

PHYS 501: Mathematical Physics I

Fall 2014

Homework #2

(Due: October 15, 2014)

In all cases, turn in the program or script you have written, whether or not it works!

1. An electrical network consists of N interconnected nodes. Each pair of nodes (i, j) is connected by a resistor of resistance $R_{ij} = \min(i, j) + 2 \max(i, j)$, for $i, j = 1, \dots, N$. Let V_i be the electrical potential of node i , and choose the zero level of potential to set $V_1 = 0$. Then Kirchhoff's laws for the other nodes in the network can be conveniently written as

$$\sum_{\substack{j=1 \\ j \neq i}}^N \frac{V_j - V_i}{R_{ij}} = I_i,$$

for $i = 2, \dots, N$, where I_i is the current flowing from node i to some external circuit. Suppose $N = 100$ and the external connection is such that current flows out of node 2 and back into node 1, so $I_1 = -1$, $I_2 = 1$, and $I_i = 0$ for $i > 2$. By solving the above $(N - 1)$ -dimensional matrix equation (e.g. using the *Numerical Recipes* routine `gaussj`, or `solve` in Python, or `linsolve` in Matlab), calculate the total resistance between nodes 1 and 2.

2. The data file <http://www.physics.drexel.edu/students/courses/physics-501/hw2.2.dat> on the course Web page contains (hypothetical) experimental data on the measurement of a function $y(x)$. The N data points are arranged, one measurement per line, in the format

$$\mathbf{x}_i \qquad \qquad \mathbf{y}_i \text{ (measured)} \qquad \qquad \sigma_i$$

where σ_i is an estimate of the uncertainty in the i -th measurement. It is desired to find the least-square fit to the data by polynomials of the form

$$y(x) = \sum_{j=1}^m a_j x^{j-1},$$

for specified values of m , by minimizing the quantity

$$\chi^2 = \sum_{i=1}^N \left[\frac{y_i - \sum_{j=1}^m a_j x_i^{j-1}}{\sigma_i} \right]^2.$$

As discussed in class (and in *Numerical Recipes*, pp 671–676), write down the overdetermined design matrix equation that results from writing $y(x_i) = y_i$,

$$\mathbf{A}\mathbf{a} = \mathbf{b},$$

where $A_{ij} = x_i^{j-1}/\sigma_i$, $b_i = y_i/\sigma_i$ (so the measurement uncertainties are included in each row), and \mathbf{a} is the vector of unknown coefficients. Solve this system using singular value decomposition (`svdcmp` in Numerical Recipes, `svd` in Python or Matlab) to obtain the best fitting polynomial for each of the cases $m = 2, 4, 7$, and 13 . For each m , give the values of a_j and χ^2 , and plot the data and the best fit on a single graph.

3. We wish to approximate the energy eigenfunctions of a one-dimensional square well by expanding them in terms of a *finite* (N -dimensional) subset of harmonic oscillator wavefunctions. The square well is defined by the potential

$$V(x) = \begin{cases} 0 & (|x| < a), \\ V_0 & (|x| > a). \end{cases}$$

The harmonic oscillator potential is $V_{ho}(x) = \frac{1}{2}kx^2$, where we will take $k = 2V_0/a^2$ here. As discussed in class, solving the problem entails diagonalization (e.g. using the *Numerical Recipes* functions `trred2` and `trqli`) of the Hamiltonian matrix $H = (h_{nm})$, where

$$h_{nm} = \langle n|H|m\rangle = \int dx \phi_n^*(x) \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \phi_m(x)$$

and $\phi_n(x)$ is the n -th harmonic oscillator wavefunction:

$$\phi_n(x) = \left(\frac{\beta^2}{\pi} \right)^{1/4} \frac{1}{\sqrt{2^n n!}} e^{-\frac{1}{2}\beta^2 x^2} H_n(\beta x),$$

with $\beta^4 = mk/\hbar^2$.

Use the recurrence relations given in Riley & Hobson, p. 373, to generate the H_n , and the differential relations (same page) along with the trapezoidal rule, where needed, to compute the matrix elements h_{nm} .

Hence, by diagonalizing the matrix H , determine the first (and only) two energy levels E_0 and E_1 of a square well with $V_0 a^2 = 2\hbar^2/m$, for three different values of N : (a) use ϕ_0, \dots, ϕ_4 as a basis ($N = 5$); (b) use ϕ_0, \dots, ϕ_9 ($N = 10$); and (c) use ϕ_0, \dots, ϕ_{19} ($N = 20$). In each case, compare your answers with the exact values

$$E_0 = 0.53 \frac{\hbar^2}{ma^2}, \quad E_1 = 1.80 \frac{\hbar^2}{ma^2}.$$