Numerical differentiation

数値微分

Fundamental of numerical analysis:
Differential => Difference (差分法)

Differential (微分) $\frac{dy}{dx}$ => approximated by difference (差分) $\frac{\Delta y}{\Delta x}$

The following terms will often appear.

Difference (差分) : $\Delta x = x_i - x_j,\ \Delta y = y_i - y_j$

Divided difference (差分商) : $\frac{\Delta y}{\Delta x}$

Forward difference (前進差分): $\frac{y_{i+1} - y_i}{x_{i+1} - x_i}$ $\quad (x_i < x_{i+1})$

Backward difference (後退差分): $\frac{y_i - y_{i-1}}{x_i - x_{i-1}}$ $\quad (x_{i-1} < x_i)$

Central difference (中心差分): $\frac{y_{i+1} - y_{i-1}}{x_{i+1} - x_{i-1}}$ $\quad (x_{i+1} - x_i = x_i - x_{i-1} = h > 0)$

Numerical differentiation (数値微分)

To calculate $\frac{dy}{dx}$ by computer,

replace the differential '*d*' with finite difference 'Δ' (for small Δ*x*)

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

Accuracy can be improved by decreasing *h*

⇔ But limited by the error of cancellation of significant digits

at least $h < 0.01v$ (v: a representative value to be handled)

32bit floating point (~7 digits) : $h > 10^{-5}v$ (should be much larger)

64bit floating point (~16 digits): $h > 10^{-14}v$ (should be much larger)

$$f(x+h)=f(x)+\frac{df(x)}{dx}h+\frac{1}{2}\frac{d^2f(x)}{dx^2}h^2+O(h^3)$$

$$\frac{f(x+h)-f(x)}{h}=\frac{df(x)}{dx}+\boxed{\frac{1}{2}\frac{d^2f(x)}{dx^2}\underline{h}+O(h^2)}$$

Error ∝ h^1

(Difference error, 差分誤差)

Numerical differentiation: Effect of *h*

$f(x) = x^3 \qquad df/dx = 3x^2$

		h=	1	0.1	0.01	0.001	1.00E-06
x	**f(x)**	**df(x)/dx**	**Δf(x)/Δx**				
0	0	**0**	**1**	**0.01**	**0.0001**	**0.000001**	**1E-12**
0.1	0.001	**0.03**	**1.33**	**0.07**	**0.0331**	**0.030301**	**0.0300003**
0.2	0.008	**0.12**	**1.72**	**0.19**	**0.1261**	**0.120601**	**0.1200006**
0.3	0.027	**0.27**	**2.17**	**0.37**	**0.2791**	**0.270901**	**0.2700009**
0.4	0.064	**0.48**	**2.68**	**0.61**	**0.4921**	**0.481201**	**0.4800012**
0.5	0.125	**0.75**	**3.25**	**0.91**	**0.7651**	**0.751501**	**0.7500015**
0.6	0.216	**1.08**	**3.88**	**1.27**	**1.0981**	**1.081801**	**1.0800018**
0.7	0.343	**1.47**	**4.57**	**1.69**	**1.4911**	**1.472101**	**1.4700021**
0.8	0.512	**1.92**	**5.32**	**2.17**	**1.9441**	**1.922401**	**1.9200024**
0.9	0.729	**2.43**	**6.13**	**2.71**	**2.4571**	**2.432701**	**2.4300027**
1	1	**3**	**7**	**3.31**	**3.0301**	**3.003001**	**3.000003**
1.1	1.331	**3.63**	**7.93**	**3.97**	**3.6631**	**3.633301**	**3.6300033**
1.2	1.728	**4.32**	**8.92**	**4.69**	**4.3561**	**4.323601**	**4.3200036**
1.3	2.197	**5.07**	**9.97**	**5.47**	**5.1091**	**5.073901**	**5.070003899**
1.4	2.744	**5.88**	**11.08**	**6.31**	**5.9221**	**5.884201**	**5.8800042**
1.5	3.375	**6.75**	**12.25**	**7.21**	**6.7951**	**6.754501**	**6.750004499**
1.6	4.096	**7.68**	**13.48**	**8.17**	**7.7281**	**7.684801**	**7.680004799**
1.7	4.913	**8.67**	**14.77**	**9.19**	**8.7211**	**8.675101**	**8.6700051**
1.8	5.832	**9.72**	**16.12**	**10.27**	**9.7741**	**9.725401**	**9.720005399**
1.9	6.859	**10.83**	**17.53**	**11.41**	**10.8871**	**10.8357**	**10.8300057**
2	8	**12**	**19**	**12.61**	**12.0601**	**12.006**	**12.000006**

How to improve accuracy?: Take average

$$\frac{df(x)}{dx} \sim \frac{f(x+h)-f(x)}{h}$$ **Asymmetric equation with respect to '*x*'**

Error: $$\frac{f(x+h)-f(x)}{h} = \frac{df(x)}{dx} \boxed{+\frac{1}{2}\frac{d^2f(x)}{dx^2}h + \frac{1}{3!}\frac{d^3f(x)}{dx^3}h^2 + O(h^3)}$$

1st order error (hに関して一次の誤差)

Average => Symmetric formula: Three-point formula (3点公式, 中点則)

$$\frac{df(x)}{dx} \sim \left[\frac{f(x+h)-f(x)}{h} + \frac{f(x)-f(x-h)}{h}\right]/2 = \boldsymbol{\frac{f(x+h)-f(x-h)}{2h}}$$

$$f(x+h) = f(x) + \frac{df(x)}{dx}h + \frac{1}{2}\frac{d^2f(x)}{dx^2}h^2 + \frac{1}{3!}\frac{d^3f(x)}{dx^3}h^3 + O(h^4)$$

$$f(x-h) = f(x) - \frac{df(x)}{dx}h + \frac{1}{2}\frac{d^2f(x)}{dx^2}h^2 - \frac{1}{3!}\frac{d^3f(x)}{dx^3}h^3 + O(h^4)$$

Error: $$\frac{f(x+h)-f(x-h)}{2h} = \frac{df(x)}{dx} + \boxed{\frac{1}{3!}\frac{d^3f(x)}{dx^3}\underline{h^2} + O(h^3)}$$

2nd order error $\propto \boldsymbol{h^2}$ (二次の誤差)

How to improve accuracy?: Take average

Three-point formula: Symmetric equation, better

$$\frac{df(x)}{dx} \sim \left[\frac{f(x+h)-f(x)}{h} + \frac{f(x)-f(x-h)}{h}\right]/2 = \frac{f(x+h)-f(x-h)}{2h}$$

$f(x) = x^3$ $\quad$ $df(x)/dx = 3x^2$

		h=	1	1	0.01	0.01
x	f(x)	df(x)/dx(exact)	(f(x+h)-f(x))/h	(f(x+h)-f(x-h))/(2h)	(f(x+h)-f(x))/h	(f(x+h)-f(x-h))/(2h)
0	0	0	1	1	0.0001	0.0001
0.2	0.008	0.12	1.72	1.12	0.1261	0.1201
0.4	0.064	0.48	2.68	1.48	0.4921	0.4801
0.6	0.216	1.08	3.88	2.08	1.0981	1.0801
0.8	0.512	1.92	5.32	2.92	1.9441	1.9201
1	1	3	7	4	3.0301	3.0001
1.2	1.728	4.32	8.92	5.32	4.3561	4.3201
1.4	2.744	5.88	11.08	6.88	5.9221	5.8801
1.6	4.096	7.68	13.48	8.68	7.7281	7.6801
1.8	5.832	9.72	16.12	10.72	9.7741	9.7201
2	8	12	19	13	12.0601	12.0001

Higher order formula

Three-point formula (3点公式)

$$
\begin{aligned}
f'(a) &= \frac{1}{h}\left\{\frac{1}{2}f(a+h) - \frac{1}{2}f(a-h)\right\} \\
&+ \frac{1}{6}f^{(3)}(a)\underline{h^2} + \cdots
\end{aligned}
$$

Five-point formula (5点公式)

$$
\begin{aligned}
f'(a) &= \frac{1}{h}\left\{-\frac{1}{12}f(a+2h) + \frac{2}{3}f(a+h) - \frac{2}{3}f(a-h) + \frac{1}{12}f(a-2h)\right\} \\
&+ \frac{1}{30}f^{(5)}(a)\underline{h^4} + \cdots
\end{aligned}
$$

Seven-point formula (7点公式)

$$
\begin{aligned}
f'(a) &= \frac{1}{h}\left\{\frac{1}{60}f(a+3h) - \frac{3}{20}f(a+2h) + \frac{3}{4}f(a+h) - \frac{3}{4}f(a-h)\right. \\
&+ \left.\frac{3}{20}f(a-2h) - \frac{1}{60}f(a-3h)\right\} \\
&+ \frac{1}{140}f^{(7)}(a)\underline{h^6} + \cdots
\end{aligned}
$$

Numerical error

$$\left.\frac{d}{dx}\exp(x)\right|_{x=1}$$

Analytic solution (解析解)**:**

exp(1.0) = 2.71828182845905

N_{div}	h	2-point	3-point	5-point	7-point
1	0.5	8.09E-01	1.15E-01	-5.83E-03	3.18E-04
2	0.25	3.70E-01	2.84E-02	-3.57E-04	4.80E-06
3	0.125	1.77E-01	7.08E-03	-2.22E-05	7.43E-08
4	0.0625	8.67E-02	1.77E-03	-1.38E-06	1.16E-09
5	0.03125	4.29E-02	4.42E-04	-8.64E-08	1.81E-11
6	0.015625	2.13E-02	1.11E-04	-5.40E-09	2.64E-13
7	0.007813	1.06E-02	2.77E-05	-3.38E-10	4.44E-15
8	0.003906	5.32E-03	6.91E-06	-2.11E-11	-7.90E-14
9	0.001953	2.66E-03	1.73E-06	-1.37E-12	-3.51E-14
10	0.000977	1.33E-03	4.32E-07	-1.23E-13	-3.65E-13
11	0.000488	6.64E-04	1.08E-07	-8.42E-13	-5.70E-13
12	0.000244	3.32E-04	2.70E-08	-2.36E-13	7.04E-13
13	0.000122	1.66E-04	6.75E-09	1.28E-12	5.52E-13
14	6.1E-05	8.30E-05	1.69E-09	-2.36E-13	-1.93E-12
15	3.05E-05	4.15E-05	4.19E-10	-5.09E-12	-1.69E-12
16	1.53E-05	2.07E-05	1.06E-10	-7.51E-12	1.63E-11
17	7.63E-06	1.04E-05	1.92E-11	-1.48E-11	3.64E-12
18	3.81E-06	5.18E-06	-9.94E-12	-4.87E-11	-9.94E-12
19	1.91E-06	2.59E-06	-9.94E-12	-2.93E-11	-2.18E-12

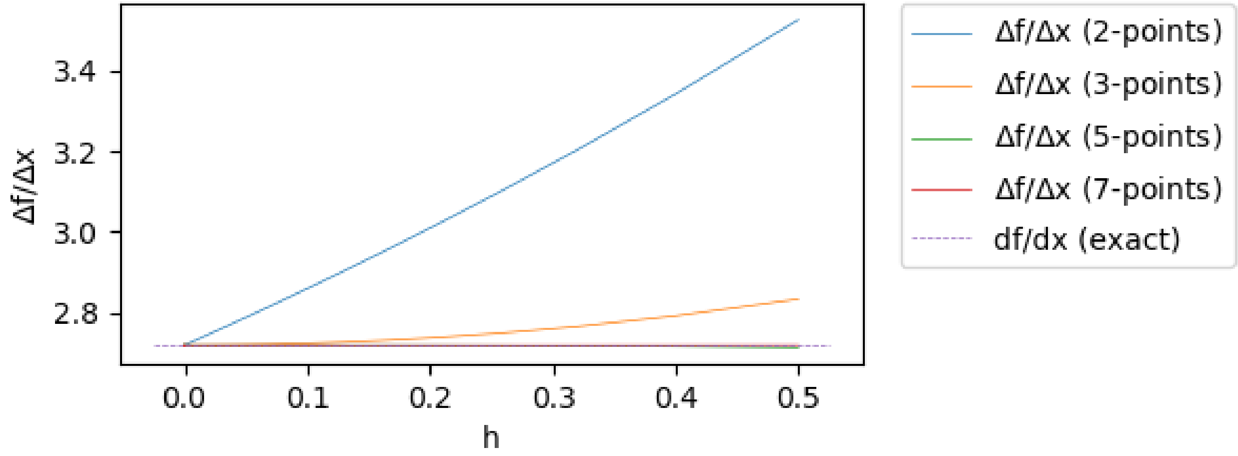
Program: diff_order.py

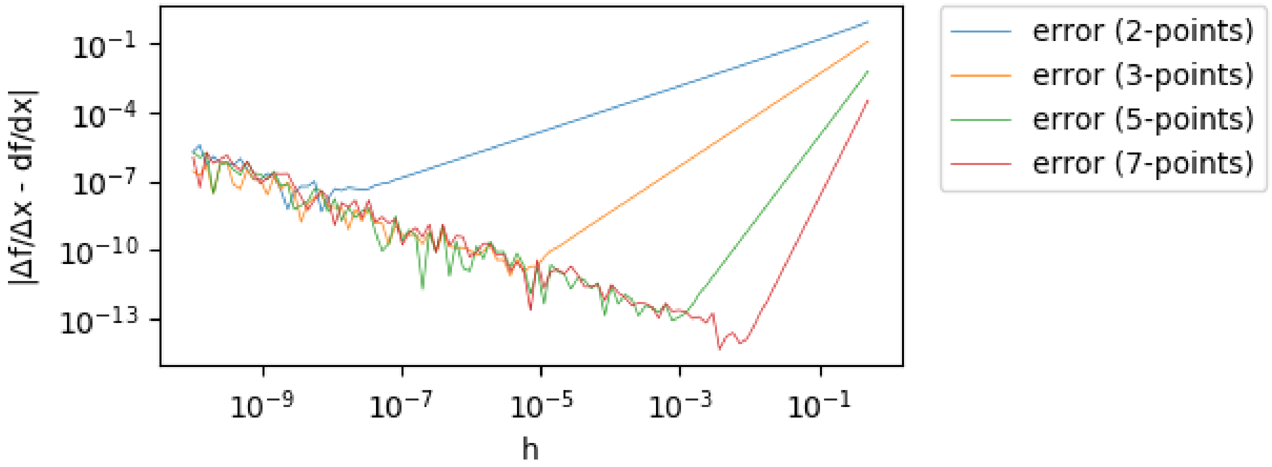
$$\frac{d}{dx}\exp(x)\Big|_{x=1}$$

Analytic solution (解析解)**:**

$$\frac{d}{dx}\exp(x)\Big|_{x=1} = \exp(1.0) = 2.71828182845905$$

run: python diff_order.py





Richardson extrapolation differentiation

(リチャードソン補外)

森正武，FORTRAN 77 数値計算プログラミング、岩波書店 (1987年増補版)

- **Start from the three-point formula (中点則), and then iteratively repeat the following formula that updates the calculation precision until a required precision will be satisfied.**

(中点則から出発し、高次の微分に相当する公式を自動的に適用し、要求精度を満たすまで繰り返す)

1. **Calc by three-point formula $D_0^{(0)} = (f(x+h) - f(x-h)) / (2h)$ at the x mesh $h = h_0$.**
2. **Reduce the mesh to a half $h_k = (1/2)^k h$, and the calculate $D_0^{(k)}$ by the three-point fomula.**
3. **Calculate next quantity**

$$D_m^{(k)} = \frac{4^m D_{m-1}^{(k+1)} - D_{m-1}^{(k)}}{4^m - 1}$$

4. **Iteration will be terminated if $|D_m^{(0)} - D_{m-1}^{(0)}|$ becomes smaller than the required precision.**

Numerial error

$$\left.\frac{d}{dx}\exp(x)\right|_{x=1}$$

Analytic solution (解析解):

exp(1) = 2.71828182845905

N_{div}	h	2-point	3-point	5-point	7-point	Richardson extrapolation		
1	**0.5**	8.09E-01	1.15E-01	-5.83E-03	3.18E-04			
2	**0.25**	3.70E-01	2.84E-02	-3.57E-04	4.80E-06	-3.57E-04		
3	**0.125**	1.77E-01	7.08E-03	-2.22E-05	7.43E-08			
4	**0.0625**	8.67E-02	1.77E-03	-1.38E-06	1.16E-09	2.06E-09		
5	**0.03125**	4.29E-02	4.42E-04	-8.64E-08	1.81E-11			
6	**0.015625**	2.13E-02	1.11E-04	-5.40E-09	2.64E-13			
7	**0.007813**	1.06E-02	2.77E-05	-3.38E-10	4.44E-15			
8	**0.003906**	5.32E-03	6.91E-06	-2.11E-11	-7.90E-14	-1.38E-14		
9	**0.001953**	2.66E-03	1.73E-06	-1.37E-12	-3.51E-14			
10	**0.000977**	1.33E-03	4.32E-07	-1.23E-13	-3.65E-13			
11	**0.000488**	6.64E-04	1.08E-07	-8.42E-13	-5.70E-13			
12	**0.000244**	3.32E-04	2.70E-08	-2.36E-13	7.04E-13			
13	**0.000122**	1.66E-04	6.75E-09	1.28E-12	5.52E-13			
14	**6.1E-05**	8.30E-05	1.69E-09	-2.36E-13	-1.93E-12			
15	**3.05E-05**	4.15E-05	4.19E-10	-5.09E-12	-1.69E-12			
16	**1.53E-05**	2.07E-05	1.06E-10	-7.51E-12	1.63E-11	-3.11E-15		
17	**7.63E-06**	1.04E-05	1.92E-11	-1.48E-11	3.64E-12			
18	**3.81E-06**	5.18E-06	-9.94E-12	-4.87E-11	-9.94E-12	4.52E-13		
19	**1.91E-06**	2.59E-06	-9.94E-12	-2.93E-11	-2.18E-12	1.69E-12		

For non-constant $h_i = x_{i+1} - x_i$

x	y
x_{-1}	y_{-1}
x_0	y_0
x_1	y_1

Rough method: Take average (maybe good but not best)

$$y'(x_0) = \frac{1}{2}\left[\frac{y_1 - y_0}{x_1 - x_0} + \frac{y_0 - y_{-1}}{x_0 - x_{-1}}\right]$$

Polynomial method: Lagrange polynomial (ラングランジュ多項式)

$$P_{n-1}(x) = f(x_0)\phi_0(x) + f(x_1)\phi_1(x) + \cdots f(x_{n-1})\phi_{n-1}(x)$$

$$\phi_i(x) = \frac{\prod_{k\neq i}^{n-1}(x - x_k)}{\prod_{k\neq i}^{n-1}(x_i - x_k)} = \prod_{k\neq i}^{n-1}\frac{(x - x_k)}{(x_i - x_k)}$$

$$y(x) = y_{-1}\frac{(x - x_0)(x - x_1)}{(x_{-1} - x_0)(x_{-1} - x_1)} + y_0\frac{(x - x_{-1})(x - x_1)}{(x_0 - x_{-1})(x_0 - x_1)} + y_1\frac{(x - x_{-1})(x - x_0)}{(x_1 - x_{-1})(x_1 - x_0)}$$

$$y'(x) = y_{-1}\frac{2x - (x_0 + x_1)}{(x_{-1} - x_0)(x_{-1} - x_1)} + y_0\frac{2x - (x_{-1} + x_1)}{(x_0 - x_{-1})(x_0 - x_1)} + y_1\frac{2x - (x_{-1} + x_0)}{(x_1 - x_{-1})(x_1 - x_0)}$$

Second differential (二階微分)

If calculate 2nd differential using forward differences both for the 1st and the 2nd differentials …

(一階微分を前進差分で計算してから二階微分を前進差分で計算すると･･･)

$$\frac{d^2 f(t)}{dx^2} = \frac{\frac{df}{dx}(x+\Delta x) - \frac{df}{dx}(x)}{\Delta t}$$

$$\sim \frac{\frac{f(x+2\Delta x)-f(x+\Delta x)}{\Delta x} - \frac{f(x+\Delta x)-f(x)}{\Delta x}}{\Delta x} = \frac{f(x+2\Delta x)-2f(x+\Delta x)+f(x)}{\Delta x^2} \quad (1)$$

If use backward differentials only for the 1st differentials (but logically inconsistent):

$$\frac{d^2 f(t)}{dx^2} \sim \frac{\frac{f(x+\Delta x)-f(x)}{\Delta x} - \frac{f(x)-f(x-\Delta x)}{\Delta x}}{\Delta x}$$

$$\boldsymbol{\frac{d^2 f(x)}{dx^2} \sim \frac{f(x+\Delta x)-2f(x)+f(x-\Delta x)}{\Delta x^2}} \quad \textbf{(2)}$$

Symmetric formula w.r.t. $x + \Delta x$ and $x - \Delta x$ is obtained

($x + \Delta x$, $x - \Delta x$ について対称になる式が取れ、精度が上がる)

Note: x value of eq. (1) is shifted by one Δx from eq. (2)

(eq.(1)では、横軸がΔxひとつ分ずれているために精度が落ちる)

Second differential by central differences

If $\dfrac{d^2f(x)}{dx^2}$ is approximated by the central difference of $\dfrac{df}{dx}$:

$$\frac{d^2f(x)}{dx^2} = \frac{\frac{df}{dx}(x+\Delta x) - \frac{df}{dx}(x-\Delta x)}{2\Delta x}$$

$$\sim \frac{\frac{f(x+2\Delta x)-f(x)}{2\Delta x} - \frac{f(x)-f(x-2\Delta x)}{2\Delta x}}{2\Delta x} = \frac{f(x+2\Delta x)-2f(x)+f(x-2\Delta x)}{(2\Delta x)^2}$$

$$\boldsymbol{\frac{d^2f(t)}{dx^2} = \frac{f(x+\Delta x')-2f(x)+f(x-\Delta x')}{\Delta x'^2}}$$

Symmetric formula w.r.t. $x + \Delta x$ and $x - \Delta x$ is obtained again

(前進差分を使ったときと同様、

$x + \Delta x$, $x - \Delta x$ について対称になる式が取れ、精度が上がる)