

**Total Diferential** For a function  $f = f(x, y, z, \dots)$ , its total derivative is defined as

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

## Identity Involving Partial Derivative

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The Jacobian of  $[u(x, y), v(x, y)]$  with respect to  $(x, y)$  is defined by

$$\frac{\partial(u, v)}{\partial(x, y)} = \begin{vmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} \\ \frac{\partial v}{\partial x} & \frac{\partial v}{\partial y} \end{vmatrix}$$

Here are some identity relating the Jacobian with partial derivative.

**Unity.** Unity as in one

$$\frac{\partial(u, v)}{\partial(x, y)} = 1$$

*Proof.* Trivial

$$\frac{\partial(x, y)}{\partial(x, y)} = \begin{vmatrix} \frac{\partial x}{\partial x} & \frac{\partial x}{\partial y} \\ \frac{\partial y}{\partial x} & \frac{\partial y}{\partial y} \end{vmatrix} = \frac{\partial x}{\partial x} \frac{\partial y}{\partial y} - \frac{\partial x}{\partial y} \frac{\partial y}{\partial x} = 1 \quad \blacksquare$$

**Change of order.** It can be proved that change of order cost the minus sign

$$\frac{\partial(u, v)}{\partial(x, y)} = -\frac{\partial(v, u)}{\partial(x, y)} = -\frac{\partial(u, v)}{\partial(y, x)}$$

*Proof.* Those three terms literally have the same value when evaluated

$$\begin{aligned} \frac{\partial(u, v)}{\partial(x, y)} &= \begin{vmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} \\ \frac{\partial v}{\partial x} & \frac{\partial v}{\partial y} \end{vmatrix} = \frac{\partial u}{\partial x} \frac{\partial v}{\partial y} - \frac{\partial u}{\partial y} \frac{\partial v}{\partial x} \\ -\frac{\partial(v, u)}{\partial(x, y)} &= -\begin{vmatrix} \frac{\partial v}{\partial x} & \frac{\partial v}{\partial y} \\ \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} \end{vmatrix} = \frac{\partial v}{\partial y} \frac{\partial u}{\partial x} - \frac{\partial v}{\partial x} \frac{\partial u}{\partial y} \\ \frac{\partial(u, v)}{\partial(y, x)} &= -\begin{vmatrix} \frac{\partial u}{\partial y} & \frac{\partial u}{\partial x} \\ \frac{\partial v}{\partial y} & \frac{\partial v}{\partial x} \end{vmatrix} = \frac{\partial u}{\partial x} \frac{\partial v}{\partial y} - \frac{\partial u}{\partial y} \frac{\partial v}{\partial x} \end{aligned}$$

See?  $\blacksquare$

**Jacobian.** In terms of Jacobian, partial derivative of  $u$  with respect to  $x$  can be written as

$$\left. \frac{\partial u}{\partial x} \right|_y = \frac{\partial(u, y)}{\partial(x, y)}$$

*Proof.* Just evaluate the Jacobian

$$\frac{\partial(u, y)}{\partial(x, y)} = \begin{vmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} \\ \frac{\partial y}{\partial x} & \frac{\partial y}{\partial y} \end{vmatrix} = \frac{\partial u}{\partial x} \frac{\partial y}{\partial y} - \frac{\partial u}{\partial y} \frac{\partial y}{\partial x} = \frac{\partial u}{\partial x} \quad \blacksquare$$

**Chain rule for partial derivative.** The expression is

$$\frac{\partial(u, y)}{\partial(x, y)} = \frac{\partial(u, y)}{\partial(w, z)} \frac{\partial(w, z)}{\partial(x, y)}$$

*Proof.* The total differential of  $u$  and  $v$  as function  $w$  and  $z$  read

$$du = \frac{\partial u}{\partial w} dw + \frac{\partial u}{\partial v} dz \quad \wedge \quad dv = \frac{\partial v}{\partial w} dw + \frac{\partial v}{\partial z} dz$$

We can therefore evaluate the Jacobian

$$\begin{aligned} \frac{\partial(u, y)}{\partial(x, y)} &= \begin{vmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} \\ \frac{\partial v}{\partial x} & \frac{\partial v}{\partial y} \end{vmatrix} = \begin{vmatrix} \frac{\partial u}{\partial w} \frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \frac{\partial z}{\partial x} & \frac{\partial u}{\partial w} \frac{\partial w}{\partial y} + \frac{\partial u}{\partial z} \frac{\partial z}{\partial y} \\ \frac{\partial v}{\partial w} \frac{\partial w}{\partial x} + \frac{\partial v}{\partial z} \frac{\partial z}{\partial x} & \frac{\partial v}{\partial w} \frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} \frac{\partial z}{\partial y} \end{vmatrix} \\ &= \begin{vmatrix} \left( \frac{\partial u}{\partial w} & \frac{\partial u}{\partial z} \right) & \left( \frac{\partial w}{\partial x} & \frac{\partial w}{\partial y} \right) \\ \left( \frac{\partial v}{\partial w} & \frac{\partial v}{\partial z} \right) & \left( \frac{\partial z}{\partial x} & \frac{\partial z}{\partial y} \right) \end{vmatrix} = \begin{vmatrix} \frac{\partial u}{\partial w} & \frac{\partial u}{\partial z} \\ \frac{\partial v}{\partial w} & \frac{\partial v}{\partial z} \end{vmatrix} \begin{vmatrix} \frac{\partial w}{\partial x} & \frac{\partial w}{\partial y} \\ \frac{\partial z}{\partial x} & \frac{\partial z}{\partial y} \end{vmatrix} \end{aligned}$$

$$\frac{\partial(u, y)}{\partial(x, y)} = \frac{\partial(u, y)}{\partial(w, z)} \frac{\partial(w, z)}{\partial(x, y)} \quad \blacksquare$$

**The real chain rule.** We have

$$\left. \frac{\partial x}{\partial z} \right|_y = \frac{\partial z}{\partial x} \bigg|_y = 1$$

*Proof.* Trivial

$$1 = \frac{\partial(x, y)}{\partial(x, y)} = \frac{\partial(x, y)}{\partial(z, y)} \frac{\partial(z, y)}{\partial(x, y)} = \left. \frac{\partial x}{\partial z} \right|_y \left. \frac{\partial z}{\partial x} \right|_y \quad \blacksquare$$

**Yet another chain rule...** Even more chain rule...

$$\left. \frac{\partial x}{\partial y} \right|_w = \left. \frac{\partial x}{\partial z} \right|_w \left. \frac{\partial z}{\partial y} \right|_w$$

*Proof.* Trivial

$$\left. \frac{\partial x}{\partial y} \right|_w = \frac{\partial(x, w)}{\partial(y, w)} = \frac{\partial(x, w)}{\partial(z, w)} \frac{\partial(z, w)}{\partial(y, w)} = \left. \frac{\partial x}{\partial z} \right|_w \left. \frac{\partial z}{\partial y} \right|_w$$

**Cyclic rule.** This is chain rule all over again...

$$\left. \frac{\partial x}{\partial z} \right|_y \left. \frac{\partial z}{\partial y} \right|_x \left. \frac{\partial y}{\partial x} \right|_z = -1$$

*Proof.* Trivial

$$\begin{aligned} 1 &= \frac{\partial(x, y)}{\partial(x, y)} = \frac{\partial(x, y)}{\partial(z, y)} \frac{\partial(z, y)}{\partial(z, x)} \frac{\partial(z, x)}{\partial(x, y)} = -\frac{\partial(x, y)}{\partial(z, y)} \frac{\partial(y, z)}{\partial(x, z)} \frac{\partial(z, x)}{\partial(y, x)} \\ &= -\left. \frac{\partial x}{\partial z} \right|_y \left. \frac{\partial y}{\partial x} \right|_z \left. \frac{\partial z}{\partial y} \right|_x \quad \blacksquare \end{aligned}$$

## Application in Thermodynamics

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Here we will derive some useful intensive parameter used in thermodynamics. We assumed entropy function  $S$  has the form of

$$S = S(U, V, N_{i|r})$$

where  $N$  is number of chemical potential and  $N_{i|r} \equiv N_1, \dots, N_r$ . Therefore, its total differential is

$$dS = \left. \frac{\partial S}{\partial U} \right|_{V, N_{i|r}} dU + \left. \frac{\partial S}{\partial V} \right|_{U, N_{i|r}} dV + \sum_{j=1}^r \left. \frac{\partial S}{\partial N_j} \right|_{U, V, N_{i \neq r}} dN_j$$

We also assume the following quantities

$$T = \left. \frac{\partial U}{\partial S} \right|_{V, N_i} ; P = - \left. \frac{\partial U}{\partial V} \right|_{S, N_i} ; \mu_j = \left. \frac{\partial U}{\partial N} \right|_{S, V, N_{i \neq j}}$$

**First identity.** As follows.

$$\left. \frac{\partial S}{\partial U} \right|_{V, N_i} = \frac{1}{T}$$

*Proof.* We use chain rule with  $x \rightarrow U, y \rightarrow V, z \rightarrow S$ ; while keeping all the  $N_i$  constant

$$\left. \frac{\partial U}{\partial S} \right|_{V, N_i} \left. \frac{\partial S}{\partial U} \right|_{V, N_i} = 1 \implies \left. \frac{\partial S}{\partial U} \right|_{V, N_i} = \left( \left. \frac{\partial U}{\partial S} \right|_{V, N_i} \right)^{-1}$$

Then, from the definition of temperature

$$\left. \frac{\partial S}{\partial U} \right|_{V, N_i} = \frac{1}{T} \quad \blacksquare$$

**Second identity.** The identity written as

$$\left. \frac{\partial S}{\partial V} \right|_{U, N_i} = \frac{P}{T}$$

*Proof.* We invoke cyclic rule with  $x \rightarrow U, y \rightarrow V, z \rightarrow S$ ; while keeping all the  $N_i$  constant

$$1 = - \left. \frac{\partial U}{\partial S} \right|_{V, N_i} \left. \frac{\partial S}{\partial V} \right|_{U, N_i} \left. \frac{\partial V}{\partial U} \right|_{U, N_i}$$

Then, from the first identity and the definition of pressure

$$1 = T \left. \frac{\partial S}{\partial V} \right|_{U, N_i} \frac{1}{P} \implies \left. \frac{\partial S}{\partial V} \right|_{U, N_i} = \frac{P}{T} \quad \blacksquare$$

**Third Identity.** Expressed as

$$\left. \frac{\partial S}{\partial N_j} \right|_{U, N_{i \neq j}} = -\frac{P}{T}$$

*Proof.* We again invoke cyclic with  $x \rightarrow U, y \rightarrow N_j, z \rightarrow S$ ; while keeping  $V$  and all  $N$  except  $N_i$  constant

$$1 = -\frac{\partial U}{\partial S} \bigg|_{V, N_i} \frac{\partial S}{\partial N_j} \bigg|_{U, N_{i \neq j}} \frac{\partial N_j}{\partial U} \bigg|_{U, N_{i \neq j}}$$

Then, from the definition of temperature and chemical potential

$$1 = -T \frac{\partial S}{\partial N_j} \bigg|_{U, N_{i \neq j}} \frac{1}{\mu_j} \implies \frac{\partial S}{\partial N_j} \bigg|_{U, N_{i \neq j}} = -\frac{\mu_j}{T} \quad \blacksquare$$

## Lagrange Multipliers

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Let  $f(x, y, z)$  be our function that we want to optimize and  $\phi(x, y, z) = \text{const}$  be our constraint. We then set the total differential of  $f(x, y, z)$  and  $\phi(x, y, z)$  equal to zero

$$\begin{aligned} \frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy + \frac{\partial f}{\partial z} dz &= 0 \\ \frac{\partial \phi}{\partial x} dx + \frac{\partial \phi}{\partial y} dy + \frac{\partial \phi}{\partial z} dz &= 0 \end{aligned}$$

Next, we construct the function

$$F(x, y, z) = f(x, y, z) + \lambda \phi(x, y, z)$$

and set its total derivative to zero

$$\left( \frac{\partial f}{\partial x} + \lambda \frac{\partial \phi}{\partial x} \right) dx + \left( \frac{\partial f}{\partial y} + \lambda \frac{\partial \phi}{\partial y} \right) dy + \left( \frac{\partial f}{\partial z} + \lambda \frac{\partial \phi}{\partial z} \right) dz = 0$$

It follows that, for any value of  $dx, dy, dz$ , we choose  $\lambda$  such that

$$\frac{\partial f}{\partial x} + \lambda \frac{\partial \phi}{\partial x} = 0, \quad \frac{\partial f}{\partial y} + \lambda \frac{\partial \phi}{\partial y} = 0, \quad \frac{\partial f}{\partial z} + \lambda \frac{\partial \phi}{\partial z} = 0$$

Putting it all together, to optimize  $f(x, y, z)$  with constraint  $\phi(x, y, z)$ , we need to optimize  $F(x, y, z)$ , which obtained by solving three partial derivative equations and constraint equation  $\phi(x, y, z) = \text{const}$ . The equations in question are

$$\frac{\partial F}{\partial x} = 0, \quad \frac{\partial F}{\partial y} = 0,$$

$$\frac{\partial F}{\partial z} = 0, \quad \phi = \text{const}.$$

**Multiple constraint.** If there are multiple constraints, say  $\phi_1$  and  $\phi_2$ , we function  $F$  we construct instead is

$$F(x, y, z) = f(x, y, z) + \lambda_1 \phi_1(x, y, z) + \lambda_2 \phi_2(x, y, z)$$

As aside, the function that we want to optimize need not to a function of three variable  $x, y, z$ . The previous derivation can be justified for any number of variable. Of course, with more variable there are more variables.

## Leibniz' rule for Integral

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Differentiation under integral sign stated by Leibniz' rule

$$\frac{d}{dx} \int_{u(x)}^{v(x)} f(x, t) dt = \int_u^v \frac{\partial f}{\partial x} dt + f(x, v) \frac{dv}{dx} - f(x, u) \frac{du}{dx}$$

**Proof.** Suppose we want  $dI/dx$  where

$$I = \int_u^v f(t) dt$$

By the fundamental theorem of calculus

$$I = F(v) - F(u) = \mathcal{F}(v, u)$$

or  $I$  is a function of  $v$  and  $u$ . Finding  $dI/dx$  is then a partial differentiation problem. We can write

$$\frac{dI}{dx} = \frac{\partial I}{\partial v} \frac{dv}{dx} + \frac{\partial I}{\partial u} \frac{du}{dx}$$

By the fundamental theorem of calculus, we have

$$\begin{aligned} \frac{d}{dv} \int_a^v f(x) dt &= \frac{d}{dv} [F(v) - F(a)] = f(v) \\ \frac{d}{dv} \int_u^b f(x) dt &= \frac{d}{dv} [F(b) - F(u)] = -f(u) \end{aligned}$$

where  $u$  and  $v$  are a function of  $x$ , while  $a$  and  $b$  are a constant. This is the case when we consider  $\partial I/\partial v$  or  $\partial I/\partial u$ ; the other variable is constant. Then

$$\frac{d}{dx} \int_u^v f(t) dt = f(v) \frac{dv}{dx} - f(u) \frac{du}{dx}$$

Under not too restrictive conditions,

$$\frac{d}{dx} \int_a^b f(x, t) dt = \int_a^b \frac{\partial f(x, t)}{\partial x} dt$$

where, as before,  $a$  and  $b$  are constant. In other words, we can differentiate under the integral sign. It is convenient to collect these formulas into one formula known as Leibniz' rule:

$$\frac{d}{dx} \int_{u(x)}^{v(x)} f(x, t) dt = \int_u^v \frac{\partial f}{\partial x} dt + f(x, v) \frac{dv}{dx} - f(x, u) \frac{du}{dx} \quad \blacksquare$$