1 Mathematics 406, Assignment 2 Due Oct 11 th

1. **Numerical Integration:**

   Write routines to perform numerical integration of a user-defined function $f(x)$ over an interval $[a, b]$: $I = \int_a^b f(x)dx$ by means of : the Midpoint rule with N cells, the Trapezium rule with N cells, Simpson's rule with $2N$ cells and three point Gauss-Legendre quadrature in each of N cells. Use these routines to evaluate the integrals (a)-(e) below. In each case complete a table of the form:

N	Midpoint	Trapezium	Simpson	Gauss-Legendre
2				
4				
16				
32				

   and determine the rate of convergence of the algorithms by calculating the error for different values of N. Compare the performance of the different algorithms for each of the given integrals by establishing the order of the error term and using a $\log - \log$ plot. Using the error estimate derived in class try to explain the different error behaviour for each of integrands.

   (a) $I = \int_{-1}^{1} \frac{dx}{\sqrt{1+x^2}} = -2\ln(\sqrt{2}-1)$

   (b) $I = \int_0^\pi \sin^2 2x dx = \frac{\pi}{2}$

   (c) $I = \int_0^1 x^{\frac{4}{3}} dx = \frac{3}{7}$

   (d) $I = \int_0^2 x^{\frac{1}{3}} dx = \frac{3}{2^{2/3}}$

   (e) $I = \int_0^1 (-\ln x)^{\frac{1}{2}}\, dx = \frac{\pi^{1/2}}{2}$ (use only the open integration rules i.e. Midpoint and Gauss integration for this integral)

2. Repeated Richardson extrapolation applied to the Trapezium Rule is known as Romberg integration. Use the following asymptotic expansion for the error in the Trepezium rule:

$$I(0) - I(h_s) = \sum_{i=1}^{\infty} c_i h_s^{2i}$$

   to derive the recursion for Richardson extrapolants for I in which $h_{s+1} = \frac{1}{2}h_s$. If we define $a_s^{(1)} = I(h_s)$ then by eliminating the $O(h^2)$ term in the expansion show that:

$$I(0) - \left\{ a_{s+1}^{(1)} + \frac{a_{s+1}^{(1)} - a_s^{(1)}}{2^2 - 1} \right\} = \sum_{i=2}^{\infty} c_i^{(2)} h_s^{2i}$$

   where $c_i^{(2)} = \frac{c_i}{3}\left(\frac{1}{4^{(i-1)}} - 1\right)$. Now define

$$a_s^{(2)} = a_{s+1}^{(1)} + \frac{a_{s+1}^{(1)} - a_s^{(1)}}{2^2 - 1}$$

and use expressions for $a_s^{(2)}$ and $a_{s+1}^{(2)}$ to eliminate the $O(h^4)$ term. Now generalize this to obtain the following recursion for $a_s^{(m)}$ in terms of $a_s^{(m-1)}$:

$$a_s^{(m)} = a_{s+1}^{(m-1)} + \frac{a_{s+1}^{(m-1)} - a_s^{(m-1)}}{4^{m-1} - 1}$$

Modify the routine `trapez` posted on the course web site to perform repeated Richardson Extrapolation until a prescribed tolerance is reached. Call this new function

$$[\texttt{Integral}, \texttt{I}, \texttt{X}] = \texttt{Romberg}(\texttt{f}, \texttt{a}, \texttt{b}, \texttt{tol}, \texttt{kmax})$$

where the inputs are `f`=the integrand, `[a,b]`= the domain of integration, `tol` = the specified tolerance, and `kmax` = the maximum number of refinements. The outputs are: `Integral`= the approximate integral, `I`= the table of extrapolated values, and X= the sample points. Use this routine to evaluate the integral

$$I = \int_0^1 (4 + x^2)^{-1} dx = \frac{1}{2} \tan^{-1}(\frac{1}{2})$$

How many refinements are required to obtain 5 digits of precision? Plot the values of the function that are used and provide the table of extrapolated values in the form:

$$h \quad a_s^{(0)} \quad a_s^{(1)} \quad a_s^{(2)} \quad \ldots$$

3. **Singular Integrals:** Evaluate the Fresnel integral $I = \int_0^{\pi/2} x^{-\frac{1}{2}} \cos x dx$ =1.95490284858266 directly using your Midpoint code. The convergence of the numerical approximation can be improved by subtracting out the singularity as follows: $I = \int_0^{\pi/2} x^{-\frac{1}{2}} dx + \int_0^{\pi/2} x^{-\frac{1}{2}} (\cos x - 1) dx = (2\pi)^{\frac{1}{2}} + \int_0^{\pi/2} x^{-\frac{1}{2}} (\cos x - 1) dx$. Since the last integrand is no longer singular it can be evaluated without difficulty using the routines developed above. Use the repeated Trapezoidal rule to evaluate I by subtracting one and three terms in the Taylor series expansion for $\cos x$. Compare your results in the following table:

Integration Rule	$h = (\frac{\pi}{2})2^{-4}$	$h = (\frac{\pi}{2})2^{-6}$
Direct Midpoint		
Direct 3 pt Gauss		
Subtract 1 term Midpoint		
Subtract 1 term 3 pt Gauss		
Subtract 1 term Trapezium		
Subtract 3 terms Midpoint		
Subtract 3 terms 3 pt Gauss		
Subtract 3 terms Trapezium		

4. **Numerical evaluation of the Hankel transform:** The zeroth order Hankel Transform

$$\mathcal{H}_0(f;k) = \int_0^\infty f(r) J_0(kr) r dr$$

where J_0 is the zeroth order Bessel function provides an efficient way to evaluate the 2D Fourier Transform of a circularly symmetric function. For the case $f(r) = e^{-r}$ the Hankel transform is

$$\mathcal{H}_0(e^{-r};k) = \frac{1}{(1+k^2)^{3/2}}$$

Use your Romberg routine to approximate $\mathcal{H}_0(e^{-r};k)$ by the evaluating the above integral numerically for $k = 3$ and $k = 5$. Evaluate these integrals directly by dividing the integral into two parts i.e. $[0,\infty) = [0,c] \cup [c,\infty)$. Can you control the error in the discarded part? What happens if you keep increasing c? Plot $I(c)$ and complete the following table

k	3	5
$c = 4$		
$c = 8$		
$c = 10$		
$c = 12$		
Exact	0.031622776601684	0.007542928274546

How large must c be in order to achieve 4 digits of precision - derive an estimate for c?