THE UNIVERSITY OF SYDNEY
MATH3076 AND MATH3976 (ADVANCED)

Mathematical Computing	Numerical Methods	2015

Lecturer: *D. J. Ivers*

Set 4 — Numerical Quadrature

Week 11

* — tutorial question; A — advanced; S — supplementary

1* *Newton-Cotes Quadrature.*

(a) Attached is a listing of the file `$mc3nm/csr.f90`, which implements the compound Simpson's $\frac{1}{3}$-rule with s panels for $s = 1, 2, 4, 8, 16, 32, 64, 128, 512$. Copy the file `$mc3nm/csr.f90` to the file `set4q1.f90` in your directory, compile, link and run it for the integral

$$\pi = \int_0^1 \frac{4}{1+x^2}\,dx\,.$$

The program already contains the correct integrand in the function subprogram `f(x)`.

(b) Modify `set4q1.f90` to:

(*i*) implement the compound trapezoidal rule for $2s$ panels using the function evaluations for the compound Simpson's rule;

(*ii*) evaluate the integrand at most once at each node and use these values in subsequent iterations of the panel `do` loop (use the variables `sum1`, `sum2` and `sum3`, and do not use arrays);

(*iii*) tabulate the error.

Compare the accuracy of the methods. For π use `pi = acos(-1.0)`.

(c) Modify your program from Part (b) to evaluate the integral

$$-\frac{4}{9} = \int_0^1 \sqrt{x}\ln x\,dx\,.$$

The integrand has an apparent singularity at $x = 0$, which you can handle in the function subprogram `f(x)` by carefully defining the integrand.

(d) Computer algebra programs such as Mathematica can evaluate some definite integrals. Mathematica commands to evaluate the integral in Part (a) are

```
f[x_]:= 4/(1+x^2)
```

and

```
Integrate[f[x],{x,0,1}]
```

Evaluate the integrals in Parts (a) and (c) using Mathematica. (Use `Sqrt[x]` and `Log[x]`). To run Mathematica use the command

```
math
```

2* *Gauss and Gauss-Kronrod Quadrature.* This question uses subroutine `glrule`, which calculates the standard n-point Gauss-Legendre weights and nodes, and subroutine `qk15`, which implements a (7,15) Gauss-Kronrod rule with error estimate. Subroutine `qk15` is described in the prologue file `$mc3nm/qk15.pro`. A sample main program `gauss_legendre`, which calls `glrule` and `qk15`, is given in the file `$mc3nm/glgk.f90`. Copy the file, compile and link it using the command

```
f90o glgk.f90 $mc3nm/glrule.f90 $kmnlib
```

and then run it. Use the program to calculate the integrals in Question 1. How do the error estimates of `qk15` compare with the actual errors ?

3^{A*} *Trapezoidal Adaptive Quadrature.* Attached is a listing of the file `$mc3nm/adaptquad.f90`, which implements an adaptive form of the trapezoidal rule.

(a) Copy the file, compile, link and run it. Use the program to calculate the integrals in Question 1. How do the number of function evaluations compare with Question 1 ?

(b) Consider a definite integral I. If $E_3 = (T_3 - T_2)/3$ is the error estimate for the 3-point trapezoidal rule T_3 value for I, where T_2 is the 2-point trapezoidal rule value for I, show that $T_3 + E_3 = S_3$, where S_3 is the 3-point Simpson $\frac{1}{3}$-rule value for I. (So `adaptquad.f90` actually gives a Simpson $\frac{1}{3}$-rule estimate for each subinterval.)

4* *Gauss-Kronrod Adaptive Quadrature.* Subroutine `q1da` from *Numerical Methods and Software* by Kahaner, Moler & Nash implements the (7,15) Gauss-Kronrod rule in an adaptive quadrature algorithm. Subroutine `q1da` is described in the prologue file `$mc3nm/q1da.pro`. A sample main program `q1da_main` is given in the file `$mc3nm/q1da_main.f90`. Copy, compile, link and run it. Modify `q1da_main.f90` to calculate the integrals and errors in Question 1. How do the error estimates of `q1da` compare with the actual errors ? How does the number of function evaluations compare with the other methods used in the previous questions?

5. *Simpson's $\frac{1}{3}$-Formula.* Derive the formula

$$\int_a^b f(x)\,dx = \frac{b-a}{6}[f(a) + 4f(m) + f(b)] - f^{(4)}(m)\frac{(b-a)^5}{2880} + \dots .$$

6. *Compound Simpson's $\frac{1}{3}$-Formula.* Derive the formula

$$\int_a^b f(x)\,dx = \frac{h}{3}[f(a)+4f(a+h)+2f(a+2h)+4f(a+3h)+\cdots+4f(b-h)+f(b)]-$$

$$(b-a)\frac{h^4}{180}f^{(4)}(m)+\ldots.$$

7. Evaluate

$$\int_0^{\frac{\pi}{2}} \sin x\,dx$$

by the following methods:

(a) analytically;

(b) 3-point composite trapezoidal rule;

(c) 3-point Simpson's $\frac{1}{3}$-rule;

(d) 2-point Gaussian rule.

[Answers: (a) 1 ; (b) 0.9480 ; (c) 1.0023 ; (d) 0.9985 .]

8. Repeat the previous question for the integral

$$\int_0^{\alpha} \tan x\,dx\,,$$

where $\alpha = 89^\circ = 1.553343$ rad. Why are the numerical results so much worse than in the previous question ?
[Answers: (a) 4.0483 ; (b) 23.0110 ; (c) 15.8494 ; (d) 2.4209 .]

9. What singularities do the following integrals possess and how would you deal with them when evaluating the integrals numerically ?

(a) $\displaystyle\int_0^{0.7} \frac{x^2e^x}{(e^x-1)^2}\,dx\,;$ (b) $\displaystyle\int_0^1 \frac{\sin x\ln x}{\sqrt{1-x}}\,dx\,.$

10. Consider the following Gaussian quadrature rule with the weight function $x^{-1/2}$,

$$\int_0^1 \frac{f(x)}{\sqrt{x}}\,dx = w_1f(x_1)+w_2f(x_2)\,.$$

(a) State the conditions that determine the weights w_1, w_2 and the nodes x_1, x_2. Derive the equations that these conditions determine and then solve for the weights w_1, w_2 and the nodes x_1, x_2. Use your rule to evaluate the integral in Part (b) of the previous question. Generalise your rule to weight functions of the form $x^{-\alpha}$, $0<\alpha<1$.

(b)^A Find the orthogonal polynomials $\phi_0(x)$, $\phi_1(x)$ and $\phi_2(x)$, using the Gram-Schmidt method. Hence derive the 2-point rule.