HW 9 Computational Physics

October 25, 2005 Due November 1

1. Expand the function $y(x) = (\cosh 2 - x)^{-1/2}$ (for $-1 < x < 1$) in a Legendre series,

$$y(x) = \sum_{n=0}^{\infty} c_n P_n(x),$$

using the following steps.

   (a) Find the appropriate orthogonality integral for the Legendre polyomials $P_n(x)$.

   (b) Using the orthogonality integral calculate the coefficients c_n by hand (*e.g.*, with an integral table).

   (c) Check your answer by plotting both $y(x)$ and the series expansion, using the computer. Keep enough terms in the series to get reasonable agreement. Snippet:

```
x = arange(-1.,1.,0.01)
y = 1./sqrt(cosh(2.)-x)          # Original function
fit = zeros(len(x))
for n in arange(...):
  cn = ...                       # Coefficient
  pnx = special.legendre(n)(x)
  fit = fit + cn*pnx
```

2. Expand $f(x) = e^{-3x}$ (for $0 \leq x \leq \infty$) in a series of Laguerre polynomials,

$$f(x) = \sum_{n=0}^{\infty} c_n L_n(x),$$

using the same steps as follows.

   (a) Find the appropriate orthogonality integral for the Laguerre polynomials $L_n(x)$.

   (b) Calculate the coefficients c_n by hand.

   (c) Check your answer by plotting both $f(x)$ and your fit (keeping enough terms to get a reasonable match).

3. Expand the function $y(x) = (1-x^2)^{-1/2}$ (for $0 \le x < 1$) in a series of Bessel functions:

$$(1-x^2)^{-1/2} = \sum_{m=1}^{\infty} c_m J_0(s_m x).$$

Here s_m are the zeros of the zeroth order Bessel function: $J_0(s_m) = 0, m = 1, 2, \ldots$; they are approximately $s_1 = 2.405$, $s_2 = 5.520$, $s_3 = 8.654$, ….

   (a) Plot $J_0(x)$ for $0 \le x \le 40$ using `special.jn(0,x)`.

   (b) Find the lowest 50 zeros s_m using `special.jn_zeros(0,50)`. Compare with your plot from (a).

   (c) Find an appropriate orthogonality integral for the set of functions used in the series above: $J_0(s_1 x), J_0(s_2 x), J_0(s_3 x), \ldots$.

   (d) Using the orthogonality integral find the coefficients c_m by hand.

   (e) Check your answer by plotting both $y(x)$ and the series expansion, keeping 50 terms. (It won't be a great fit.)

4. Suppose I give you a new set of special functions $\clubsuit_m(x)$, $m = 0, 1, 2, \ldots$, which have the orthogonality integral:

$$\int_{-\infty}^{\infty} dx\, e^{-x^2} x^3 \clubsuit_m(x) \clubsuit_n(x) = \begin{cases} 0 & m \ne n \\ m! & m = n. \end{cases}$$

You can expand an arbitrary function $f(x)$ in these:

$$f(x) = \sum_{m=0}^{\infty} c_m \clubsuit_m(x).$$

Figure out the integral you would have to do to calculate c_m, given $f(x)$.

5. Consider the energy eigenstate problem

$$\left[-\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\psi(x), \text{ with } \psi(0) = 0 = \psi(L). \tag{1}$$

Here $L = 11$ and the potential energy is

$$\hat{V}(x) = \begin{cases} 0, & x \leq \frac{L}{2} - \frac{w}{2} \\ V_0\left[\frac{4}{w^2}\left(x - \frac{L}{2}\right)^2 - 1\right], & \frac{L}{2} - \frac{w}{2} < x < \frac{L}{2} + \frac{w}{2} \\ 0, & x \geq \frac{L}{2} + \frac{w}{2} \end{cases}$$

with $V_0 = 50, w = L/10$. In this problem you will solve this numerically by expansion in the truncated basis

$$u_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{(n+1)\pi x}{L}\right), \quad n = 0, 1, 2, \ldots, \mathrm{nmax} - 1.$$

You will use this approach to calculate the three lowest eigenfunctions and their corresponding eigenvalues. Work through the following steps.

(a) Show that the expansion

$$\psi(x) = \sum_{n=0}^{\mathrm{nmax}-1} c_n\, u_n(x) \tag{2}$$

turns the eigenfunction problem in Eq. (1) into the eigenvector problem

$$Hc = Ec.$$

Here c is a column vector and H is a square matrix with

$$H_{nm} = \varepsilon_n \delta_{nm} + V_{nm}$$

for $n, m = 0, 1, 2, \ldots, \mathrm{nmax} - 1$, with

$$\begin{aligned} \varepsilon_n &= \left(\frac{(n+1)\pi}{L}\right)^2 \\ V_{nm} &= \int_0^L dx\, u_n^*(x) V(x) u_m(x). \end{aligned}$$

(b) Write a code to evaluate and print matrix H for nmax=5. Display only a few digits using something like `print round(H,5)`. You did essentially this in Homework 6; see the on-line solutions for another code.

(c) Modify your code to:

   i. Calculate the eigenvalues and eigenvectors of matrix H. Print all the eigenvalues but not the eigenvectors.

   ii. Identify the three lowest eigenvalues. Use their corresponding eigenvectors to calculate the eigenfunctions $\psi_i(x)$, $i = 0, 1, 2$, using Eq. (2). Careful: the lowest three eigenvalues may not be the first three eigenvalues in your list. Snippet:

```
psi = 0*x
i = ...
print "Energy is",evals[i]
for n in arange(nmax):
   cn =evecs[i][n]
   un = sqrt(2./L)*sin((n+1)*pi*x/L)
   psi = psi + cn*un
```

   iii. Plot $\psi_i(x)$, for $i = 0, 1, 2$, along with $V(x)/V_0$, all on one plot.

   Debug using a small value of nmax. When your code is working choose nmax large enough to get accurate results.