y^T y) = \left(\frac{\partial}{\partial y}y^T\right)y = Iy$

⑤ $\frac{\partial}{\partial B}B^T X^T X B = 2X^T X B.$

pf. $\frac{\partial}{\partial B}(B^T X^T X B) = A + B = IX^T X B + IX^T X B = 2X^T X B.$

$$A = \left(\frac{\partial}{\partial B} B^T\right) X^T X B = I X^T X B.$$

$$B = \left(\frac{\partial}{\partial B}\right)\left(\underline{B^T X^T X B}\right) = \left(\frac{\partial}{\partial B}\right)\left(B^T X^T X B\right) = I X^T X B.$$

$$\text{loss} = (y - XB)^T (y - XB)$$

$$= y^T y - y^T X B - B^T X^T y + B^T X^T X B.$$

$$\frac{\partial}{\partial B}\text{loss} = 0 - \frac{\partial}{\partial B} y^T X B - \frac{\partial}{\partial B} B^T X^T y + \frac{\partial}{\partial B} B^T X^T X B$$

$$= 0 - X^T y - X^T y + 2X^T X B$$

$$\therefore \frac{\partial}{\partial B}\text{loss} = 0 \iff 2X^T y = 2X^T X B.$$

$$\therefore \hat{B} = (X^T X)^{-1} X^T y.$$