Adaptive Quadrature

Your work should be presented in the form of a typed report using clear and properly punctuated English. Where appropriate include full program listing and output. If you choose to work in a group of two, please turn in independently prepared reports.

1. Let f be continuously differentiable on the interval $[a, b]$ and denote the integral and trapezoid formula, respectively, by

$$I_{ab} = \int_a^b f(x)dx \qquad \text{and} \qquad T_{ab} = \frac{f(a) + f(b)}{2}(b - a).$$

It is known that

$$I_{ab} = T_{ab} - \frac{f''(\xi_1)}{12}(b - a)^3 \qquad \text{for some} \qquad \xi_1 \in [a, b].$$

Denote the midpoint of the interval $[a, b]$ by $c = (a + b)/2$. Show that

$$I_{ab} = T_{ac} + T_{cb} - \frac{f''(\xi_2)}{48}(b - a)^3 \qquad \text{for some} \qquad \xi_2 \in [a, b].$$

2. Find I_{ab} for $a = 1$, $b = 2$ and $f(x) = x \cos x$ using integration by parts. Express your answer exactly in terms of sine and cosine functions.

3. Simpson's formula is

$$S_{ab} = \frac{4T_{ac} + 4T_{cb} - T_{ab}}{3} = \frac{f(a) + 4f(c) + f(b)}{6}(b - a)$$

Write a program to calculate

$$\Big|I_{ab} - S_{ab}\Big|, \quad \Big|I_{ab} - T_{ac} - T_{cb}\Big| \quad \text{and} \quad \Big|S_{ab} - T_{ac} - T_{cb}\Big|$$

for $a = 1$, $b = 2$ and $f(x) = x \cos x$.

4. It is known that

$$I_{ab} = S_{ab} - \frac{f''''(\xi_3)}{2880}(b - a)^5 \qquad \text{for some} \qquad \xi_3 \in [a, b].$$

If $b - a$ is small and f'''' is reasonably behaved, then the error in S_{ab} is much smaller than the error in $T_{ac} + T_{cb}$. In particular

$$\Big|I_{ab} - S_{ab}\Big| \ll \Big|I_{ab} - T_{ac} - T_{cb}\Big| \approx \Big|S_{ab} - T_{ac} - T_{cb}\Big|.$$

Are the calculations for $a = 1$, $b = 2$ and $f(x) = x \cos x$ in part 3 consistent with the above inequality. Repeat and comment on this inequality when $b = 1.1$, when $b = 1.01$ and when $b = 10$.

5. Fix $n \in \mathbf{N}$, let $h = (b-a)/n$ and let $x_i = a + ih$. Denote

$$T_i = T_{x_i x_{i+1/2}} + T_{x_{i+1/2}, x_{i+1}} \qquad \text{and} \qquad S_i = S_{x_i, x_{i+1}}.$$

Let

$$S = \sum_{i=0}^{n-1} S_i \qquad \text{and} \qquad E = \sum_{i=0}^{n-1} \big| S_i - T_i \big|$$

and use part 4 to show that $|I_{ab} - S| \ll E$.

6. Write a C computer program to compute S, $|I_{ab} - S|$ and E for $a = 1$, $b = 10$ and $f(x) = x \cos x$ when $n = 10, 20, 50$ and 100.

7. To guarantee $E < \epsilon$ it is sufficient that $|S_i - T_i| < \epsilon/n$ for $i = 0, \ldots, n-1$. Write a recursive function $\text{quad}(a, b, \epsilon)$ defined as

$$\text{quad}(a,b,\epsilon) = \begin{cases} S_{ab} & \text{if } |S_{ab} - T_{ac} - T_{cb}| < \epsilon \\ \text{quad}(a, c, \epsilon/2) \\ \qquad + \text{quad}(c, b, \epsilon/2) & \text{otherwise} \end{cases}$$

and then use the formula

$$\sum_{i=0}^{n-1} \text{quad}(x_i, x_{i+1}, \epsilon/n)$$

to approximate I_{ab} to precision $\epsilon = 10^{-7}$ for $a = 1$, $b = 10$ and $f(x) = x \cos x$. Run your program with $n = 10$. How does the initial choice of n affect your results? What is a good way of choosing n?

8. [Extra Credit and Math/CS 666]. Show that

$$R_{ab} = \frac{16 S_{ac} + 16 S_{cb} - S_{ab}}{15} = I_{ab} + \mathcal{O}\big((b-a)^7\big)$$

and use the error estimate $|I_{ab} - R_{ab}| \ll |R_{ab} - S_{ac} - S_{cb}|$ to create a higher order adaptive quadrature routine. Write your program in a way to minimize the number of function calls by reusing previously computed values of $f(x)$ where possible. Test your routine under the same conditions as part 7 and determine its efficiency by comparing how many function calls are used by each method to achieve the same accuracy. Make up an additonal test problem by choosing new values for f, a, b, ϵ and n and compare the results.