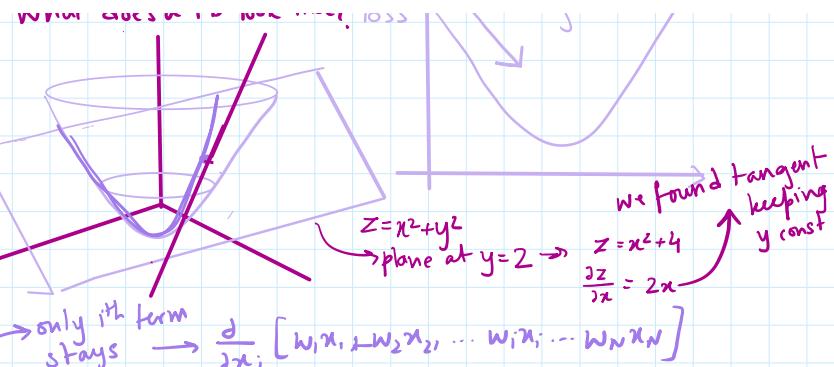


o/p: scalar - jump/run

$$y = w_1x_1 + w_2x_2 + \dots + w_Nx_N \\ = \sum_{i=1}^N w_i x_i$$

$$\Rightarrow \nabla y = \left[\frac{\partial y}{\partial x_1}, \frac{\partial y}{\partial x_2}, \dots, \frac{\partial y}{\partial x_N} \right] \\ = [w_1, w_2, \dots, w_N] \\ = \frac{\partial}{\partial x_i} \left(\sum_{i=1}^N w_i x_i \right) = (w_i)$$



Matrix I/P, Scalar O/P

vector calculus
matrix calculus
Here, we're moving from derivative of one fn ($f(\bar{x})$) to derivative of many functions ($f(W)$)

function of a matrix instead of a vector

$$f(W), W = \begin{bmatrix} w_{11} & w_{12} & w_{13} \\ w_{21} & w_{22} & w_{23} \\ w_{31} & w_{32} & w_{33} \end{bmatrix}$$

Demonstration: $g(x,y) = 2x + y^2$

$$f(x,y) = 3x^2y$$

$$\frac{\partial g}{\partial x} = \frac{\partial}{\partial x} (2x + y^2) = 2$$

$$\frac{\partial g}{\partial y} = \frac{\partial}{\partial y} (2x + y^2) = 8y^2$$

$$\nabla g(x,y) = \begin{bmatrix} \frac{\partial g}{\partial x}, \frac{\partial g}{\partial y} \end{bmatrix} \\ = [2, 8y^2]$$

$$\frac{\partial f}{\partial x} = \frac{\partial}{\partial x} (3x^2y) = 6xy$$

$$\frac{\partial f}{\partial y} = \frac{\partial}{\partial y} (3x^2y) = 3x^2$$

$$\nabla f(x,y) = \begin{bmatrix} \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y} \end{bmatrix} \\ = [6xy, 3x^2]$$

$$\Rightarrow \frac{\partial f}{\partial W} = \begin{bmatrix} \frac{\partial f}{\partial w_{11}}, \frac{\partial f}{\partial w_{12}}, \frac{\partial f}{\partial w_{13}} \\ \vdots \\ \frac{\partial f}{\partial w_{31}}, \frac{\partial f}{\partial w_{32}}, \frac{\partial f}{\partial w_{33}} \end{bmatrix}$$

Before: single f^n , vector I/P

Now: multiple functions, matrix I/P

organize their gradients.

$$J = \begin{bmatrix} \frac{\partial f_1}{\partial x_1}, \frac{\partial f_1}{\partial x_2}, \dots, \frac{\partial f_1}{\partial x_n} \\ \vdots \\ \frac{\partial f_m}{\partial x_1}, \frac{\partial f_m}{\partial x_2}, \dots, \frac{\partial f_m}{\partial x_n} \end{bmatrix} \Rightarrow J = \begin{bmatrix} \nabla f_1(x, y) \\ \vdots \\ \nabla f_m(x, y) \end{bmatrix} = \begin{bmatrix} 6xy & 3x^2 \\ 2 & 8y^2 \end{bmatrix}$$

So far:

- ① gradient of f^n w/ scalar o/p = gradient- vector
- ② gradient of f^n w/ vector o/p = Jacobian

Our input was a set of vectors + our o/p (Jacobian) was also a set of vectors.

HESSIAN

Matrix of 2nd Order Derivatives

$$\bar{y} = f(\bar{x}), |\bar{x}| = n$$

each f_i, f^n here can return a scalar

Special case of an IDENTITY fn:

$$\bar{y} = f(\bar{x})$$

$$\rightarrow |\bar{x}| = n$$

$$\rightarrow |\bar{y}| = m$$

$$\frac{\partial \bar{y}}{\partial \bar{x}} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \dots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \dots & \frac{\partial f_m}{\partial x_n} \end{bmatrix} = \begin{bmatrix} \frac{\partial^2 f_1}{\partial x_1^2} & \dots & \frac{\partial^2 f_1}{\partial x_1 \partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f_m}{\partial x_1^2} & \dots & \frac{\partial^2 f_m}{\partial x_1 \partial x_n} \end{bmatrix}$$

$$(Y_1) = f_1(\bar{x})$$

$$\text{NOT VECTOR } (Y_2) = f_2(\bar{x})$$

$$\vdots$$

$$(Y_m) = f_m(\bar{x})$$

- ① $f_i(\bar{x})$ or y_i is scalar!!
- ② Diff' each scalar wrt vector

$$\text{Ex 1: } f(x,y) = xy$$

$$\frac{\partial f}{\partial x} = y \quad \frac{\partial f}{\partial y} = x \quad [\nabla f = (y, x)]$$

$$\frac{\partial^2 f}{\partial x^2} = 0 \quad \frac{\partial^2 f}{\partial y^2} = 0$$

$$\frac{\partial^2 f}{\partial x \partial y} = 1 \quad \frac{\partial^2 f}{\partial y \partial x} = 1$$

$$H = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix}$$

$$\frac{\partial \bar{y}}{\partial \bar{x}} = \begin{bmatrix} \nabla f_1(\bar{x}) \\ \nabla f_2(\bar{x}) \\ \vdots \\ \nabla f_m(\bar{x}) \end{bmatrix} = \begin{bmatrix} \frac{\partial}{\partial \bar{x}} f_1(\bar{x}) \\ \frac{\partial}{\partial \bar{x}} f_2(\bar{x}) \\ \vdots \\ \frac{\partial}{\partial \bar{x}} f_m(\bar{x}) \end{bmatrix}$$

① $f_i(\bar{x})$ or y_i is scalar!!
② Diff' each scalar wrt vector
= vector

sounds like a ... GRADIENT!!!

Back to solving:

$$\frac{\partial \bar{y}}{\partial \bar{x}} = \begin{bmatrix} \frac{\partial f_1(\bar{x})}{\partial x_1} & \frac{\partial f_1(\bar{x})}{\partial x_2} & \dots & \frac{\partial f_1(\bar{x})}{\partial x_n} \\ \vdots & & & \\ \frac{\partial f_m(\bar{x})}{\partial x_1} & \frac{\partial f_m(\bar{x})}{\partial x_2} & \dots & \frac{\partial f_m(\bar{x})}{\partial x_n} \end{bmatrix}$$

J { vector in
vector out }

$$= \begin{bmatrix} \frac{\partial x_1}{\partial x_1} & 0 & \dots & 0 \\ \vdots & & & \frac{\partial x_n}{\partial x_n} \\ 0 & \dots & & \\ 0 & 0 & \dots & 0 \\ \vdots & & & \\ 0 & 0 & \dots & 0 \end{bmatrix} \rightarrow \frac{\partial x_i}{\partial x_j} = 0, \text{ when } i \neq j$$

$$= \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & \dots & 0 \\ \vdots & & & & \\ 0 & 0 & 0 & \dots & 1 \end{bmatrix} = I \text{ (identity matrix)}$$

$$H = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}_{n \times n}$$

- ① Grad: vector of n dimensions
② H: $n \times n$ matrix

$$|x| = n$$

Single Variable Chain Rule

*forward diff"

$$x \rightarrow y \\ \frac{dy}{dx} = \frac{du}{dx} \cdot \frac{dy}{du}$$

*backward diff"

$$y \rightarrow x \\ \frac{dy}{dx} = \frac{dy}{du} \cdot \frac{du}{dx}$$

There's only a single dataflow path from x to y

+ none of intermediate functions have more than one param.

How to :

- ① Introduce intermediate variables.
- ② Compute derivative wrt parameters.
- ③ Combine all derivatives of interm. variables.
- ④ Substitute intermediate values.

$$\text{Ex. 1: } f(x) = \ln(\sin(x^3)^2)$$

$$\textcircled{1} \quad u = x^3$$

$$v = \sin u$$

$$w = v^2$$

$$y = \ln w$$

$$\textcircled{2} \quad \frac{dy}{dx} = \frac{dy}{du} \cdot \frac{du}{dw} \cdot \frac{dw}{dv} \cdot \frac{dv}{du} \cdot \frac{du}{dx} \\ = \frac{1}{w} \cdot 2v \cdot \cos u \cdot 3x^2$$

$$\textcircled{3} \quad \frac{dy}{dx} = \frac{1}{v^2} \cdot 2v \cdot \cos u^3 \cdot 3x^2 \\ = \frac{2}{\sin x^3} \cdot \cos x^3 \cdot 3x^2 \\ = \underline{\underline{6x^2 \cdot \cos x^3}}$$

$$\textcircled{4}$$

$$\text{Ex. 1: } y = f(g(u)) = \sin(u^2)$$

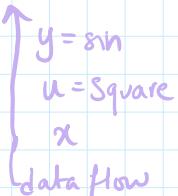
$$\textcircled{1} \quad u = x^2$$

$$\rightarrow y = \sin u$$

$$\textcircled{2} \quad \frac{du}{dx} = 2x \quad \frac{dy}{du} = \cos u$$

$$\textcircled{3} \quad \frac{dy}{dx} = \frac{dy}{du} \cdot \frac{du}{dx} = 2x \cos u.$$

$$\textcircled{4} \quad \frac{dy}{dx} = 2x \cos u^2$$



$$y = \sin$$

$$u = \text{Square}$$

$$x$$

data flow

Single variable total Derivative Chain Rule.

Case study: $y = f(u) = u + u^2$
after fixing u

$$\frac{dy}{du} = 1 + 2u \quad (\text{using the usual rules})$$

But let's try it w/
single variable chain rule.

$$u_1(x) = x^2$$

$$y = u_2(x) = u + u^2,$$

$$\frac{du_2}{du_1} = 0 + 1 = 1$$

$$\frac{du_1}{dx} = 2x$$

Now solve old case: $y = u + u^2$

→ direct + indirect.

$x \rightarrow \oplus$
Multiple paths
for single
But why?

Law of total derivative → "To compute $\frac{dy}{dx}$, we need to sum up all the contributions from x to y ."

But why?
for single var. ch. rule, we only had a single path of data flow.

$\frac{dy}{dx} = \frac{du_1}{dx} \cdot \frac{du_2}{du_1} \cdots \frac{du_n}{du_{n-1}} \cdot \frac{dy}{du_n}$
 $= (1)(2x) = 2x \times$
can we try w/ PD?

$$\begin{aligned}\frac{dy}{dx} &= \frac{\partial f(x)}{\partial x} = \frac{\partial u_2(x, u_1)}{\partial x} \\ &= \frac{\partial u_2}{\partial x} \cdot \frac{\partial x}{\partial x} + \frac{\partial u_2}{\partial u_1} \cdot \frac{\partial u_1}{\partial x}\end{aligned}$$

Ex: $f(x) = \sin(x+u^2)$

① Intermediate variables.

Notice how we're
treating:
 $u_1(x) = x^2$
 $u_2(x, u_1) = x + u_1$
 $u_3(u_2) = \sin(u_2)$
like a Russian doll but w/ fn's.

② Taking partials:

$$\frac{\partial}{\partial x} u_1(x) = 2x$$

$$\begin{aligned}\frac{\partial}{\partial x} u_2(x, u_1) &= \frac{\partial u_2}{\partial x} + \frac{\partial u_2}{\partial u_1} \cdot \frac{\partial u_1}{\partial x} \\ &= 1 + (1 \cdot 2x) \\ &= 1 + 2x\end{aligned}$$

$$\begin{aligned}\frac{\partial}{\partial x} u_3(u_2) &= \frac{\partial u_3}{\partial u_2} + \frac{\partial u_3}{\partial u_2} \cdot \frac{\partial u_2}{\partial x} \\ &\text{first diff w/ whoever came first outside} \\ &= 0 + \cos(u_2) \cdot (1 + 2x)\end{aligned}$$

③ Put it all together:

$$\begin{aligned}\frac{\partial f}{\partial x} &= \cos(u_2) \cdot (1 + 2x) \\ &= (1 + 2x) \cos(x + u_1) \\ &= (1 + 2x) \cos(x + x^2)\end{aligned}$$

Vector Chain Rule.

Deals w/ vectors of variables + functions!

$\bar{y} = f(x)$ → \bar{y} is a vector
function is a vector.

$$\begin{bmatrix} y_1(x) \\ y_2(x) \end{bmatrix} = \begin{bmatrix} h(x) \\ f_2(x) \end{bmatrix} \rightarrow \text{here, vectors are like accordions}$$

" u_2 is a fn of $x + u_1$.
 u_1 is a fn of x ."



To remember: Total derivative ALWAYS sums

Eg: $y = x \cdot x^2$
① $u_1(x) = x^2$
 $u_2(x, u_1) = x \cdot u_1$

② $\frac{\partial u_1}{\partial x} = 2x$
 $\frac{\partial u_2}{\partial x, u_1} = \frac{\partial u_2}{\partial x} + \frac{\partial u_2}{\partial u_1} \cdot \frac{\partial u_1}{\partial x}$
 $= u_1 + x \cdot 2x$
 $= u_1 + 2x^2$

③ $\frac{\partial y}{\partial x} = u_1 + 2x^2$
 $= x^2 + 2x^2$
 $= 3x^2 \checkmark$

Eg: $\frac{\partial u_3}{\partial x} = \frac{\partial u_3}{\partial u_2} \cdot \frac{\partial u_2}{\partial x}$

w/ extra steps to include u_2

- simplify chain rule
- AUTOMATIC DIFFN IN NN (well, numerics it)

$$\begin{bmatrix} y_1(x) \\ y_2(x) \end{bmatrix} = \begin{bmatrix} f_1(x) \\ f_2(x) \end{bmatrix}$$

Assumption: If \mathbf{P} is a vector of functions of a single variable.



Let $\bar{y} = \bar{f}(x)$

$$\begin{bmatrix} y_1(x) \\ y_2(x) \end{bmatrix} = \begin{bmatrix} f_1(x) \\ f_2(x) \end{bmatrix} = \begin{bmatrix} \ln(x^2) \\ \sin(3x) \end{bmatrix}$$

All single variable.

vector of functions
w.r.t column vector

$$② \frac{\partial \bar{y}}{\partial x} = \begin{bmatrix} \frac{\partial f_1(\bar{g})}{\partial x} \\ \frac{\partial f_2(\bar{g})}{\partial x} \end{bmatrix}$$

* Components of vector \bar{y} are computed using single var total deriv chain rule.

$$\frac{\partial \bar{y}}{\partial x} = \begin{bmatrix} \frac{\partial}{\partial x} f_1(g_1, g_2) \\ \frac{\partial}{\partial x} f_2(g_1, g_2) \end{bmatrix}$$

* Derivative of vector \bar{y} w.r.t scalar x

↓ COLUMN VECTOR

$$\frac{\partial \bar{y}}{\partial x} = \begin{bmatrix} \frac{\partial y}{\partial x} \\ \frac{\partial y_2}{\partial x} \\ \vdots \\ \frac{\partial y_n}{\partial x} \end{bmatrix}$$

① We introduce two intermediate variables, $g_1 + g_2 \rightarrow \bar{g} = [g_1, g_2]$
How?

$$\bar{y} = \bar{f}(x) = \bar{f}(\bar{g}(x))$$

$$\Rightarrow \begin{bmatrix} g_1(x) \\ g_2(x) \end{bmatrix} = \begin{bmatrix} x^2 \\ 3x \end{bmatrix}$$

$$\Rightarrow \begin{bmatrix} f_1(g) \\ f_2(g) \end{bmatrix} = \begin{bmatrix} \ln(g_1) \\ \sin(g_2) \end{bmatrix}$$

$$\frac{\partial \bar{y}}{\partial x} = \begin{bmatrix} \frac{\partial f_1}{\partial g_1} \cdot \frac{\partial g_1}{\partial x} + \frac{\partial f_1}{\partial g_2} \cdot \frac{\partial g_2}{\partial x} \\ \frac{\partial f_2}{\partial g_1} \cdot \frac{\partial g_1}{\partial x} + \frac{\partial f_2}{\partial g_2} \cdot \frac{\partial g_2}{\partial x} \end{bmatrix} = \begin{bmatrix} \frac{1}{g_1} \cdot 2x + 0 \\ 0 + \cos(g_2) \cdot 3 \end{bmatrix} = \begin{bmatrix} 2x/x^2 \\ 3\cos(3x) \end{bmatrix} = \begin{bmatrix} 2/x \\ 3\cos(3x) \end{bmatrix}$$

BUT WE'VE DONE!

To note: Vector Rule

$$\frac{\partial}{\partial x} \bar{f}(g(x))$$

↓
vector
 $= \frac{\partial \bar{f}}{\partial \bar{g}} \cdot \frac{\partial \bar{g}}{\partial x}$

We can write this as a matrix-vector oper'n !!

$$\frac{\partial \bar{y}}{\partial x} = \frac{\partial \bar{f}(\bar{g}(x))}{\partial x} = \begin{bmatrix} \frac{\partial f_1(\bar{g})}{\partial x} \\ \frac{\partial f_2(\bar{g})}{\partial x} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial g_1} & \frac{\partial f_1}{\partial g_2} \\ \frac{\partial f_2}{\partial g_1} & \frac{\partial f_2}{\partial g_2} \end{bmatrix} \begin{bmatrix} \frac{\partial g_1}{\partial x} \\ \frac{\partial g_2}{\partial x} \end{bmatrix} = \frac{\partial \bar{f}}{\partial \bar{g}} \cdot \frac{\partial \bar{g}}{\partial x}$$

and then multiply \bar{f} w.r.t \bar{g}

Generalization Time!

Assumptions: $\bar{x}, \bar{g}, \bar{f}$ are vectors.

$$|\bar{x}| = n \quad |\bar{g}| = k \quad |\bar{f}| = m$$

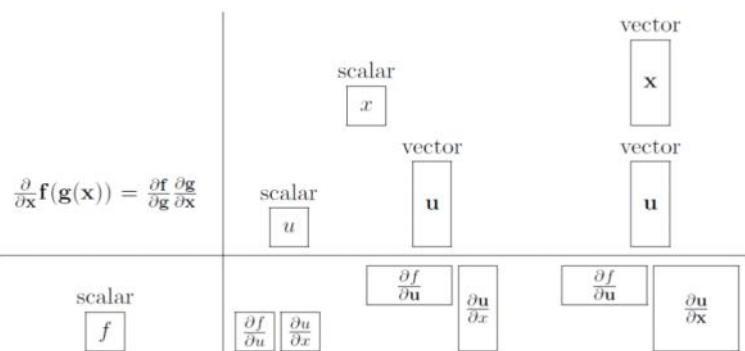
Jacobian = $m \times n$ matrix

for $\frac{\partial}{\partial \bar{x}} \bar{f}(\bar{g}(\bar{x}))$

$$\frac{\partial}{\partial \bar{x}} \bar{f}(\bar{g}(\bar{x})) = \begin{bmatrix} \frac{\partial f_1}{\partial g_1} \cdot \frac{\partial g_1}{\partial x_1} & \dots & \frac{\partial f_1}{\partial g_k} \cdot \frac{\partial g_k}{\partial x_1} \\ \vdots & & \vdots \\ \frac{\partial f_m}{\partial g_1} \cdot \frac{\partial g_1}{\partial x_1} & \dots & \frac{\partial f_m}{\partial g_k} \cdot \frac{\partial g_k}{\partial x_1} \end{bmatrix} \begin{bmatrix} \frac{\partial g_1}{\partial x_1} \cdot \frac{\partial g_1}{\partial x_2} \dots \frac{\partial g_1}{\partial x_n} \\ \vdots \\ \frac{\partial g_k}{\partial x_1} \cdot \frac{\partial g_k}{\partial x_2} \dots \frac{\partial g_k}{\partial x_n} \end{bmatrix}$$

$$\begin{aligned} \bar{f} &= \bar{f}(\bar{g}) \\ \bar{g} &: \mathbb{R}^m \rightarrow \mathbb{R}^k \\ \bar{f} &= \bar{f}(\bar{x}) \text{ thru' } \bar{g} \\ \bar{F} &: \mathbb{R}^k \rightarrow \mathbb{R}^n \end{aligned}$$

vector in → Jacobian → vector out



$$\frac{\partial \mathbf{f}}{\partial \mathbf{x}} \mathbf{f}(\mathbf{g}(\mathbf{x})) = \frac{\partial \mathbf{f}}{\partial \mathbf{g}} \frac{\partial \mathbf{g}}{\partial \mathbf{x}}$$

scalar

f

vector

\mathbf{f}

scalar

x

vector

\mathbf{u}

vector

\mathbf{x}

vector

\mathbf{u}

scalar

u

vector

\mathbf{u}

$\frac{\partial f}{\partial u}$

$\frac{\partial u}{\partial x}$

$\frac{\partial u}{\partial x}$

$\frac{\partial f}{\partial \mathbf{u}}$

$\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$

$\frac{\partial f}{\partial \mathbf{u}}$

$\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$

$- \mathbf{u} \cdot$

$- \mathbf{j} \times$

$- \mathbf{j} \mathbf{k} \cdot$

$- \mathbf{o} \mathbf{n}_1$

$- \mathbf{o} \mathbf{n}_2$

$- \mathbf{o} \mathbf{n}_3$