UNIVERSITY OF LEICESTER

Computational Project

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Course: *MA2252 Introduction to Computing*
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1. Topic 1

Answer. To get the second-order accurate forward, backward and centered finite difference schemes for finding the derivative.[2] 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 $f(x-3h)$

$$\begin{aligned} f(x+h) &= f(x) + h\frac{f'(x)}{1!} + h^2\frac{f''(x)}{2!} \\ f(x-h) &= f(x) - h\frac{f'(x)}{1!} + h^2\frac{f''(x)}{2!} \\ f(x+2h) &= f(x) + 2h\frac{f'(x)}{1!} + 4h^2\frac{f''(x)}{2!} \\ f(x-2h) &= f(x) - 2h\frac{f'(x)}{1!} + 4h^2\frac{f''(x)}{2!} \\ f(x+3h) &= f(x) + 3h\frac{f'(x)}{1!} + 9h^2\frac{f''(x)}{2!} \\ f(x-3h) &= f(x) - 3h\frac{f'(x)}{1!} + 9h^2\frac{f''(x)}{2!} \end{aligned} \tag{1.1}$$

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

$$\begin{aligned} \frac{f'(x)}{1!} = f'(x) = \frac{1}{h}(a_0 f(x) + \\ &a_1 f(x) + a_1 f'(x)h + a_1 f''(x)h^2 \\ &a_2 f(x) + 2a_2 f'(x)h + 4a_2 f''(x)h^2 + \mathcal{O}(h^3)) \end{aligned} \tag{1.2}$$

Which is equivalent to solving a linear system

$$\left(\begin{array}{ccc|c} 1 & 1 & 1 & 0 \\ 0 & 1 & 2 & 1 \\ 0 & 1 & 4 & 0 \end{array}\right) \tag{1.3}$$

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

$$f'(x) = \frac{-\frac{3}{2}f(x) + 2f(x+h) - \frac{1}{2}f(x+2h)}{h} + \mathcal{O}(h^2) \tag{1.4}$$

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

1. Second order accurate centered difference approximations:
$$\begin{aligned} f'(x) &:(f(x+h) - f(x-h))/(2h) \\ f''(x) &:(f(x+h) - 2f(x) + f(x-h))/h^2 \end{aligned} \tag{1.5}$$
2. Second order accurate forward difference approximations:
$$\begin{aligned} f'(x) &:(-3f(x) + 4f(x+h) - f(x+2h))/(2h) \\ f''(x) &:(2f(x) - 5f(x+h) + 4f(x+2h) - f(x+3h))/h^2 \end{aligned} \tag{1.6}$$
3. Second order accurate backward difference approximations:
$$\begin{aligned} f'(x) &:(3f(x) - 4f(x-h) + f(x-2h))/(2h) \\ f''(x) &:(2f(x) - 5f(x-h) + 4f(x-2h) - f(x-3h))/h^2 \end{aligned} \tag{1.7}$$

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

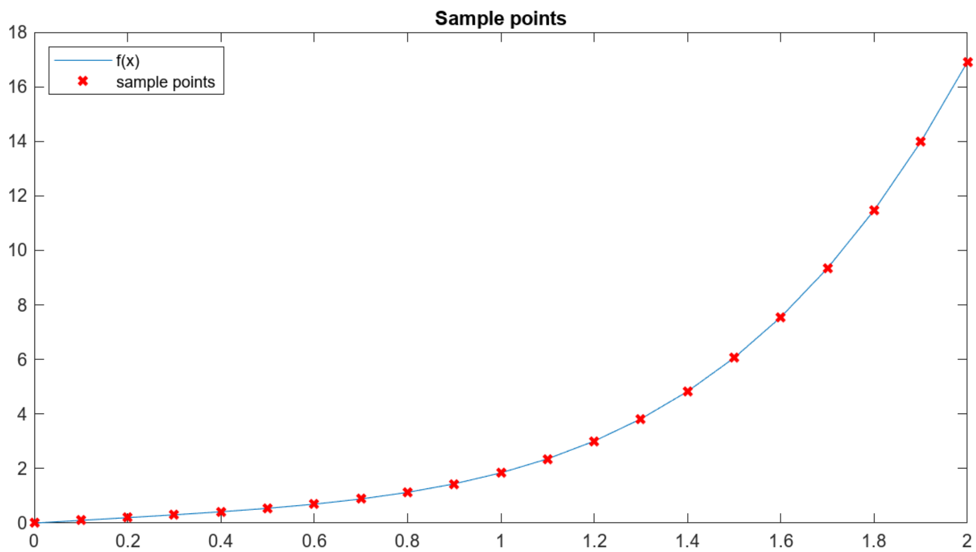

Figure 1.1: Sample Points of f(x)

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

Figure.1.2 and Figure.1.3 told us that the second-order accurate difference approximations are close to the real derivative, even their actual difference. You can find more implementation detail in the code.

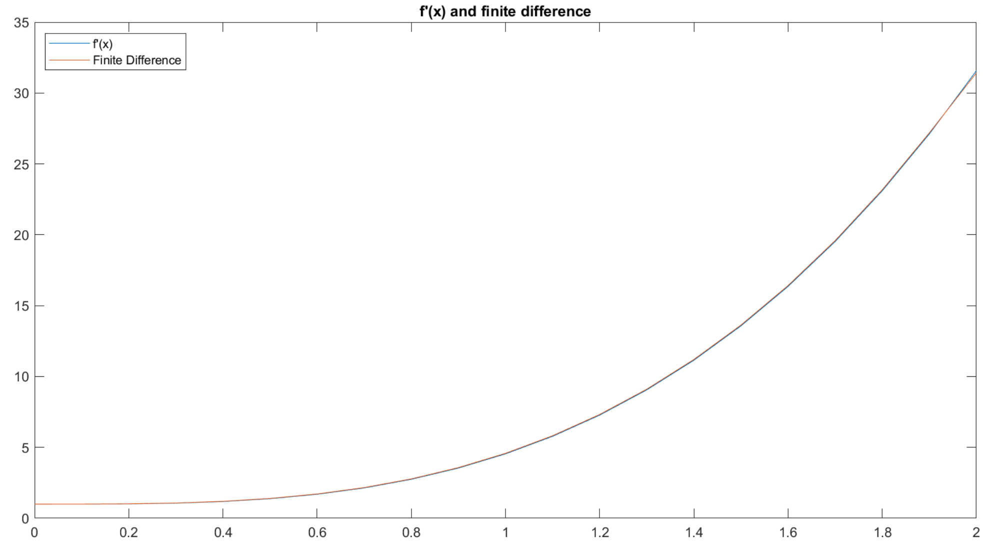

Figure 1.2: Compare real first derivative and finite difference

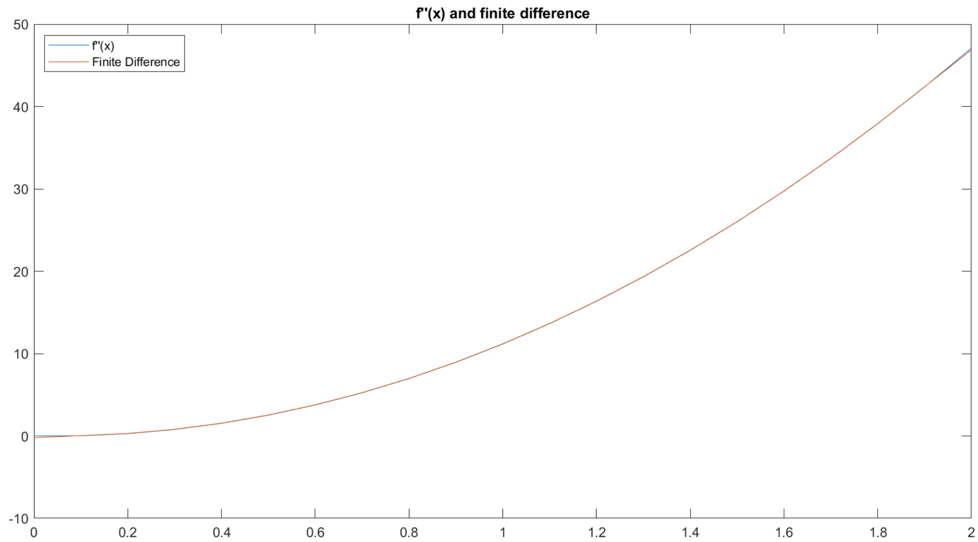

Figure 1.3: Compare real second derivative and finite difference

2. Topic 2

Answer. To evaluate double integrals which are performed on the rectangle $R = \{(x, y) \in \mathbb{R}^2 : a \leq x \leq b \text{ and } c \leq y \leq d\}$, We first consider the uniform-grid in each dimension. Let grid space of x and y be the h, which means we have $x_1, x_2, \ldots, x_{n_x}$ and $y_1, y_2, \ldots, y_{n_y}$.[1]

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

$$\begin{aligned} g(y) &= \int_a^b f(x,y)\,dx \\ &= \sum_{i=1}^{n_x-1} \frac{1}{2}[f(x_i)+f(x_{i+1})]h \\ &= \frac{h}{2}[f(x_0,y)+f(x_{n_x},y)+2\sum_{i=2}^{n_x-1} f(x_i,y)] \\ &= \frac{h}{2}[f(a,y)+f(b,y)+2\sum_{i=2}^{n_x-1} f(x_i,y)] \end{aligned} \tag{2.1}$$

Finally we get $g(y)=\frac{h}{2}[f(a,y)+f(b,y)+2\sum_{i=2}^{n_x-1} f(x_i,y)]$

Task 2 After integrate x, we now integrate y,

$$\begin{aligned} I &= \int_c^d g(y)\,dy \\ &= \sum_{i=1}^{n_y-1} \frac{1}{2}[g(y_i)+g(y_{i+1})]h \\ &= \frac{h}{2}[g(c)+g(d)+2\sum_{j=2}^{n_y-1} g(y_j)] \end{aligned} \tag{2.2}$$

Substituting eq.(2.1) into eq.(2.2) we have

$$\begin{aligned} I = \frac{h}{2}\{&\frac{h}{2}[f(a,c)+f(b,c)+2\sum_{i=2}^{n_x-1} f(x_i,c)] \\ &+\frac{h}{2}[f(a,d)+f(b,d)+2\sum_{i=2}^{n_x-1} f(x_i,d)] \\ &+\frac{h}{2}2\sum_{j=2}^{n_y-1}[f(a,y_j)+f(b,y_j)+2\sum_{i=2}^{n_x-1} f(x_i,y_j)]\} \end{aligned} \tag{2.3}$$

Now we can simplify eq.(2.3) as much as possible

$$\begin{aligned} I = (\frac{h}{2})^2[&f(a,c)+f(b,c)+f(a,d)+f(b,d) \\ &+2\sum_{i=2}^{n_x-1}[f(x_i,c)+f(x_i,d)] \\ &+2\sum_{j=2}^{n_y-1}[f(a,y_j)+f(b,y_j)] \\ &+4\sum_{j=2}^{n_y-1}\sum_{i=2}^{n_x-1} f(x_i,y_j)] \end{aligned} \tag{2.4}$$

Table 2.1: Accuracy of difference h with function $y^4 + \sin(x)$

	a=0;b=1;c=2;d=4;h=0.1	a=0;b=1;c=2;d=4;h=0.5
my_integral2	199.505289	203.962661
real	199.319395	199.319395
error	**0.0933%**	**2.3296%**

Table 2.2: Accuracy of difference R with function $y^4 + \sin(x)$

	a=0;b=1;c=2;d=4;h=0.1	a=0;b=1;c=0;d=10;h=0.1
my_integral2	199.505289	20007.926445
real	199.319395	20004.596977
error	**0.0933%**	**0.0166%**

Implement. Here is the implemented code with Matlab. I compared Matlab's original function with an extra h parameter for testing how different the final integration result would be with different accuracy of the partition. Then use for-loop to accumulate multiple times and finally output the result of integration

```
function I=my_integral2(f, a, b, c, d, h)
  x=a:h:b;
  y=c:h:d;
  n_x=length(x);
  n_y=length(y);
  I=f(a, c)+f(b,c)+f(a,d)+f(b,d);
  for i=2:n_x-1
    I = I + 2*(f(x(i),c)+f(x(i),d));
  end
  for j=2:n_y-1
    I = I + 2*(f(a, y(j))+f(b, y(j)));
  end
  for i=2:n_x-1
    for j=2:n_y-1
      I = I + 4*f(x(i), y(j));
    end
  end
  I = h^2/4*I;
end
```

After doing some experiments, I found that the finer the segmentation and the larger the rectangle, the higher the accuracy can be obtained. You can see more detailed data in the following two tables (Table 2.1) (Table 2.2). Here I use the formula $\frac{|my\_integral2 - real|}{|real|}$ to calculate the error.

References

[1] David Keffer. Numerical techniques for the evaluation of multi-dimensional integral equations. http://utkstair.org/clausius/docs/che505/pdf/IE_eval_N-Dints.pdf, September 1999.

[2] Alice C. Yew. Numerical differentiation: finite differences. https://www.dam.brown.edu/people/alcyew/handouts/numdiff.pdf, Spring 2011.