Adaptive Quadrature method Simpson's method

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Abstract: Composite formulas for solving numerical integration are ineffective because of large computation time due to small equally-spaced step-size (h). This is inappropriate when a function has both large and small functional variations in an interval. So adaptive step-size quadrature methods were introduced. This report describes the working of procedural way of derivation of adaptive technique for the Simpson's 1/3 method and explains it using pseudo-code and an example. The operation can be extrapolated to other methods like trapezoidal and mid-point methods also.

INTRODUCTION

Numerical integration is the approximate computation of an integral using numerical techniques. The simplest way is to divide the interval into very small steps h and calculate the area under the curve over individual steps. But functions that vary fast need a better refinement of h while for slowly varying functions, it would be a waste of computational power.

Using adaptive method one can dynamically set h and set coarse mesh for slowly varying function and finer mesh for fast varying functions. Let's discuss how:

THEORY

Since the Simpson's $\frac{1}{3}$ rule is the most widely used methods which works under sufficiently less number of iterations, we discuss this in detail.

Suppose that we want to approximate $\int_a^b f(x)dx$ within tolerance $\varepsilon > 0$.

$$\int_a^b f(x)dx = S(a,b) - h^4 \frac{(b-a)}{180} f^{(4)}(\xi) \quad \text{for some } \xi \text{ in } (a,b) \tag{1}$$

Here, the general formula for error in Simpson's rule is used. The proof for equation (1) can be obtained using Taylor expansion. The complete proof of this equation is beyond the scope of this report. See reference [1] and [3].

Let's get back to our method. The first step is to apply Simpson's rule with step size $h = \frac{(b-a)}{2}$. This produces (see figure 1)

$$\int_a^b f(x)dx = S(a,b) - \frac{h^5}{90} f^{(4)}(\xi) \tag{2}$$

where we denote the Simpson's rule approximation on $[a,b]$ by $S(a,b)$, and the second term gives the error in the quadrature.

$$S(a,b) = \frac{h}{3}[f(a) + 4f(a+h) + f(b)] \tag{3}$$

The next step is to determine an accuracy approximation that does not require $f^{(4)}(\xi)$. To do this, we apply the Composite Simpson's rule with $n = 4$ and step size $\frac{(b-a)}{4} = \frac{(h)}{2}$. This makes the integral $\int_a^b f(x)dx$

$$= \frac{h}{6}\left[f(a) + 4f\left(a+\frac{h}{2}\right) + 2f(a+h) + 4f\left(a+\frac{3h}{2}\right) + f(b)\right] - \left(\frac{h}{2}\right)^4 \frac{(b-a)}{180} f^{(4)}(\bar{\xi}) \qquad \text{for some } \bar{\xi} \text{ in } (a,b) \tag{4}$$

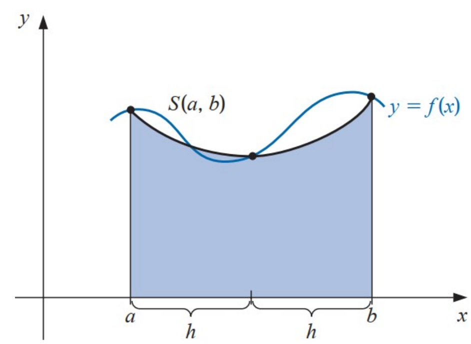

FIG. 1. *Simpson's method with 2 sub-intervals*

The above equation can be rewritten (see figure 2) as

$$\int_a^b f(x)dx = S\left(a, \frac{a+b}{2}\right) + S\left(\frac{a+b}{2}, b\right) - \frac{1}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\bar{\xi}) \tag{5}$$

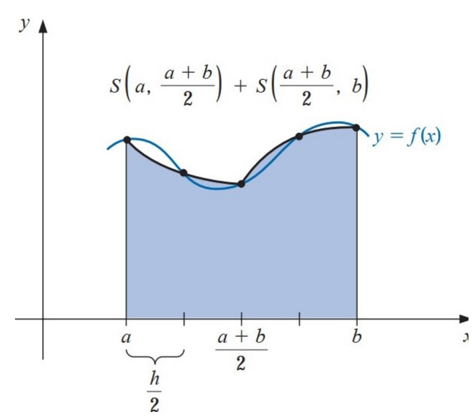

FIG. 2. *Simpson's method with 4 sub-intervals*

The error estimation is derived by assuming that $\xi \approx \bar{\xi}$ or, more precisely, that $f^{(4)}(\xi) \approx f^{(4)}(\xi)$, and the success of the technique depends on the accuracy of this assumption.

If it is accurate, then equating the integrals in Eqs. (2) and (5) gives

$$S\left(a, \frac{a+b}{2}\right) + S\left(\frac{a+b}{2}, b\right) - \frac{1}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\xi) \approx S(a,b) - \frac{h^5}{90} f^{(4)}(\xi) \tag{6}$$

Hence

$$\frac{h^5}{90} f^{(4)}(\xi) \approx \frac{16}{15}\left[S(a,b) - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right] \tag{7}$$

Using this in Eq. (5) produces the error estimation

$$\begin{aligned} &\left|\int_a^b f(x)dx - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right| \\ &\approx \frac{1}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\xi) \\ &\approx \frac{1}{15}\left|S(a,b) - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right| \end{aligned} \tag{8}$$

This implies that $S(a, \frac{(a+b)}{2}) + S(\frac{(a+b)}{2}, b)$ approximates $\int_a^b f(x)dx$ about 15 times better than it agrees with the computed value $S(a,b)$. Thus, if

$$\left|S(a,b) - S\left(a \cdot \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right| < 15\varepsilon \tag{9}$$

we expect to have

$$\left|\int_a^b f(x)dx - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right| < \varepsilon \tag{10}$$

and $S\left(a, \frac{a+b}{2}\right) + S\left(\frac{a+b}{2}, b\right)$ is assumed to be a sufficiently accurate approximation to $\int_a^b f(x)dx$.

If this does not work for any sub-interval, we again break that particular sub-interval into halves and then work out the same procedure again.

This is done until a sufficiently fine mesh is obtained and the error is under the given tolerance. This whole operation will give a non-uniform mesh and the number of iterations that have been used will be significantly less than ordinary Simpson's method for slowly varying functions.

PSEUDO CODE

Given below is the pseudo-code for adaptive step-size quadrature. The method requires recursion for execution since the end-point of of the process is not defined explicitly. The function calls itself and the successive sub-intervals are broken into halves till the required accuracy is achieved.

The parameter k in the pseudo-code represents the order of h on which the error depends, i.e., when E $\sim h^p$ then $k = 2^p - 1$.
For Simpson's method, $k = 2^4 - 1 = 15$, while for mid-point and trapezoidal method, it is $k = 2^2 - 1 = 3$.

$$k = \begin{cases} 15 & \rightarrow \text{ Simpson} \\ 3 & \rightarrow \text{ Mid-point or Trapezoidal} \end{cases}$$

f : function, $[a,b]$: interval, ε : tolerance for error.

Compute $S_1[a,b]$ and $S_2[a,b]$ using ordinary methods of composite integration where $S_2 = S_1[a,c] + S_1[c,b]$ and $c = \frac{(a+b)}{2}$

if $|S_2 - S_1| < k\varepsilon$
    Ans $= S_2 + \left(\frac{S_2 - S_1}{k}\right)$
else
    $c = (a+b)/2$
    Left=Adaptive$(f, a, c, \varepsilon/2)$
    Right=Adaptive$(f, c, b, \varepsilon/2)$
    Ans=Left+Right
return Ans

ILLUSTRATION

Suppose we calculate the numerical integration of the function $f(x) = exp(-x)cos(5x)$ over the interval $[0,6]$ with a tolerance $\varepsilon = 10^{-6}$. The plot for $f(x)$ is shown in figure 3.

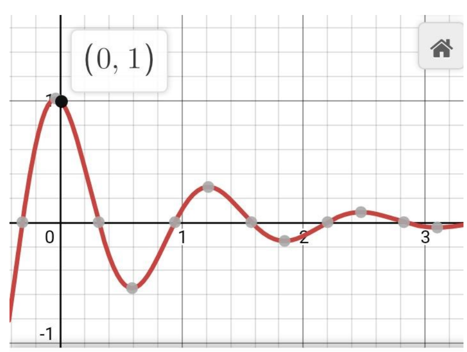

FIG. 3. *Plot for $exp(-x)cos(5x)$.* Note that the graph is varying very fastly near the origin while it decays down as it goes along the x-axis.

Solving the problem analytically yields

$$\int_0^6 e^{-x} cos(5x) dx = \left[\frac{e^{-x}\left(5\sin(5x) - \cos(5x)\right)}{26}\right]_0^6$$
$$= 0.0379758546$$

The application of ordinary Simpson's rule uses composite Simpson's rule i.e. equal step-sized method to calculate the quadrature. The error is defined by the tolerance $\varepsilon = 10^{-6}$. From this, we obtain the answer as **0.0379758284**. The number of iteration can also be calculated.

$$\varepsilon \leq \frac{(b-a)^5}{180\, N^4} \left|f^{(4)}(\xi)\right|_{max} \qquad \text{for } h = \frac{(b-a)}{N}$$
$$\implies N \geq \left(\frac{(b-a)^5}{180\,\varepsilon} \left|f^{(4)}(\xi)\right|_{max}\right)^{\frac{1}{4}}$$
$$N \geq \left(\frac{(6-0)^5}{180\,\varepsilon} 476\right)^{\frac{1}{4}} = 380$$

Hence the total number of iterations used in ordinary Simpson's method is **N=380**.

No we use the adaptive Simpson's method to find the answer. This solves to give the final value as **0.0379758504**. To find the number of iterations, we define a blank array and append the number of iteration number at each step. Finally, it's length is found to get the total number of iterations. The execution of this step is shown in the codes. This function yields the total umber of iterations as **N=63**.

This is much less than the number of iterations obtained for ordinary method, and is closer to the actual value. However, the tolerance provided has been successfully achieved so any variation beyond is easily acceptable.

RESULTS

The Simpson's $\frac{1}{3}$ rule is the most widely used method for calculating the quadrature of a function. Using adaptive step-size techniques with it makes it highly efficient. The quadrature is calculated for any function in much less number of iterations where the function is varying slowly, while it is equally efficient for fast varying functions. For better understanding and operation, please refer the python code with this report.

The numerical quadrature for mid-point and trapezoidal methods also have been calculated using adaptive methods. There is only a difference in the value of k. Refer the codes for operation.

BIBLIOGRAPHY

I would like to sincerely thank Dr. Subhasis Basak for giving the motivation to prepare this report. This report not only helped me in better understanding, but also proposed a way to calculate numerical quadrature in lesser number of iterations and estimate the error in the process.

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