

recall: for $f(x_1(t), \dots, x_n(t))$ the chain rule reads

Session 8
Feb. 26, 2020

$$\frac{df}{dt} = \sum_{i=1}^n \frac{\partial f}{\partial x_i} \frac{dx_i}{dt} = (\vec{\nabla} f) \cdot \frac{d\vec{x}}{dt}$$

Ex.: classical mechanics: $H(\vec{q}, \vec{p}) = \frac{\vec{p}^2}{2} + V(\vec{q})$ (mass $m=1$)
↳ kinetic energy ↖ potential energy

\vec{q} = particle position, $\vec{p} = \frac{d\vec{q}}{dt}$ momentum/velocity

Newton's law reads $\frac{d\vec{p}}{dt} = -\vec{\nabla} V(\vec{q})$ (force = mass · acceleration)

chain rule ↓

$$\frac{dH}{dt} = (\vec{\nabla}_{\vec{q}} H) \cdot \frac{d\vec{q}}{dt} + (\vec{\nabla}_{\vec{p}} H) \cdot \frac{d\vec{p}}{dt}$$

$$= (\vec{\nabla}_{\vec{q}} H) \cdot \vec{p} + (\vec{\nabla}_{\vec{p}} H) \cdot (-\vec{\nabla}_{\vec{q}} V(\vec{q}))$$

$$= (\vec{\nabla}_{\vec{q}} H) \cdot (\vec{\nabla}_{\vec{p}} H) + (\vec{\nabla}_{\vec{p}} H) \cdot (-\vec{\nabla}_{\vec{q}} H)$$

$= 0$, which is energy conservation!

Remark: If $x_i(t_1, \dots, t_m)$, then we have $\frac{\partial f}{\partial t_k} = \sum_{i=1}^n \frac{\partial f}{\partial x_i} \frac{\partial x_i}{\partial t_k}$

next: a few more topics/applications of many-variable derivatives

A) More on differentials

force \vec{F} , potential V are related by $\vec{F} = -\vec{\nabla}V$

- given V , we can directly compute \vec{F}
- but given \vec{F} , can we find a V ?

In other words: given a differential $dV = \frac{\partial V}{\partial x_1} dx_1 + \dots + \frac{\partial V}{\partial x_n} dx_n$, can we find V ?

If yes, we call dV an **exact differential**, if no dV is called **inexact**.

Ex.: • $df = \underbrace{y}_{\frac{\partial f}{\partial x}} dx + \underbrace{x}_{\frac{\partial f}{\partial y}} dy \Rightarrow f(x,y) = xy + c$ ($c \in \mathbb{R}$ some constant)

\Rightarrow exact differential

• $df = \underbrace{3y}_{\frac{\partial f}{\partial x}} dx + \underbrace{x}_{\frac{\partial f}{\partial y}} dy$

\hookrightarrow need $f(x,y) = 3xy + g(y)$ for some fct. g

$\Rightarrow \frac{\partial f}{\partial y} = \underbrace{3x}_{\text{factor 3 too much}} + \underbrace{\frac{dg(y)}{dy}}_{\text{fct. of } y}$

\Rightarrow inexact differential

General answer: consider $df = \underbrace{A(x,y)}_{\frac{\partial f}{\partial x}} dx + \underbrace{B(x,y)}_{\frac{\partial f}{\partial y}} dy$

$$\Rightarrow \frac{\partial}{\partial y} \frac{\partial f}{\partial x} = \frac{\partial A}{\partial y} \quad \text{and} \quad \frac{\partial}{\partial x} \frac{\partial f}{\partial y} = \frac{\partial B}{\partial x}$$

but these are equal! (due to Clairaut/Schwarz (see Session 5))

$$\Rightarrow \text{need } \frac{\partial A}{\partial y} = \frac{\partial B}{\partial x} \quad \text{as a necessary condition}$$

It turns out (here without proof) that this is also sufficient!

Generally: $df = \sum_{i=1}^n g_i(x_1, \dots, x_n) dx_i$ is exact

$$\Leftrightarrow \frac{\partial g_i}{\partial x_k} = \frac{\partial g_k}{\partial x_i} \quad \forall i, k = 1, \dots, n$$

B) Taylor series

consider the function $g(t) = f(\underbrace{\vec{a} + t\vec{h}}_{\text{many variables}})$
one variable

What is the Taylor expansion of g around 0 at $t=1$?

(this will lead us to an expansion of $f(\vec{a} + \vec{h})$)

$$\begin{aligned}
 \Rightarrow g'(t) &= (\vec{\nabla} f)(\vec{a} + t\vec{h}) \cdot \underbrace{\frac{d(\vec{a} + t\vec{h})}{dt}}_{=\vec{h}} = \underbrace{\vec{h} \cdot (\vec{\nabla} f)(\vec{a} + t\vec{h})}_{=h_1 \partial_{x_1} f + \dots + h_n \partial_{x_n} f} \\
 &\quad \uparrow \\
 &\quad \text{chain rule} \\
 &= (h_1 \partial_{x_1} + \dots + h_n \partial_{x_n}) f \\
 &= (\vec{h} \cdot \vec{\nabla}) f(\vec{a} + t\vec{h})
 \end{aligned}$$

$$\Rightarrow g''(t) = (\vec{h} \cdot \vec{\nabla}) (\vec{h} \cdot \vec{\nabla}) f(\vec{a} + t\vec{h})$$

$$\Rightarrow g^{(k)}(t) = (\vec{h} \cdot \vec{\nabla})^k f(\vec{a} + t\vec{h})$$

$$\begin{aligned}
 \Rightarrow \text{Taylor expansion } g(t) &= \sum_{k=0}^{\infty} \frac{t^k}{k!} \underbrace{g^{(k)}(0)}_{=(\vec{h} \cdot \vec{\nabla})^k f(\vec{a})} + \mathcal{R}_n(t) \\
 &= (\vec{h} \cdot \vec{\nabla})^k f(\vec{a})
 \end{aligned}$$

$$\begin{aligned}
 \Rightarrow g(1) &= \sum_{k=0}^{\infty} \frac{(\vec{h} \cdot \vec{\nabla})^k f(\vec{a})}{k!} + \mathcal{R}_n(1) \\
 &\quad \parallel \\
 &\quad f(\vec{a} + \vec{h})
 \end{aligned}$$

$$\Rightarrow f(\vec{a} + \vec{h}) = \sum_{k=0}^{\infty} \frac{(\vec{h} \cdot \vec{\nabla})^k f(\vec{a})}{k!} \text{ is the infinite Taylor series of } f \text{ around } \vec{a}$$

Note: there are expressions for the rest term, but they are a bit lengthy, so let's not write them down here.

Ex.: Second-order expansion of $f(x_1, x_2)$ around $\vec{a} = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$; cell $\vec{h} = \begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix}$

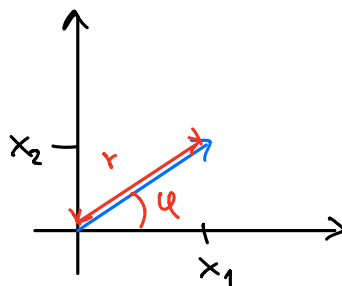
$$\begin{aligned} \Rightarrow f\left(\vec{a} + \begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix}\right) &= f(\vec{a}) + \underbrace{\left(\vec{h} \cdot \vec{\nabla}\right)}_{\begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix} \begin{pmatrix} \partial_x \\ \partial_y \end{pmatrix}} f(\vec{a}) + \frac{1}{2} \underbrace{\left(\vec{h} \cdot \vec{\nabla}\right) \left(\vec{h} \cdot \vec{\nabla}\right)}_{\left(\Delta x \partial_x + \Delta y \partial_y\right) \left(\Delta x \partial_x + \Delta y \partial_y\right)} f(\vec{a}) + \text{Rest} \\ &= \begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix} \begin{pmatrix} \partial_x \\ \partial_y \end{pmatrix} f \\ &= \Delta x \frac{\partial f}{\partial x}(\vec{a}) + \Delta y \frac{\partial f}{\partial y}(\vec{a}) \end{aligned}$$

$$\begin{aligned} \Rightarrow f\left(\vec{a} + \begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix}\right) &= f(\vec{a}) + \Delta x \frac{\partial f(\vec{a})}{\partial x} + \Delta y \frac{\partial f(\vec{a})}{\partial y} \\ &+ \frac{1}{2} \Delta x^2 \frac{\partial^2 f(\vec{a})}{\partial x^2} + \frac{1}{2} \Delta y^2 \frac{\partial^2 f(\vec{a})}{\partial y^2} + \Delta x \Delta y \frac{\partial^2 f(\vec{a})}{\partial x \partial y} + \text{Rest} \end{aligned}$$

c) Change of variables

sometimes we would like to express functions $f(x_1, x_2)$ in terms of different variables

Ex.: polar coordinates



instead of writing $f(x_1, x_2)$, we would like write $f(r, \varphi)$ with

$$x_1 = r \cos \varphi, \quad x_2 = r \sin \varphi \quad (r \geq 0, \varphi \in [0, 2\pi))$$

\Rightarrow chain rule tells us that $\frac{\partial f}{\partial r} = \frac{\partial f}{\partial x_1} \frac{\partial x_1}{\partial r} + \frac{\partial f}{\partial x_2} \frac{\partial x_2}{\partial r}$

e.g. for $f(x_1, x_2) = \sqrt{x_1^2 + x_2^2}$

$\Rightarrow f(r, \varphi) = \sqrt{(r \cos \varphi)^2 + (r \sin \varphi)^2} = r$, linear fct. in r

$\Rightarrow \frac{\partial f}{\partial r} = 1$ (much faster than computing a directional derivative)