Numerical Analysis Homework: Calculating a Double Integral Using Different Methods

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Chapter 1

Introduction

The assignment concerns the calculation of the double integral of the function $f(x, y) = x^2 + y^3$ over a domain with y limits [x,2x] and x limits [0,1]:

$$I = \int_0^1 \int_x^{2x} x^2 + y^3 \, dydx \tag{1.1}$$

Three different approaches are used: the analytical calculation, Simpson's rule, which is a numerical calculation, and Monte Carlo integration.

The specific integral defines the volume that is enclosed in the space between the surfaces: y=x, y=2x, x=0, x=1 and z=$x^2 + y^3$. Although its analytical solution is trivial, Simpson's one - third rule and Monte Carlo integration are applied, too, in order to be learned and tested.

Chapter 2

Methodology

2.1 Analytical Calculation (Exact Method)

First of all, the analytical solution of the integral I (1.1) was found. Firstly, the calculation of the inner integral was made according to the integration for y and the independence of x and y:

$$I = \int_0^1 \int_x^{2x} x^2 + y^3 = \int_0^1 \left[x^2 y + \frac{y^4}{4} \right]_x^{2x} dx = \int_0^1 x^3 + \frac{15}{4} x^4 \, dx$$

Afterwards, the integration was calculated for x:

$$I = \left[\frac{x^4}{4} + \frac{3x^5}{4} \right]_0^1$$

Finally, the result is:

$$I = 1$$

The order of integration is important because the limits of the inner integral depend on the variable x.

The result represents the volume that is included inside the surfaces y=x, y=2x, x=0, x=1, and $z=x^2+y^3$. z takes values from 0 to 9. All the dimensions happen to be on the positive side of the axes. Therefore, integral is the accurate shape's volume.

2.2 Numerical Calculation: Simpson's 1/3 rule

Simpson's rule is a classical numerical approach to an integral's value. Concerning Simpson's 1/3 rule, it is based on finding a parabola that connects three points of the function that are mended to be integrated.[1] The simplest situation is when the interval is separated into two equal segments. In that case, the equation that approaches the integral is:

$$\int_a^b f(x) = \frac{h}{3}(f_1 + 4f_2 + f_3) \tag{2.1}$$

where $h = \frac{b-a}{n}$, n the number of segments, and f_1, f_2, f_3 the values of f at a, a+(b-a)/2, and b, respectively. In general, Simpson's 1/3 rule is used for an even n number of segments with the general equation:

$$\int_a^b f(x) = \sum_1^{n-2} \frac{h}{3}(f_i + 4f_{i+1} + f_{i+2}) = \frac{h}{3}(f_1 + 4f_2 + 2f_3 + 4f_4 + ... + 2f_{n-2} + 4f_{n-1} + f_n) \tag{2.2}$$

The error is analogous to h^4 and not to h^5 as expected:

$$E = -\frac{b-a}{180}h^4 f^{(4)}(\xi) \tag{2.3}$$

with ξ inside the last segment.[3]

The exercise's integral is a double integral, with the inner integral's limits depending on x. Python was used to apply the formula to two models. The first model uses Simpson's rule for both integrations regarding y and x. The second model computes analytically the inner integral and numerically the outer integral.

First Model

In this case, the implementation of Simpson's 1/3 rule was made for both y integration and x integration. Firstly, a function with the f(x,y) function was defined. Secondly, Simpson's 1/3 rule for two segments was defined as a function called *simpsons13(y,dy,dx)* based on the equation 2.1. This function is called for nx=ny segments. The results were summarized. The total procedure took place in a function called *doubleintegral(nx)*. There, the step dx was calculated as 1/nx. x took values from zero to one with the dx step, and y took values for each x, 1.5x, and 2x.

The implementation was made for nx=2, 50, 100, and 1000 in order to investigate the method's convergence.

Second Model

By using sympy Python's library and the sp.integrate tool, the inner integral was calculated with accuracy as follows:

$$\frac{15x^4}{4} + x^3$$

using a function *innerintegral*. After that, a new Simpson's rule function was defined based on the equation 2.2, called *simpsons1*. Finally, the outer integral was calculated using both *innerintegral* and *simpsons1*.

2.3 Monte Carlo

Monte Carlo integration is a numerical technique for integration using arbitrary numbers. It randomly chooses points near the area in which the integral is evaluated. It can be easily applied to double integrals and higher - dimensional integrals.[2]

Concerning the particular integral 1.1, it represents a 3D shape 'A' that has for sides the surfaces y=x, y=2x, x=0, x=1, and $z=x^2+y^3$. The hole shape 'A' is included in a 3D parallelogram with x sides equal to 1, y sides equal to 2, z sides equal to 9, and volume V=1*2*9=18. Therefore, the integral's value can be approached as the percentage of the arbitrary points that are inside the shape 'A' over those that belong to the 3D parallelogram.

The steps that were followed during the computation are:

- Drawing N random numbers (x_i, y_i, z_i by using the function "numpy.random.random()". This function draws random float numbers in the interval [0, 1]. Therefore, it is significant to use proper coefficients for x, y, z: 1, 2, 9. As a results, the points could be anywhere inside the parallelogram.
- Counting how many points are inside the shape 'A'. In order to achieve this, the following if condition was applied: if ((Zrand≤Xrand**2+Yrand**3) & (Yrand≥Xrand) & (Yrand≤2*Xrand))
- Calculating the integral as: I=V A/N

For research purposes, N was defined as an 1x4 array: [100,1000,10000,100000]. The target was to investigate the convergence of the method.

Chapter 3

Results

Having already solved the integral in the Analytical Calculation part, it is known that the result is 1. Simpson's rule and Monte Carlo integration were also able to sufficiently approach the correct number.

First of all, Simpson's rule's results differed between the first and second models. Of course, the second model had faster convergence. The result in that case was 1.0313 for two segments. The reason for this is that the inner integral was precisely calculated. The error occurred due to the rule's application to compute the outer integral, and it is analogous to the h^4, error at simple integrals (equation 2.3). Hence, the result was immediately accurate with only two segments.

On the other hand, two segments were not enough in the first model. The result was completely insufficient (2.555), with an error of more than 200%. To have the same accuracy as in the previous model, about one hundred segments were needed. As it can be clearly seen in the graph 3.1, for 100 segments, the result was 1.024, while for 1000 segments, the result was 1.002.

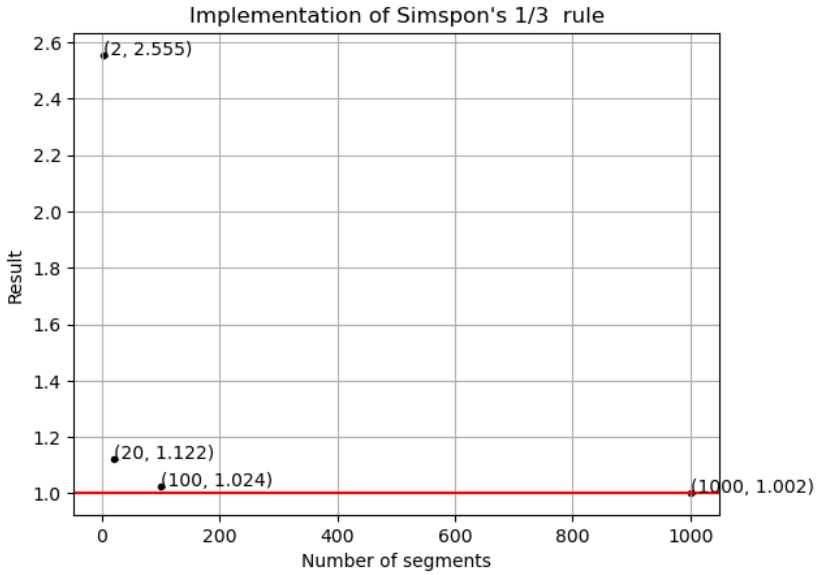

Figure 3.1: Results of the first model: implementation of Simpson's rule for the inner and outer integrals for 2, 20, 100, and 1000 segments at each axes. The accuracy is extremely improved for N≤100. The horizontal red line is the Result=1. In other words, it represents the integral's solution.

Table 3.1: Monte Carlo Integration: Approaches for different numbers of points

Number of points	Result
100	0.9
1000	0.81
10000	0.999
100000	1.002

Finally, Monte Carlo's results were different every time the program ran, but close to the target value. For instance, table 3.1 shows the results that occurred in one compilation.

Chapter 4

Discussion

Compering the results to which the above approaches led, a few aspects occurred. One important observation is the big difference that the first model's convergence has compared to that of the second model's. The first model implements Simpson's rule for both the inner and outer integrals. That is the explanation why it has larger errors than the second model, failures in the computation of the inner integral are transferred to the computation of the second integral and added to the second integral's errors. As a result, the uncertainty becomes analogous to the $(h_x h_y)^4$.

Another significant note that has to be taken into consideration is the convergence of Monte Carlo integration. Although the results for small N (100-1000) do not converge, for larger N, the error becomes smaller. For N about 10000, the result becomes accurate for three decimal digits. The method's uncertainty for smaller N is a consequence of the method's nature. It is based on randomness, and it requires a huge number of points in order to limit the results nearer the one.

Chapter 5

Conclusion

In conclusion, comparing the first and second models, the first one, although it has greater errors, uses the requested method more properly. Additionally, coding Simpson's had many difficulties. There are a good many numerical integration methods that might be more efficient for double integration, such as the trapezoidal rule. However, the assignment's integral has x to the power of 2 and y to the power of 3, which combined with the trapezoidal rule would lead to greater errors than the Simpson's rule does. Finally, Monte Carlo integration was easy to code and had sufficient accuracy for large Ns. Therefore, should a higher - dimensional integral be numerically approached, Monte Carlo integration is recommended.

Bibliography

[1] Introduction to Numerical Analysis with applications in Physics, K. D. Kokkotas

[2] Monte Carlo Integration

[3] Course's notes, Lecture 5, K. Kosmidis