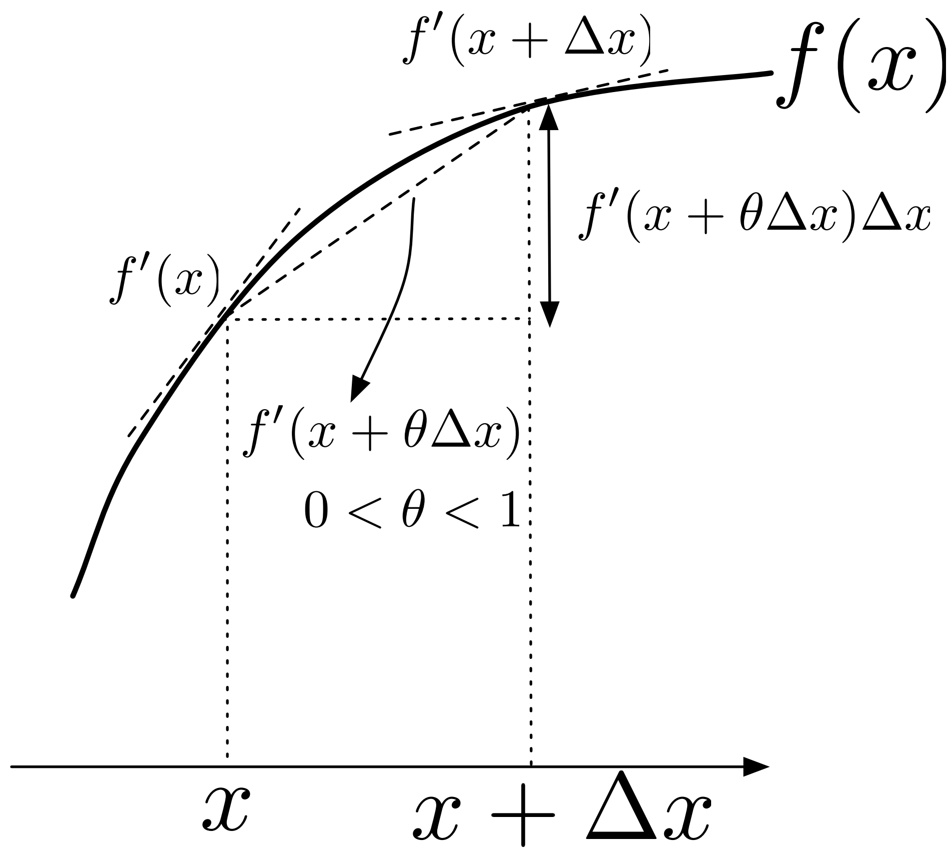
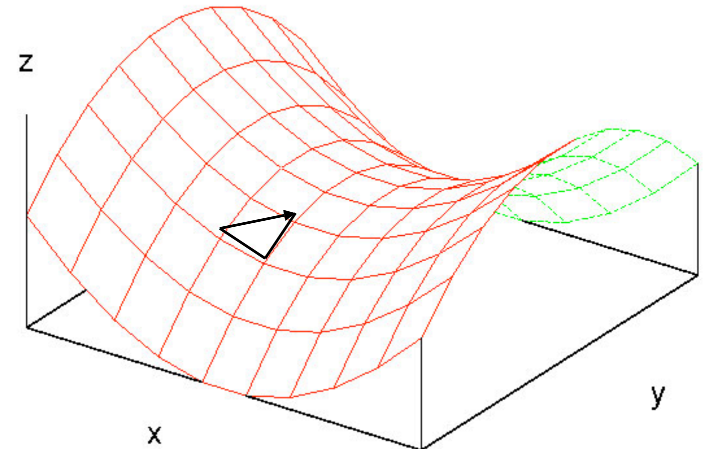
微分　differentiation

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



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

Total 全微分 and Partial Differentials 偏微分



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

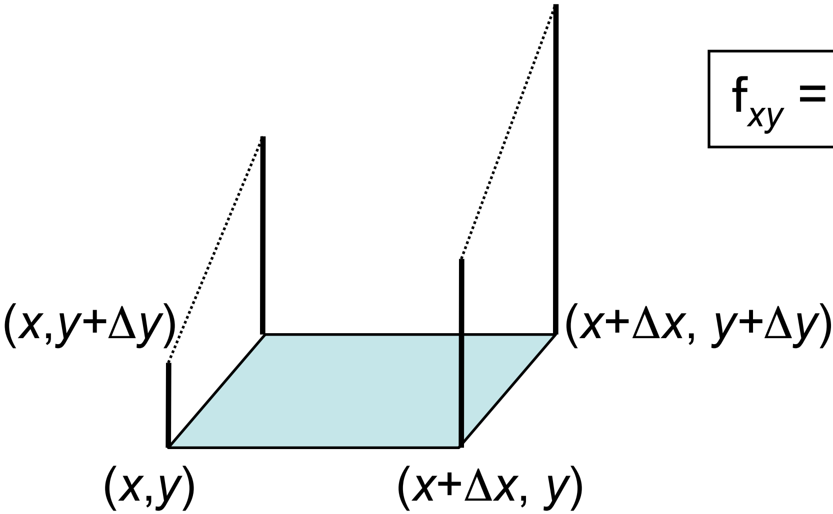
$$
\begin{aligned}
f_x &= \frac{\partial f}{\partial x} = \lim_{\Delta x\to 0}\frac{f(x+\Delta x, y) - f(x,y)}{\Delta x} \\
f_y &= \frac{\partial f}{\partial y} = \lim_{\Delta y\to 0}\frac{f(x, y+\Delta y) - f(x,y)}{\Delta y} \\
\epsilon_1 &\equiv f_x(x+\theta_1\Delta x, y+\Delta y) - f_x(x,y) \\
\epsilon_2 &\equiv f_y(x, y+\theta_2\Delta y) - f_y(x,y)
\end{aligned}
$$

$$
df = f_x(x,y)dx + f_y(x,y)dy = \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial y}dy
$$

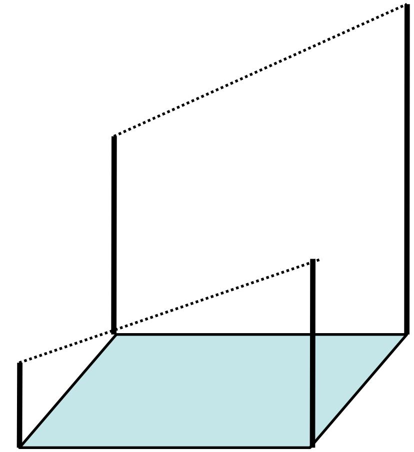
全微分（第一階全微分）

$f_{xy} = f_{yx}$ の証明

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



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



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

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

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

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

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

高次の展開（ここは省略可）

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

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

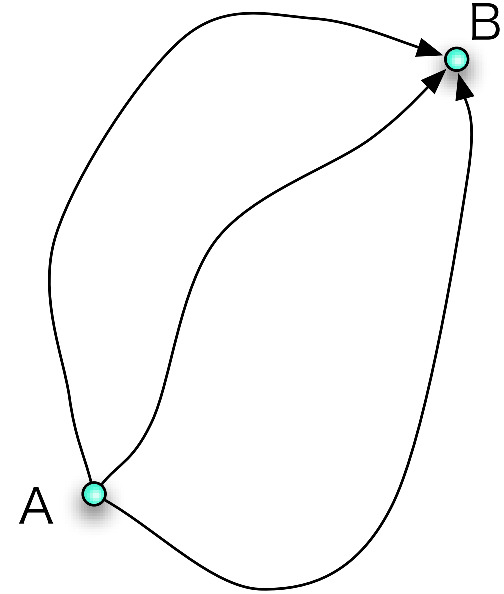
$$\begin{aligned}\Delta f &= \left\{ \Delta x f_x(x,y) + \Delta y f_y(x,y) \right\} \\ &\quad + \frac{1}{2} \Big\{ (\Delta x)^2 f_{xx}(x+\theta_1 \Delta x, y+\Delta y) + 2 \Delta x \Delta y f_{xy}(x, y+\theta_2 \Delta y) \\ &\quad + (\Delta y)^2 f_{yy}(x, y+\theta_3 \Delta y) \Big\}\end{aligned}$$

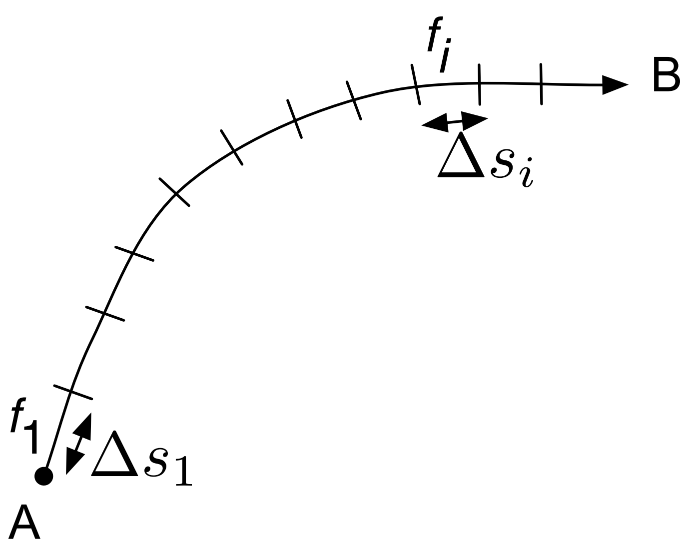
$$\begin{aligned}\Delta f &= df + \frac{1}{2} d^2 f \\ df &= \frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy \\ d^2 f &= \frac{\partial^2 f}{\partial x^2} dx^2 + 2 \frac{\partial^2 f}{\partial xy} dx dy + \frac{\partial^2 f}{\partial y^2} dy^2 \qquad \rightarrow \text{第二階全微分}\end{aligned}$$

線積分 line integral

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

$$f_i = f(x_i, y_i)$$





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

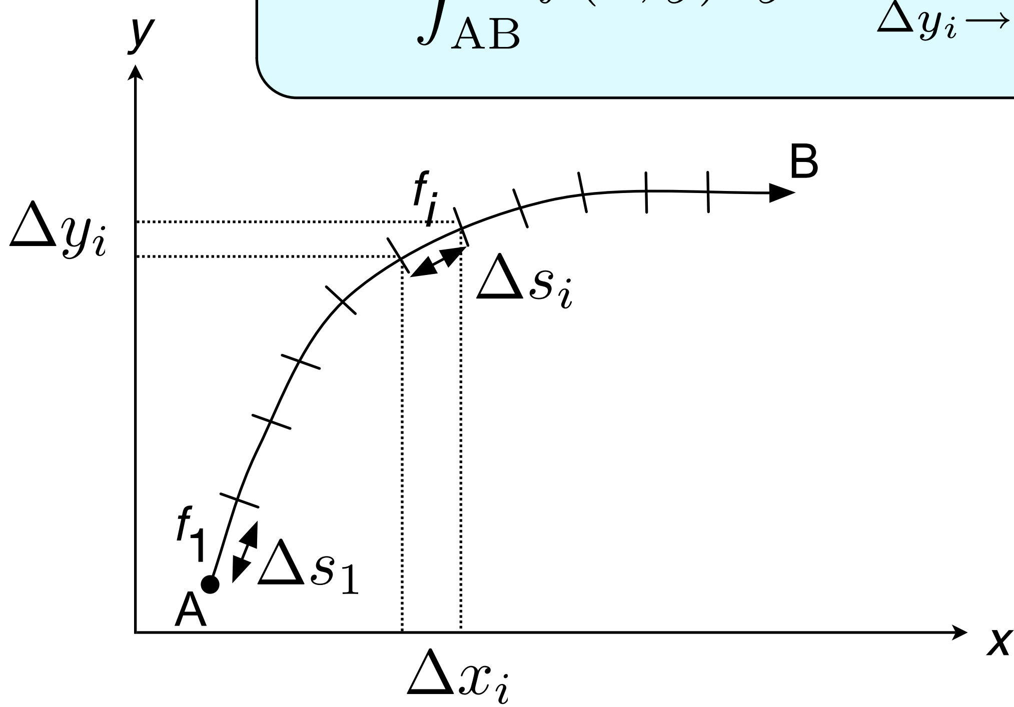
線積分 line integral

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，

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

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

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



で，*x*軸，*y*軸上への射影の線積分を定義する。

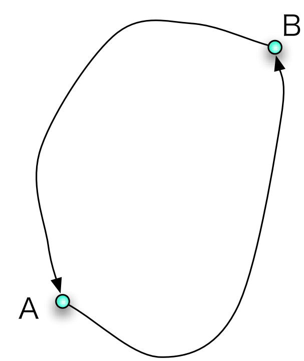
完全微分，不完全微分

exact differential, nonexact (imperfect) differential

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

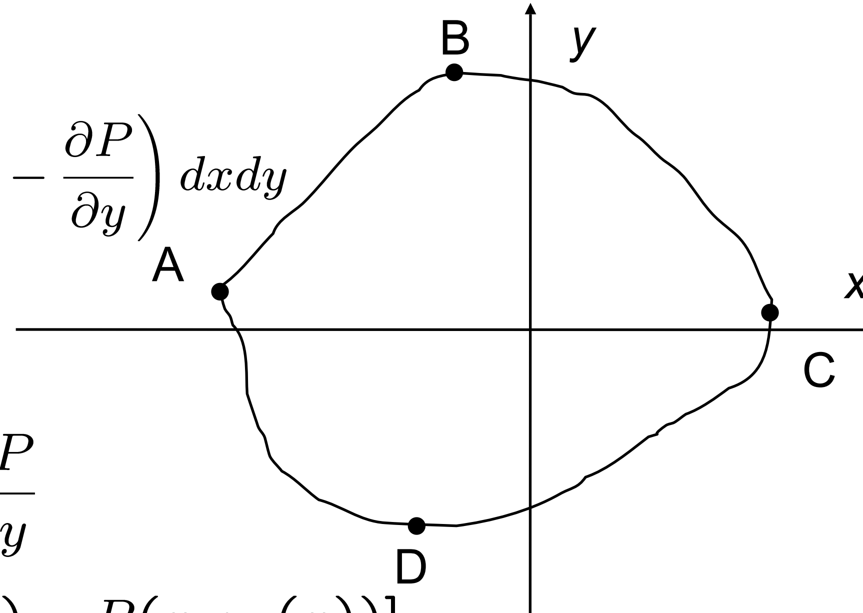
をある点Aから点Bまで*x*軸，*y*軸上への射影の線積分をする。
経路は，２次元平面内で自由にとれるが，積分が経路に依らないならば，
経路を任意にとってもとに戻る積分経路（経路が閉曲線）での
線積分はゼロになる。 経路が閉曲線の場合，線積分を
以下のように書く。

$$\oint df$$



Green's Theorem

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



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

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

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

$$\int\int \frac{\partial Q}{\partial x} dxdy = \int_{y_D}^{y_B} dy \int_{x_2(y)}^{x_1(y)} dx \frac{\partial Q}{\partial x}$$
$$= \int_{y_D}^{y_B} dxQ(x_1(y), y) - Q(x_2(y), y)$$
$$= \oint dyQ, \quad (C \text{ is a counterclockwise direction})$$

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

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

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

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

$$\rightarrow \ \text{nonexact}$$

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

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

$$\rightarrow \ \text{exact}$$