

1 変数の微分 differentiation

$$\frac{df(x)}{dx} = f'(x) = \lim_{\Delta x \rightarrow 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

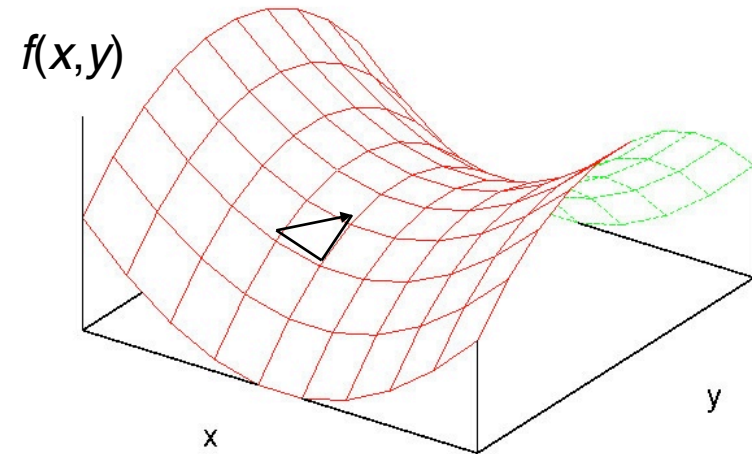
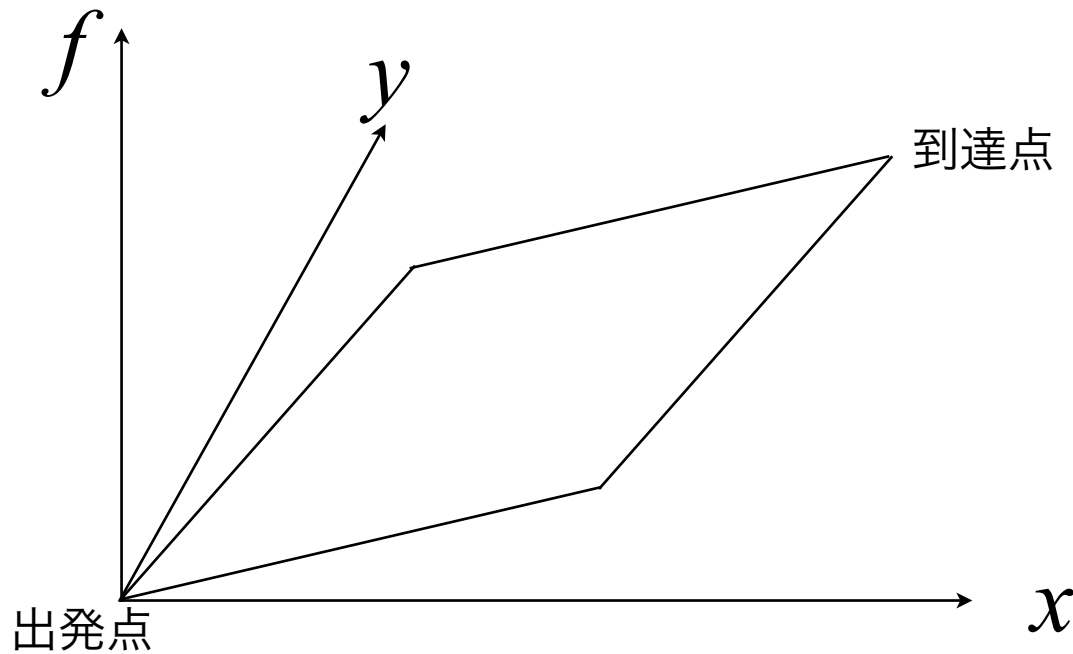
$$f(x + \Delta x) \simeq f(x) + \frac{df}{dx} \Delta x$$

$$f(x + \Delta x) - f(x) \simeq \frac{df}{dx} \Delta x \quad (1)$$

2次元系

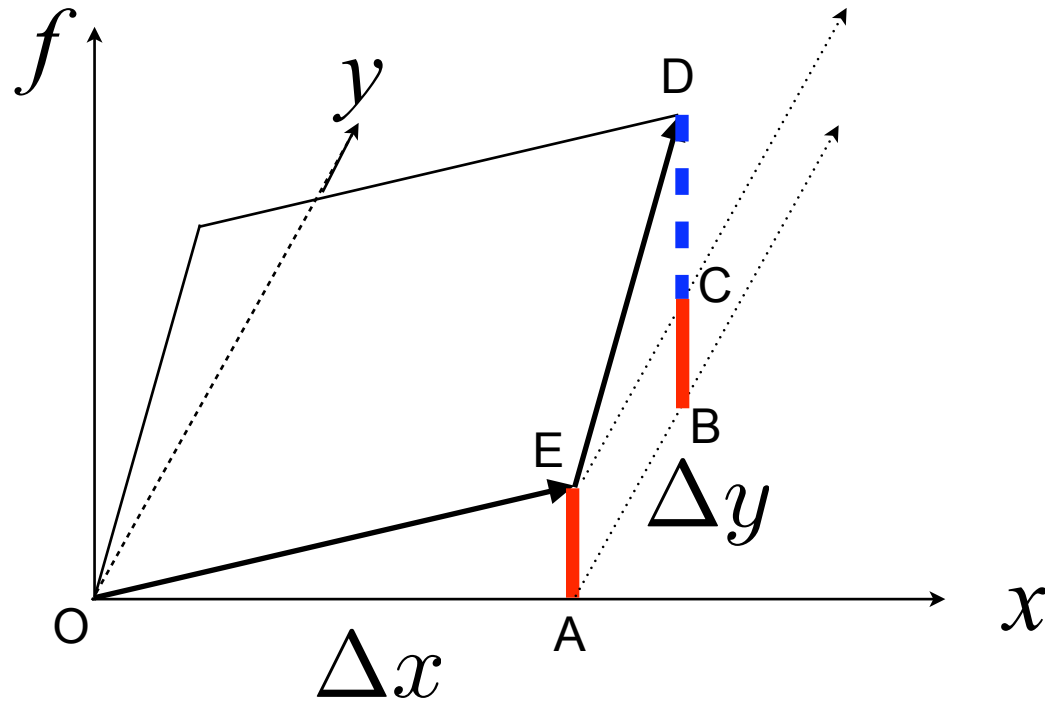
ある出発点から坂をのぼって到達点に登る

x : 東西方向 y : 南北方向



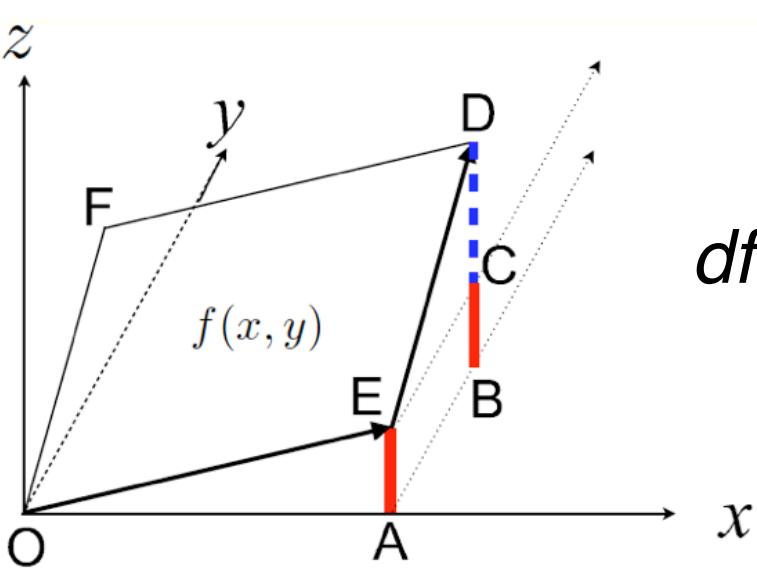
$f(x,y)$: x,y 地点での標高

$$\text{---} + \text{---} = \Delta f = f(x + \Delta x, y + \Delta y) - f(x, y)$$



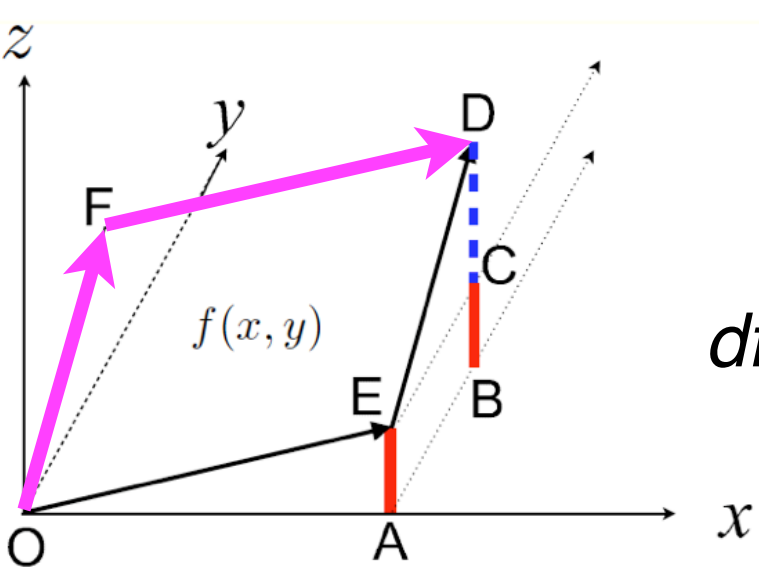
高さ = 傾き × 距離

$$\begin{aligned} df &= |BD| = |BC| + |CD| = |AE| + |CD| \\ &= \text{slope}(\vec{OE})|OA| + \text{slope}(\vec{ED})|EC| \end{aligned}$$



$$\begin{aligned}
 df &= |BD| = |BC| + |CD| = |AE| + |CD| \\
 &= \text{slope}(\vec{OE})|OA| + \text{slope}(\vec{ED})|EC|
 \end{aligned}$$

$$\begin{aligned}
 df &= \left(\frac{\partial f}{\partial x} \right)_y dx + \left(\frac{\partial f}{\partial y} \right)_{x+dx} dy \\
 &\simeq \left(\frac{\partial f}{\partial x} \right)_y dx + \left\{ \left(\frac{\partial f}{\partial y} \right)_x + \left[\frac{\partial}{\partial x} \left(\frac{\partial f}{\partial y} \right)_x \right]_y dx \right\} dy \\
 &= \left(\frac{\partial f}{\partial x} \right)_y dx + \left(\frac{\partial f}{\partial y} \right)_x dy + \left[\frac{\partial}{\partial x} \left(\frac{\partial f}{\partial y} \right)_x \right]_y dx dy \\
 &= \left(\frac{\partial f}{\partial x} \right)_y dx + \left(\frac{\partial f}{\partial y} \right)_x dy + \left(\frac{\partial f_y}{\partial x} \right)_y dx dy
 \end{aligned}$$



$$df = \text{slope}(\vec{OF})|AB| + \text{slope}(\vec{FD})|OA|$$

$$df = \left(\frac{\partial f}{\partial y} \right)_x dy + \left(\frac{\partial f}{\partial x} \right)_{y+dy} dx$$

$$\simeq \left(\frac{\partial f}{\partial y} \right)_x dy + \left\{ \left(\frac{\partial f}{\partial x} \right)_y + \left[\frac{\partial}{\partial y} \left(\frac{\partial f}{\partial x} \right)_y \right]_x dy \right\} dx$$

$$= \left(\frac{\partial f}{\partial x} \right)_y dx + \left(\frac{\partial f}{\partial y} \right)_x dy + \left[\frac{\partial}{\partial y} \left(\frac{\partial f}{\partial x} \right)_y \right]_x dx dy$$

$$= \left(\frac{\partial f}{\partial x} \right)_y dx + \left(\frac{\partial f}{\partial y} \right)_x dy + \left(\frac{\partial f_x}{\partial y} \right)_x dx dy$$

同じ df を与えるには,

$$\left(\frac{\partial f_x}{\partial y} \right)_x = \left(\frac{\partial f_y}{\partial x} \right)_y$$

$$\left[\frac{\partial}{\partial y} \left(\frac{\partial f}{\partial x} \right)_y \right]_x = \left[\frac{\partial}{\partial x} \left(\frac{\partial f}{\partial y} \right)_x \right]_y$$

別解

式を変形する。Eq.(1)を使う。

$$\begin{aligned}\Delta f &= f(x + \Delta x, y + \Delta y) - f(x, y) \\ &= f(x + \Delta x, y + \Delta y) - f(x + \Delta x, y) \\ &\quad + f(x + \Delta x, y) - f(x, y) \\ &\simeq f_y(x + \Delta x, y)\Delta y + f_x(x, y)\Delta x \\ &\simeq [f_y(x, y) + f_{yx}(x, y)\Delta x]\Delta y + f_x(x, y)\Delta x \\ &= f_x(x, y)\Delta x + f_y(x, y)\Delta y + f_{yx}(x, y)\Delta x\Delta y\end{aligned}\tag{2}$$

ここで以下の関係を使った

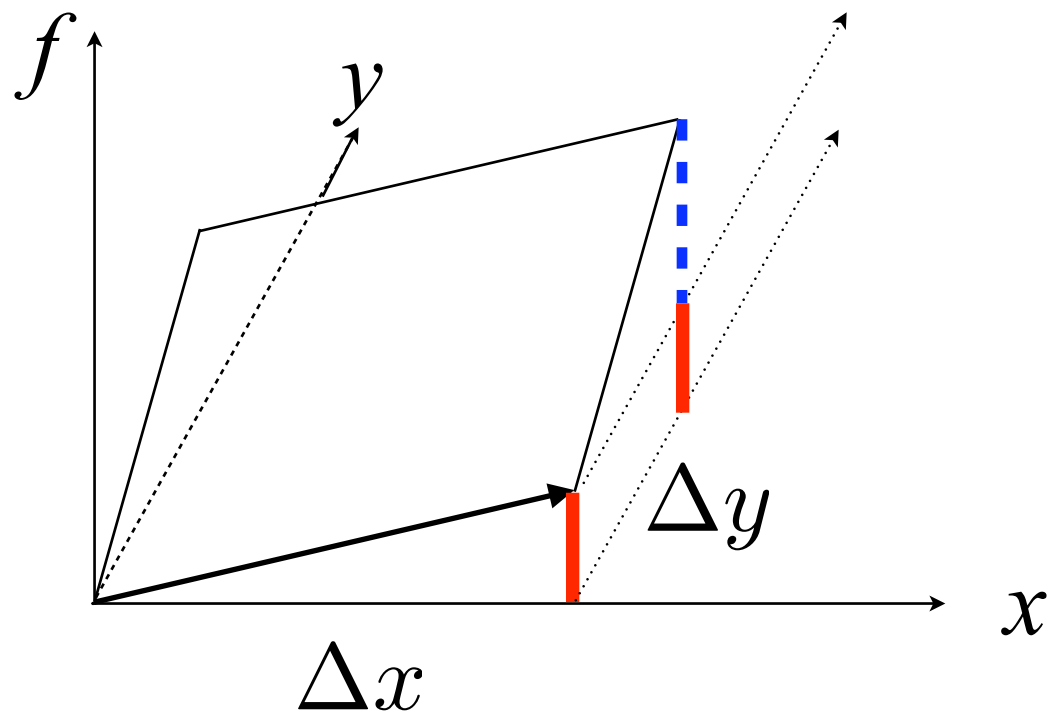
$$f_x(x, y) \equiv \left. \frac{\partial f}{\partial x} \right|_y = \left(\frac{\partial f}{\partial x} \right)_y$$

$$f_y(x, y) \equiv \left. \frac{\partial f}{\partial y} \right|_x = \left(\frac{\partial f}{\partial y} \right)_x$$

$$f_{yx}(x, y) \equiv \frac{\partial}{\partial x} \left[\left(\frac{\partial f}{\partial y} \right)_x \right]_y$$

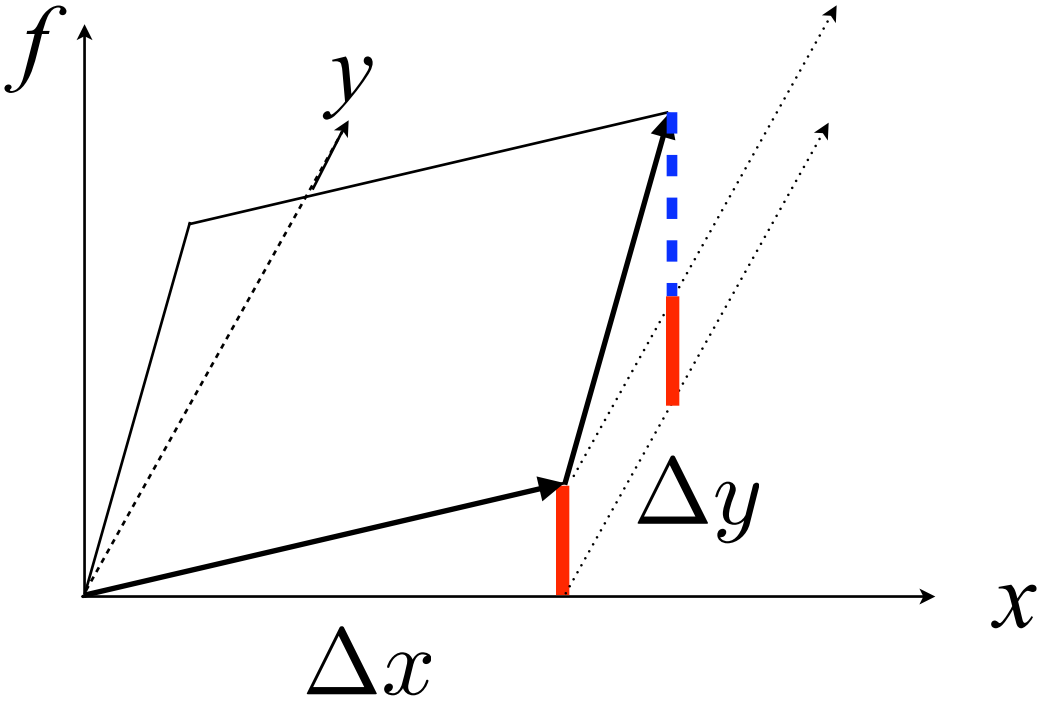
意味を図示しよう。

$$\text{—} = f_x(x, y) \Delta x = \left(\frac{\partial f}{\partial x} \right)_y \Delta x$$

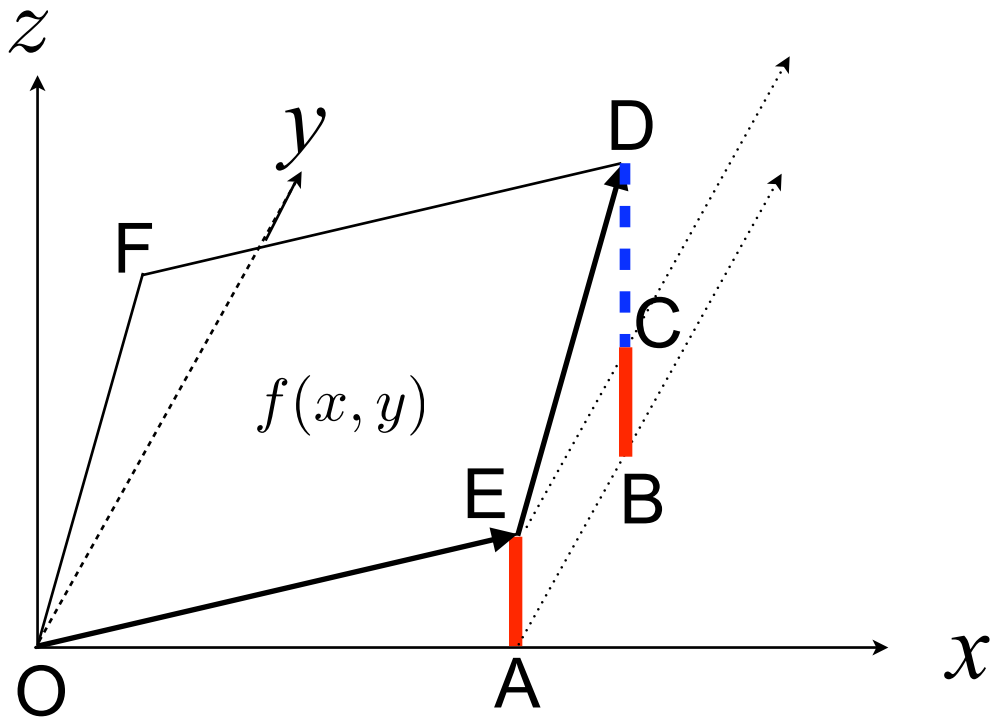


意味を図示しよう。

$$\text{---} = f_y(x, y) \Delta y = \left(\frac{\partial f}{\partial y} \right)_x \Delta y$$



問題1 Fig.1 に示した平面 OEDF を表す方程式が $z = f(x, y)$ で与えられる。全微分 $df = (\frac{\partial f}{\partial x})_y dx + (\frac{\partial f}{\partial y})_x dy$ の意味を図を使って説明せよ。 x 軸上にある OA の長さを dx , y 軸に平行な AB の長さを dy , z 軸に平行な BD の長さを df とする。また, AE の長さ と BC の長さは等しいものとする。ヒント: BD の長さを, AE と CD の長さに分けて考えよ。

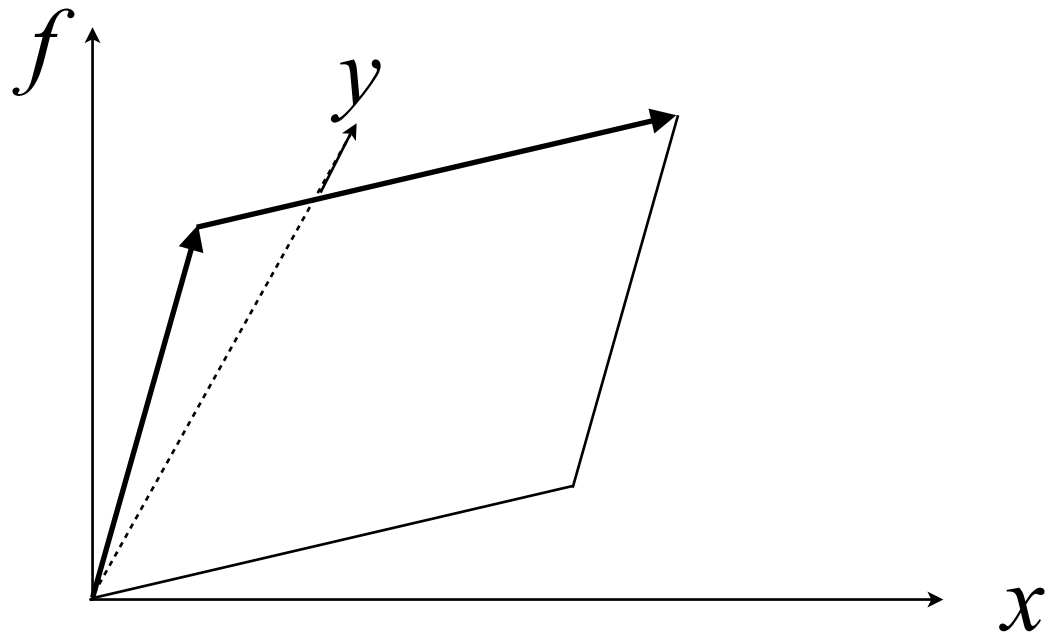


全微分と偏微分

total and partial total differentiation

$$df = \left(\frac{\partial f}{\partial x} \right)_y dx + \left(\frac{\partial f}{\partial y} \right)_x dy$$

another route? もあるはず。



以前と同じように式を変形する。Eq.(1)を使う。

$$\begin{aligned}\Delta f &= f(x + \Delta x, y + \Delta y) - f(x, y) \\ &= f(x + \Delta x, y + \Delta y) - f(x, y + \Delta y) \\ &\quad + f(x, y + \Delta y) - f(x, y) \\ &\simeq f_x(x, y + \Delta y)\Delta x + f_y(x, y)\Delta y \\ &\simeq [f_x(x, y) + f_{xy}(x, y)\Delta y]\Delta x + f_y(x, y)\Delta y \\ &= f_x(x, y)\Delta x + f_y(x, y)\Delta y + f_{xy}(x, y)\Delta x\Delta y\end{aligned}\tag{3}$$

$$f_{xy}(x, y) \equiv \frac{\partial}{\partial y} \left[\left(\frac{\partial f}{\partial x} \right)_y \right]_x$$

$$df = \left(\frac{\partial f}{\partial x} \right)_y dx + \left(\frac{\partial f}{\partial y} \right)_x dy$$

Eq. (2) と (3) の比較により

$$f_{xy}(x, y) = f_{yx}(x, y)$$

meaning of grad f : 2D system

vector :

$$d\mathbf{r} = dx\mathbf{i} + dy\mathbf{j} = (dx, dy)$$

vector :

$$\text{grad } f = \nabla f \equiv \frac{\partial f}{\partial x}\mathbf{i} + \frac{\partial f}{\partial y}\mathbf{j} = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y} \right)$$

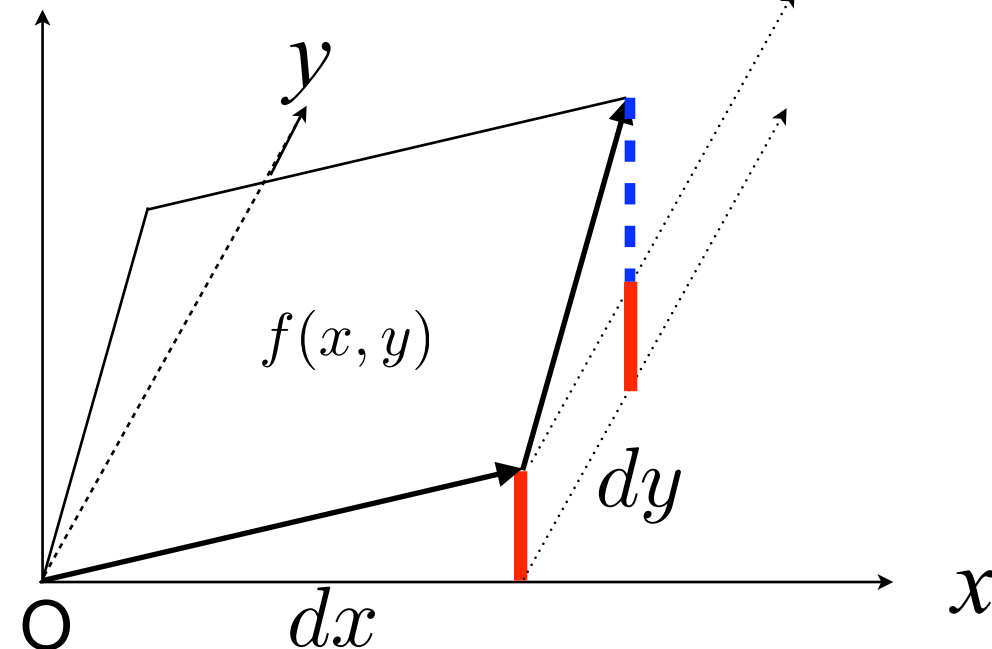
inner product :

$$\text{grad } f \cdot d\mathbf{r} = \nabla f \cdot d\mathbf{r} = \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial y}dy = df$$

under the condition that $d\mathbf{r} = \text{const.}$,

$\nabla f \parallel d\mathbf{r}$ gives the maximum of df ,

this means ∇f is the steepest descent direction.



状態関数 と 完全微分

状態関数：経路によらず2つの状態間の差で決まる。

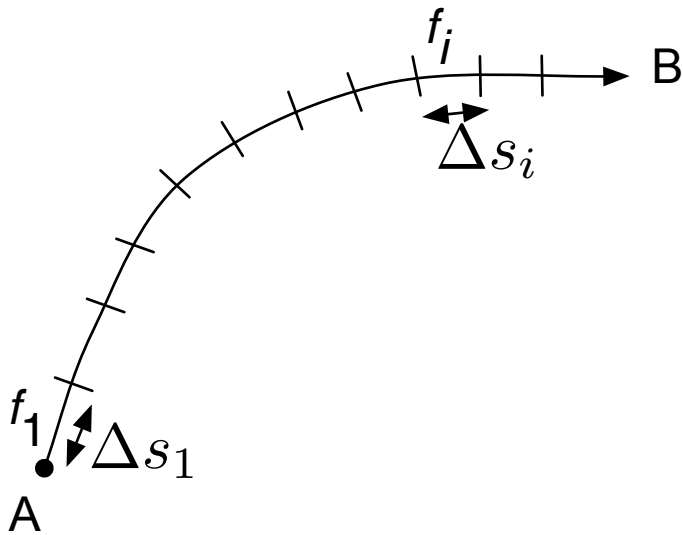
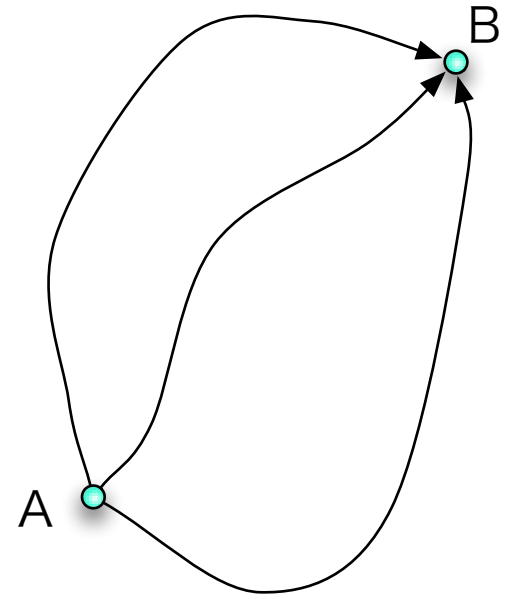
例：内部エネルギー

経路によるばあい

例：熱

線積分 line integral

$$\int_C f(x, y) ds = \lim_{\Delta s_i \rightarrow 0} \sum_i f_i \Delta s_i$$
$$f_i = f(x_i, y_i)$$



曲線を微小な弧に分割して、
それぞれの長さを、 $\Delta s_1, \Delta s_2, \dots, \Delta s_i, \dots$
とする。

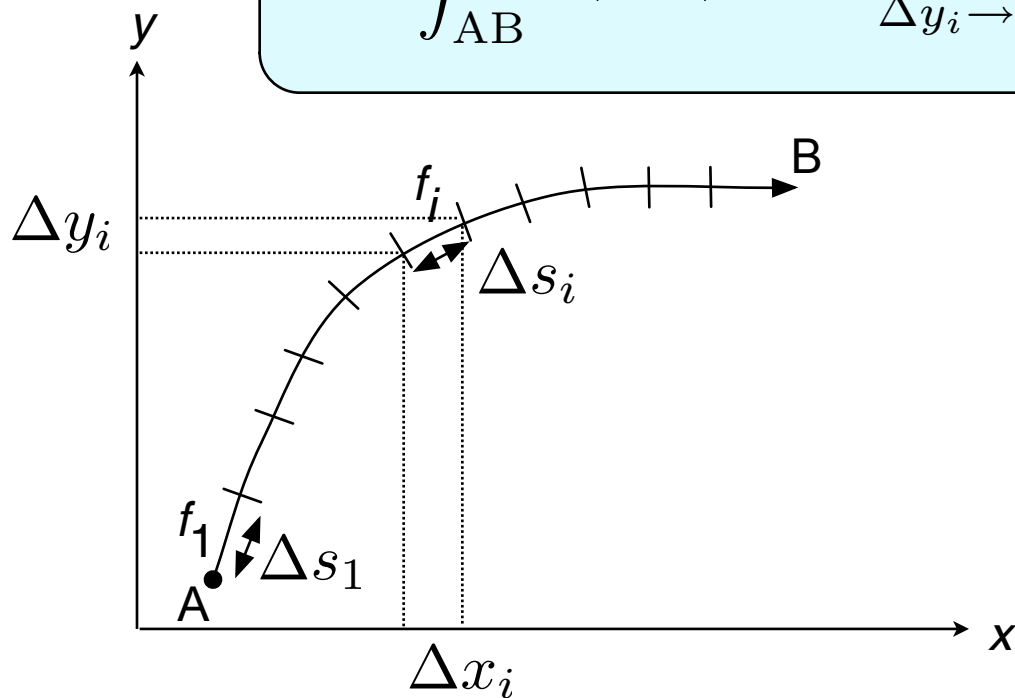
線積分 line integral

今, Δs_i の x 軸, y 軸への射影を $\Delta x_i, \Delta y_i$ とする。 x 軸と Δs_i のなす角を α とすると,

$$\Delta x_i = \cos \alpha \Delta s_i, \Delta y_i = \sin \alpha \Delta s_i$$

$$\int_{AB} f(x, y) dx \equiv \lim_{\Delta x_i \rightarrow 0} \sum_i f_i \Delta x_i$$

$$\int_{AB} f(x, y) dy \equiv \lim_{\Delta y_i \rightarrow 0} \sum_i f_i \Delta y_i$$



で, x 軸, y 軸上への射影の線積分を定義する。

完全微分, 不完全微分

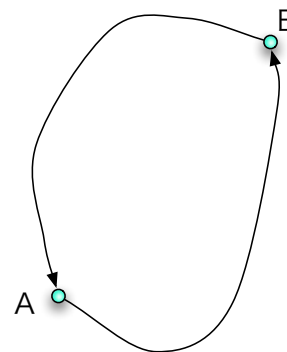
exact differential, nonexact (imperfect) differential

$$df = P(x, y)dx + Q(x, y)dy$$

をある点Aから点Bまでx軸, y軸上への射影の線積分をする。

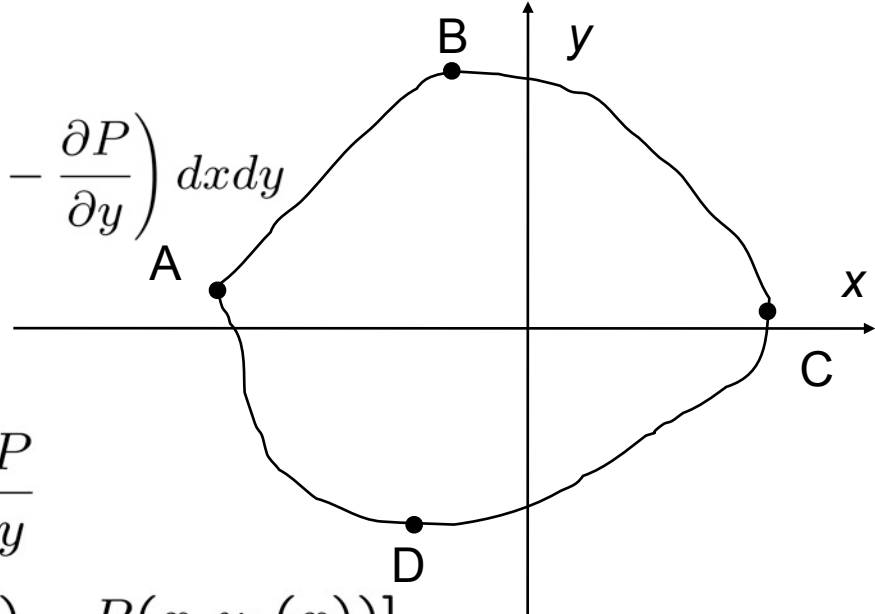
経路は, 2次元平面内で自由にとれるが, 積分が経路に依らないならば, 経路を任意にとってもとに戻る積分経路(経路が閉曲線)での線積分はゼロになる。経路が閉曲線の場合, 線積分を以下のように書く。

$$\oint df$$



Green's Theorem

$$\oint_C [P(x, y)dx + Q(x, y)dy] = \iint_R \left(\frac{\partial Q}{\partial x} - \frac{\partial P}{\partial y} \right) dx dy$$



ABC: $y_2(x)$, ADC: $y_1(x)$

$$\begin{aligned} \iint \frac{\partial P}{\partial y} dx dy &= \int_{x_A}^{x_C} dx \int_{y_1(x)}^{y_2(x)} dy \frac{\partial P}{\partial y} \\ &= \int_{x_A}^{x_C} dx [P(x, y_2(x)) - P(x, y_1(x))] \\ &= - \oint dx P, \quad (C \text{ is a counterclockwise direction}) \end{aligned}$$

DAB: $x_2(y)$, DCB: $x_1(y)$

$$\begin{aligned} \iint \frac{\partial Q}{\partial x} dx dy &= \int_{y_D}^{y_B} dy \int_{x_2(y)}^{x_1(y)} dx \frac{\partial Q}{\partial x} \\ &= \int_{y_D}^{y_B} dx Q(x_1(y), y) - Q(x_2(y), y) \\ &= \oint dy Q, \quad (C \text{ is a counterclockwise direction}) \end{aligned}$$

$$\frac{\partial P}{\partial y} = \frac{\partial Q}{\partial x}$$

なら, $\oint df = 0$ となる。

$$\begin{aligned} df &= P(x, y)dx + Q(x, y)dy \\ &= \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial y}dy \end{aligned}$$

と書けるなら, 完全微分が成立する上の式は

$$\frac{\partial}{\partial y} \frac{\partial f}{\partial x} = \frac{\partial}{\partial x} \frac{\partial f}{\partial y}$$

となる。

不完全微分 nonexact (imperfect) differential の例は

あるのか？

McQuarrie and Simon, Appendix H.10

$$dx = C_V(T)dT + \frac{nRT}{V}dV$$

$$\partial C_V(T)/\partial V = 0, \quad \partial(nRT/V)/\partial T = nR/V$$

→ nonexact

$$\frac{dx}{T} = \frac{C_V(T)}{T}dT + \frac{nR}{V}dV$$

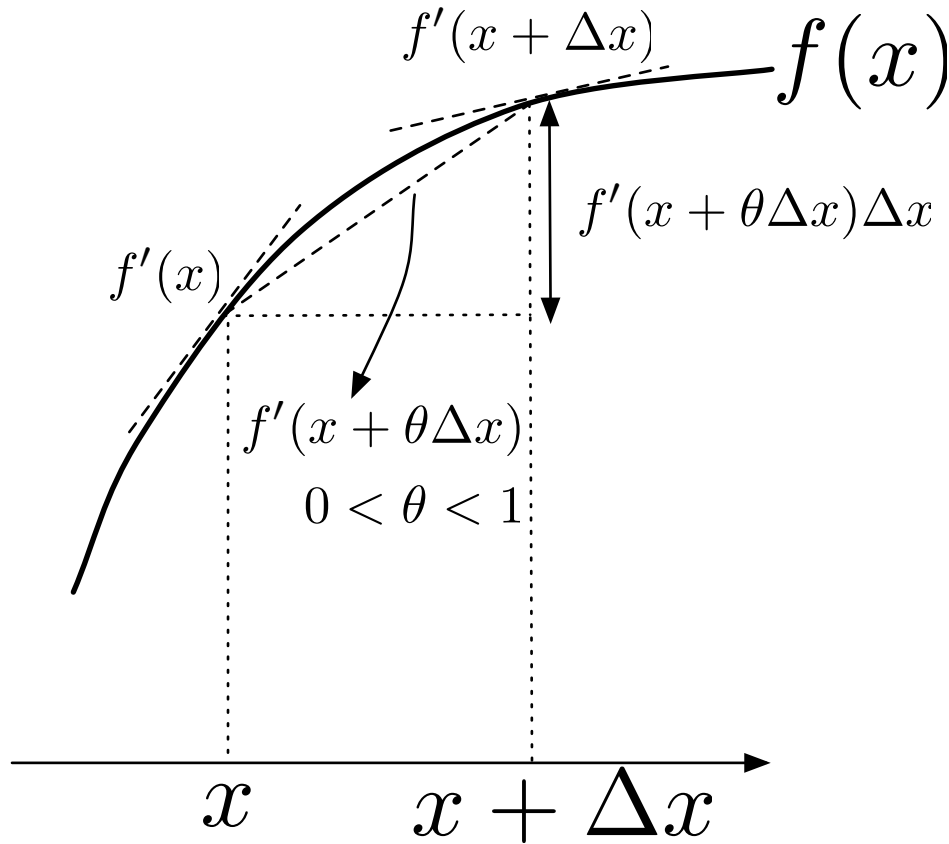
$$\partial[C_V(T)T^{-1}]/\partial V = \partial(nR/V)/\partial T = 0$$

→ exact

より厳密には

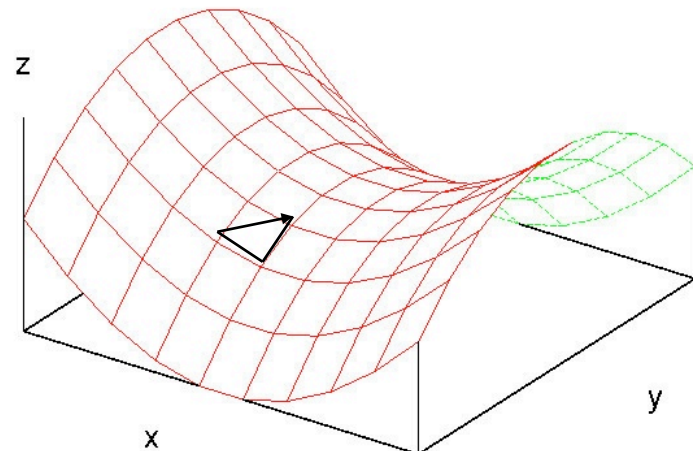
微分 differentiation

$$\frac{df(x)}{dx} = f'(x) = \lim_{\Delta x \rightarrow 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}$$



$$f(x + \Delta x) - f(x) \simeq f'(x + \theta\Delta x)\Delta x$$

Total 全微分 and Partial Differentials 偏微分



$$\begin{aligned}\Delta f &= f(x + \Delta x, y + \Delta y) - f(x, y) \\ &= [f(x + \Delta x, y + \Delta y) - f(x, y + \Delta y)] + [f(x, y + \Delta y) - f(x, y)] \\ &= f_x(x + \theta_1 \Delta x, y + \Delta y) \Delta x + f_y(x, y + \theta_2 \Delta y) \Delta y, \quad (0 < \theta_1, \theta_2 < 1) \\ &= f_x(x, y) \Delta x + f_y(x, y) \Delta y + \epsilon_1 \Delta x + \epsilon_2 \Delta y\end{aligned}$$

$$f_x = \frac{\partial f}{\partial x} = \lim_{\Delta x \rightarrow 0} \frac{f(x + \Delta x, y) - f(x, y)}{\Delta x}$$

$$f_y = \frac{\partial f}{\partial y} = \lim_{\Delta y \rightarrow 0} \frac{f(x, y + \Delta y) - f(x, y)}{\Delta y}$$

$$\epsilon_1 \equiv f_x(x + \theta_1 \Delta x, y + \Delta y) - f_x(x, y)$$

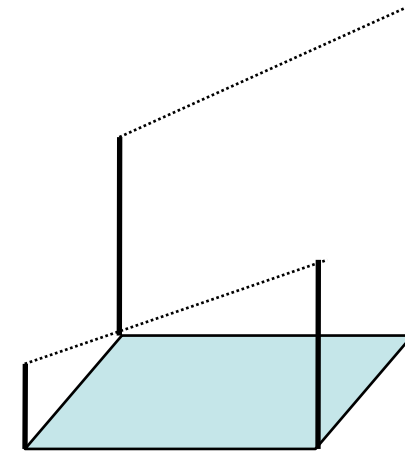
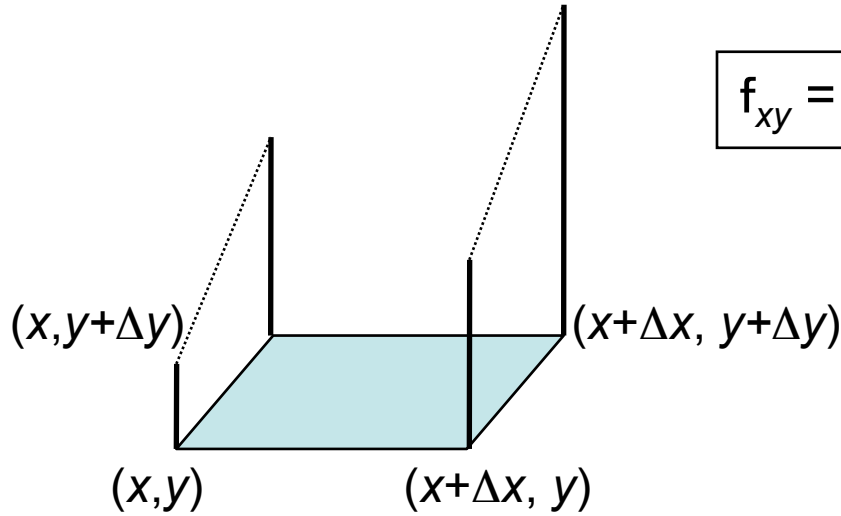
$$\epsilon_2 \equiv f_y(x, y + \theta_2 \Delta y) - f_y(x, y)$$

$$df = f_x(x, y)dx + f_y(x, y)dy = \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial y}dy \quad \text{全微分(第一階全微分)}$$

$$F = f(x + \Delta x, y + \Delta y) - f(x + \Delta x, y) - [f(x, y + \Delta y) - f(x, y)]$$

$$F = f(x + \Delta x, y + \Delta y) - f(x, y + \Delta y) - [f(x + \Delta x, y) - f(x, y)]$$

$f_{xy} = f_{yx}$ の証明



$$\begin{aligned} \varphi(x) &= f(x, y + \Delta y) - f(x, y) \\ \varphi'(x) &= f_x(x, y + \Delta y) - f_x(x, y) \end{aligned}$$

$$\begin{aligned} \phi(y) &= f(x + \Delta x, y) - f(x, y) \\ \phi'(y) &= f_y(x + \Delta x, y) - f_y(x, y) \end{aligned}$$

$$\begin{aligned} F &= \varphi(x + \Delta x) - \varphi(x) \\ &= \Delta x \varphi'(x + \theta \Delta x) \\ &= \Delta x \{f_x(x + \theta \Delta x, y + \Delta y) - f_x(x + \theta \Delta x, y)\} \\ &= \Delta x \Delta y f_{xy}(x + \theta \Delta x, y + \theta' \Delta y) \end{aligned}$$

$$\begin{aligned} F &= \phi(y + \Delta y) - \phi(y) \\ &= \Delta y \phi'(y + \theta_1 \Delta y) \\ &= \Delta y \{f_y(x + \Delta x, y + \theta_1 \Delta y) - f_y(x, y + \theta_1 \Delta y)\} \\ &= \Delta x \Delta y f_{yx}(x + \theta'_1 \Delta x, y + \theta_1 \Delta y) \end{aligned}$$

$$\Delta x, \Delta y \rightarrow 0, \quad f_{xy} = f_{yx}$$

高次の展開 (ここは省略可)

$$\begin{aligned}\Delta f &= f(x + \Delta x, y + \Delta y) - f(x, y) \\ &= [f(x + \Delta x, y + \Delta y) - f(x, y + \Delta y)] \\ &\quad + [f(x, y + \Delta y) - f(x, y)]\end{aligned}$$

$$\begin{aligned}f(x + \Delta x, y + \Delta y) - f(x, y + \Delta y) &= \Delta x f_x(x, y + \Delta y) + \frac{(\Delta x)^2}{2} f_{xx}(x + \theta_1 \Delta x, y + \Delta y) \\ &= \Delta x \{f_x(x, y) + \Delta y f_{xy}(x, y + \theta_2 \Delta y)\} \\ &\quad + \frac{(\Delta x)^2}{2} f_{xx}(x + \theta_1 \Delta x, y + \Delta y)\end{aligned}$$

$$f(x, y + \Delta y) - f(x, y) = \Delta y f_y(x, y) + \frac{(\Delta y)^2}{2} f_{yy}(x, y + \theta_3 \Delta y)$$

$$\begin{aligned}\Delta f &= \{\Delta x f_x(x, y) + \Delta y f_y(x, y)\} \\ &\quad + \frac{1}{2} \left\{ (\Delta x)^2 f_{xx}(x + \theta_1 \Delta x, y + \Delta y) + 2\Delta x \Delta y f_{xy}(x, y + \theta_2 \Delta y) \right. \\ &\quad \left. + (\Delta y)^2 f_{yy}(x, y + \theta_3 \Delta y) \right\}\end{aligned}$$

$$\Delta f = df + \frac{1}{2} d^2 f$$

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

$$d^2 f = \frac{\partial^2 f}{\partial x^2} dx^2 + 2 \frac{\partial^2 f}{\partial xy} dx dy + \frac{\partial^2 f}{\partial y^2} dy^2 \quad \rightarrow \text{第二階全微分}$$