UNIVERSITY OF LEICESTER

Computational Project

Student name: *Junbiao Li*

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Name: Junbiao Li
Signed: Junbiao Li
Date: March 28th, 2022

Topic 1

Answer. In order to get the second order accurate forward, backward and centered finite difference schemes for finding the derivative. We first write down the Taylor series expansions of $f(x+h)$, $f(x-h)$, $f(x+2h)$, $f(x-2h)$, $f(x+3h)$ and $f(x-3h)$

$$
\begin{aligned}
f(x+h) &= f(x) + h\frac{f'(x)}{1!} + h^2\frac{f''(x)}{2!} \\
f(x-h) &= f(x) - h\frac{f'(x)}{1!} + h^2\frac{f''(x)}{2!} \\
f(x+2h) &= f(x) + 2h\frac{f'(x)}{1!} + 4h^2\frac{f''(x)}{2!} \\
f(x-2h) &= f(x) - 2h\frac{f'(x)}{1!} + 4h^2\frac{f''(x)}{2!} \\
f(x+3h) &= f(x) + 3h\frac{f'(x)}{1!} + 9h^2\frac{f''(x)}{2!} \\
f(x-3h) &= f(x) - 3h\frac{f'(x)}{1!} + 9h^2\frac{f''(x)}{2!}
\end{aligned}
$$

For the second order accurate forward difference, we want to find out $f'(x) = \frac{1}{h}(a_0 f(x) + a_1 f(x+h) + a_2 f(x+2h) + O(h^3))$ where a_0, a_1, a_2 are all constant. Hence, we have

$$
\begin{aligned}
\frac{f'(x)}{1!} = f'(x) = \frac{1}{h}(a_0 f(x) + & \\
& a_1 f(x) + a_1 f'(x)h + a_1 f''(x)h^2 \\
& a_2 f(x) + 2a_2 f'(x)h + 4a_2 f''(x)h^2 + O(h^3))
\end{aligned}
$$

Which is equivalent to solve a linear system

$$\left(\begin{array}{ccc|c} 1 & 1 & 1 & 0 \\ 0 & 1 & 2 & 1 \\ 0 & 1 & 4 & 0 \end{array}\right)$$

Hence, $a_0 = -\frac{3}{2}$, $a_1 = 2$ and $a_3 = -\frac{1}{2}$, and

$$f'(x) = \frac{-\frac{3}{2}f(x) + 2f(x+h) - \frac{1}{2}f(x+2h)}{h} + O(h^2)$$

With the same process, We can calculate second order accurate forward, backward and centered finite difference schemes for first derivative and second derivative:

1. Second order accurate centered difference approximations:

$$f'(x) : (f(x+h) - f(x-h))/(2h)$$
$$f''(x) : (f(x+h) - 2f(x) + f(x-h))/h^2$$

2. Second order accurate forward difference approximations:

$$f'(x) : (-3f(x) + 4f(x+h) - f(x+2h))/(2h)$$
$$f''(x) : (2f(x) - 5f(x+h) + 4f(x+2h) - f(x+3h))/h^2$$

3. Second order accurate backward difference approximations:

$$f'(x) : (3f(x) - 4f(x-h) + f(x-2h))/(2h)$$
$$f''(x) : (2f(x) - 5f(x-h) + 4f(x-2h) - f(x-3h))/h^2$$

Implement. I chose $x^4 + \sin(x)$ as test function, with $0 \leq x \leq 2$ and $h = 0.1$

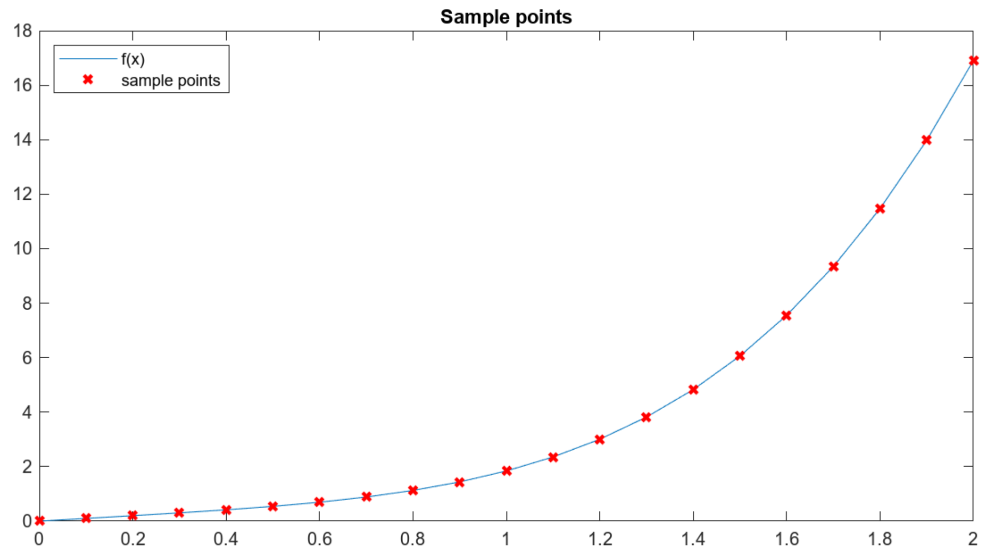
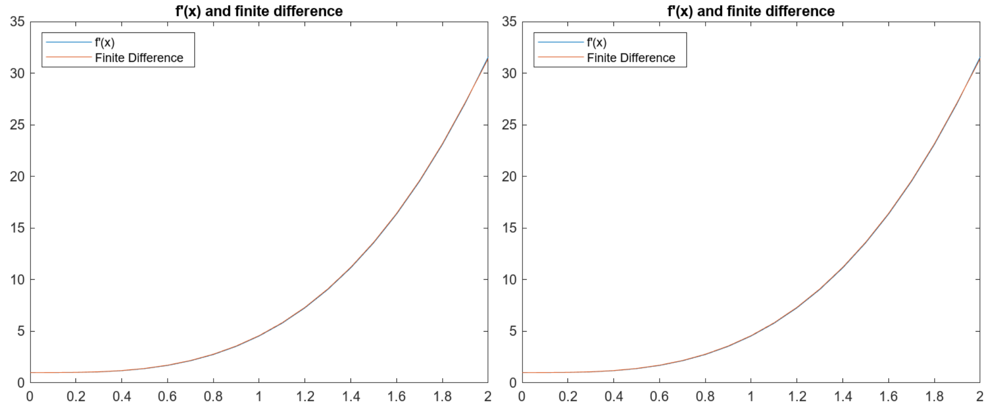


Figure 1: Sample Points of f(x)

After applying second order accurate difference approximations, I draw $f'(x)$ and $f''(x)$ to check the difference between real derivative and finite difference schemes.

Figure.2 told us that the second order accurate difference approximations is really close to the real derivative, even their actually difference. You can find more implement detail in the code.



(a) f′(x) (b) f″(x)

Figure 2: Compare real derivative and finite difference

Topic 2

Answer. In order to evaluate double integrals which is perform on the rectangle $R = \{(x, y) \in \mathbb{R}^2 : a \leq x \leq bandc \leq y \leq d\}$, We first consider the uniform-grid in each dimension. Let grid space of x and y be the h, which means we have $x_1, x_2, \cdots, x_{n_x}$ and $y_1, y_2, \cdots, y_{n_y}$.

Task 1 Now apply trapezoidal rule to calculate the integral with respect to x with fixed y.

$$\begin{aligned} g(y) &= \int_a^b f(x, y)\, dx \\ &= \sum_{i=1}^{n_x - 1} \frac{1}{2}[f(x_i) + f(x_{i+1})]h \\ &= \frac{h}{2}[f(x_0, y) + f(x_{n_x}, y) + 2\sum_{i=2}^{n_x - 1} f(x_i, y)] \\ &= \frac{h}{2}[f(a, y) + f(b, y) + 2\sum_{i=2}^{n_x - 1} f(x_i, y)] \end{aligned}$$

Finally we get $g(y) = \frac{h}{2}[f(a, y) + f(b, y) + 2\sum_{i=2}^{n_x} f(x_i, y)]$

Task 2 After integrate x, we now integrate y,

$$\begin{aligned} I &= \int_c^d g(y)\, dy \\ &= \sum_{i=1}^{n_y} \frac{1}{2}[g(y_i) + g(y_{i+1})]h \\ &= \frac{h}{2}[g(c) + g(d) + 2\sum_{i=2}^{n_y} g(y_i) + g(y_{i+1})] \end{aligned}$$

Substituting into

$$
\begin{aligned}
I = \frac{h}{2}\{ & \frac{h}{2}[f(a,c)+f(b,c)+2\sum_{i=2}^{n_x} f(x_i,c)] \\
& +\frac{h}{2}[f(a,d)+f(b,d)+2\sum_{i=2}^{n_x} f(x_i,d)] \\
& +\frac{h}{2}[f(a,y)+f(b,y)+2\sum_{i=2}^{n_x} f(x_i,y)]\}
\end{aligned}
$$