Nantes Université
Department of Earth Sciences
http://www.univ-nantes.fr/sciences/dptstu

Let f be C^{n+1} on an open interval containing x_i. The Taylor expansion of f about x_i with the Lagrange form of the remainder is

$$f(x_i+\delta x) = f(x_i) + \delta x\, f'(x_i) + \frac{(\delta x)^2}{2!} f''(x_i) + \cdots + \frac{(\delta x)^n}{n!} f^{(n)}(x_i) + R_{n+1}(x_i,\delta x), \tag{1}$$

where the remainder (Lagrange form) is

$$R_{n+1}(x_i,\delta x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}\,(\delta x)^{n+1} \qquad \text{for any } \xi \text{ in the interval } x_i \text{ and } x_i+\delta x.$$

Using big-O notation,

$$R_{n+1}(x_i,\delta x) = O\big((\delta x)^{n+1}\big) \quad \text{as } \delta x \to 0, \tag{2}$$

because the Lagrange form shows the remainder is proportional to $(\delta x)^{n+1}$, up to a factor depending on the $(n+1)$-th derivative.

A short proof that the Lagrange remainder implies the O-bound

Proof. Suppose $f \in C^{n+1}$ on a closed interval I containing the segment between x_i and $x_i+\delta x$. Then $f^{(n+1)}$ is continuous on I and therefore bounded: there exists $M>0$ such that

$$\big|f^{(n+1)}(t)\big| \le M \qquad \text{for all } t \in I.$$

The Lagrange remainder definition can be then written as,

$$R_{n+1}(x_i,\delta x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}\,(\delta x)^{n+1}$$

for some $\xi \in I$. Taking absolute values and using the bound on $f^{(n+1)}$ gives

$$\big|R_{n+1}(x_i,\delta x)\big| \le \frac{M}{(n+1)!}\,|\delta x|^{n+1}.$$

If we introduce $C := M/(n+1)!$, then for all sufficiently small $|\delta x|$, says for all $|\delta x|$ such that $x_i+\delta x \in I$), we have

$$\big|R_{n+1}(x_i,\delta x)\big| \le C\,|\delta x|^{n+1}.$$

This is precisely the definition of $R_{n+1}(x_i,\delta x) = O\big((\delta x)^{n+1}\big)$ as $\delta x \to 0$. □

Remark. The same type of bound extends to multivariable Taylor expansions: if all partial derivatives of total order $n+1$ are continuous (hence bounded on a compact set), the multivariate remainder can be bounded by a constant times the appropriate power of the grid spacing(s) (*e. g.* $|\delta x|^p|\delta y|^q$ or, in typical symmetric statements, by $\|(\delta x,\delta y)\|^{n+1}$), yielding a corresponding $O(\cdot)$ statement.

1 1-D Taylor Expansions at position x_i

Let introduce the shortcuts $f_i = f(x_i)$ and $f_{i\pm1} = f(x_i \pm \delta x)$. Expanding f in Taylor series around x_i, up to the fourth order,

$$f_{i+1} = f_i + \delta x\, f'(x_i) + \tfrac{(\delta x)^2}{2} f''(x_i) + \tfrac{(\delta x)^3}{6} f^{(3)}(x_i) + \tfrac{(\delta x)^4}{24} f^{(4)}(x_i) + O(\delta x^5), \tag{3}$$

$$f_{i-1} = f_i - \delta x\, f'(x_i) + \tfrac{(\delta x)^2}{2} f''(x_i) - \tfrac{(\delta x)^3}{6} f^{(3)}(x_i) + \tfrac{(\delta x)^4}{24} f^{(4)}(x_i) + O(\delta x^5). \tag{4}$$

1.1 First Derivative definitions

Forward Difference

$$\boxed{f'(x_i) \approx \frac{f_{i+1} - f_i}{\delta x}} \qquad \text{Error: } O(\delta x).$$

Backward Difference

$$\boxed{f'(x_i) \approx \frac{f_i - f_{i-1}}{\delta x}} \qquad \text{Error: } O(\delta x).$$

Central Difference Subtracting eq. (4) from eq. (3) to eliminate even derivatives,

$$f_{i+1} - f_{i-1} = 2\delta x\, f'(x_i) + O(\delta x^2),$$

so

$$\boxed{f'(x_i) \approx \frac{f_{i+1} - f_{i-1}}{2\delta x}} \qquad \text{Error: } O(\delta x^2).$$

1.2 Second Derivative (central)

Adding the two expansions eq. (3) and eq. (4),

$$f_{i+1} + f_{i-1} = 2f_i + (\delta x)^2 f''(x_i) + O(\delta x^2), \tag{5}$$

which gives

$$\boxed{f''(x_i) \approx \frac{f_{i+1} - 2f_i + f_{i-1}}{(\delta x)^2}} \qquad \text{Error: } O(\delta x^2).$$

2 2-D Finite Differences

Let use the notation $f_{i,j} = f(x_i, y_j)$, we denote the partial derivatives at first order by f_x, f_y such as

$$f_x = \frac{\partial f(x,y)}{\partial x} \quad \text{and} \quad f_y = \frac{\partial f(x,y)}{\partial y}.$$

For a given point at position (x_i, y_j), this implies that $\dfrac{\partial f(x_i,y_j)}{\partial x}$ is now written $f_x(x_i, y_j)$ and the same for a derivation with respect to y, $\dfrac{\partial f(x_i,y_j)}{\partial y}$ that becomes $f_y(x_i, y_j)$.

The same notation is used for the second order partial derivatives,

$$\frac{\partial^2 f(x_i,y_j)}{\partial x^2} = f_{xx}(x_i, y_j), \quad \frac{\partial^2 f(x_i,y_j)}{\partial y^2} = f_{yy}(x_i, y_j) \quad \text{and} \quad \frac{\partial^2 f(x_i,y_j)}{\partial x \partial y} = f_{xy}(x_i, y_j).$$

An for the third order derivatives,

$$\frac{\partial^3 f(x_i,y_j)}{\partial x^3} = f_{xxx}(x_i, y_j) \quad \text{and} \quad \frac{\partial^3 f(x_i,y_j)}{\partial y^3} = f_{yyy}(x_i, y_j).$$

2-D Taylor expansions (central points and neighbours)

$$f_{i+1,j} = f_{i,j} + \delta x\, f_x + \tfrac{(\delta x)^2}{2} f_{xx} + \tfrac{(\delta x)^3}{6} f_{xxx} + O(\delta x^4), \tag{6}$$

$$f_{i-1,j} = f_{i,j} - \delta x\, f_x + \tfrac{(\delta x)^2}{2} f_{xx} - \tfrac{(\delta x)^3}{6} f_{xxx} + O(\delta x^4), \tag{7}$$

$$f_{i,j+1} = f_{i,j} + \delta y\, f_y + \tfrac{(\delta y)^2}{2} f_{yy} + \tfrac{(\delta y)^3}{6} f_{yyy} + O(\delta y^4), \tag{8}$$

$$f_{i,j-1} = f_{i,j} - \delta y\, f_y + \tfrac{(\delta y)^2}{2} f_{yy} - \tfrac{(\delta y)^3}{6} f_{yyy} + O(\delta y^4). \tag{9}$$

For corner points (including leading mixed term):

$$f_{i+1,j+1} = f_{i,j} + \delta x f_x + \delta y f_y + \delta x \delta y f_{xy} + \frac{(\delta x)^2}{2} f_{xx} + \frac{(\delta y)^2}{2} f_{yy} + O(\delta x^3, \delta y^3).$$

2.1 2-D Finite Difference defintions

First partial derivatives (central)

$$\boxed{f_x(x_i, y_j) \approx \frac{f_{i+1,j} - f_{i-1,j}}{2\delta x}} \quad \text{and} \quad \boxed{f_y(x_i, y_j) \approx \frac{f_{i,j+1} - f_{i,j-1}}{2\delta y}}.$$

Second partial derivatives (central)

$$\boxed{f_{xx}(x_i, y_j) \approx \frac{f_{i+1,j} - 2f_{i,j} + f_{i-1,j}}{(\delta x)^2}} \quad \text{and} \quad \boxed{f_{yy}(x_i, y_j) \approx \frac{f_{i,j+1} - 2f_{i,j} + f_{i,j-1}}{(\delta y)^2}}.$$

Mixed partial f_{xy} (central)

$$\begin{aligned} &f_{i+1,j+1} - f_{i+1,j-1} - f_{i-1,j+1} + f_{i-1,j-1} \\ &\quad = 4\,\delta x\,\delta y\, f_{xy}(x_i, y_j) + O(\delta x^3 \delta y,\ \delta x \delta y^3), \end{aligned}$$

hence

$$\boxed{f_{xy}(x_i, y_j) \approx \frac{f_{i+1,j+1} - f_{i+1,j-1} - f_{i-1,j+1} + f_{i-1,j-1}}{4\,\delta x\,\delta y}}.$$

3 Summary

Derivative	Formula	Error Order
$f'(x_i)$	$\frac{f_{i+1} - f_i}{\delta x}$	$O(\delta x)$
$f'(x_i)$	$\frac{f_i - f_{i-1}}{\delta x}$	$O(\delta x)$
$f'(x_i)$	$\frac{f_{i+1} - f_{i-1}}{2\delta x}$	$O(\delta x^2)$
$f''(x_i)$	$\frac{f_{i+1} - 2f_i + f_{i-1}}{(\delta x)^2}$	$O(\delta x^2)$
$f_x(x_i, y_j)$	$\frac{f_{i+1,j} - f_{i-1,j}}{2\delta x}$	$O(\delta x^2)$
$f_y(x_i, y_j)$	$\frac{f_{i,j+1} - f_{i,j-1}}{2\delta y}$	$O(\delta y^2)$
$f_{xx}(x_i, y_j)$	$\frac{f_{i+1,j} - 2f_{i,j} + f_{i-1,j}}{(\delta x)^2}$	$O(\delta x^2)$
$f_{yy}(x_i, y_j)$	$\frac{f_{i,j+1} - 2f_{i,j} + f_{i,j-1}}{(\delta y)^2}$	$O(\delta y^2)$
$f_{xy}(x_i, y_j)$	$\frac{f_{i+1,j+1} - f_{i+1,j-1} - f_{i-1,j+1} + f_{i-1,j-1}}{4\,\delta x\,\delta y}$	$O(\delta x^2 + \delta y^2)$

4 Take home message

- The $O(\cdot)$ truncation-error statements above are justified directly by the Lagrange remainder formula; the constant hidden in the O-notation is controlled by a bound on the appropriate derivative.
- Central differences are preferred for interior points because they cancel lower-order error terms and achieve higher order.
- Forward/backward differences are used at boundaries, but higher-order one-sided formulas may be derived from Taylor expansions - see the lecture on uncentering operations for derivatives.