Applied Mathematics 2130 Lab 2006W-3A

This laboratory is about numerical integration. We seek to generate a reasonable process to deal numerically with the expression

$$\int_a^b f(x)\,dx\,.$$

To a large extent, definite integrals can be treated rather well by machine. Even convergent improper integrals can usually be handled, provided necessary cautionary steps are taken.

Since the expression $\int_a^b f(x)\,dx$ is nothing more than the limiting value of a Riemann sum, it makes perfect sense that one should be able to approximate

$$\int_a^b f(x)\,dx \qquad \text{by} \qquad \sum_{i=1}^{N} a_i f(x_i)$$

for suitably chosen (a_i, x_i). One would like to have the limit as $N \to \infty$, of the sum displayed above, equal to the value of the integral. What is not clear is how one might go about finding suitable coefficients (a_i, x_i) to do the job, and indeed several approaches can be taken. The sum that is used to approximate the integral is normally referred to as a *quadrature rule.*

Classical techniques for numerical integration replace $f(x)$ in the integrand by a polynomial $p(x)$ which approximates $f(x)$ and integrate $p(x)$ instead of $f(x)$. This approach is termed *interpolatory quadrature.*

Now let us look at the particular case where $N = 1$, $x_0 = a$, $x_1 = b$. Since the linear interpolant to the data $(x_0, f(x_0))$, $(x_1, f(x_1))$ can be written as

$$p(x) = \frac{x-b}{a-b} f(a) + \frac{x-a}{b-a} f(b)\,,$$

then computing $\int_a^b p(x)\,dx$ gives

$$\int_a^b f(x)\,dx \approx \frac{b-a}{2}[f(a) + f(b)]\,. \tag{1}$$

This case is known as the *Trapezoidal Rule.* You must provide a mathematical explanation of how equation (1) is obtained. Include a suitable figure to illustrate the rule.

Similarly, we can consider the case $N = 2$, $x_0 = a$, $x_1 = \frac{a+b}{2}$ and $x_2 = b$. We use a quadratic polynomial to interpolate $(x_0, f(x_0))$, $(x_1, f(x_1))$, $(x_2, f(x_2))$. The result is:

$$\int_a^b f(x)\,dx \approx \frac{b-a}{6}[f(x_0) + 4f(x_1) + f(x_2)]\,. \tag{2}$$

This case is known as *Simpson's Rule.* You must provide a mathematical explanation of this formula also. You can use Maple to do the tedious calculations. *Lagrange's Interpolation*

Formula can be used to find the unique polynomial of degree 2 passing through three given points. You should include a suitable graph to illustrate the rule.

Higher order integration rules can be derived in a similar way by making use of interpolating polynomials with larger values of N. These are known as *Newton-Côtes Quadrature Rules* and their formulae are also well known. These techniques are not quite as popular because a preferred tactic is to subdivide the given interval $[a, b]$ into smaller partitions and use low degree approximation over each sub-interval. This would lead to a *composite* quadrature rule.

Thus if we subdivide the interval $[a, b]$ into N equally-spaced intervals $[x_i, x_{i+1}]$ for $i = 0, 1, \ldots, N-1$, define $h := \frac{b-a}{N}$, and note that

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_1} f(x)\,dx + \ldots + \int_{x_{N-1}}^{x_N} f(x)\,dx\,,$$

we can use equation (1) on each interval $[x_i, x_{i+1}]$ and do a little more algebra to obtain a *Composite Trapezoidal Rule*

$$\int_a^b f(x)\,dx \approx \frac{h}{2}\left[f(x_0) + 2f(x_1) + \ldots + 2f(x_{N-1}) + f(x_N)\right]. \tag{3}$$

To obtain a *Composite Simpson's Rule* we begin with the observation that, when N is even, we have

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_2} f(x)\,dx + \ldots + \int_{x_{N-2}}^{x_N} f(x)\,dx\,,$$

so that, using (2) on each $[x_i, x_{i+2}]$, we get

$$\int_a^b f(x)\,dx \approx \frac{h}{3}\left[f(x_0) + 4f(x_1) + 2f(x_2) + \ldots + 2f(x_{N-2}) + 4f(x_{N-1}) + f(x_N)\right]. \tag{4}$$

Note that the coefficients 4 and 2 alternate along this sum. You must provide mathematical explanations of how both the Composite Trapezoidal Rule and the Composite Simpson's Rule are obtained. Include suitable graphics.

Finally with each integration formula, it is possible to derive expressions for an error term. For the Composite Trapezoidal Rule (3) we can derive

$$\int_a^b f(x)\,dx - [\text{COMPOSITE TRAPEZOIDAL RULE}] = \frac{(a-b)h^2}{12} f''(\zeta), \tag{5}$$

whereas for the Composite Simpson's Rule

$$\int_a^b f(x)\,dx - [\text{COMPOSITE SIMPSON'S RULE}] = \frac{(a-b)h^4}{180} f^{(4)}(\zeta). \tag{6}$$

In each case, the quantity ζ is unknown, except that it lies somewhere within the interval of integration. Again, you will need to provide mathematical explanations of how the error formulae (5) and (6) are obtained, and how they are used.

Write programs that will implement the Composite Trapezoidal and Simpson's Rules. Your programs should accept as input the number $\boldsymbol{N}$ of points to be used in the approximation as well as the values of $\boldsymbol{a}$ and $\boldsymbol{b}$ that define the interval of integration. Use your programs to approximate the following integrals to at least four significant figures:

(a) $\int_0^1 e^{x^2}\,dx$ (b) $\int_{-1}^1 x^4\,dx$ (c) $\int_{-1}^3 \sin x^2\,dx$ (d) $\int_0^e x \ln x\,dx.$

You must use the suggested quadrature rules to get approximate values. Differential Calculus techniques may be used for deriving and checking the error bounds; otherwise, all calculations must be done numerically.

You should consider the error behavior of each method as $\boldsymbol{N}$ increases. Appropriate tables should be included, indicating maximum errors for each $\boldsymbol{N}$ chosen. If you had to make a recommendation on which method is better for the problem at hand, which one would you choose? Explain your reasoning.

Prepare a report discussing the effectiveness of the numerical integration methods considered in this lab. Include suitable graphics describing and supporting your conclusions.
Supporting mathematical reasoning is essential.