Math 225: Scientific Computing II

Problem Set 4

Numerical Integration and Numerical Differentiation

Part A: Due Tuesday, 25 February 2003

1. Consider the numerical integration schemes based on left- and right-hand Riemann sums. If one wants to approximate $I(f) = \int_a^b f(x)\,dx$, the left-hand Riemann scheme (LHR) is specified by $h = (b-a)/n$, $x_k = a + kh$ with $k = 0, 1, 2, \ldots, n$, $f_k = f(x_k)$, and $L_n(f) = h\sum_{k=0}^{n-1} f_k$, where $L_n(f)$ approximates $I(f)$. In the right-hand Riemann scheme (RHR), $R_n(f) = h\sum_{k=1}^{n} f_k$.

(a) For the LHR:

- Derive the error formula for a single application:
$E_1(f) = I(f) - L_1(f)$.

- Derive the error formula for the composite scheme:
$E_n(f) = I(f) - L_n(f)$.

- Derive the asymptotic error formula.

- Explain geometrically the forms and signs of the errors.

- Determine the degree of precision.

- Construct a specific example of the composite LHR that illustrates the error, the order of the error, and agreement with the asymptotic error.

- Also in your example, use the empirical formula based on Aitken extrapolation to approximate the order of the error, to approximate the asymptotic constant, and to obtain a closer approximation to $I(f)$.

(b) For the RHR:

- Derive the error formula for a single application:
$E_1(f) = I(f) - R_1(f)$.

- Derive the error formula for the composite scheme:
$E_n(f) = I(f) - R_n(f)$.

- Derive the asymptotic error formula.

- Describe how and why these results differ from those for the LHR.

2. Simpson's rule takes advantage of a felicitous cancellation to obtain an order of convergence that is two orders higher than that of the trapezoidal rule. Verify that cancellation. Let $c(x)$ be an arbitrary cubic polynomial defined on $[a, b]$, and let $q(x)$ be the second-order interpolating polynomial to that cubic that has equally-spaced nodes on $[a, b]$. Show that $\int_a^b (c(x) - q(x))\, dx = 0$.

Part B: Due Tuesday, 4 March 2003

3. Let $f(x) = \operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-s^2}\, ds$. Write programs that you need from scratch; use double-precision arithmetic.

   You can check your results and estimate error by means of comparisons with published tables or by making use of the alternating series that one gets by expanding the integrand in its Maclaurin series and integrating term by term. In an alternating series, one knows from elementary calculus that the magnitude of the error is less than the magnitude of the first term of the series that is neglected. The alternating series is

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n x^{2n+1}}{(2n+1)n!}. \qquad (1)$$

   (a) Use the composite trapezoidal rule and its error formula to estimate $f(2)$ with error magnitude less than 10^{-8}.

   (b) Use the composite Simpson's rule and its error formula to estimate $f(2)$ with error magnitude less than 10^{-8}.

   (c) Based on the number of subintervals required for parts (a) and (b), and on other pertinent considerations, how do the computational costs of the two methods compare?

   (d) Let n be the number of subintervals used in an application of either Simpson's rule or the Trapezoidal rule to find $f(2)$. For both methods, obtain plots of the base-ten logarithm of an estimate of the magnitude of the error, as a function of the base-ten logarithm of n. Relate the resulting plots to the expected orders of convergence and to the asymptotic error formulas. For sufficiently large n the effects of floating point arithmetic may become apparent.

   (e) Discuss whether your estimates of $f(2)$ in parts (a) and (b) are likely to have been significantly influenced by floating point errors.

   (f) For both Simpson's rule and the trapezoidal rule, use the formula based on Aitken extrapolation to estimate the order of convergence and the coefficient of the asymptotic error, and compare your results with the actual values. Also, obtain a better value for $f(2)$ based on the extrapolation formula. Write a simple program to apply the formula. Choose n sufficiently large for good results.

(g) Use the extrapolation formula, the procedure of part (f), and estimates of $f(x)$ for $x \in [0,2]$ based on Simpson's rule and the trapezoidal rule to produce graphs that estimate $p(x)$ and $k(x)$ for $x \in [0,2]$, where p is the order of convergence and k is the coefficient of the asymptotic error. For n sufficiently large, both p and k should approximate horizontal lines.

(The programs that you write for parts (f) and (g) may be useful to you throughout your career for estimating errors incurred in numerical procedures. We will use them later for evaluating some methods for ODEs.)

(h) Use Romberg integration (based on the trapezoidal rule) to estimate $f(2)$ with error magnitude less than 10^{-8}. Write an efficient program, based on Atkinson's treatment on pages 297-299, to perform the integration. Considering both the conservative error test in Atkinson's pseudo-code, and your previous estimates for $f(2)$, how many subintervals are needed to obtain your estimate? Compare this number of subintervals with the number of subintervals used in parts (a) and (b).

4. Numerical differentiation may be used to gain information about data of unknown accuracy or quality, or about data from an unknown source. In my public html directory

   `www.math.duke.edu/~layton/225/DataPS3/`

   you will find five files of data that represent functions f_i ($i = 1$, 2, 3, 4, 5) defined on $[0,1]$; each file (D1, D2, D3, D4, and D5) may be down-loaded by affixing its name to the end of the directory name and then saving the file.

   (a) Write a program that numerically approximates derivatives $f_i^{(n)}$ of these functions with error $O(h^2)$.

   (b) Identify the functions f_i by examining the results of successive applications of the numerical derivative. The identifications should include explicit formulas with explicit coefficients, where possible.

   (c) Also, write a program that uses the trapezoidal rule to approximate $F_i^{+1}(x) = 1 + \int_0^x f_i(s)\, ds$ on $[0,1]$, $F_i^{+2} = 1 + \int_0^x F_i^{+1}(s)\, ds$, etc.

(d) Can useful information be obtained by successive integrations? Why, or why not?

(Hint: One of these functions is the exponential function. The others are pretenders: a trigonometric function, a polynomial, a piecewise-defined polynomial, and some simulated experimental data.)