

§ 10 Chain Rule

In single variable calculus, we have

Theorem 10.1 (Chain Rule in Single Variable Calculus)

Let $A, B \subseteq \mathbb{R}$ and let $x_0 \in A$.

Suppose that $f: B \rightarrow \mathbb{R}$ and $g: A \rightarrow \mathbb{R}$ are functions such that

1) $g(A) \subseteq B$ (guarantee $f \circ g: A \rightarrow \mathbb{R}$ is well-defined)

2) g is differentiable at $x_0 \in A$

3) f is differentiable at $g(x_0) \in B$

then the composite function $(f \circ g): A \rightarrow \mathbb{R}$ defined by $(f \circ g)(x) = f(g(x))$ is differentiable at x_0 and $(f \circ g)'(x_0) = f'(g(x_0)) \cdot g'(x_0)$

Furthermore, suppose that both $f: B \rightarrow \mathbb{R}$ and $g: A \rightarrow \mathbb{R}$ are differentiable.

Then, $(f \circ g): A \rightarrow \mathbb{R}$ is also differentiable.

If we let $u = g(x)$ and $y = f(u)$, then $y = f(g(x))$ is a function of x and

the chain rule can be rephrased as $\frac{dy}{dx} = \frac{dy}{du} \frac{du}{dx}$.

Example 10.1

Let $f: B = (0, \infty) \rightarrow \mathbb{R}$ defined by $f(x) = \ln x$, and let $g: A = (0, \pi) \rightarrow \mathbb{R}$ defined by $g(x) = \sin x$.

Note that $g(A) = (0, 1] \subseteq B$, so $f \circ g: (0, \pi) \rightarrow \mathbb{R}$ is well-defined, which is $f \circ g(x) = f(g(x)) = \ln(\sin x)$.

Also, if $x \in A = (0, \pi)$, g is differentiable at x and f is differentiable at $g(x) = \sin x$, so

$$(f \circ g)'(x) = f'(g(x)) g'(x) = \frac{1}{(\sin x)} \cos x = \cot x.$$

Theorem 10.2 (Chain Rule)

Let $A \subseteq \mathbb{R}^n$, $B \subseteq \mathbb{R}^k$ and let $\bar{x}_0 \in A$.

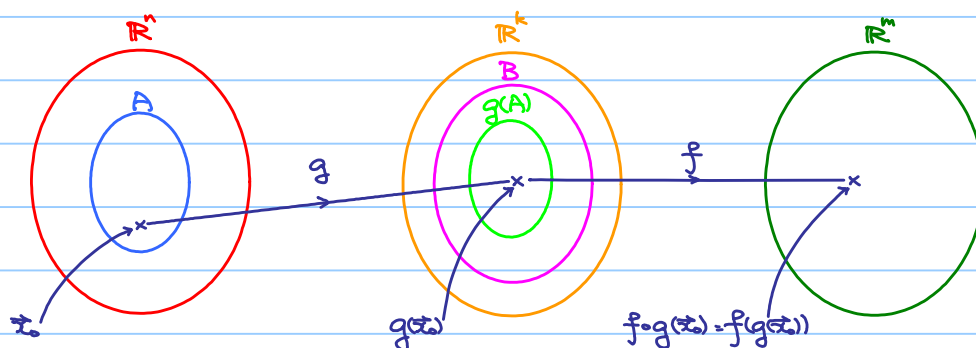
Suppose that $f: B \rightarrow \mathbb{R}^m$ and $g: A \rightarrow \mathbb{R}^k$ are functions such that

1) $g(A) \subseteq B$

2) g is differentiable at $\bar{x}_0 \in A$, i.e. $Dg(\bar{x}_0) \in M_{k \times n}(\mathbb{R})$ is well-defined

3) f is differentiable at $g(\bar{x}_0) \in B$, i.e. $Df(g(\bar{x}_0)) \in M_{m \times k}(\mathbb{R})$ is well-defined

then the composite function $(f \circ g): A \rightarrow \mathbb{R}^m$ defined by $(f \circ g)(x) = f(g(x))$ is differentiable at \bar{x}_0 and $D(f \circ g)(\bar{x}_0) = Df(g(\bar{x}_0)) \cdot Dg(\bar{x}_0) \in M_{m \times n}(\mathbb{R})$.



Remark: If $n = k = m = 1$, then $\bar{x}_0 = x_0 \in \mathbb{R}$

$$D(f \circ g)(\bar{x}_0) = [(f \circ g)'(x_0)] \in M_{1 \times 1}(\mathbb{R})$$

$$Df(g(\bar{x}_0)) = [f'(g(x_0))] \in M_{1 \times 1}(\mathbb{R})$$

$$Dg(\bar{x}_0) = [g'(x_0)] \in M_{1 \times 1}(\mathbb{R})$$

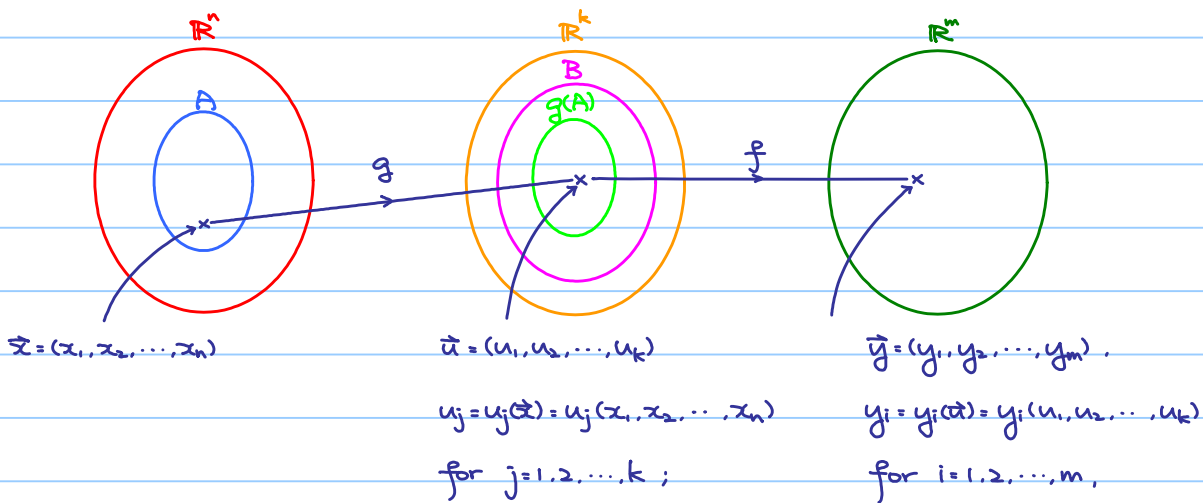
$$D(f \circ g)(\bar{x}_0) = Df(g(\bar{x}_0)) \cdot Dg(\bar{x}_0) \Rightarrow [(f \circ g)'(x_0)] = [f'(g(x_0))] \cdot [g'(x_0)]$$

$$= [f'(g(x_0))g'(x_0)] \in M_{1 \times 1}(\mathbb{R})$$

which is the chain rule in single variable calculus.

Furthermore, suppose that both $f: B \rightarrow \mathbb{R}^m$ and $g: A \rightarrow \mathbb{R}^k$ are differentiable.

Then $(f \circ g): A \rightarrow \mathbb{R}^m$ is differentiable.



If we write $\vec{y} = (y_1, y_2, \dots, y_m)$, $\vec{u} = (u_1, u_2, \dots, u_k)$ and $\vec{x} = (x_1, x_2, \dots, x_n)$

where $\vec{u} = g(\vec{x})$ and $\vec{y} = f(\vec{u}) = f(g(\vec{x}))$,

then $u_j = u_j(x_1, x_2, \dots, x_n)$ for $j = 1, 2, \dots, k$; $y_i = y_i(u_1, u_2, \dots, u_k)$ for $i = 1, 2, \dots, m$,

so $y_i = y_i(x_1, x_2, \dots, x_n) = y_i(u_1(x_1, x_2, \dots, x_n), u_2(x_1, x_2, \dots, x_n), \dots, u_k(x_1, x_2, \dots, x_n))$.

The chain rule is :

$$\begin{bmatrix} \frac{\partial y_1}{\partial x_1}(\vec{x}) & \dots & \frac{\partial y_1}{\partial x_n}(\vec{x}) \\ \vdots & & \vdots \\ \frac{\partial y_m}{\partial x_1}(\vec{x}) & \dots & \frac{\partial y_m}{\partial x_n}(\vec{x}) \end{bmatrix} = \begin{bmatrix} \frac{\partial y_1}{\partial u_1}(g(\vec{x})) & \dots & \frac{\partial y_1}{\partial u_k}(g(\vec{x})) \\ \vdots & & \vdots \\ \frac{\partial y_m}{\partial u_1}(g(\vec{x})) & \dots & \frac{\partial y_m}{\partial u_k}(g(\vec{x})) \end{bmatrix} \begin{bmatrix} \frac{\partial u_1}{\partial x_1}(\vec{x}) & \dots & \frac{\partial u_1}{\partial x_n}(\vec{x}) \\ \vdots & & \vdots \\ \frac{\partial u_k}{\partial x_1}(\vec{x}) & \dots & \frac{\partial u_k}{\partial x_n}(\vec{x}) \end{bmatrix}$$

$$D(f \circ g)(\vec{x}) \in M_{m \times n}(\mathbb{R}) \quad Df(g(\vec{x})) \in M_{m \times k}(\mathbb{R}) \quad Dg(\vec{x}) \in M_{k \times n}(\mathbb{R})$$

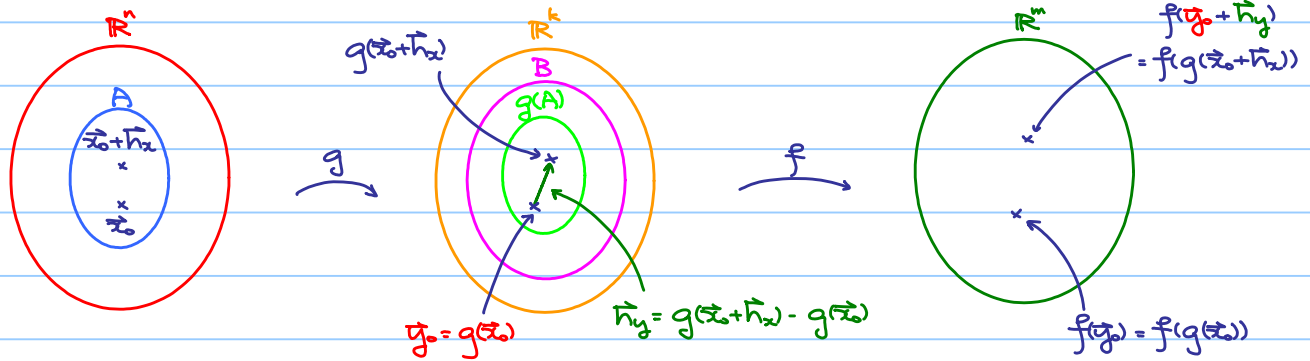
$$\text{For } 1 \leq i \leq m, 1 \leq j \leq n, \frac{\partial y_i}{\partial x_j}(\vec{x}) = \sum_{k=1}^k \frac{\partial y_i}{\partial u_k}(g(\vec{x})) \cdot \frac{\partial u_k}{\partial x_j}(\vec{x})$$

(OR write $\frac{\partial (y_1, \dots, y_m)}{\partial (x_1, \dots, x_n)} = \frac{\partial (y_1, \dots, y_m)}{\partial (u_1, \dots, u_k)} \frac{\partial (u_1, \dots, u_k)}{\partial (x_1, \dots, x_n)}$, so it looks like $\frac{dy}{dx} = \frac{dy}{du} \frac{du}{dx}$ in single variable calculus.)

💡 Idea: Let $\varepsilon_g(\tilde{h}_x) = g(\tilde{x}_0 + \tilde{h}_x) - g(\tilde{x}_0) - Dg(\tilde{x}_0) \cdot \tilde{h}_x$

$$\varepsilon_f(\tilde{h}_y) = f(\tilde{y}_0 + \tilde{h}_y) - f(\tilde{y}_0) - Df(\tilde{y}_0) \cdot \tilde{h}_y$$

where $\lim_{\tilde{h}_x \rightarrow 0} \frac{|\varepsilon_g(\tilde{h}_x)|}{|\tilde{h}_x|} = 0$ and $\lim_{\tilde{h}_y \rightarrow 0} \frac{|\varepsilon_f(\tilde{h}_y)|}{|\tilde{h}_y|} = 0$.



Put $\tilde{y}_0 = g(\tilde{x}_0)$ and $\tilde{h}_y = g(\tilde{x}_0 + \tilde{h}_x) - g(\tilde{x}_0) = Dg(\tilde{x}_0) \cdot \tilde{h}_x + \varepsilon_g(\tilde{h}_x)$ we have

$$\varepsilon_f(\tilde{h}_y) = f(\tilde{y}_0 + \tilde{h}_y) - f(\tilde{y}_0) - Df(\tilde{y}_0) \cdot \tilde{h}_y$$

$$= f(g(\tilde{x}_0) + (g(\tilde{x}_0 + \tilde{h}_x) - g(\tilde{x}_0))) - f(g(\tilde{x}_0)) - Df(g(\tilde{x}_0)) \cdot (Dg(\tilde{x}_0) \cdot \tilde{h}_x + \varepsilon_g(\tilde{h}_x))$$

$$= f(g(\tilde{x}_0 + \tilde{h}_x)) - f(g(\tilde{x}_0)) - [Df(g(\tilde{x}_0)) \cdot Dg(\tilde{x}_0)] \cdot \tilde{h}_x - Df(g(\tilde{x}_0)) \cdot \varepsilon_g(\tilde{h}_x)$$

$$\therefore \underbrace{Df(g(\tilde{x}_0)) \cdot \varepsilon_g(\tilde{h}_x)}_{\varepsilon_{f \circ g}(\tilde{h}_x)} + \varepsilon_f(\tilde{h}_y) = f(g(\tilde{x}_0 + \tilde{h}_x)) - f(g(\tilde{x}_0)) - \underbrace{[Df(g(\tilde{x}_0)) \cdot Dg(\tilde{x}_0)] \cdot \tilde{h}_x}_{\text{linear transformation on } \tilde{h}_x}$$

If $\lim_{\tilde{h}_x \rightarrow 0} \frac{|\varepsilon_{f \circ g}(\tilde{h}_x)|}{|\tilde{h}_x|} = 0$, then $D(f \circ g)(\tilde{x}_0) = Df(g(\tilde{x}_0)) \cdot Dg(\tilde{x}_0)$

Example 10.2

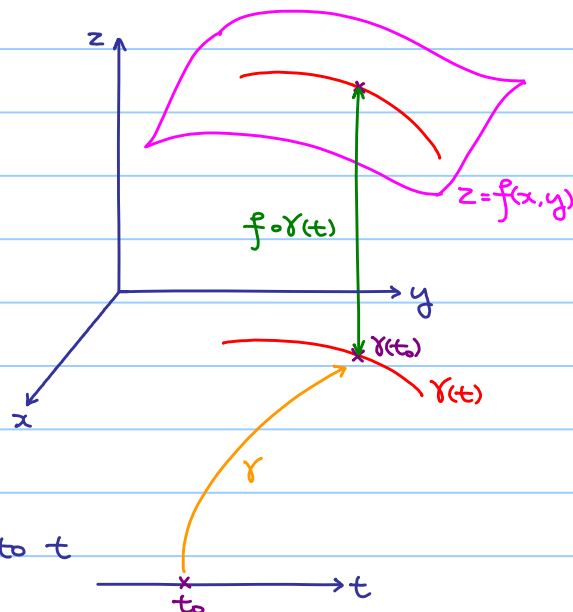
Let $f: \mathbb{R}^2 \rightarrow \mathbb{R}$ defined by $f(x,y) = x^2y$ and $\gamma: \mathbb{R} \rightarrow \mathbb{R}^2$ defined by $\gamma(t) = (x(t), y(t)) = (t, t^3)$.

Then $f \circ \gamma: \mathbb{R} \rightarrow \mathbb{R}$.

Note γ is a curve in \mathbb{R}^2 ,

i.e. given $t \in \mathbb{R}$, $\gamma(t) = (x(t), y(t))$ gives a point in \mathbb{R}^2 .

Then, the point $\gamma(t)$ is inputted into f and a real number $f \circ \gamma(t) \in \mathbb{R}$ is outputted.



Question: As t changes, how does $f \circ \gamma(t)$ change?

We write $z = f(x,y)$, then $z(t) = f(\gamma(t)) = f(x(t), y(t))$.

so $\frac{dz}{dt}$ is the rate of change of z with respect to t

Note $Df \in M_{1 \times 2}(\mathbb{R})$, $D\gamma \in M_{2 \times 1}(\mathbb{R})$ and $D(f \circ \gamma) \in M_{1 \times 1}(\mathbb{R})$.

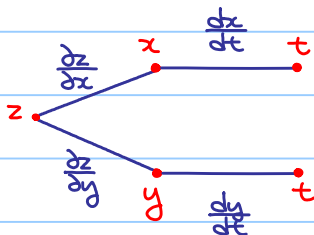
$$Df(\gamma(t)) = \left[\frac{\partial z}{\partial x} \quad \frac{\partial z}{\partial y} \right] = [2xy \quad x^2], \quad D\gamma(t) = \begin{bmatrix} \frac{dx}{dt} \\ \frac{dy}{dt} \end{bmatrix} = \begin{bmatrix} 1 \\ 3t^2 \end{bmatrix}$$

$$D(f \circ \gamma)(t) = \left[\frac{dz}{dt} \right] = [2xy \quad x^2] \begin{bmatrix} 1 \\ 3t^2 \end{bmatrix} = [2xy + 2x^2t] = [4t^3]$$

Verification: $z = f(\gamma(t)) = f(t, t^3) = (t)^2(t^3) = t^4$ and so $\frac{dz}{dt} = 4t^3$.

Find it difficult? Try this:

Tree diagram:



$$\frac{dz}{dt} = \frac{\partial z}{\partial x} \frac{dx}{dt} + \frac{\partial z}{\partial y} \frac{dy}{dt}$$

Example 10.3

Let $f: \mathbb{R}^3 \rightarrow \mathbb{R}$ defined by $w = f(x, y, z) = x^2 + xy + yz$ and

$g: \mathbb{R} \rightarrow \mathbb{R}^3$ defined by $g(t) = (x(t), y(t), z(t)) = (t, t^2, t^3)$

Note $Df \in M_{1 \times 3}(\mathbb{R})$, $Dg \in M_{3 \times 1}(\mathbb{R})$ and $D(f \circ g) \in M_{1 \times 1}(\mathbb{R})$.

$$D(f \circ g)(t) = Df(g(t)) \cdot Dg(t)$$

$$\left[\frac{dw}{dt} \right] = \left[\frac{\partial w}{\partial x} \quad \frac{\partial w}{\partial y} \quad \frac{\partial w}{\partial z} \right] \begin{bmatrix} \frac{dx}{dt} \\ \frac{dy}{dt} \\ \frac{dz}{dt} \end{bmatrix}$$

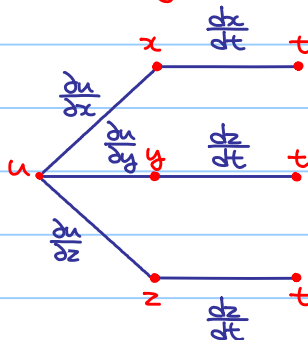
$$= \left[\frac{\partial w}{\partial x} \frac{dx}{dt} + \frac{\partial w}{\partial y} \frac{dy}{dt} + \frac{\partial w}{\partial z} \frac{dz}{dt} \right]$$

$$\therefore \frac{dw}{dt} = (2x+y)(1) + (x+z)(2t) + (y)(3t^2)$$

$$= (2t+t^2)(1) + (t+t^3)(2t) + (t^2)(3t^2)$$

$$= 5t^4 + 3t^2 + 2t$$

Tree diagram:



Example 10.4

Let $u = u(x, y)$, $x = x(s, t)$ and $y = y(s, t)$ be differentiable functions.

Therefore $(s, t) \mapsto (x(s, t), y(s, t)) \mapsto u(x(s, t), y(s, t))$

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

Then,

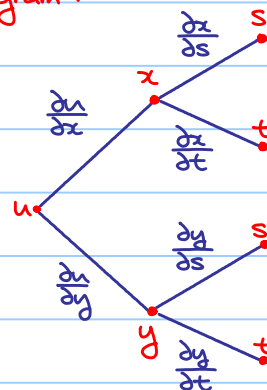
$$\left[\frac{\partial u}{\partial s} \quad \frac{\partial u}{\partial t} \right] = \left[\frac{\partial u}{\partial x} \quad \frac{\partial u}{\partial y} \right] \begin{bmatrix} \frac{\partial x}{\partial s} & \frac{\partial x}{\partial t} \\ \frac{\partial y}{\partial s} & \frac{\partial y}{\partial t} \end{bmatrix}$$

$$M_{1 \times 2}(\mathbb{R}) \quad M_{1 \times 2}(\mathbb{R}) \quad M_{2 \times 2}(\mathbb{R})$$

$$\frac{\partial u}{\partial s} = \frac{\partial u}{\partial x} \frac{\partial x}{\partial s} + \frac{\partial u}{\partial y} \frac{\partial y}{\partial s}$$

$$\frac{\partial u}{\partial t} = \frac{\partial u}{\partial x} \frac{\partial x}{\partial t} + \frac{\partial u}{\partial y} \frac{\partial y}{\partial t}$$

Tree diagram:



Compute $\frac{\partial u}{\partial s}$. Sum of paths end at s.

Exercise 10.1

Let $u = x^2 - 2xy + 2y^3$ where $x = s^2 \ln t$ and $y = 2st^3$.

Find $\frac{\partial u}{\partial s}$ and $\frac{\partial u}{\partial t}$.

$$\text{Ans: } \frac{\partial u}{\partial s} = (2s^2 \ln t - 4st^3)(2s \ln t) + (-2s^2 \ln t + 24s^2 t^6)(2t^3)$$

$$\frac{\partial u}{\partial t} = (2s^2 \ln t - 4st^3) \left(\frac{s^2}{t} \right) + (-2s^2 \ln t + 24s^2 t^6)(6st^2)$$

Example 10.5

Let $u = u(x, y, z)$, $x = x(r, s, t)$, $y = y(s, t)$ and $z = z(r, t)$ be differentiable functions.

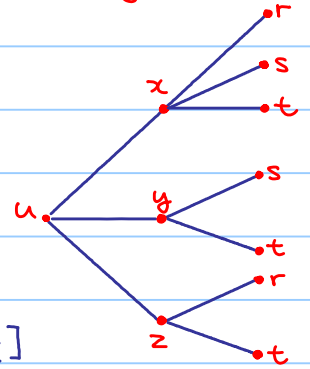
$$\frac{\partial u}{\partial r} = \frac{\partial u}{\partial x} \frac{\partial x}{\partial r} + \frac{\partial u}{\partial z} \frac{\partial z}{\partial r}$$

$$\frac{\partial u}{\partial s} = \frac{\partial u}{\partial x} \frac{\partial x}{\partial s} + \frac{\partial u}{\partial y} \frac{\partial y}{\partial s}$$

$$\frac{\partial u}{\partial t} = \frac{\partial u}{\partial x} \frac{\partial x}{\partial t} + \frac{\partial u}{\partial y} \frac{\partial y}{\partial t} + \frac{\partial u}{\partial z} \frac{\partial z}{\partial t}$$

$$\begin{bmatrix} \frac{\partial u}{\partial r} & \frac{\partial u}{\partial s} & \frac{\partial u}{\partial t} \end{bmatrix} = \begin{bmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} & \frac{\partial u}{\partial z} \end{bmatrix} \begin{bmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial s} & \frac{\partial x}{\partial t} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial s} & \frac{\partial y}{\partial t} \\ \frac{\partial z}{\partial r} & \frac{\partial z}{\partial s} & \frac{\partial z}{\partial t} \end{bmatrix} \quad (\because \frac{\partial y}{\partial r} = \frac{\partial z}{\partial s} = 0)$$

Tree diagram :



$$= \left[\frac{\partial u}{\partial x} \frac{\partial x}{\partial r} + \frac{\partial u}{\partial z} \frac{\partial z}{\partial r} \quad \frac{\partial u}{\partial x} \frac{\partial x}{\partial s} + \frac{\partial u}{\partial y} \frac{\partial y}{\partial s} \quad \frac{\partial u}{\partial x} \frac{\partial x}{\partial t} + \frac{\partial u}{\partial y} \frac{\partial y}{\partial t} + \frac{\partial u}{\partial z} \frac{\partial z}{\partial t} \right]$$

Implicit Differentiation

Example 10.6

Let \mathcal{C} be the circle defined by $x^2 + y^2 - 1 = 0$. Find $\frac{dy}{dx}$.

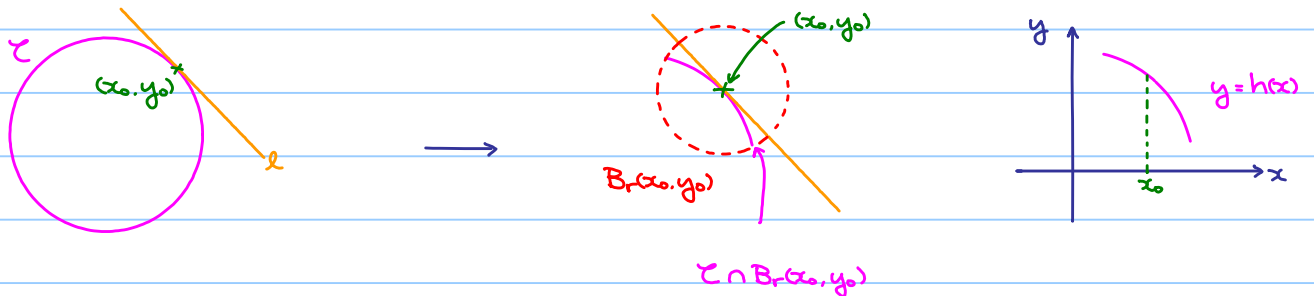
Differentiate both sides with respect to x :

$$2x + 2y \frac{dy}{dx} = 0 \quad \leftarrow \text{Why can it be done?}$$

$$\frac{dy}{dx} = -\frac{x}{y}$$

Let $F(x, y) = x^2 + y^2 - 1$. Then the circle \mathcal{C} is just defined by $F(x, y) = 0$.

Suppose that (x_0, y_0) lying on \mathcal{C} such that $y_0 \neq 0$.



If $r > 0$ is sufficiently small, $\mathcal{C} \cap B_r(x_0, y_0)$ is a small piece of arc of the circle \mathcal{C} , which is the graph of some function $y = h(x)$ and $\frac{dy}{dx}$ means $h'(x)$.

In general, suppose that

- 1) $F(x, y)$ is differentiable;
- 2) $F(x_0, y_0) = 0$;
- 3) there exists $r > 0$ such that $\{(x, y) : F(x, y) = 0\} \cap B_r(x_0, y_0)$ can be regarded as graph of a differentiable function $y = h(x)$.

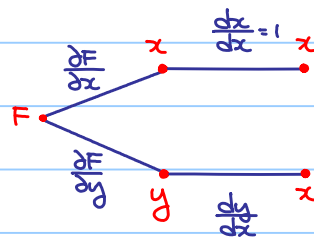
Then,

$$F(x, y) = 0$$

$$\frac{\partial F}{\partial x} \frac{dx}{dx} + \frac{\partial F}{\partial y} \frac{dy}{dx} = 0 \quad (\text{Chain Rule})$$

$$\therefore \frac{\partial F}{\partial x} \cdot 1 + \frac{\partial F}{\partial y} \frac{dy}{dx} = 0$$

$$\text{At } (x_0, y_0), \quad \frac{\partial F}{\partial x}(x_0, y_0) + \frac{\partial F}{\partial y}(x_0, y_0) \cdot \left. \frac{dy}{dx} \right|_{x=x_0} = 0$$



$$\text{if } \frac{\partial F}{\partial y}(x_0, y_0) \neq 0, \text{ then } \left. \frac{dy}{dx} \right|_{x=x_0} = -\left(\frac{\frac{\partial F}{\partial x}(x_0, y_0)}{\frac{\partial F}{\partial y}(x_0, y_0)} \right).$$

Remark: Implicit function theorem:

$\frac{\partial F}{\partial y}(x_0, y_0) \neq 0$ if and only if condition (3) holds. (Discuss later!)

§ 11 More on Gradient

Gradient and Directional Derivatives

Proposition 11.1

Let $D \subseteq \mathbb{R}^n$ be an open subset, let $\vec{x}_0 \in D$ and let $f: D \rightarrow \mathbb{R}$.

If f is differentiable at \vec{x}_0 , then the directional derivative exists along any nonzero vector \vec{v} and we have $\nabla_{\vec{v}} f(\vec{x}_0) = \nabla f(\vec{x}_0) \cdot \frac{\vec{v}}{|\vec{v}|}$.

proof:

f is differentiable at $\vec{x}_0 \Rightarrow$ there exists $\vec{L} \in \mathbb{R}^n$ such that $\lim_{\vec{h} \rightarrow \vec{0}} \frac{f(\vec{x}_0 + \vec{h}) - (f(\vec{x}_0) + \vec{L} \cdot \vec{h})}{|\vec{h}|} = 0$
(in fact, $\vec{L} = \nabla f(\vec{x}_0)$.)

In particular, take $\vec{h} = h\hat{v}$, where $\hat{v} = \frac{\vec{v}}{|\vec{v}|}$,

$$\lim_{h \rightarrow 0} \frac{f(\vec{x}_0 + h\hat{v}) - (f(\vec{x}_0) + \nabla f(\vec{x}_0) \cdot h\hat{v})}{|h\hat{v}|} = 0$$

$$\lim_{h \rightarrow 0} \frac{f(\vec{x}_0 + h\hat{v}) - (f(\vec{x}_0) + \nabla f(\vec{x}_0) \cdot h\hat{v})}{|h|} = 0$$

$$\Rightarrow \lim_{h \rightarrow 0} \frac{f(\vec{x}_0 + h\hat{v}) - (f(\vec{x}_0) + \nabla f(\vec{x}_0) \cdot h\hat{v})}{h} = 0$$

$$\lim_{h \rightarrow 0} \frac{f(\vec{x}_0 + h\hat{v}) - f(\vec{x}_0)}{h} = \nabla f(\vec{x}_0) \cdot \hat{v}, \text{ so } \nabla_{\vec{v}} f(\vec{x}_0) = \nabla f(\vec{x}_0) \cdot \hat{v} = \nabla f(\vec{x}_0) \cdot \frac{\vec{v}}{|\vec{v}|}$$

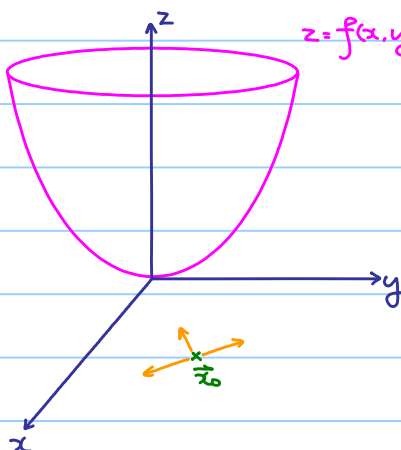
Example 11.1

Let $f(x, y) = xy$ and $\vec{v} = (1, 2) \in \mathbb{R}^2$.

Then $\hat{v} = \frac{\vec{v}}{|\vec{v}|} = \frac{1}{\sqrt{5}}(1, 2)$ and f is differentiable on \mathbb{R}^2 , $\nabla f(x, y) = (y, x)$.

$$\nabla_{\vec{v}} f(\vec{x}_0) = \nabla f(\vec{x}_0) \cdot \frac{\vec{v}}{|\vec{v}|} = \frac{2}{\sqrt{5}}x + \frac{1}{\sqrt{5}}y \quad (\text{Compare with example 8.4})$$

Geometrical Meaning of Gradient



$z = f(x, y) = x^2 + y^2$ Question: If we move away from \vec{x}_0 , then the value of f changes.

However, which direction shall we go to increase / decrease f most rapidly?

Since $\nabla_{\vec{v}} f(\vec{x}_0)$ is the rate of change of f at \vec{x}_0 along \vec{v} , our question is equivalent to maximize / minimize $\nabla_{\vec{v}} f(\vec{x}_0)$ among all possible direction \vec{v} .

Let $D \subseteq \mathbb{R}^n$ be an open subset, let $\vec{x}_0 \in D$ and let $f: D \rightarrow \mathbb{R}$.

Suppose that f is differentiable at \vec{x}_0 . If $\vec{v} \in \mathbb{R}^n$ and $|\vec{v}| = 1$, i.e. $\hat{v} = \vec{v}$, then $\nabla_{\vec{v}} f(\vec{x}_0) = \nabla f(\vec{x}_0) \cdot \vec{v}$.

$$\begin{aligned} |\nabla_{\vec{v}} f(\vec{x}_0)| &= |\nabla f(\vec{x}_0) \cdot \vec{v}| \\ &= |\nabla f(\vec{x}_0)| |\vec{v}| |\cos \theta|, \text{ where } \theta \text{ is the angle between } \nabla f(\vec{x}_0) \text{ and } \vec{v} \\ &\stackrel{(*)}{\leq} |\nabla f(\vec{x}_0)| \cdot |\vec{v}| \\ &= |\nabla f(\vec{x}_0)| \quad (\because |\vec{v}| = 1) \end{aligned}$$

$$\therefore -|\nabla f(\vec{x}_0)| \leq \nabla_{\vec{v}} f(\vec{x}_0) \leq |\nabla f(\vec{x}_0)|$$

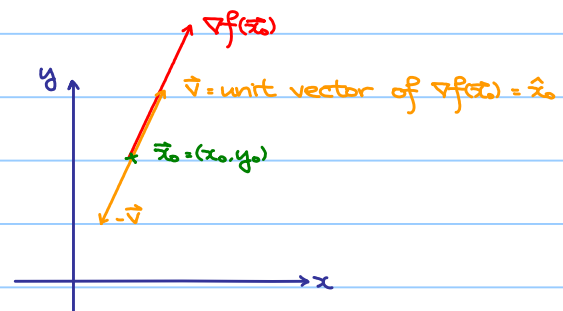
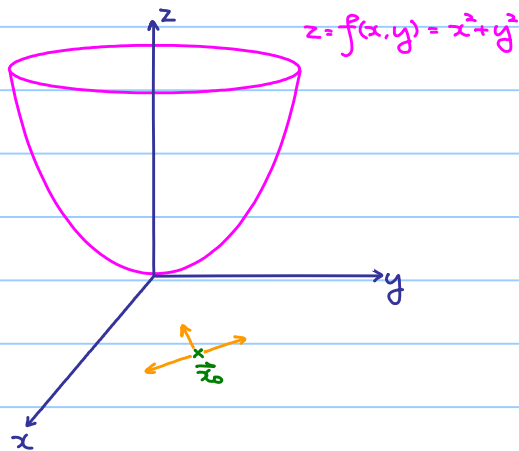
Furthermore, equality of $(*)$ holds if and only if $\theta = 0$ or π , i.e. $\vec{v} \parallel \nabla f(\vec{x}_0)$

Therefore, if f changes most rapidly if we move along the direction of $\nabla f(\vec{x}_0)$ or $-\nabla f(\vec{x}_0)$.

Example 11.2

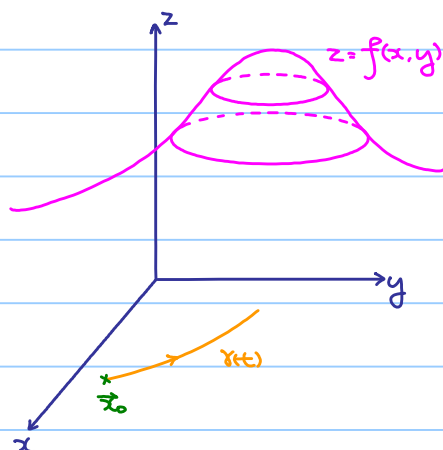
Let $f(x, y) = x^2 + y^2$. Then, $\nabla f(x, y) = (2x, 2y)$.

\therefore For any $\vec{x}_0 = (x_0, y_0)$, $\nabla f(\vec{x}_0) = 2\vec{x}_0$



f changes most rapidly if we move along the direction of $\nabla f(\vec{x}_0)$ or $-\nabla f(\vec{x}_0)$.

Remark.



Idea: If we start from \vec{x}_0 and move along the curve $\gamma(t)$ such that $\gamma(0) = \vec{x}_0$ and $\dot{\gamma}(t) = \nabla f(\gamma(t))$, i.e. always moves along the gradient direction.

Eventually, we arrive extreme points of f !
 (Gradient flow, useful in optimization)

Gradient and Level Set

Let $D \subseteq \mathbb{R}^n$ be an open subset, let $\vec{x}_0 \in D$ and let $f: D \rightarrow \mathbb{R}$ be a smooth function.

Suppose that $L_c(f) = \{\vec{x} \in D : f(\vec{x}) = c\}$ and $\nabla f(\vec{x}) \neq \vec{0}$ for all points $\vec{x} \in L_c(f)$ ($\Rightarrow L_c(f)$ is a smooth $(n-1)$ -dimensional manifold in \mathbb{R}^n) and $\vec{x}_0 \in L_c(f)$ i.e. $f(\vec{x}_0) = c$.

Let $\gamma: (-\varepsilon, \varepsilon) \rightarrow D$ be a differentiable curve such that γ lies on $L_c(f)$,

$\gamma(0) = \vec{x}_0$ and $\gamma'(0)$ is nonzero. Then $\gamma'(0)$ is a vector tangent to $L_c(f)$ at \vec{x}_0 .

Furthermore, since γ lies on $L_c(f)$, we have $f(\gamma(t)) = c$ for all $t \in (-\varepsilon, \varepsilon)$.

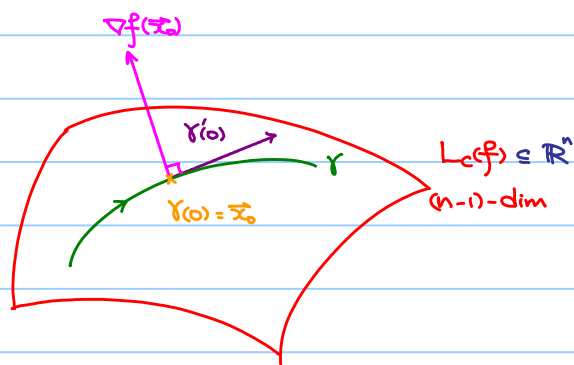
Then, $\frac{d}{dt} f(\gamma(t)) = \nabla f(\gamma(t)) \cdot \gamma'(t) = 0$ (Chain Rule).

In particular, put $t=0$, we have

$$\nabla f(\gamma(0)) \cdot \gamma'(0) = \nabla f(\vec{x}_0) \cdot \gamma'(0) = 0$$

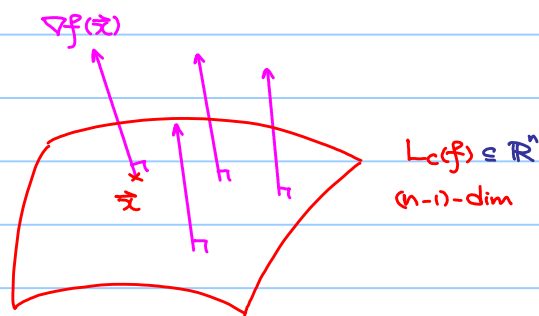
Therefore, $\nabla f(\vec{x}_0)$ is orthogonal to every vector tangent to $L_c(f)$ at \vec{x}_0 ,

and $\nabla f(\vec{x}_0)$ gives a normal of $L_c(f)$ at \vec{x}_0 .



For every point $\vec{x} \in L_c(f)$, we draw

$\nabla f(\vec{x})$, then we will see this:

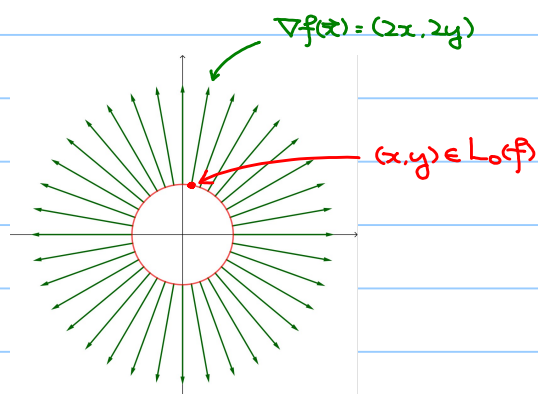


Example 11.3

Let $f: \mathbb{R}^2 \rightarrow \mathbb{R}$ defined by $f(x, y) = x^2 + y^2 - 1$.

$L_0(f) = \{(x, y) \in \mathbb{R}^2 : x^2 + y^2 - 1 = 0\}$ which is the unit circle centered at the origin.

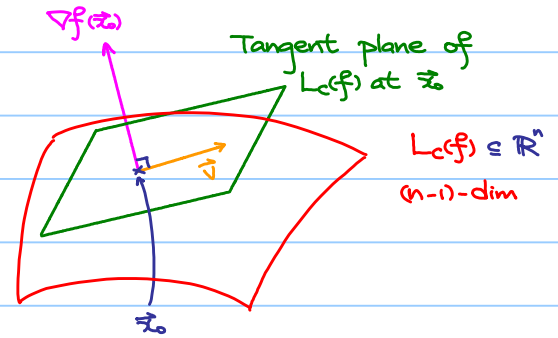
$$\nabla f(\vec{x}) = \left(\frac{\partial f}{\partial x}(\vec{x}), \frac{\partial f}{\partial y}(\vec{x}) \right) = (2x, 2y)$$



Summary

Fix $\vec{z}_0 \in L_c(f)$ (i.e. $f(\vec{z}_0) = c$), assume $\nabla f(\vec{z}_0)$ is nonzero.

- 1) if we move along any direction on the tangent plane of $L_c(f)$ at \vec{z}_0 , the value of f does not change:
- 2) if we move along the normal direction of the tangent plane of $L_c(f)$ at \vec{z}_0 , the value of f changes mostly rapidly.



§ 12 Taylor's Theorem

Taylor's Polynomial for Two variables

Let $D \subseteq \mathbb{R}^2$ be an open set, and let $f: D \rightarrow \mathbb{R}$ be a function such that partial derivatives of all order exist, i.e. $\frac{\partial^k f}{\partial x^{k_1} \partial y^{k_2}}$ exists for any positive integer k with integers $k_1, k_2 \geq 0$ and $k_1 + k_2 = k$.

Let $\vec{a} = (a_1, a_2) \in D$.

💡 Idea: Can we approximate $f(x, y)$ around \vec{a} by a polynomial $P_n(x, y)$ of degree n such that f and P_n agree up to n -th order at \vec{a} , i.e.

$$\frac{\partial^k f}{\partial x^{k_1} \partial y^{k_2}}(a_1, a_2) = \frac{\partial^k P_n}{\partial x^{k_1} \partial y^{k_2}}(a_1, a_2), \text{ for } k_1 + k_2 = k, 0 \leq k \leq n?$$

Let $P_n(x, y) = C_{0,0}$

$$+ C_{1,0}(x-a_1) + C_{0,1}(y-a_2)$$

$$+ C_{2,0}(x-a_1)^2 + C_{1,1}(x-a_1)(y-a_2) + C_{0,2}(y-a_2)^2 + \dots$$

$$+ C_{n,0}(x-a_1)^n + C_{n-1,1}(x-a_1)^{n-1}(y-a_2) + \dots + C_{0,n}(y-a_2)^n$$

$$= \sum_{k=0}^n \sum_{k_1+k_2=k} C_{k_1, k_2} (x-a_1)^{k_1} (y-a_2)^{k_2}$$

Determine C_{k_1, k_2} 's:

$$\bullet P_n(a_1, a_2) = f(a_1, a_2) \Rightarrow C_{0,0} = f(a_1, a_2)$$

$$\bullet \frac{\partial P_n}{\partial x}(a_1, a_2) = \frac{\partial f}{\partial x}(a_1, a_2) \Rightarrow C_{1,0} = \frac{\partial f}{\partial x}(a_1, a_2) \quad \frac{\partial P_n}{\partial y}(a_1, a_2) = \frac{\partial f}{\partial y}(a_1, a_2) \Rightarrow C_{0,1} = \frac{\partial f}{\partial y}(a_1, a_2)$$

$$\bullet \frac{\partial^2 P_n}{\partial x^2}(a_1, a_2) = \frac{\partial^2 f}{\partial x^2}(a_1, a_2) \Rightarrow C_{2,0} = \frac{1}{2} \frac{\partial^2 f}{\partial x^2}(a_1, a_2)$$

$$\frac{\partial^2 P_n}{\partial y^2}(a_1, a_2) = \frac{\partial^2 f}{\partial y^2}(a_1, a_2) \Rightarrow C_{0,2} = \frac{1}{2} \frac{\partial^2 f}{\partial y^2}(a_1, a_2)$$

$$\frac{\partial^2 P_n}{\partial x \partial y}(a_1, a_2) = \frac{\partial^2 f}{\partial x \partial y}(a_1, a_2) \Rightarrow C_{1,1} = \frac{\partial^2 f}{\partial x \partial y}(a_1, a_2)$$

$$\bullet \text{In general, } C_{k_1, k_2} = \frac{1}{k_1! k_2!} \frac{\partial^k f}{\partial x^{k_1} \partial y^{k_2}}(a_1, a_2) \text{ with } k = k_1 + k_2.$$

Definition 12.1

Let D be an open subset in \mathbb{R}^2 , let $\vec{a} = (a_1, a_2) \in D$.

and let $f: D \rightarrow \mathbb{R}$ be a function such that partial derivatives

of f exist up to n -th order at \vec{a} . Then,

$$P_n(x, y) = \sum_{k=0}^n \sum_{k_1+k_2=k} \left(\frac{1}{k_1! k_2!} \frac{\partial^k f}{\partial x^{k_1} \partial y^{k_2}}(a_1, a_2) \right) (x-a_1)^{k_1} (y-a_2)^{k_2}$$

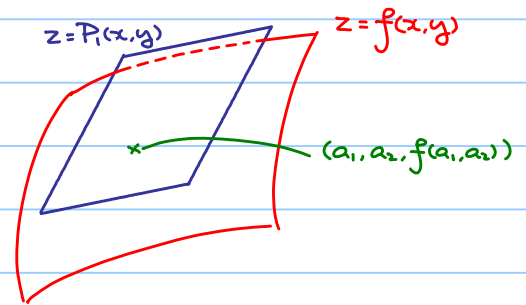
is said to be the Taylor polynomial of degree n generated by $f(x, y)$ at \vec{a} .

In particular, $z = P_1(x, y) = f(a_1, a_2) + \left(\frac{\partial f}{\partial x}(a_1, a_2)\right)(x - a_1) + \left(\frac{\partial f}{\partial y}(a_1, a_2)\right)(y - a_2)$

gives the tangent plane of f at \vec{a} .

Also, $P_1(x, y)$ is exactly the linearization of f at $\vec{a} = (a_1, a_2)$

(see example 9.3)



$$P_2(x, y) = f(a_1, a_2) + \left(\frac{\partial f}{\partial x}(a_1, a_2)\right)(x - a_1) + \left(\frac{\partial f}{\partial y}(a_1, a_2)\right)(y - a_2) + \left(\frac{1}{2} \frac{\partial^2 f}{\partial x^2}(a_1, a_2)\right)(x - a_1)^2 + \left(\frac{\partial^2 f}{\partial x \partial y}(a_1, a_2)\right)(x - a_1)(y - a_2) + \left(\frac{1}{2} \frac{\partial^2 f}{\partial y^2}(a_1, a_2)\right)(y - a_2)^2$$

Example 12.1

Let $f(x, y) = e^{x^2+y}$.

Let $P_n(x, y)$ be the Taylor polynomial of degree n generated by $f(x, y)$ at $(0, 0)$.

• $f(0, 0) = 1$

• $\frac{\partial f}{\partial x} = 2xe^{x^2+y} \Rightarrow \frac{\partial f}{\partial x}(0, 0) = 0$ $\frac{\partial f}{\partial y} = e^{x^2+y} \Rightarrow \frac{\partial f}{\partial y}(0, 0) = 1$

• $\frac{\partial^2 f}{\partial x^2} = (2+4x^2)e^{x^2+y} \Rightarrow \frac{\partial^2 f}{\partial x^2}(0, 0) = 2$ $\frac{\partial^2 f}{\partial x \partial y} = 2xe^{x^2+y} \Rightarrow \frac{\partial^2 f}{\partial x \partial y}(0, 0) = 0$ $\frac{\partial^2 f}{\partial y^2} = e^{x^2+y} \Rightarrow \frac{\partial^2 f}{\partial y^2}(0, 0) = 1$

• $\frac{\partial^3 f}{\partial x^3} = (2x+8x^3)e^{x^2+y} \Rightarrow \frac{\partial^3 f}{\partial x^3}(0, 0) = 0$ $\frac{\partial^3 f}{\partial x^2 \partial y} = (2+4x^2)e^{x^2+y} \Rightarrow \frac{\partial^3 f}{\partial x^2 \partial y}(0, 0) = 0$

$\frac{\partial^3 f}{\partial x \partial y^2} = (2+4x^2)e^{x^2+y} \Rightarrow \frac{\partial^3 f}{\partial x \partial y^2}(0, 0) = 2$ $\frac{\partial^3 f}{\partial y^3} = e^{x^2+y} \Rightarrow \frac{\partial^3 f}{\partial y^3}(0, 0) = 1$

$P_0(x, y) = f(0, 0) = 1$

$P_1(x, y) = f(0, 0) + \frac{\partial f}{\partial x}(0, 0)x + \frac{\partial f}{\partial y}(0, 0)y = 1 + y$

$P_2(x, y) = f(0, 0) + \frac{\partial f}{\partial x}(0, 0)x + \frac{\partial f}{\partial y}(0, 0)y + \frac{1}{2} \frac{\partial^2 f}{\partial x^2}(0, 0)x^2 + \frac{\partial^2 f}{\partial x \partial y}(0, 0)xy + \frac{1}{2} \frac{\partial^2 f}{\partial y^2}(0, 0)y^2$
 $= 1 + y + x^2 + \frac{1}{2}y^2$

$P_3(x, y) = f(0, 0) + \frac{\partial f}{\partial x}(0, 0)x + \frac{\partial f}{\partial y}(0, 0)y + \frac{1}{2} \frac{\partial^2 f}{\partial x^2}(0, 0)x^2 + \frac{\partial^2 f}{\partial x \partial y}(0, 0)xy + \frac{1}{2} \frac{\partial^2 f}{\partial y^2}(0, 0)y^2$
 $+ \frac{1}{6} \frac{\partial^3 f}{\partial x^3}(0, 0)x^3 + \frac{1}{2} \frac{\partial^3 f}{\partial x^2 \partial y}(0, 0)x^2y + \frac{1}{2} \frac{\partial^3 f}{\partial x \partial y^2}(0, 0)xy^2 + \frac{1}{6} \frac{\partial^3 f}{\partial y^3}(0, 0)y^3$
 $= 1 + y + x^2 + \frac{1}{2}y^2 + x^2y + \frac{1}{6}y^3$

Frequently used Taylor series :

$$1) \frac{1}{1-x} = 1+x+x^2+\dots+x^n+\dots = \sum_{n=0}^{\infty} x^n, \quad |x| < 1$$

$$2) \frac{1}{1+x} = 1-x+x^2-\dots+(-x)^n+\dots = \sum_{n=0}^{\infty} (-x)^n, \quad |x| < 1$$

$$3) e^x = 1+x+\frac{x^2}{2!}+\dots+\frac{x^n}{n!}+\dots = \sum_{n=0}^{\infty} \frac{x^n}{n!}, \quad x \in \mathbb{R}$$

$$4) \sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \dots + (-1)^n \frac{x^{2n+1}}{(2n+1)!} + \dots = \sum_{n=0}^{\infty} \frac{(-1)^n x^{2n+1}}{(2n+1)!}, \quad x \in \mathbb{R}$$

$$5) \cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \dots + (-1)^n \frac{x^{2n}}{(2n)!} + \dots = \sum_{n=0}^{\infty} \frac{(-1)^n x^{2n}}{(2n)!}, \quad x \in \mathbb{R}$$

$$6) \ln(1+x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \dots + (-1)^{n+1} \frac{x^n}{n} + \dots = \sum_{n=1}^{\infty} \frac{(-1)^{n+1} x^n}{n}, \quad -1 < x \leq 1$$

Example 12.1 (Cont.)

$$\begin{aligned} e^{x^2+y} &= 1 + (x^2+y) + \frac{1}{2!}(x^2+y)^2 + \frac{1}{3!}(x^2+y)^3 + \dots \\ &= 1 + (x^2+y) + \frac{1}{2}(x^4+2xy+y^2) + \frac{1}{6}(x^6+3x^4y+3x^2y^2+y^3) + \dots \\ &= 1 + y + x^2 + \frac{1}{2}y^2 + x^2y + \frac{1}{6}y^3 + \dots \\ &\quad \parallel \text{higher order terms} \\ &\quad \parallel P_3(x,y) \end{aligned}$$

OR :

$$\begin{aligned} e^{x^2+y} &= e^{x^2} \cdot e^y \\ &= (1+x^2+\dots)(1+y+\frac{1}{2}y^2+\frac{1}{6}y^3+\dots) \\ &= 1 + y + x^2 + \frac{1}{2}y^2 + x^2y + \frac{1}{6}y^3 + \dots \\ &\quad \parallel \text{higher order terms} \\ &\quad \parallel P_3(x,y) \end{aligned}$$

Example 12.2

$$\begin{aligned} \sin(e^y + x - 1) &= \sin\left(\left(1+y+\frac{1}{2}y^2+\frac{1}{6}y^3+\dots\right) + x - 1\right) \\ &= \sin\left(x+y+\frac{1}{2}y^2+\frac{1}{6}y^3+\dots\right) \\ &= \left(x+y+\frac{1}{2}y^2+\frac{1}{6}y^3+\dots\right) - \frac{1}{3!}\left(x+y+\frac{1}{2}y^2+\frac{1}{6}y^3+\dots\right)^3 + \frac{1}{5!}\left(x+y+\frac{1}{2}y^2+\frac{1}{6}y^3+\dots\right)^5 - \dots \\ &= \left(x+y+\frac{1}{2}y^2+\frac{1}{6}y^3+\dots\right) - \frac{1}{6}(x^3+3x^2y+3xy^2+y^3+\dots) + \dots \\ &= x+y+\frac{1}{2}y^2 - \frac{1}{6}x^3 - \frac{1}{2}x^2y - \frac{1}{2}xy^2 + \dots \\ &\quad \parallel \text{higher order terms} \\ &\quad \parallel P_3(x,y) \end{aligned}$$

Example 12.3

$$\ln(1+x+y) = \ln(1+(x+y))$$

$$= (x+y) - \frac{(x+y)^2}{2} + \frac{(x+y)^3}{3} + \dots$$

$$= x+y - \frac{1}{2}(x^2+2xy+y^2) + \frac{1}{3}(x^3+3x^2y+3xy^2+y^3) + \dots$$

\parallel
 $P_3(x,y)$

higher order terms

In particular, there is a very compact way to write down $P_2(x,y)$ which is very useful later!

We have

$$P_2(x,y) = f(a_1, a_2) + \left(\frac{\partial f}{\partial x}(a_1, a_2)\right)(x-a_1) + \left(\frac{\partial f}{\partial y}(a_1, a_2)\right)(y-a_2)$$

$$+ \left(\frac{1}{2} \frac{\partial^2 f}{\partial x^2}(a_1, a_2)\right)(x-a_1)^2 + \left(\frac{\partial^2 f}{\partial x \partial y}(a_1, a_2)\right)(x-a_1)(y-a_2) + \left(\frac{1}{2} \frac{\partial^2 f}{\partial y^2}(a_1, a_2)\right)(y-a_2)^2$$

$$= f(a_1, a_2) + \begin{bmatrix} \frac{\partial f}{\partial x}(a_1, a_2) & \frac{\partial f}{\partial y}(a_1, a_2) \end{bmatrix} \begin{bmatrix} x-a_1 \\ y-a_2 \end{bmatrix} + \frac{1}{2} \begin{bmatrix} x-a_1 & y-a_2 \end{bmatrix} \begin{bmatrix} \frac{\partial^2 f}{\partial x^2}(a_1, a_2) & \frac{\partial^2 f}{\partial x \partial y}(a_1, a_2) \\ \frac{\partial^2 f}{\partial y \partial x}(a_1, a_2) & \frac{\partial^2 f}{\partial y^2}(a_1, a_2) \end{bmatrix} \begin{bmatrix} x-a_1 \\ y-a_2 \end{bmatrix}$$

$$(\because \frac{\partial^2 f}{\partial x \partial y}(a_1, a_2) = \frac{\partial^2 f}{\partial y \partial x}(a_1, a_2))$$

$$= f(\vec{a}) + \nabla f(\vec{a}) (\vec{x}-\vec{a}) + \frac{1}{2} (\vec{x}-\vec{a})^T H(\vec{a}) (\vec{x}-\vec{a})$$

$$\text{where } \vec{x}-\vec{a} = \begin{bmatrix} x-a_1 \\ y-a_2 \end{bmatrix}, \nabla f(\vec{x}) = \begin{bmatrix} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial y} \end{bmatrix}, H(\vec{x}) = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix} \text{ called Hessian matrix.}$$

Taylor's Theorem for Two Variables

Theorem 12.1 (Taylor's Theorem for Two Variables)

Let D be an open convex set in \mathbb{R}^2 , let $\vec{a} = (a_1, a_2) \in D$

and let $f: D \rightarrow \mathbb{R}$ be a C^{n+1} function on D . Then,

$$f(\vec{x}) = f(x,y) = \sum_{k=0}^n \sum_{k_1+k_2=k} \left(\frac{1}{k_1! k_2!} \frac{\partial^{k_1+k_2} f}{\partial x^{k_1} \partial y^{k_2}}(a_1, a_2) \right) (x-a_1)^{k_1} (y-a_2)^{k_2} + R_n(\vec{x}) \quad \text{for } \vec{x} \in D$$

\parallel
 $P_n(x,y)$

$$\text{where } R_n(\vec{x}) = \sum_{k_1+k_2=n+1} \left(\frac{1}{k_1! k_2!} \frac{\partial^{k_1+k_2} f}{\partial x^{k_1} \partial y^{k_2}}(\vec{c}) \right) (x-a_1)^{k_1} (y-a_2)^{k_2} \quad \text{for some } \vec{c} = t\vec{a} + (1-t)\vec{x}, t \in (0,1).$$

Theorem 12.2 (Taylor's Theorem)

Let D be an open convex set in \mathbb{R}^m , let $\vec{a} = (a_1, a_2, \dots, a_m) \in D$.

and let $f: D \rightarrow \mathbb{R}$ be a C^{n+1} function on D . Then,

$$f(\vec{x}) = \sum_{k=0}^n \sum_{k_1+k_2+\dots+k_m=k} \left(\frac{1}{k_1!k_2!\dots k_m!} \frac{\partial^{k_p} f}{\partial x_1^{k_1} \partial x_2^{k_2} \dots \partial x_m^{k_m}}(\vec{a}) (x_1-a_1)^{k_1} (x_2-a_2)^{k_2} \dots (x_m-a_m)^{k_m} \right) + R_n(\vec{x}) \text{ for } \vec{x} \in D$$

" $P_n(\vec{x})$

where $R_n(\vec{x}) = \sum_{k_1+k_2+\dots+k_m=n+1} \left(\frac{1}{k_1!k_2!\dots k_m!} \frac{\partial^{k_p} f}{\partial x_1^{k_1} \partial x_2^{k_2} \dots \partial x_m^{k_m}}(\vec{c}) \right) (x_1-a_1)^{k_1} (x_2-a_2)^{k_2} \dots (x_m-a_m)^{k_m}$

for some $\vec{c} = t\vec{a} + (1-t)\vec{x}$, $t \in (0, 1)$.