Adaptive Quadrature-Simpson's Method

P346 - Computational Physics DIY Project

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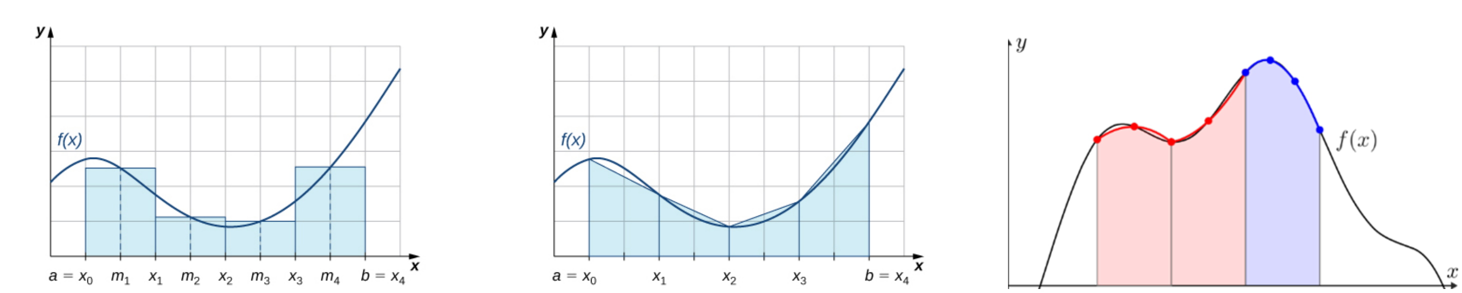
This project describes the need of adaptive quadrature when the techniques of dividing equal widths in case of midpoint, trapezoidal and Simpson's method increases computational power and time complexity. The adaptive method carefully divides the intervals into sub-intervals based on the tolerance level to give the integral value. In our case, adaptive Simpson's method was studied for the function e^{-x} for the interval [0,4].

Introduction

Quadrature means to calculate the area under the curve. Hence calculating definite integrals is also called quadrature. In mid-point integration rule, the integral is estimated within a range by dividing the sub-intervals of equal width and the mid points of each sub-intervals. The function is continuous in the interval $[a, b]$, then they are divided into equal parts of width w, $w = (b - a)/N$, and mid points of these intervals, m are calculated. The total sum of all such area of rectangle approximates to $M_n = \sum_{i=1}^{n} f(m_i)w$ and with $\lim_{x\to\infty} M_n = \int_a^b f(x)$.

Like mid-point integration rule, trapezoidal rule also follows similar rule, with the fact that instead of rectangles, trapezoids of equal size is used to calculate the area under the curve. The area of each trapezoid is calculated as $\frac{h(f(x_{n-1})+f(x_n))}{2}$ and summing over this area to get the integral, as $\lim_{n\to\infty} \frac{h}{2}(f(x_0) + 2[\sum_{i=1}^{n-1} f(x_i)] + f(x_n)) = \int_a^b f(x)$.

In Simpson's 1/3 rule, the area under the curve is calculated by quadratic interpolation. The area under the curve is calculated by $\lim_{n\to\infty} \frac{h}{3}(f(x_0) + 2[\sum_{i=1}^{n-1} f(x_{2i})] + 4[\sum_{j=1}^{n-1} f(x_{2j+1})] + f(x_n)) = \int_a^b f(x)$.



(a) Integration by mid-point rule
(b) Integration by trapezoidal rule
(c) Integration by Simpson's rule

Figure 1: Depiction of area under curve for different integration rules

The Problem and Solution

Simpson's method is more accurate in determining the integrals as it uses quadratic approximations but the other two methods, midpoint and trapezoidal rules just uses linear approximations where the area under the curve has to be compromised with adding or ignoring the areas where the function doesn't lie. It is evident as shown in Figure(1).

With for different functions, it is unimportant to have a uniform intervals for every case, as it increases the computational power and time complexity to compute the integrals. This is where adaptive quadrature kicks in. It carefully divides and refines the intervals into sub-intervals using static quadrature rules. The psuedo code for the adaptive quadrature for Simpson's rule is as follows.

```
#integrate by simpson's method
def adaptive_simpson(f,a,b,tolerance):  # f=function, a,b= limits
        error_est=(simpson(f,a,b,N1)-simpson(f,a,b,N2))
        if error_est<15*tolerance:
                I=simpson(f,a,b,N2)+(simpson(f,a,b,N2)-simpson(f,a,b,N1))/15
        else:
                m=(a+b)/2
                I=adaptive_simpson(f,a,m,tolerance/2)+
                adaptive_simpson(f,m,b,tolerance/2)
return I
```

In the pseudo code, 15 is multiplied to the tolerance as it is the termination criterion suggested by J.N. Lyness.

Case Study

We have considered function as e^{-x} in the interval [0,4] and studied how the convergence of integrals varies with the number of iterations. The tolerance was already given as input in the adaptive Simpson's function giving outputs with integral and number of iterations to achieve that precision. To compare with the Simpson's method we dealt in class, the maximum number was obtained to achieve the required precision by applying ceil function to N, as shown in following equation:

$$\text{Precision} <= \frac{(b-a)^5.|f''''(x)|_{max}}{180.N^4} \tag{1}$$

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(a) Convergence of integral adaptive Simpson's method

(b) Convergence of integral with Simpson's method

Figure 2: Convergence of Adaptive Simpson's and Simpson's methods for function e^{-x} for limit ranging from [0,4]

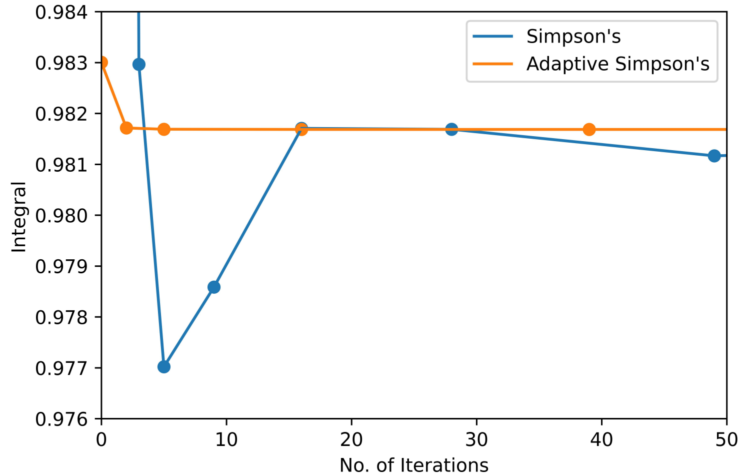

Figure 3: Convergence of integral with Simpsons and Adaptive Simpson's method

It is seen that Adaptive Simpson's method maintains stable integral value with different precision with with the iterations, whereas in case of Simpson's method, the integral value starts to deviate as seen Figure(3). The actual value of integral is 0.9816843611. The intervals are divided based on the need, in adaptive Simpson's method, to give the desired result, hereby reducing the computational costs and time complexity to become efficient function to determine the integral.

Acknowledgement

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References

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