Computional Homework9 Report

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1 Derivation of the Five-Point Second-order Derivative Difference Formula

The five-point formula is derived using the Lagrange interpolation polynomial on five nodes x_0, x_1, x_2, x_3, x_4. The interpolating polynomial is:

$$P_4(x) = \sum_{k=0}^{4} f(x_k) L_k(x)$$

where the Lagrange basis is

$$L_k(x) = \prod_{\substack{i=0 \\ i \neq k}}^{4} \frac{x - x_i}{x_k - x_i}$$

The first derivative of the interpolation polynomial is given by

$$P_4'(x) = \sum_{k=0}^{4} f(x_k) L_k'(x)$$

$$P_4'(x) = \sum_{k=0}^{4} f(x_k) \frac{\sum_{i=0}^{4} \prod_{\substack{j=0 \\ j \neq i}}^{4} (x - x_j)}{\prod_{\substack{i=0 \\ i \neq k}}^{4} (x_k - x_i)}$$

Similarly, the second derivative of the interpolation polynomial is:

$$P_4''(x) = \sum_{k=0}^{4} f(x_k) L_k''(x)$$

$$P_4''(x) = \sum_{k=0}^{4} f(x_k) \frac{\displaystyle\sum_{m=0}^{4}\sum_{i=0}^{4} \prod_{\substack{j=0 \\ j\neq i, j\neq m}}^{4} (x - x_j)}{\displaystyle\prod_{\substack{i=0 \\ i\neq k}}^{4} (x_k - x_i)}$$

For the five-point second derivative formula at x_2 (uniform grid, $x_k = x_2 + (k-2)h$):

For $k = 0$:

$$\frac{f(x_0)\,[(x_2 - x_1)(x_2 - x_3) + (x_2 - x_1)(x_2 - x_4) + (x_2 - x_3)(x_2 - x_4)] \times 2}{(x_0 - x_1)(x_0 - x_2)(x_0 - x_3)(x_0 - x_4)}$$

$$= \frac{f(x_0)\,[h(-h) + h(-2h) + (-h)(-2h)] \times 2}{(-h)(-2h)(-3h)(-4h)}$$

$$= \frac{f(x_0)(-h^2 - 2h^2 + 2h^2) \times 2}{24h^4} = \frac{f(x_0)(-h^2) \times 2}{24h^4}$$

$$= -\frac{f(x_0)}{12h^2}$$

For $k = 1$:

$$\frac{f(x_1)\,[(x_2 - x_0)(x_2 - x_3) + (x_2 - x_0)(x_2 - x_4) + (x_2 - x_3)(x_2 - x_4)] \times 2}{(x_1 - x_0)(x_1 - x_2)(x_1 - x_3)(x_1 - x_4)}$$

$$= \frac{f(x_1)\,[2h(-h) + 2h(-2h) + (-h)(-2h)] \times 2}{(h)(-h)(-2h)(-3h)}$$

$$= \frac{f(x_1)[-2h^2 - 4h^2 + 2h^2] \times 2}{-6h^4} = \frac{f(x_1)(-4h^2) \times 2}{-6h^4}$$

$$= \frac{8f(x_1)}{6h^2} = \frac{16f(x_1)}{12h^2}$$

For $k = 2$:

$$\frac{f(x_2)\begin{bmatrix} (x_2-x_0)(x_2-x_1)+(x_2-x_0)(x_2-x_3)+(x_2-x_0)(x_2-x_4) \\ +\,(x_2-x_1)(x_2-x_3)+(x_2-x_1)(x_2-x_4)+(x_2-x_3)(x_2-x_4) \end{bmatrix}\times 2}{(x_2-x_0)(x_2-x_1)(x_2-x_3)(x_2-x_4)}$$

$$= \frac{f(x_2)\,[2h(h)+2h(-h)+2h(-2h)+h(-h)+h(-2h)+(-h)(-2h)]\times 2}{(2h)(h)(-h)(-2h)}$$

$$= \frac{f(x_2)[2h^2-2h^2-4h^2-h^2-2h^2+2h^2]\times 2}{-4h^4}$$

$$= \frac{f(x_2)(-5h^2)\times 2}{-4h^4}$$

$$= -\frac{30f(x_2)}{12h^2}$$

For $k = 3$:

$$\frac{f(x_3)\,[(x_2-x_0)(x_2-x_1)+(x_2-x_0)(x_2-x_4)+(x_2-x_1)(x_2-x_4)]\times 2}{(x_3-x_0)(x_3-x_1)(x_3-x_2)(x_3-x_4)}$$

$$= \frac{f(x_3)\,[(2h)(h)+(2h)(-2h)+(h)(-2h)]\times 2}{(3h)(2h)(h)(-h)}$$

$$= \frac{f(x_3)[2h^2-4h^2-2h^2]\times 2}{-6h^4}$$

$$= \frac{f(x_3)(-4h^2)\times 2}{-6h^4}$$

$$= \frac{8f(x_3)}{6h^2} = \frac{16f(x_3)}{12h^2}$$

For $k = 4$:

$$\frac{f(x_4)\,[(x_2-x_0)(x_2-x_1)+(x_2-x_0)(x_2-x_3)+(x_2-x_1)(x_2-x_3)]\times 2}{(x_4-x_0)(x_4-x_1)(x_4-x_2)(x_4-x_3)}$$

$$= \frac{f(x_4)\,[(2h)(h)+(2h)(-h)+(h)(-h)]\times 2}{(4h)(3h)(2h)(h)}$$

$$= \frac{f(x_4)[2h^2-2h^2-h^2]\times 2}{24h^4}$$

$$= \frac{-2f(x_4)h^2}{24h^4}$$

$$= -\frac{f(x_4)}{12h^2}$$

Then, we can get the five-point formula for the second derivative:

$$f''(x_2) = P_4''(x_2) \approx \frac{1}{12h^2}\left[-f(x_0) + 16f(x_1) - 30f(x_2) + 16f(x_3) - f(x_4)\right]$$

2 Truncation Error Derivation for the Five-Point Second Derivative Formula

Given the five-point stencil:

$$f''(x_2) \approx \frac{1}{12h^2}\left[-f(x_0) + 16f(x_1) - 30f(x_2) + 16f(x_3) - f(x_4)\right]$$

where $x_k = x_2 + (k-2)h$, for $k = 0, 1, 2, 3, 4$.

To derive the truncation error, expand each $f(x_k)$ in a Taylor series about x_2:

$$\begin{aligned} f(x_2 + mh) = f(x_2) + mhf'(x_2) + \frac{(mh)^2}{2}f''(x_2) + \frac{(mh)^3}{6}f'''(x_2) \\ + \frac{(mh)^4}{24}f^{(4)}(x_2) + \frac{(mh)^5}{120}f^{(5)}(x_2) + \frac{(mh)^6}{720}f^{(6)}(\xi_m) \end{aligned}$$

where $m = -2, -1, 0, 1, 2$ and ξ_m lies between x_2 and $x_2 + mh$.

Now, substitute this into the five-point formula:

$$S = -f(x_0) + 16f(x_1) - 30f(x_2) + 16f(x_3) - f(x_4)$$

Identify $x_0 = x_2 - 2h$, $x_1 = x_2 - h$, x_2, $x_3 = x_2 + h$, $x_4 = x_2 + 2h$ and set m accordingly.

Write the Taylor expansions for each:

$$\begin{aligned} f(x_2 - 2h) &= f(x_2) - 2hf' + 2h^2f'' - \frac{4h^3}{3}f''' + \frac{2h^4}{3}f^{(4)} - \frac{4h^5}{15}f^{(5)} + \frac{4h^6}{45}f^{(6)} - \frac{8h^7}{315}f^{(7)}(\xi_0) \\ f(x_2 - h) &= f(x_2) - hf' + \frac{h^2}{2}f'' - \frac{h^3}{6}f''' + \frac{h^4}{24}f^{(4)} - \frac{h^5}{120}f^{(5)} + \frac{h^6}{720}f^{(6)} - \frac{h^7}{5040}f^{(7)}(\xi_1) \\ f(x_2) &= f(x_2) \\ f(x_2 + h) &= f(x_2) + hf' + \frac{h^2}{2}f'' + \frac{h^3}{6}f''' + \frac{h^4}{24}f^{(4)} + \frac{h^5}{120}f^{(5)} + \frac{h^6}{720}f^{(6)} - \frac{h^7}{5040}f^{(7)}(\xi_3) \\ f(x_2 + 2h) &= f(x_2) + 2hf' + 2h^2f'' + \frac{4h^3}{3}f''' + \frac{2h^4}{3}f^{(4)} + \frac{4h^5}{15}f^{(5)} + \frac{4h^6}{45}f^{(6)} - \frac{8h^7}{315}f^{(7)}(\xi_4) \end{aligned}$$

Apply the coefficients:

$$S = -f(x_2 - 2h) + 16f(x_2 - h) - 30f(x_2) + 16f(x_2 + h) - f(x_2 + 2h)$$

For $f(x_2)$:

$$-1 + 16 - 30 + 16 - 1 = 0$$

For $f'(x_2)$:

$$[2 - 16 + 16 - 2]h = 0$$

For $f''(x_2)$:

$$[-1 \cdot 2 + 16 \cdot \frac{1}{2} - 30 \cdot 0 + 16 \cdot \frac{1}{2} - 1 \cdot 2]h^2 = (-2 + 8 + 0 + 8 - 2)h^2 = 12h^2$$

For $f'''(x_2)$:

$$[-1 \cdot (-\frac{4}{3}) + 16 \cdot (-\frac{1}{6}) + 16 \cdot (\frac{1}{6}) - 1 \cdot \frac{4}{3}]h^3$$
$$= \left(\frac{4}{3} - \frac{16}{6} + \frac{16}{6} - \frac{4}{3}\right) h^3 = 0$$

For $f^{(4)}(x_2)$:

$$[-1 \cdot \frac{2}{3} + 16 \cdot \frac{1}{24} + 16 \cdot \frac{1}{24} - 1 \cdot \frac{2}{3}]h^4$$
$$= \left(-\frac{2}{3} + \frac{2}{3} + \frac{2}{3} - \frac{2}{3}\right) h^4 = 0$$

For $f^{(5)}(x_2)$:

$$[-1 \cdot \left(-\frac{4}{15}\right) + 16 \cdot \left(-\frac{1}{120}\right) + 0 + 16 \cdot \left(\frac{1}{120}\right) - 1 \cdot \left(\frac{4}{15}\right)]h^5$$
$$= \left(\frac{4}{15} - \frac{16}{120} + \frac{16}{120} - \frac{4}{15}\right) h^5 = 0$$

For $f^{(6)}(x_2)$:

$$[-1 \cdot \frac{4}{45} + 16 \cdot \frac{1}{720} + 16 \cdot \frac{1}{720} - 1 \cdot \frac{4}{45}]h^6$$

$$= \left(-\frac{4}{45} + \frac{16}{720} + \frac{16}{720} - \frac{4}{45}\right) h^6 = -\frac{2}{15}h^6$$

The truncation error comes from the $f^{(6)}$ term in the Taylor expansion:

Truncation error derivation:

$$\text{Coefficient of } f^{(6)}(x_2): \quad -\frac{2}{15}h^6$$

In the finite difference formula, we divide by $12h^2$:

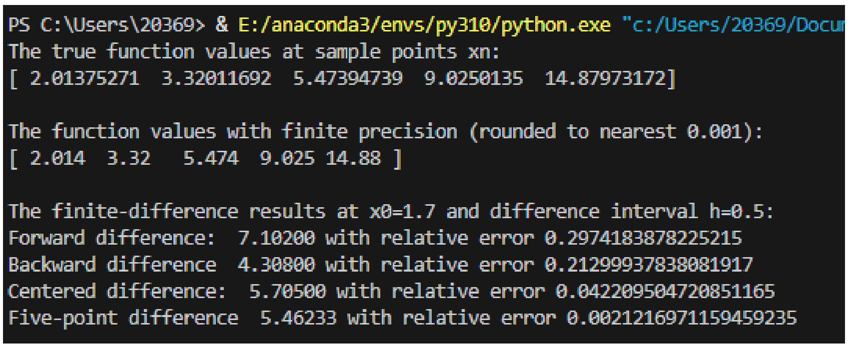
$$\text{Truncation error} = \frac{-\frac{2}{15}h^6}{12h^2} f^{(6)}(\xi) = -\frac{2h^4}{180} f^{(6)}(\xi) = -\frac{h^4}{90} f^{(6)}(\xi)$$

where $\xi \in [x_2 - 2h, x_2 + 2h]$.

3 Comparison of Different Finite Precision Difference Formulas

To test the effect of numerical precision, we set $\epsilon = 10^{-3}$, so that every $f(x_i)$ used in calculating differences is rounded to three decimal places.

Since we are calculating the derivative of e^x, $f(x)$ denotes both the original function and its analytic derivative.



```
PS C:\Users\20369> & E:/anaconda3/envs/py310/python.exe "c:/Users/20369/Docu
The true function values at sample points xn:
[ 2.01375271  3.32011692  5.47394739  9.0250135  14.87973172]

The function values with finite precision (rounded to nearest 0.001):
[ 2.014  3.32   5.474  9.025 14.88 ]

The finite-difference results at x0=1.7 and difference interval h=0.5:
Forward difference:  7.10200 with relative error 0.2974183878225215
Backward difference  4.30800 with relative error 0.21299937838081917
Centered difference:  5.70500 with relative error 0.042209504720851165
Five-point difference  5.46233 with relative error 0.0021216971159459235
```

Figure 1 **Demonstration of the effect of three-digit precision ($\epsilon = 0.001$) in function values at grid points for computing the derivative of $f(x) = e^x$ at $x_2 = 1.7$ with $h = 0.5$. The plot shows true and rounded values for $f(x_i)$, as well as the results of each finite difference formula under these conditions.**

```python
def f(x):
    return np.exp(x)

class Diff:
    def __init__(self,f,x0,h,e=1e-3):
        self.f=f
        self.x0=x0
        self.h=h
        xn=np.array([self.x0-n*self.h for n in range(2,-3,-1)])
```

```
        yn=self.f(xn)
        print(f"The true function values at sample points xn:\n{yn}")
        self.yn=np.round(yn/e)*e
        print(f"The function values with finite precision (rounded to nearest {e}):\n{self.yn}")
```

3.1 Finite Difference Methods

We consider four finite difference formulas for approximating $f'(x_2)$:

- **Forward Difference:**

$$f'(x_2) = \frac{f(x_3) - f(x_2)}{h}$$

```
    def cal_diff(self,mode="forward"):
        diff=(self.yn[3]-self.yn[2])/(self.h)
```

- **Backward Difference:**

$$f'(x_2) = \frac{f(x_2) - f(x_1)}{h}$$

```
        if mode=="backward":
            diff=(self.yn[2]-self.yn[1])/(self.h)
```

- **Centered Difference:**

$$f'(x_2) = \frac{f(x_3) - f(x_1)}{2h}$$

```
        elif mode=="centered":
            diff=(self.yn[3]-self.yn[1])/(2*self.h)
```

- **Five-Point Difference:**

$$f'(x_2) = \frac{f(x_0) - 8f(x_1) + 8f(x_3) - f(x_4)}{12h}$$

```
        elif mode=="five-point":
            diff=(self.yn[0]-8*self.yn[1]+8*self.yn[3]-self.yn[4])/(12*self.h)
        return diff
```

3.2 Numerical Results for Different h

Note: $x_2 = 1.7$, f and f' are evaluated at x_2.

h	Forward Value (Rel. Err.)	Backward Value (Rel. Err.)	Centered Value (Rel. Err.)	Five-point Value (Rel. Err.)
0.5	7.10200(0.29742)	4.30800(0.21300)	5.70500(0.04221)	5.46233(0.00212)
0.2	6.06000(0.10706)	4.96000(0.09389)	5.51000(0.00659)	5.47292(0.00019)
0.1	5.76000(0.05226)	5.21000(0.04822)	5.48500(0.00202)	5.47667(0.00050)
0.05	5.40000(0.01351)	5.40000(0.01351)	5.40000(0.01351)	5.36667(0.01960)
0.01	5.00000(0.08658)	6.00000(0.09610)	5.50000(0.00476)	5.50000(0.00476)

Table 1 Comparison of finite difference formulas for $f'(1.7)$ with various h. Each entry shows value (relative error).

3.3 Error Curves for All h

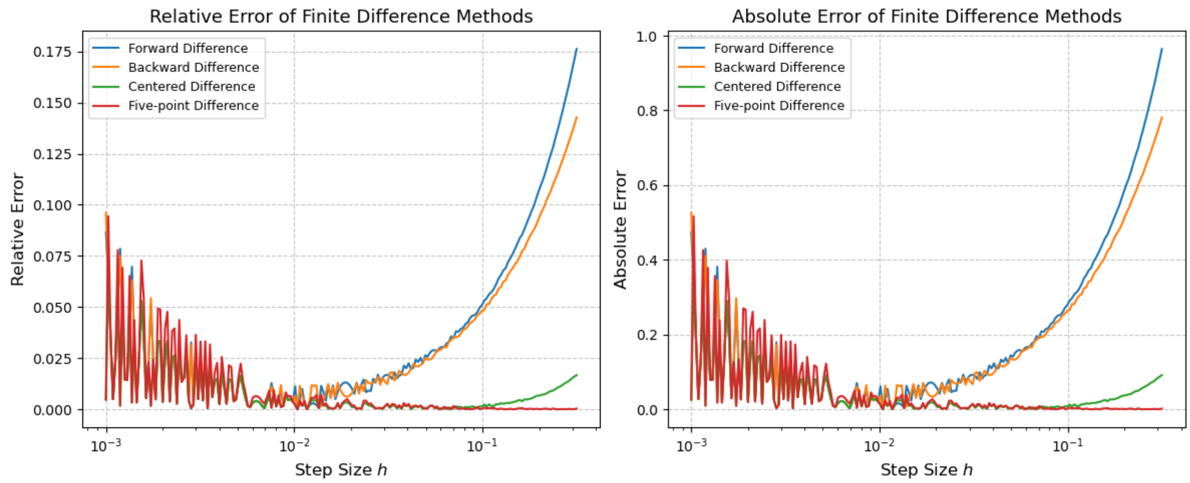


Figure 2 Relative and absolute errors for four finite difference derivative formulas (forward, backward, centered, and five-point) at $x = 1.7$, using the true value $f'(x)$ for reference, shown as a function of step size h (logarithmic scale).

As shown in Fig. 2, the forward and backward formulas have noticeably larger errors than the centered and five-point formulas.

The five-point difference formula consistently offers the smallest error for a wide range of h.

For all methods, the error generally decreases as h becomes smaller, reaches a minimum, and then increases again for very small h. This U-shaped behavior is due to the trade-off between discretization (truncation) error, which decreases with h, and rounding error, which increases as h is made too small.