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Slaybaugh NucE 155

Assignment 3

1. (10 points) Using Taylor's theorem and the points $(x_i - 2h), (x_i - h)$, and x_i derive the $O(h^2)$ backward difference formula for $f''(x_i)$. This means find a, b, c, and an expression for the truncation error E such that

$$f''(x_i) = af(x_i - 2h) + bf(x_i - h) + cf(x_i) + E\,.$$

Backwards difference for $O(h^2)$: combine the point and the next two points backwards:

$$f'(x_i) = \frac{3f(x_i) - 4f(x_i - h) + f(x_i - 2h)}{2h} + \frac{1}{3}h^2 f'''(\mu)$$

$$af(x_i) + bf(x_i - h) + cf(x_i - 2h) = f''(x_i)$$

$$=af(x_i) + b\left[f(x_i) - hf'(x_i) + \frac{h^2 f''(x_i)}{2} - \frac{h^3 f'''(x_i)}{6}\right] + c\left[f(x_i) - 2hf'(x_i) + 2h^2 f''(x_i) - \frac{4}{3}h^3 f'''(x_i)\right] = f''(x_i) = (a+b+c)f(x_i) + f'(x_i)[-bh - 2hc] + f''(x_i)\left[\frac{bh^2}{2} + 2h^2 c\right] + f'''(x_i)\left[-\frac{bh^3}{6} - \frac{c4h^3}{3}\right] = f''(x_i)$$

$$=(a+b+c)f(x_i) + f'(x_i)[-bh - 2hc] + f''(x_i)\left[\frac{bh^2}{2} + 2h^2 c\right\} + f'''(x_i)\left[-\frac{bh^3}{6} - \frac{c4h^3}{3}\right] + f''''(x_i)\left[\frac{bh^4}{24} + \frac{c2}{3}h^4\right]$$

a + b + c = 0
-bh = 2hc → b = -2c
$bh^2/2 + 2h^2c = 1$

$$-\frac{2ch^2}{2} + 2ch^2 = 1 = 1ch^2; c = \frac{1}{h^2}, b = -\frac{2}{h^2}, a = \frac{1}{h^2}$$

first error: $-\frac{2}{h^2} * \frac{h^4}{24} + \frac{1}{h^2} * h^4 * \frac{2}{3} = -\frac{h^2}{12} + \frac{2h^2}{3} = \frac{7}{12}h^2$

second error: $-\frac{2}{h^2} * \frac{h^4}{24} + \frac{1}{h^2}h^4 * \frac{2}{3} = -\frac{h^2}{12} + \frac{2h^2}{3} = \frac{7}{12}h^2$

$$f''(x_i) = \frac{1}{h^2}f(x_i - 2h) - \frac{2}{h^2}f(x_i - h) + \frac{1}{h^2}f(x_i) - hf'''(\mu) + \frac{7}{12}h^2 f''''(\mu)$$

2. (15 points) Consider the following four equally-spaced points on the interval $[x_0, x_3]$:

$$x_j = x_0 + jh \qquad j = 0,1,2,3 \qquad h = (x_3 - x_0)/3\,.$$

Using the formula for the interpolating polynomial $P_3(x)$ you used in Question 1b of Homework 2, integrate $P_3(x)$ to derive the following Newton-Cotes formula, often referred to as **Simpson's three-eights rule:**

$$I(f(x)) \approx I_3(f(x)) = \frac{3h}{8}\Big[f(x_0) + 3f(x_0 + h) + 3f(x_0 + 2h) + f(x_0 + 3h)\Big]$$

Note that you can substitute h in for the xs in P_3 because we are explicitly stating that the points are equally spaced.
For this problem, don't worry about an error term.

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2) $P_3(x) = f(x_0)\cdot\frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)} + f(x_1)\cdot\frac{(x-x_0)(x-x_2)(x-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)} + f(x_2)\frac{(x-x_0)(x-x_1)(x-x_3)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)}$

$+ f(x_3)\frac{(x-x_0)(x-x_1)(x-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)}$

$$P_3(x) = f(x_0)\cdot\frac{\left(\frac{x_3-x_0}{3}-x_0-h\right)\left(\frac{x_3-x_0}{3}-x_0-2h\right)\left(\frac{x_3-x_0}{3}-x_0-3h\right)}{(x_0-x_0-h)(x_0-x_0-2h)(x_0-x_0-3h)} = \frac{f(x_0)\left(\frac{x_3-4x_0}{3}-h\right)\left(\frac{x_3-4x_0}{3}-2h\right)\left(\frac{x_3-4x_0}{3}-3h\right)}{\underbrace{(-h)(-2h)(-3h)}_{\to -6h^3}}$$

$$+ f(x_1)\frac{\left(\frac{x_3-x_0}{3}-x_0\right)\left(\frac{x_3-x_0}{3}-x_0-2h\right)\left(\frac{x_3-x_0}{3}-x_0-3h\right)}{(\cancel{x_0}+h-\cancel{x_0})(\cancel{x_0}+h-x_0-2h)(x_0+h-x_0-3h)} = \frac{f(x_1)\left(\frac{x_3-4x_0}{3}\right)\left(\frac{x_3-4x_0}{3}-2h\right)\left(\frac{x_3-4x_0}{3}-3h\right)}{\underbrace{(h)(-h)(-2h)}_{\to (2h^3)}}$$

$$+ f(x_2)\frac{\left(\frac{x_3-x_0}{3}-x_0\right)\left(\frac{x_3-x_0}{3}-x_0-h\right)\left(\frac{x_3-x_0}{3}-x_0-3h\right)}{(\cancel{x_0}+2h-\cancel{x_0})(\cancel{x_0}+2h-\cancel{x_0}-h)(\cancel{x_0}+2h-x_0-3h)} = \frac{f(x_2)\left(\frac{x_3-4x_0}{3}\right)\left(\frac{x_3-4x_0}{3}-h\right)\left(\frac{x_3-4x_0}{3}-3h\right)}{\underbrace{(2h)(h)(-h)}_{\to 2h^3}}$$

$$+ f(x_3)\frac{\left(\frac{x_3-x_0}{3}-x_0\right)\left(\frac{x_3-x_0}{3}-x_0-h\right)\left(\frac{x_3-x_0}{3}-x_0-2h\right)}{(\cancel{x_0}+3h-\cancel{x_0})(\cancel{x_0}+3h-x_0-h)(\cancel{x_0}+3h-x_0-2h)} = \frac{f(x_3)\left(\frac{x_3-4x_0}{3}\right)\left(\frac{x_3-4x_0}{3}-h\right)\left(\frac{x_3-4x_0}{3}-2h\right)}{\underbrace{(3h)(2h)(h)}_{\to 6h^3}}$$

$$P_3(x) = \frac{f(x_0)}{-6h^3}\left[(-x_0)(-x_0-h)(-x_0-2h)\right] + \frac{f(x_0+h)}{2h^3}\left[(h-x_0)(-x_0-h)(-x_0-2h)\right] - \frac{f(x_0+2h)}{2h^3}\left[(h-x_0)(-x_0)(-x_0-2h)\right]$$
$$+ \frac{f(x_0+3h)}{6h^3}\left[(h-x_0)(-x_0)(-x_0-h)\right]$$

$$P_3(x) = -\frac{f(x_0)}{6h^3}(x-x_0-h)(x-x_0-2h)(x-x_0-3h) + \frac{f(x_0+h)}{2h^3}(x-x_0)(x-x_0-2h)(x-x_0-3h) - \frac{f(x_0+2h)}{2h^3}(x-x_0)(x-x_0-h)(x-x_0-3h)$$
$$+ \frac{f(x_0+3h)}{6h^3}(x-x_0)(x-x_0-h)(x-x_0-2h)$$

1^{st} integral

$$= -\frac{f(x_0)}{6h^3}\left(-6h^3+11h^2x-11h^2x_0-6hx^2+12hx\cdot x_0-6hx_0^2+x^3-3x^2x_0+3xx_0^2-x_0^3\right)$$

integrate: $-\frac{f(x_0)}{6h^3}\left(-6h^3x+\frac{11}{2}h^2x^2-11h^2x_0x-2hx^3+6hx^2x_0-6hx_0^2x+\frac{1}{4}x^4-x^3x_0+\frac{3}{2}x^2x_0^2-x_0^3x\right)\Big|_{x_0}^{x_0+3h}$

$$= -\frac{f(x_0)}{6h^3}\Big(-6h^3x_0-18h^4+\frac{11}{2}h^2x_0^2+33h^3x_0+\frac{99}{2}h^4-11h^2x_0^2-33h^3x_0-[\text{illegible}]-54h^4$$
$$-54h^3x_0+18h^2x_0^2-2hx_0^3+54h^3x_0+36h^2x_0^2+6hx_0^3-18h^2x_0^2-6hx_0^3+\frac{81}{4}h^4+27h^3x_0+\frac{27}{2}h^2x_0^2$$
$$+3hx_0^3+\frac{1}{4}x_0^4-27h^3x_0-27h^2x_0^2-9hx_0^3-x_0^4+\frac{27}{2}h^2x_0^2+9hx_0^3+\frac{3}{2}x_0^4-3hx_0^3-x_0^4$$
$$+6h^3x_0-\frac{11}{2}h^2x_0^2+11h^2x_0^2+2hx_0^3-6hx_0^3+6hx_0^3-\frac{x_0^4}{4}+x_0^4-\frac{3}{2}x_0^4+x_0^4\Big)$$

$$= -\frac{f(x_0)}{6h^3}\left[0-\frac{9}{4}h^4+0+0+0\right] = \frac{f(x_0)}{6h^3}\left(\frac{9}{4}h^4\right) = \frac{f(x_0)}{8}3h$$

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2nd integral: $\frac{f(x_0+h)}{2h^3}(x-x_0)(x-x_0-2h)(x-x_0-3h)$

$u=x-x_0$: $\frac{f(x_0+h)}{2h^3}\int_0^{3h}(u)(u-2h)(u-3h)\,du = \frac{f(x_0+h)}{2h^3}\int_0^{3h}(u^3-5hu^2+6h^2u)\,du$

$= \frac{f(x_0+h)}{2h^3}\left[\frac{1}{4}u^4-\frac{5}{3}hu^3+3h^2u^2\right]\Big|_0^{3h}$

$= \frac{f(x_0+h)}{2h^3}\left(\frac{1}{4}(3h)^4-\frac{5}{3}h(3h)^3+3h^2(3h)^2\right)$

$= \frac{f(x_0+h)}{2h^3}\left[\frac{81h^4}{4}-45h^4+27h^4\right]$

$= \frac{f(x_0+h)}{2h^3}\left[\frac{9}{4}h^4\right] = \frac{f(x_0+h)}{8}\cdot 9h$

3rd integral: $-\frac{f(x_0+2h)}{2h^3}(x-x_0)(x-x_0-h)(x-x_0-3h)$; $u=x-x_0$:

$-\frac{f(x_0+2h)}{2h^3}\int_0^{3h}(u)(u-h)(u-3h)\,du = -\frac{f(x_0+2h)}{2h^3}\int_0^{3h}(u^3-4hu^2+3h^2u)\,du$

$= -\frac{f(x_0+2h)}{2h^3}\left[\frac{1}{4}u^4-\frac{4}{3}hu^3+\frac{3}{2}h^2u^2\right]\Big|_0^{3h}$

$= -\frac{f(x_0+2h)}{2h^3}\left[\frac{81}{4}h^4-36h^4+\frac{27}{2}h^4\right] = -\frac{f(x_0+2h)}{2h^3}\left[-\frac{9}{4}h^4\right] = \frac{f(x_0+2h)}{8}\cdot 9h$

4th integral: $\frac{f(x_0+3h)}{6h^3}(x-x_0)(x-x_0-h)(x-x_0-2h)$; $u=x-x_0$:

$\frac{f(x_0+3h)}{6h^3}\int_0^{3h}(u)(u-h)(u-2h)\,du = -\frac{f(x_0+2h)}{6h^3}\int_0^{3h}(u^3-3hu^2+2h^2u)\,du$

$= -\frac{f(x_0+2h)}{6h^3}\left[\frac{1}{4}u^4-hu^3+h^2u^2\right]\Big|_0^{3h}$

$= \frac{f(x_0+2h)}{6h^3}\left[\frac{81}{4}h^4-27h^4+9h^4\right] = \frac{f(x_0+2h)}{6h^3}\left[\frac{9}{4}\right]h^4 = \frac{f(x_0+2h)}{8}3h$

Total: $\frac{f(x_0)}{8}\cdot 3h + \frac{f(x_0+h)}{8}\cdot 9h + \frac{f(x_0+2h)}{8}\cdot 9h + \frac{f(x_0+3h)}{8}3h \approx I_3(f(x))$

Which can be rewritten as: $I_3(f(x)) \approx \frac{3h}{8}\left(f(x_0)+3f(x_0+h)+3f(x_0+2h)+f(x_0+3h)\right)$

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3. (20 points) Using a general interpolant $I_3(f(x))$ (that is, there is no need for equally spaced points as this is not a fundamental part of the derivation):

   (a) (5 points) Compute an *expression* for the error term, $E_3(x) = I(f(x)) - I_3(f(x))$. Recall, this requires constructing $R_3(x)$ (what we called $err(x)$ in the last homework; this can stay in integral form).

   (b) (7 points) Given
   $$f(x) = \sin(\frac{\pi}{2}x) + \frac{x^2}{4},$$
   use information about the function to bound the expression for $E_3(x)$ (you may use the result you got in Homework 2 to help you).
   You may use a mathematical package for help with the integration.

   (c) (2 points) Use the values $x_0 = 0, x_1 = 2, x_2 = 3$, and $x_3 = 4$ to get a bounded value for $E_3(x)$ over this interval.

   (d) (2 points) What is the maximum value of R_3 at $x = 1$? What about E_3?

   (e) (4 points) What is the maximum value of R_3 at $x = 5$?
   How does that compare to $x = 1$ and what insight can you draw from that?
   Can you make any comments about E_3 in this case?

a) Error term: $E_3(x) = I(f(x) - I_3(f(x))$

$$R_3(x) = \frac{f^{n+1}(\xi)}{(n+1)!}\prod_{i=0}^{n}(x - x_i),$$

hence: $R_3(x) = \dfrac{f^{iv}(\xi)}{4!}(x-x_0)(x-x_1)(x-x_2)(x-x_3)$

The error expression is:

$$E_3(x) = I\big(f(x)\big) - I_3\big(f(x)\big) = \int_{x_0}^{x_3} \frac{f^{iv}(c)}{4!}(x-x_0)(x-x_1)(x-x_2)(x-x_3)$$

b) $f(x) = \sin\left(\frac{\pi}{2}x\right) + \frac{x^2}{4}$, $\quad f'(x) = \frac{\pi}{2}\cos\left(\frac{\pi}{2}x\right) + \frac{1}{2}x$

$$f''(x) = -\left(\frac{\pi}{2}\right)^2 \sin\left(\frac{\pi}{x}x\right) + \frac{1}{2}$$

$$f'''(x) = -\left(\frac{\pi}{2}\right)^3 \cos\left(\frac{\pi}{2}x\right)$$

$$f^{iv}(x) = \left(\frac{\pi}{2}\right)^4 \sin\left(\frac{\pi}{2}x\right)$$

$$R_3(x) = \frac{\left(\frac{\pi}{2}\right)^4 \sin\left(\frac{\pi}{2}\xi\right)}{24}(x-x_0)(x-x_1)(x-x_2)(x-x_3).\, E_3 = \int_{x_0}^{x_3} R_3(x)$$

*The maximum value of f^{iv} is @ $\xi = 1 \rightarrow \sin\left(\frac{\pi}{2}\right) = 1$

$$\therefore E_3 = \frac{\pi^4}{16} * \frac{1}{24}\int_{x_0}^{x_3}(x-x_0)(x-x_1)(x-x_2)(x-x_3)dx < -the\ \mathrm{max}\ bound$$

c) $x_0 = 0, x_1 = 2, x_2 = 3, x_3 = 4$

$$E_3(x) = \int_0^4 \frac{\left(\frac{\pi}{2}\right)^4 \sin\left(\frac{\pi}{2}c\right)}{24}(x)(x-2)(x-3)(x-4)dx$$

$$= \frac{\left(\frac{\pi}{2}\right)^4 \sin\left(\frac{\pi}{2}c\right)}{24}\int_0^4 x(x-2)(x^2-7x+12)dx$$

$$= \frac{\left(\frac{\pi}{2}\right)^4 \sin\left(\frac{\pi}{2}c\right)}{24}\int_0^4 (x^4-9x^3+26x^2-24x)dx$$

$$= \frac{\left(\frac{\pi}{2}\right)^4 \sin\left(\frac{\pi}{2}c\right)}{24}\left[\frac{1}{5}x^5 - \frac{9}{4}x^4 + \frac{26}{3}x^3 - 12x^2\right]\Big|_0^4$$

$$= \frac{\left(\frac{\pi}{2}\right)^4 \sin\left(\frac{\pi}{2}c\right)}{24}(-8.5333)$$

when c = 1: $-\left(\frac{\pi}{2}\right)^4\left(\frac{1}{24}\right)(8.5333)$

and when c = 3: $\left(\frac{\pi}{2}\right)^4\left(\frac{1}{24}\right)(8.5333)$

d) x = 1: $R_3 = \frac{\left(\frac{\pi}{2}\right)^4 \sin\left(\frac{\pi}{2}\xi\right)}{24}(1)(1-2)(1-3)(1-4) = \frac{\left(\frac{\pi}{2}\right)^4 \sin\left(\frac{\pi}{2}\xi\right)}{24}(-6) = -\frac{\left(\frac{\pi}{2}\right)^4 \sin\left(\frac{\pi}{2}\xi\right)}{4}$
from 0 to 4, the maximum value is at $\xi = 1$ where R_3 = -1.522

For $E_3 = \frac{\left(\frac{\pi}{2}\right)^4 \sin\left(\frac{\pi}{2}\xi\right)}{24}\int_0^4 (-1)(-2)(-3)dx = \frac{\left(\frac{\pi}{2}\right)^4 \sin\left(\frac{\pi}{2}\xi\right)}{24}(-6x)|_0^4$
The maximum value is at $\xi = 1$: $E_3 = \left(\frac{\pi}{2}\right)^4 \sin\left(\frac{\pi}{2}\right) = -\left(\frac{\pi}{2}\right)^4 = 6.088$

e) x = 5:

$$R_3 = \frac{\left(\frac{\pi}{2}\right)^4 \sin\left(\frac{\pi}{2}\xi\right)}{24}(5)(3)(2)(1) = \frac{30}{24} * \frac{\pi^4}{16}\sin\left(\frac{\pi}{2}\xi\right)$$

From 0 to 4, the max value is @ $\xi = 1$: $R_3 = \frac{30}{24} * \frac{\pi^4}{16} = 7.61$

For the error term, $\frac{\left(\frac{\pi}{2}\right)^4 \sin\left(\frac{\pi}{2}\xi\right)}{24}\int_0^4 30dx = 30.44\sin\left(\frac{\pi}{2}\right) \rightarrow maximum\ is\ E_3 = 30.44$

The maximum value of R_3 @ x = 5 is five times greater than @ x = 1. The reason why the error is much larger at x = 5 is because x = 5 is far away compared to x = 1. You are given more points near x= 1. Also, 5 is out of the range of 0 to 4, therefore E_3 has a large error.

4. (20 points) Consider the following integral

$$I = \int_2^4 \frac{x}{\sqrt{x^2-1}} dx \, .$$

(a) (6 points) Compute the integral exactly by hand.

(b) (8 points) Write a code that performs Composite Simpson's 3/8 rule to compute the integral. I advise something like
`I = CompSimp38(a,b,n)`
where `a` and `b` are the endpoints and `n` is the number of points to use in the integration (which must be divisible by 3!).

(c) (6 points) Experimentally determine the rate of convergence as a function of `h`.

a) $I = \int_2^4 \frac{x}{\sqrt{x^2-1}} dx = \int_2^4 x(x^2-1)^{-\frac{1}{2}} dx = (x^2-1)^{\frac{1}{2}} |_2^4 = (16-1)^{1/2} - (4-1)^{\frac{1}{2}} = 15^{\frac{1}{2}} - 3^{\frac{1}{2}}$

3.873 – 1.732 = 2.141

b)

Composite_simpson_rule.py

```
import numpy as np
import matplotlib.pyplot as plt

x = []

def fun(x):
    '''
    This step is to define the function we are intregrating
    '''
    return x / np.sqrt(x ** 2 - 1)

def x_axis_tool(n, a=2, b=4):
    '''
    This step creates an axis that will be used to perform Simpson's
Rule
    '''
    x = np.linspace(a, b, (6 * n) + 2)
    return x

def CompSimp38(n, a = 2, b = 4):
    '''
    This is the Composite Simpson's 3/8th rule for the function defined
above.
    n has to be a whole number in order for the function to run
accurately.
    '''
    x = x_axis_tool(n, a, b)
    y = []
    for i in x:
        y.append(fun(i))
    results = []
```

```
    results.append(y[0])
    i = 1
    while i < len(x) - 1:
        if i % 3 == 0:
            results.append(2 * y[i])
        else:
            results.append(3 * y[i])
        i += 1
    i += 1
    results.append(y[len(x)-1])
    h = (b-a)/(6*n)
    return (3/8)*h*sum(results)

i = 450
while i < 500:
    print('For n = {}'.format(6*i))
    print(CompSimp38(i))
    i+=5

print(CompSimp38(500))
```

```
Returns:
For n = 2994
2.14147513446
```

c)

If we use the method where $p \approx \frac{\log\left(\frac{e_{new}}{e_{old}}\right)}{\log\left(\frac{h_{new}}{h_{old}}\right)}$ where p is used to find the rate of convergence of a discretization method:

Compsite_simpson_rule.py

```
def convergence(value1, value2, h1, h2):
    exact = 2.141
    e1 = np.abs(value1 - exact)
    e2 = np.abs(value2 - exact)
    return (np.log(e2/e1))/(np.log(h2/h1))

value1 = CompSimp38(1)
value2 = CompSimp38(2)

print(convergence(value1[0],value2[0], value1[1], value2[1]))

value1 = CompSimp38(2)
value2 = CompSimp38(4)

print(convergence(value1[0],value2[0], value1[1], value2[1]))
```

```
1.00024898395
1.00051539016
```

Both of these returned values round to one. Hence the rate of convergence is 1.