二階偏微分の非対角項における高精度数値差分法

森 渉

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1 二階偏微分の数値差分

2 変数テイラーの定理より

$$f(a+h_x, b+h_y) = f(a,b)$$
$$+\hat{D}(h_x,h_y)f + \frac{1}{2!}\hat{D}^2(h_x,h_y)f + \frac{1}{3!}\hat{D}^3(h_x,h_y)f + \frac{1}{4!}\hat{D}^4(h_x,h_y)f + \frac{1}{5!}\hat{D}^5(h_x,h_y)f + \dots$$

但し $\hat{D}(h_x,h_y) = (h_x\frac{\partial}{\partial x} + h_y\frac{\partial}{\partial y}) = (\hat{X}+\hat{Y})$ を表す
$\hat{D}(h_x,h_y)$ について

$$\begin{aligned}\hat{D}^2(h_x,h_y) &= (h_x\frac{\partial}{\partial x} + h_y\frac{\partial}{\partial y})^2 \\ &= (h_x^2\frac{\partial^2}{\partial x^2} + 2h_yh_x\frac{\partial^2}{\partial y\partial x} + h_y^2\frac{\partial^2}{\partial y^2}) \qquad (1)\end{aligned}$$

$$\hat{D}(ah_x,ah_y) = (ah_x\frac{\partial}{\partial x} + ah_y\frac{\partial}{\partial y}) = a\hat{D}(h_x,h_y) \ (a \text{ は定数}) \qquad (2)$$

$$\hat{D}^2(h_x,h_y) - \hat{D}^2(-h_x,h_y) = (\hat{X}+\hat{Y})^2 - (-\hat{X}+\hat{Y})^2 = 4\hat{X}\hat{Y} = 4h_xh_y\frac{\partial^2}{\partial x\partial y} \qquad (3)$$

$$\begin{aligned}\hat{D}^4(h_x,h_y) - \hat{D}^4(-h_x,h_y) &= (\hat{X}+\hat{Y})^4 - (-\hat{X}+\hat{Y})^4 = 8(\hat{X}^3\hat{Y} + \hat{X}\hat{Y}^3) \\ &= 8(h_x^3h_y\frac{\partial^4}{\partial x^3\partial y} + h_xh_y^3\frac{\partial^4}{\partial x\partial y^3}) \qquad (4)\end{aligned}$$

ここで

$$\begin{aligned}&f(a-h_x, b-h_y) = f(a,b) \\ &+\hat{D}(-h_x,-h_y)f + \frac{1}{2!}\hat{D}^2(-h_x,-h_y)f + \frac{1}{3!}\hat{D}^3(-h_x,-h_y)f + \frac{1}{4!}\hat{D}^4(-h_x,-h_y)f + \frac{1}{5!}\hat{D}^5(-h_x,-h_y)f + \dots \\ &= f(a,b) - \hat{D}(h_x,h_y)f + \frac{1}{2!}\hat{D}^2(h_x,h_y)f - \frac{1}{3!}\hat{D}^3(h_x,h_y)f + \frac{1}{4!}\hat{D}^4(h_x,h_y)f - \frac{1}{5!}\hat{D}^5(h_x,h_y)f + \dots \qquad (5)\end{aligned}$$

$f(a+h_x,b+h_y)$ と $f(a-h_x,b-h_y)$ の和を求める

$$f(a+h_x,b+h_y) + f(a-h_x,b-h_y) = 2f(a,b) + 2\frac{1}{2!}\hat{D}^2(h_x,h_y)f + 2\frac{1}{4!}\hat{D}^4(h_x,h_y)f + \dots \qquad (6)$$

$$f(a-h_x,b+h_y) + f(a+h_x,b-h_y) = 2f(a,b) + 2\frac{1}{2!}\hat{D}^2(-h_x,h_y)f + 2\frac{1}{4!}\hat{D}^4(-h_x,h_y)f + \dots \qquad (7)$$

(6) と (7) の差 $F(h_x,h_y)$ を取る

$$
\begin{aligned}
F(h_x,h_y) &= f(a+h_x,b+h_y)+f(a-h_x,b-h_y)-(f(a-h_x,b+h_y)+f(a+h_x,b-h_y)) \quad (8)\\
&= 2\frac{1}{2!}(\hat{D}^2(h_x,h_y)-\hat{D}^2(-h_x,h_y))f+2\frac{1}{4!}(\hat{D}^4(h_x,h_y)-\hat{D}^4(-h_x,h_y))f+\dots\\
&= 4h_xh_y\frac{\partial^2}{\partial x\partial y}f+2\frac{1}{4!}8(h_x^3h_y\frac{\partial^4}{\partial x^3\partial y}+h_xh_y^3\frac{\partial^4}{\partial x\partial y^3})f+O(h_x^6)\\
\therefore \frac{\partial^2}{\partial x\partial y}f &= \frac{F(h_x,h_y)}{4h_xh_y}+O(h_x^2) \quad (9)
\end{aligned}
$$

よって結論のは h_x^2 オーダーで正確。

2 高精度数値差分

1 変数の四点微分法同様にして高精度にする。
$F(2h_x,2h_y)$ について

$$
\begin{aligned}
F(2h_x,2h_y) &= 4(2h_x)(2h_y)\frac{\partial^2}{\partial x\partial y}f+2\frac{1}{4!}8((2h_x)^3 2h_y\frac{\partial^4}{\partial x^3\partial y}+(2h_x)(2h_y)^3\frac{\partial^4}{\partial x\partial y^3})f+\dots\\
&= 16h_xh_y\frac{\partial^2}{\partial x\partial y}f+16*2\frac{1}{4!}8(h_x^3h_y\frac{\partial^4}{\partial x^3\partial y}+h_xh_y^3\frac{\partial^4}{\partial x\partial y^3})f+\dots \quad (10)
\end{aligned}
$$

$16F(h_x,h_y)-F(2h_x,2h_y)$ について第二項は打ち消すので

$$
\begin{aligned}
16F(h_x,h_y)-F(2h_x,2h_y) &= 16*4h_xh_y\frac{\partial^2}{\partial x\partial y}f \quad -16h_xh_y\frac{\partial^2}{\partial x\partial y}f+\dots\\
&= 48h_xh_y\frac{\partial^2}{\partial x\partial y}f \quad +\dots \quad (11)\\
\therefore \frac{\partial^2}{\partial x\partial y}f &= \frac{16F(h_x,h_y)-F(2h_x,2h_y)}{48h_xh_y}+O(h_x^4) \quad (12)\\
F(h_x,h_y) &= f(a+h_x,b+h_y)+f(a-h_x,b-h_y)-(f(a-h_x,b+h_y)+f(a+h_x,b-h_y))
\end{aligned}
$$

非対角項は 8 点で計算すれば高精度の数値微分計算が可能となる。