

CSCI 567 - LINEAR ALGEBRA DISCUSSION II

① DERIVATIVES, GRADIENTS AND JACOBIAN

$$f: \mathbb{R}^1 \rightarrow \mathbb{R}^1$$

eg. $f(x)$

$$\nabla f = \frac{df}{dx} = \frac{\partial f}{\partial x} = f_x$$

1×1 derivative

$$f: \mathbb{R}^2 \rightarrow \mathbb{R}^1$$

eg. $f(x, y)$

$$\nabla f = \left[\frac{\partial f}{\partial x} \quad \frac{\partial f}{\partial y} \right]_{1 \times 2}$$

gradient (row vector)

$$\vec{f}: \mathbb{R}^1 \rightarrow \mathbb{R}^2$$

eg. $\begin{bmatrix} a(x) \\ b(x) \end{bmatrix}$

$$\nabla f = \begin{bmatrix} \frac{\partial a}{\partial x} \\ \frac{\partial b}{\partial x} \end{bmatrix} = \begin{bmatrix} a_x \\ b_x \end{bmatrix}$$

2×1 Jacobian

$$\vec{f}: \mathbb{R}^2 \rightarrow \mathbb{R}^3$$

eg. $\begin{bmatrix} a(x, y) \\ b(x, y) \\ c(x, y) \end{bmatrix}$

$$\nabla f = \begin{bmatrix} \frac{\partial a}{\partial x} & \frac{\partial a}{\partial y} \\ \frac{\partial b}{\partial x} & \frac{\partial b}{\partial y} \\ \frac{\partial c}{\partial x} & \frac{\partial c}{\partial y} \end{bmatrix}$$

3×2 Jacobian

functions are always column vectors.

★ The usual derivative is a special case of gradients which itself is a special case of jacobians.

☆ We always represent gradients as row vectors.
This is the numerator layout.

Exercise: Find the dimension of the jacobian/gradient

i) $f: \mathbb{R} \rightarrow \mathbb{R}$ 1×1

ii) $f: \mathbb{R}^5 \rightarrow \mathbb{R}$ 1×5

iii) $\vec{f}: \mathbb{R} \rightarrow \mathbb{R}^3$ 3×1

iv) $\vec{f}: \mathbb{R}^7 \rightarrow \mathbb{R}^{10}$ 10×7

② CHAIN RULE

Ⓐ $f: \mathbb{R} \rightarrow \mathbb{R}$

$g: \mathbb{R} \rightarrow \mathbb{R}$

$h = f \circ g: \mathbb{R} \rightarrow \mathbb{R}$

$h(x) = f(g(x))$

} Single variable

$$\nabla h = \frac{dh}{dx} = \frac{df}{dg} \cdot \frac{dg}{dx} = f'(g) g'$$

$$\nabla h = \nabla_g f \cdot \nabla_x g$$

$$\textcircled{b} \quad f: \mathbb{R} \rightarrow \mathbb{R} \quad \longrightarrow \quad 1 \times 1$$

$$g: \mathbb{R}^2 \rightarrow \mathbb{R} \quad \xrightarrow{\text{e.g. } g(x,y)} \quad 1 \times 2$$

$$h: f \circ g: \mathbb{R}^2 \rightarrow \mathbb{R} \quad \longrightarrow$$

$$h(x,y) = f(g(x,y))$$

$$\underline{\underline{\nabla h}} = [h_x \quad h_y] = \begin{bmatrix} \frac{\partial h}{\partial x} & \frac{\partial h}{\partial y} \end{bmatrix}$$

$$\underline{\underline{\frac{\partial h}{\partial x}}} = \underline{\underline{\frac{\partial f}{\partial g} \cdot \frac{\partial g}{\partial x}}} \quad \text{and} \quad \underline{\underline{\frac{\partial h}{\partial y}}} = \underline{\underline{\frac{\partial f}{\partial g} \cdot \frac{\partial g}{\partial y}}}$$

$$\underline{\underline{\nabla h}} = \left[\left(\frac{\partial f}{\partial g} \right) \frac{\partial g}{\partial x} \quad \left(\frac{\partial f}{\partial g} \right) \frac{\partial g}{\partial y} \right] = \begin{bmatrix} \frac{\partial f}{\partial g} \end{bmatrix}_{1 \times 1} \begin{bmatrix} \frac{\partial g}{\partial x} & \frac{\partial g}{\partial y} \end{bmatrix}_{1 \times 2}$$

$$\rightarrow \nabla h = \nabla_g f \cdot \nabla_{(x,y)} g \quad h' = \underbrace{f'(g)}_{\nabla f} \underbrace{g'}_{\nabla g}$$

$$\textcircled{c} \quad \vec{f}: \mathbb{R} \rightarrow \mathbb{R}^2 \quad \text{e.g. } \vec{f}(x) = \begin{bmatrix} a(x) \\ b(x) \end{bmatrix}$$

$$g: \mathbb{R} \rightarrow \mathbb{R} \quad \text{e.g. } g(x)$$

$$h = f \circ g: \mathbb{R} \rightarrow \mathbb{R}^2 \quad \longrightarrow \quad \underline{\underline{\mathbb{Z} \times 1}}$$

$$h(x) = f(g(x)) = \begin{bmatrix} a(g(x)) \\ b(g(x)) \end{bmatrix}$$

$$\nabla h = \begin{bmatrix} \frac{\partial a}{\partial x} \\ \frac{\partial b}{\partial x} \end{bmatrix} = \begin{bmatrix} \frac{\partial a}{\partial g} & \frac{\partial g}{\partial x} \\ \frac{\partial b}{\partial g} & \frac{\partial g}{\partial x} \end{bmatrix}$$

2×1
 2×1

$$= \begin{bmatrix} \frac{\partial a}{\partial g} \\ \frac{\partial b}{\partial g} \end{bmatrix} \begin{bmatrix} \frac{\partial g}{\partial x} \end{bmatrix}$$

2×1
 1×1

$$\nabla h = \nabla_g f \cdot \nabla_x g$$

2×1
 2×1
 1×1

④ $f: \mathbb{R}^3 \rightarrow \mathbb{R} \rightarrow 1 \times 3$

$\vec{g}: \mathbb{R}^2 \rightarrow \mathbb{R}^3 \rightarrow 3 \times 2$

$h = f \circ g: \mathbb{R}^2 \rightarrow \mathbb{R} \rightarrow \underline{1 \times 2}$

$$f = f(p, q, r) \quad \vec{g} = g(x, y) = \begin{bmatrix} p(x, y) \\ q(x, y) \\ r(x, y) \end{bmatrix}$$

$$\frac{\partial h}{\partial x} = \frac{\partial f}{\partial p} \frac{\partial p}{\partial x} + \frac{\partial f}{\partial q} \frac{\partial q}{\partial x} + \frac{\partial f}{\partial r} \frac{\partial r}{\partial x}$$

$$\frac{\partial h}{\partial y} = \frac{\partial f}{\partial p} \frac{\partial p}{\partial y} + \frac{\partial f}{\partial q} \frac{\partial q}{\partial y} + \frac{\partial f}{\partial r} \frac{\partial r}{\partial y}$$

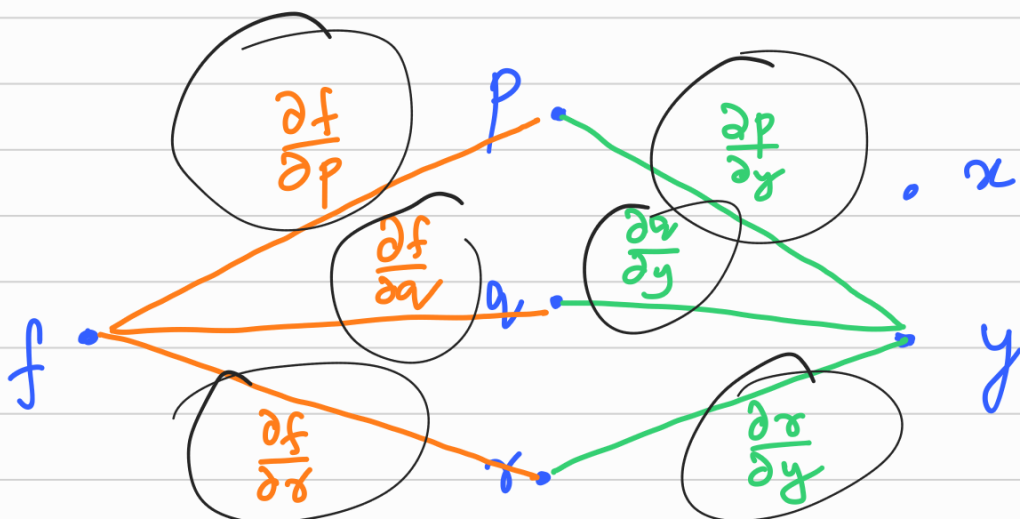
$$\nabla h = \left[\frac{\partial h}{\partial x} \quad \frac{\partial h}{\partial y} \right]_{1 \times 2}$$

$$\left[\frac{\partial f}{\partial p} \frac{\partial p}{\partial x} + \frac{\partial f}{\partial q} \frac{\partial q}{\partial x} + \frac{\partial f}{\partial r} \frac{\partial r}{\partial x} \quad \frac{\partial f}{\partial p} \frac{\partial p}{\partial y} + \frac{\partial f}{\partial q} \frac{\partial q}{\partial y} + \frac{\partial f}{\partial r} \frac{\partial r}{\partial y} \right]_{1 \times 2}$$

$$= \left[\frac{\partial f}{\partial p} \quad \frac{\partial f}{\partial q} \quad \frac{\partial f}{\partial r} \right]_{1 \times 3} \begin{bmatrix} \frac{\partial p}{\partial x} & \frac{\partial p}{\partial y} \\ \frac{\partial q}{\partial x} & \frac{\partial q}{\partial y} \\ \frac{\partial r}{\partial x} & \frac{\partial r}{\partial y} \end{bmatrix}_{3 \times 2}$$

$$\nabla h = \nabla f(p, q) \cdot \nabla \vec{g}(x, y)$$

1×3
 3×2



$$\frac{\partial h}{\partial y} = \frac{\partial f}{\partial p} \frac{\partial p}{\partial y} + \frac{\partial f}{\partial q} \frac{\partial q}{\partial y} + \frac{\partial f}{\partial r} \frac{\partial r}{\partial y}$$

(e) $\vec{f}: \mathbb{R}^2 \rightarrow \mathbb{R}^3, \rightarrow 3 \times 2$
 $\vec{g}: \mathbb{R}^3 \rightarrow \mathbb{R}^2 \rightarrow 2 \times 3$
 $\vec{h} = \vec{f} \circ \vec{g}: \mathbb{R}^3 \rightarrow \mathbb{R}^3 \rightarrow 3 \times 3$

e.g. $\vec{f} = f(p, q) = \begin{bmatrix} a(p, q) \\ b(p, q) \\ c(p, q) \end{bmatrix}$

$$\vec{g} = g(x, y, z) = \begin{bmatrix} p(x, y, z) \\ q(x, y, z) \end{bmatrix}$$

$$h = \begin{bmatrix} a(p(x, y, z), q(x, y, z)) \\ b(p(x, y, z), q(x, y, z)) \\ c(p(x, y, z), q(x, y, z)) \end{bmatrix}$$

$$\nabla h(x, y, z) = \begin{bmatrix} \frac{\partial a}{\partial x} & \frac{\partial a}{\partial y} & \frac{\partial a}{\partial z} \\ \frac{\partial b}{\partial x} & \frac{\partial b}{\partial y} & \frac{\partial b}{\partial z} \\ \frac{\partial c}{\partial x} & \frac{\partial c}{\partial y} & \frac{\partial c}{\partial z} \end{bmatrix}$$

3 x 3

$$= \begin{bmatrix} \frac{\partial a}{\partial p} \frac{\partial p}{\partial x} + \frac{\partial a}{\partial q} \frac{\partial q}{\partial x} & \frac{\partial a}{\partial p} \frac{\partial p}{\partial y} + \frac{\partial a}{\partial q} \frac{\partial q}{\partial y} & \frac{\partial a}{\partial p} \frac{\partial p}{\partial z} + \frac{\partial a}{\partial q} \frac{\partial q}{\partial z} \\ \frac{\partial b}{\partial p} \frac{\partial p}{\partial x} + \frac{\partial b}{\partial q} \frac{\partial q}{\partial x} & \frac{\partial b}{\partial p} \frac{\partial p}{\partial y} + \frac{\partial b}{\partial q} \frac{\partial q}{\partial y} & \frac{\partial b}{\partial p} \frac{\partial p}{\partial z} + \frac{\partial b}{\partial q} \frac{\partial q}{\partial z} \\ \frac{\partial c}{\partial p} \frac{\partial p}{\partial x} + \frac{\partial c}{\partial q} \frac{\partial q}{\partial x} & \frac{\partial c}{\partial p} \frac{\partial p}{\partial y} + \frac{\partial c}{\partial q} \frac{\partial q}{\partial y} & \frac{\partial c}{\partial p} \frac{\partial p}{\partial z} + \frac{\partial c}{\partial q} \frac{\partial q}{\partial z} \end{bmatrix}$$

3 x 3

$$= \begin{bmatrix} \frac{\partial a}{\partial p} & \frac{\partial a}{\partial q} \\ \frac{\partial b}{\partial p} & \frac{\partial b}{\partial q} \\ \frac{\partial c}{\partial p} & \frac{\partial c}{\partial q} \end{bmatrix} \begin{bmatrix} \frac{\partial p}{\partial x} & \frac{\partial p}{\partial y} & \frac{\partial p}{\partial z} \\ \frac{\partial q}{\partial x} & \frac{\partial q}{\partial y} & \frac{\partial q}{\partial z} \end{bmatrix}$$

3 x 2

2 x 3

$$\Rightarrow \nabla \vec{h}(x, y, z) = \nabla \vec{f}(p, q) \cdot \nabla \vec{g}(x, y, z)$$

3×3 3×2 2×3

5.5 Consider the following functions:

$$f_1(\mathbf{x}) = \sin(x_1) \cos(x_2), \quad \mathbf{x} \in \mathbb{R}^2 \leftarrow 1 \times 2$$

$$f_2(\mathbf{x}, \mathbf{y}) = \mathbf{x}^\top \mathbf{y}, \quad \mathbf{x}, \mathbf{y} \in \mathbb{R}^n \quad 1 \times 2n$$

$$\underline{f_3(\mathbf{x}) = \mathbf{x}\mathbf{x}^\top}, \quad \mathbf{x} \in \mathbb{R}^n \quad \underline{(n \times n) \times n}$$

Draft (2024-01-15) of "Mathematics for Machine Learning". Feedback: <https://mml-book.com>.

Exercises

171

- What are the dimensions of $\frac{\partial f_i}{\partial \mathbf{x}}$?
- Compute the Jacobians.

(a) $f_1: \mathbb{R}^2 \rightarrow \mathbb{R}^1, \nabla f_1 \in \mathbb{R}^{1 \times 2}$

$f_2: \mathbb{R}^{2n} \rightarrow \mathbb{R}^1, \nabla f_2 \in \mathbb{R}^{1 \times 2n}$

$f_3: \mathbb{R}^n \rightarrow \mathbb{R}^{n \times n}, \nabla f_3 \in \mathbb{R}^{(n \times n) \times n}$

3D matrix OR
3rd order tensor

$$(b) \quad f_1(x_1, x_2) = \sin(x_1) \cos(x_2)$$

$$\nabla f_1 = \left[\frac{\partial f_1}{\partial x_1} \quad \frac{\partial f_1}{\partial x_2} \right]$$

$$= \left[\cos(x_1) \cos(x_2) \quad -\sin(x_1) \sin(x_2) \right]$$

$$f_2 = \mathbf{x}^T \mathbf{y} \quad \text{Let } \mathbf{x}, \mathbf{y} \in \mathbb{R}^2$$

$$f_2(x_1, x_2, y_1, y_2) = [x_1, x_2] \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

$$= x_1 y_1 + x_2 y_2$$

$$\nabla f_2 = \left[\frac{\partial f_2}{\partial x_1} \quad \frac{\partial f_2}{\partial x_2} \quad \frac{\partial f_2}{\partial y_1} \quad \frac{\partial f_2}{\partial y_2} \right]$$

$$= \left[y_1 \quad y_2 \quad x_1 \quad x_2 \right]$$

$$\therefore \text{in general, } \nabla f_2 = \left[\vec{y} \quad ; \quad \vec{x} \right]$$

$$f_3 = x x^T, \text{ let } x \in \mathbb{R}^2$$

$$f_3 = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_{2 \times 1} \begin{bmatrix} x_1 & x_2 \end{bmatrix}_{1 \times 2} = \begin{bmatrix} & \\ & \end{bmatrix}_{2 \times 2}$$

$$= \begin{bmatrix} x_1^2 & x_1 x_2 \\ x_2 x_1 & x_2^2 \end{bmatrix}_{2 \times 2}$$

$$\nabla f_3 = \begin{bmatrix} \frac{\partial x_1^2}{\partial x_1} & \frac{\partial (x_1 x_2)}{\partial x_1} \\ \frac{\partial (x_2 x_1)}{\partial x_1} & \frac{\partial x_2^2}{\partial x_1} \end{bmatrix} \begin{bmatrix} \frac{\partial x_1^2}{\partial x_2} & \frac{\partial (x_1 x_2)}{\partial x_2} \\ \frac{\partial (x_2 x_1)}{\partial x_2} & \frac{\partial x_2^2}{\partial x_2} \end{bmatrix}$$

2x2x2

$$= \begin{bmatrix} 0 & x_1 \\ x_1 & 2x_2 \end{bmatrix} \begin{bmatrix} 2x_1 & x_2 \\ x_2 & 0 \end{bmatrix}$$

Can be generalized when $x \in \mathbb{R}^n$
(we will skip this)

RESULTS TO REMEMBER

① $f(\vec{x}) = \underline{a^T x}$ $\nabla f(x) = \underline{a^T}$ ←
 $f: \mathbb{R}^n \rightarrow \mathbb{R}$ gradient always a
row vector
 $x \in \mathbb{R}^n$
 $f(x) = [a_1 \ a_2] \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \underbrace{(a_1 x_1 + a_2 x_2)}_{[a_1 \ a_2] \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}}$

② $f(\vec{x}) = \underline{x^T a}$ $\nabla f(x) = \underline{a^T}$
 $f: \mathbb{R}^n \rightarrow \mathbb{R}$
 $x \in \mathbb{R}^n$

③ $\vec{f}(\vec{x}) = A x$ $\nabla f = A$
 $A \in \mathbb{R}^{m \times n}$ $f: \mathbb{R}^n \rightarrow \mathbb{R}^m$
 $x \in \mathbb{R}^n$

Ex: $A = \begin{bmatrix} a & b \\ c & d \\ e & f \end{bmatrix}_{3 \times 2}$ $x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_{2 \times 1}$

$$f(x) = A x = \begin{bmatrix} ax_1 + bx_2 \\ cx_1 + dx_2 \\ ex_1 + fx_2 \end{bmatrix} \quad 3 \times 1$$

$$\nabla f = \begin{bmatrix} \frac{\partial}{\partial x_1} (ax_1 + bx_2) & b \\ c & \frac{\partial}{\partial x_2} (cx_1 + dx_2) \\ e & f \end{bmatrix}$$

3x2

$$= A$$

COROLLARY $\bar{f}(\bar{x}) = \bar{x} = \mathbf{I} \bar{x}$

then $\nabla f = \mathbf{I}$

$$x = \mathbf{I} x$$

$$A = \mathbf{I}$$

$$A x \rightarrow A = \mathbf{I}$$

④ $\vec{f}(x) = x^T A$ is a row vector

But vector functions are always
column vectors by convention.

So we convert $\vec{f}(x)$ into a column vector
first.

$$\vec{f}(x) = (x^T A)^T = A^T x$$

$$\nabla f = \underline{A^T}$$

$$\underline{x^T a} \rightarrow a^T$$
$$\underline{x^T A x} = A^T$$

⑤ $f(x) = x^T A x \leftarrow$ Quadratic Form

Let $g(x) = Ax$, $\nabla g = A$

$$f(x) = x^T g$$

$$\nabla f = g^T + x^T \nabla g \quad (\text{product rule})$$

$$= (Ax)^T + x^T A \quad (fg)' = f'g + f \cdot g'$$

$$= x^T A^T + x^T A \quad \underline{f'g + g'f}$$

$$= \underline{x^T (A^T + A)} \leftarrow \text{row vector}$$

COROLLARY

$$\underline{\|x\|^2} = x^T x = x^T I x$$

$$\nabla \|x\|^2 = x^T (I + I^T) = \underline{2x^T}$$

Q3 $f(w) = \|Xw - y\|_2^2 + w^T M w, w \in \mathbb{R}^d$

Find $\underline{w^*} = \arg \min f(w)$

$$f \in \mathbb{R}^d \rightarrow \mathbb{R}^1$$

Solⁿ

$$\text{Set } \nabla f = 0$$

$$w \in \mathbb{R}^d$$

$$\nabla f = \underline{\nabla \|z\|^2} + \underline{\nabla (w^T M w)}$$

$$= 2z^T \nabla z + \underline{w^T (M + M^T)}$$

$$= \underline{2z^T X} + w^T (M + M^T)$$

$$= 2(Xw - y)^T X + w^T (M + M^T)$$

$$= \underline{2(w^T X^T X - y^T X) + w^T (M + M^T)}$$

$$\underline{\nabla f = 0} \Rightarrow w^T (2X^T X + M + M^T) = 2y^T X$$

$$\Rightarrow (2X^T X + M^T + M) w = 2X^T y$$

$$\Rightarrow \left(X^T X + \frac{M^T + M}{2} \right) w = X^T y$$

$$\Rightarrow w^* = \left(X^T X + \frac{M^T + M}{2} \right)^{-1} X^T y$$

$$\|z\|^2 \rightarrow 2z^T \nabla z$$

Solⁿ 2

$$f(w) = \underline{\|Xw - y\|_2^2} + w^T M w$$

$$\nabla f = \nabla \|Xw - y\|_2^2 + \nabla (w^T M w)$$

$$= \nabla \|Xw - y\|_2^2 + w^T (M + M^T)$$

$\|z\|_2^2 = z^T z$

$$\|Xw - y\|_2^2 = \underline{(Xw - y)^T (Xw - y)}$$

$$= (w^T X^T - y^T) (Xw - y)$$

$$= w^T X^T X w - w^T X^T y - y^T X w + y^T y$$

$$\Rightarrow \nabla \|Xw - y\|_2^2 = w^T (X^T X + X^T X) - y^T X - y^T X + 0$$

$$= 2w^T X^T X - 2y^T X$$

$$\therefore \nabla f = 2w^T X^T X - 2y^T X + w^T (M + M^T)$$

$$\Rightarrow \nabla f = 0 \Rightarrow 2w^T \left(X^T X + \frac{M + M^T}{2} \right) = 2y^T X$$

$$\Rightarrow \left(X^T X + \frac{M^T + M}{2} \right) w = X^T y$$

$$\Rightarrow w^* = \left(X^T X + \frac{M^T + M}{2} \right)^{-1} X^T y \checkmark$$

COROLLARY 1: LINEAR REGRESSION (ORDINARY LEAST SQUARES)

In linear regression, $\hat{y} = Xw$ and

$$\text{error} = \|\hat{y} - y\|_2^2 = \|Xw - y\|_2^2$$

Here $M = 0$

$M = 0$

then $f(w) = \|Xw - y\|_2^2 =$ error in linear regression

$$w^* = \left(X^T X + \frac{M + M^T}{2} \right)^{-1} X^T y$$

$$w^* = (X^T X)^{-1} X^T y$$

w^* = Solution of best parameters for the linear regression model $\hat{y} = Xw$.

Note: $X^T X w = X^T y$ is called the normal equation.

w^* is a solution of the normal equation.

There could be multiple solutions based on whether $X^T X$ is invertible or not.

$$X = \begin{pmatrix} \hat{A} \\ y \end{pmatrix}$$

$$Xw = y$$

COROLLARY 2: Regularization

$$\text{If } M = \lambda I$$

$$\text{Then } f(w) = \|Xw - y\|_2^2 + \underline{w^T(\lambda I)w}$$

$$= \|Xw - y\|_2^2 + \lambda w^T I w$$

$$= \|Xw - y\|_2^2 + \lambda \underline{w^T w}$$

$$= \|Xw - y\|_2^2 + \lambda \|w\|^2 \swarrow$$

Regularizer to control model complexity.

$$\text{Then } w^* = \left[X^T X + \frac{\lambda I + (\lambda I)^T}{2} \right]^{-1} X^T y$$

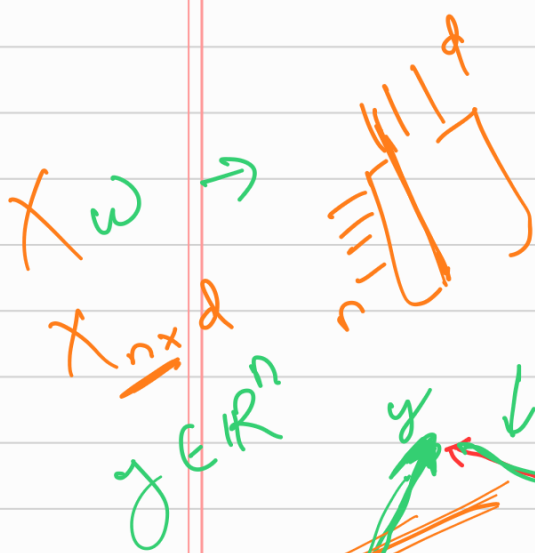
$$= \underline{\underline{(X^T X + \lambda I)^{-1} X^T y}}$$

GEOMETRIC INTERPRETATION OF OLS / LINEAR REGRESSION SOLUTION

$$\hat{y} = Xw$$

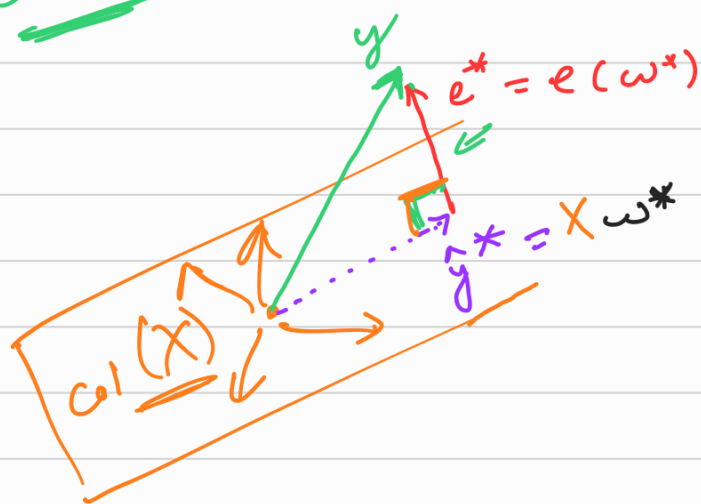
$$\vec{e} = y - \hat{y} = y - Xw$$

$$w^* = \operatorname{argmin} \|Xw - y\|_2^2 = \|r\|^2$$



$$X = \begin{bmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{bmatrix}$$

$$y = \begin{bmatrix} 10 \\ 11 \\ 12 \end{bmatrix}$$



Clearly, $\underline{e^*} \perp \underline{\operatorname{Colspace}(X)}$ $(X^T X)^{-1} X^T y$

$$\Rightarrow \underline{y - \hat{y}^*} \perp \underline{\text{each column of } X}$$

$$\Rightarrow \underline{X^T (y - \hat{y}^*)} = 0$$

$$\Rightarrow X^T (y - Xw^*) = 0$$

$$\Rightarrow X^T y - X^T X w^* = 0$$

$$\Rightarrow X^T X w^* = X^T y \quad (\text{normal eq}^n)$$

$$\Rightarrow w^* = (X^T X)^{-1} X^T y$$