CSE/MATH 455, Arnold　　Lab 10　　December 5, 1997

Quadrature rules with uniform spacing, regular and singular integrands

Due date: Friday, December 12

Preparation: Copy the files `trapez.m`, `simp.m`, `f.m` from `~dna2` to your directory.

In this lab we will investigate the accuracy of the trapezoidal rule and Simpson's rule with equally spaced points for various integrals. The programs are simple enough to write, but to save time you can use `trapez.m` and `simp.m`. (Look at the routines.) For example, to compute $\int_0^1 \exp(-x^2)\,dx$ using the trapezoidal rule with 16 subintervals (17 function evaluations), you would use `trapez('f',0,1,16)` where `'f'` refers to the Matlab function `f(x)` defined in the file `f.m`. The call `simp('f',a,b,n)` works similarly. For Simpson, the number `n` *must* be even (again $n+1$ is the number of function evaluations).

The test integrals are:

$$\int_0^1 \exp(-x^2)\,dx = 0.74682413281242702\ldots,$$

$$\int_0^3 |\cos x| \exp(-x/10)\,dx = 1.61523492777325443\ldots,$$

$$\int_0^2 \cos x \exp(-\sqrt{x})\,dx = 0.49060485069310796\ldots.$$

1. The first integrand is a smooth function on the interval $[0,1]$ of integration. Plot it. Complete the following table. (The first two rows are completed for you to check your methodology.) For the rate use the formula $\log(e_{n/2}/e_n)/\log 2$ where e_n is the error with n subintervals.

$\int_0^1 \exp(-x^2)\,dx$	TRAPEZOIDAL			SIMPSON		
subints	error	rel. error	rate	error	rel. error	rate
2	1.55e-02	2.07e-02	*na*	-3.56e-04	-4.77e-04	*na*
4	3.84e-03	5.14e-03	2.01	-3.12e-05	-4.18e-05	3.51
8						
16						
32						
64						
128						

For this example, the trapezoidal rule converges as what power of h? ___________
How about Simpson's rule? ___________ How many subintervals are needed with the trapezoidal rule to achieve a relative error of 10^{-4}? ___________
With Simpson's rule? ___________ By what factor is Simpson's rule more accurate than the trapezoidal rule with 128 subintervals in this example? __________________________

2. The second integrand has a jump discontinuity in its first derivative at $\pi/2$. Plot it. Complete the table, or at least enough to answer the questions below it.

$\int_0^3 \lvert\cos x\rvert \exp(-x/10)\, dx$	TRAPEZOIDAL			SIMPSON		
subints	error	rel. error	rate	error	rel. error	rate
2	2.24e-01	1.39e-01	*na*	6.27e-01	3.88e-01	*na*
4	3.42e-02	2.12e-02	2.71	-2.90e-02	-1.79e-02	4.43
8						
16						
32						
64						
128						

For this example, the trapezoidal rule converges as what power of h? ___________
How about Simpson's rule? ___________ How many subintervals are needed with the trapezoidal rule to achieve a relative error of 10^{-4}? ___________
With Simpson's rule? ___________ By what factor is Simpson's rule more accurate than the trapezoidal rule with 128 subintervals in this example? __________________________

3. The third integrand has an infinite derivative at 0. Plot it. Complete the table, or at least enough to answer the questions below it.

$\int_0^2 \cos x \exp(-\sqrt{x})\, dx$	TRAPEZOIDAL			SIMPSON		
subints	error	rel. error	rate	error	rel. error	rate
2			*na*			*na*
4						
8						
16						
32						
64						
128						

For this example, the trapezoidal rule converges as what power of h? ___________
How about Simpson's rule? ___________ How many subintervals are needed with the trapezoidal rule to achieve a relative error of 10^{-4}? ___________
With Simpson's rule? ___________ By what factor is Simpson's rule more accurate than the trapezoidal rule with 128 subintervals in this example? _________________________

The second and third integrands are *singular*. They are not smooth enough for the convergence results we proved in class to apply, and consequently numerical quadrature rules converge more slowly for them. There are various ways to improve the situation, depending on the particular integral. In the next three problems we explore some of these.

4. The approach to integrands like the second one is simple. Break up the integral into two pieces so the jump in the derivative occurs at an endpoint: $\int_0^3 = \int_0^{\pi/2} + \int_{\pi/2}^3$. For a fair comparison, in the first row compare the result of Simpson's rule with four subintervals on $[0, 3]$ with the result of using Simpson's rule with two subintervals on $[0, \pi/2]$ and two subintervals on $[\pi/2, 3]$. Fill out the other rows similarly.

subints	Simpson's rule error	error after splitting interval
4		
8		
16		
32		

5. There are various approaches to improve the accuracy with singularities like that of the third integral. One approach is to "subtract off the singularity". Specifically, write

$$\int_a^b f(x)\,dx = \int_a^b [f(x) - g(x)]\,dx + \int_a^b g(x)\,dx,$$

where $g(x)$ is chosen so that (a) the function $f(x) - g(x)$ does not have an infinite derivative, and (b) the integral of $g(x)$ can be computed analytically. In our case we can take $g(x) = \exp(-\sqrt{x})$. Using the substitution $u = \sqrt{x}$ and then integrating by parts leads to $\int_0^2 g(x)\,dx = 2 - (2 + 2\sqrt{2})/\exp(\sqrt{2})$. Use Simpson's rule to evaluate the integral of $f - g$ and add in this exact value to compute the entire integral. Record the errors in column 3 of the table.

subints	Simpson's rule error	err. after subtracting sing.	err. after changing variable
4			
8			
16			
32			

6. Another approach which often works is a cleverly selected change of variable. In the case of the third integral, the change of variable $u = \sqrt{x}$ leads to a nicer integral. Perform the change of variable, compute the resulting integral by Simpson's rule and record the errors in the last column of the above table.