PHYSICS 115/242

Homework 2

Due in class, Monday, April 14.

Note: As always, the answers to the questions must include the computer code and output, in addition to any writing that might be needed. If you are not sure what is required please ask me.

1. *This exercise requires you to perform a numerical integration for a problem where you know the answer and to determine the form of the truncation errors.*
   Consider the evaluation of the integral

   $$I = \int_0^1 \frac{1}{1+x}$$

   by the Trapezium Rule. Obtain estimates for the integral with n, the number of intervals, successively equal to 2, 4, 8 etc.

   (a) Print out the values of h (the width of one interval), your estimate for the integral, and the error in that estimate divided by h^2. (Determine the error by subtracting from your estimate the exact value of the the integral determined analytically).

   (b) Your results for error/h^2 should tend to a constant for h moderately small. Show that the value of this constant corresponds to the leading error in the trapezium rule,

   $$I - T_n = -\frac{h^2}{12}\left[f'(b) - f'(a)\right] + \cdots ,$$

   where $f(x)$ is the integrand, a is the lower limit and b the upper limit.

   Note: You need to cover a broad range of h so you should choose h–values which vary in a geometric manner. e.g. successively divide by 2.

2. Evaluate

   $$\int_0^2 \exp(-x)\sin(x)\,dx$$

   to 4 decimal places using Simpson's Rule.
   Start with two intevals and keep doubling the number. Print out the answer at each stage.
   Note: You *must* explain how you determined that the desired accuracy had been obtained.

3. Use Romberg integration to determine

   $$\int_0^1 \exp(-x^2/2)\,dx$$

   to six decimal places.
   Print out successive Romberg estimates.
   Note: Again you must explain how you determined that you had achieved the desired accuracy.

4. Show that the integral

$$I = \int_a^b f(x)\, dx$$

is given approximately by the Midpoint Rule with n intervals as follows:

$$M_n = h(f_{1/2} + f_{3/2} + \cdots + f_{n-3/2} + f_{n-1/2}),$$

where $f_k = f(a + kh)$ and $h = (b - a)/n$, with an error given by

$$I - M_n = \frac{h^2}{24} \left[f'(b) - f'(a) \right] + \cdots ,$$

Hint: To obtain the error for one interval it might be useful to Taylor expand $f(x)$ about the midpoint of that interval.

5. *This is a physically motivated problem which involves a change of variables to evaluate the integral numerically* .
Consider a simple pendulum of length l. It is oscillating with a maximum angle of from the vertical of θ_m. You know that if θ_m is *small* the pendulum undergoes simple harmonic motion with period $T_0 = 2\pi\sqrt{l/g}$, where g is the acceleration due to gravity. Here we investigate how the period changes when the amplitude is *no longer small.*

   (a) From conservation of the energy, E, where

   $$E = \frac{1}{2} m \left(l\dot{\theta} \right)^2 + mgl(1 - \cos\theta),$$

   show that the period of oscillation, $T(\theta_m)$, is related to the period for small oscillations T_0 by the following integral

   $$\frac{T(\theta_m)}{T_0} = \frac{\sqrt{2}}{\pi} \int_0^{\theta_m} \frac{d\theta}{\sqrt{\cos\theta - \cos\theta_m}} \quad .$$

   You *must* show your working.

   (b) This expression is not, however, very convenient because of the square root divergence when $\theta \to \theta_m$. Show that we can rewrite the integral in a way which does not have this singularity by firstly using the relation $\cos\theta = 1 - 2\sin^2(\theta/2)$, which gives

   $$\frac{T(\theta_m)}{T_0} = \frac{1}{\pi} \int_0^{\theta_m} \frac{d\theta}{\sqrt{\sin^2(\theta_m/2) - \sin^2(\theta/2)}} \quad ,$$

   and then making the substitution $\sin\psi = \sin(\theta/2)/\sin(\theta_m/2)$ which gives

   $$\frac{T(\theta_m)}{T_0} = \frac{2}{\pi} \int_0^{\pi/2} \frac{d\psi}{\sqrt{1 - \sin^2(\theta_m/2)\sin^2(\psi)}} \quad .$$

   The integrand no longer has a singularity (except if $\theta_m = \pi$).

(c) This last integral is actually a function known in the literature as an elliptical integral. However, we will not use this information here. Expand the integrand in powers of $\sin^2(\theta_m/2)$ and integrate it term by term, to obtain the coefficients a and b in the expansion:

$$\frac{T(\theta_m)}{T_0} = 1 + a\sin^2(\theta_m/2) + b\sin^4(\theta_m/2) + \cdots .$$

(d) Evaluate $T(\theta_m)/T_0$ numerically using your favorite method (keep it simple; I suggest either the Trapezium Rule or Simpson's Rule) for $\theta_m = 0.1, 0.2, \pi/4, \pi/2$, and $3\pi/4$. Compare your answers with the results of the series expansion in the last section.

Note: Later we will see that with Mathematica we can do the integral and plot the period as a function of θ_m with a one-line command.

6. Determine numerically the integral

$$\int_0^1 \frac{\sin x}{x^{3/2}}\, dx$$

to 4 decimal places.
Hint: Perform an appropriate change of variables to remove the singularity at the lower limit. It may then be appropriate to use the Midpoint Rule.

7. *For Physics 242 students only.*
As mentioned briefly in class, there are methods for numerical integration called Gaussian quadrature, see Numerical Recipes Sec. 4.5, in which an integral of the form

$$I = \int_a^b W(x)f(x)\, dx$$

(where $W(x)$ is called a "weight function") is evaluated from

$$I \simeq \sum_{i=1}^{N} w_i f(x_i) \tag{1}$$

in which the x_i are zeroes of a function $G_N(x)$, where the the *set* of functions $G_n(x)$, with $n = 0, 1, 2, \cdots$, are *orthogonal* in the interval from a to b with the weight function $W(x)$, which means that

$$\int_a^b W(x)G_n(x)G_m(x)\, dx = 0 \qquad (n \neq m)\,.$$

The weight *factor* w_i in Eq. (1) is related to the derivative of $G_N(x)$ at the zero x_i and does *not* depend on the weight *function* $W(x_i)$ (which therefore does not appear at all in Eq,. (1)). The w_i and x_i are either stored in tables prepared in advance, or calculated "on the fly" as discussed in Numerical Recipes. Increasing N leads to higher order approximations.

Here we take a useful example of this with $a = -\infty, b = \infty, W(x) = \exp(-x^2)$, for which the functions $G_n(x)$ are Hermite polynomials (which occur in the solution of the simple harmonic oscillator in quantum mechanics). In other words

$$\int_{-\infty}^{\infty} e^{-x^2} f(x)\, dx \simeq \sum_{i=1}^{N} w_i f(x_i),$$

where you are given the following values of w_i and x_i for $N = 2, 3$ and 4.

N	i	x_i	w_i
2	1	0.7071068	0.8862269
	2	-0.7071068	0.8862269
3	1	1.2247449	0.2954090
	2	0.0000000	1.1816359
	3	-1.2247449	0.2954090
4	1	1.6506801	0.0813128
	2	0.5246476	0.8049141
	3	-0.5246476	0.8049141
	4	-1.6506801	0.0813128

(I can provide these numbers in plain text upon request.)

Note how convenient it is that the integral from $-\infty$ to ∞ can be done in a finite number of function evaluations without needing to transform the variables.

(a) Consider three choices for $f(x)$: $f(x) = x^2, x^4$ and x^6. Show that

i. with $N = 2$ the exact answer is given for x^2 but not for x^4 or x^6,

ii. with $N = 3$ the exact answer is given for x^2 and x^4 but not for x^6, and

iii. with $N = 4$ the exact answer is given for x^2, x^4 and x^6.

Note: I give you the result that

$$\int_{-\infty}^{\infty} e^{-x^2}\, dx = \sqrt{\pi},$$

and you should be able to work out, from this, the integrals $\int_{-\infty}^{\infty} x^m e^{-x^2}\, dx$ for $m = 2, 4$ and 6.

Bearing in mind that the method gives correctly the trivial result of 0 for $f(x) = x^m$ with m odd, we see that, at least for N up to 4, it works *exactly* for polynomials up to order $2N - 1$.

Note: This turns out to be true in general. The reason is that a polynomial of order $2N - 1$ has $2N$ parameters, and in Gaussian quadrature one has $2N$ parameters to choose: the N x-values, x_i, and the N weights, w_i.

(b) Evaluate

$$\int_{-\infty}^{\infty} e^{-x^2} \frac{1}{e^x + 1}\, dx$$

using Gaussian quadrature with $N = 4$.