PROBLEM SET 4 [Due Tuesday, February 19]

Physics 210– Computational Physics

The goals of this problem set are (i) to apply the "power method" to get the eigenvector of largest eigenvalue for a small, simple matrix; (ii) to learn how to use canned packages to diagonalize and invert matrices, and get a feel for how fast they run; and (iii) to use the diagonalizer to study the physics of localization in a solid.

[**1.**] Find the eigenvector of largest eigenvalue for the matrix

$$A = \begin{pmatrix} 2 & 1 & 1 & 1 \\ 1 & 3 & 1 & 1 \\ 1 & 1 & 4 & 1 \\ 1 & 1 & 1 & 5 \end{pmatrix}.$$

by the "power method". Start with the initial vector $v = (0.9, 0.8, 0.7, 0.6)$. How many iterations does it take? What is the eigenvalue? What happens if you start with different initial vectors? Could you have done this problem "by hand"?

[**2.**] Find the inverse of the matrix

$$A = \begin{pmatrix} 2 & 1 & 1 \\ 1 & 3 & 1 \\ 1 & 1 & 4 \end{pmatrix}.$$

"by hand" and then by using the subroutines provided in class.

[**3.**] Find the inverse of the matrix whose elements are given by

$$m_{ij} = 5\delta_{ij} + \frac{1}{i+j}.$$

Do it for matrices of dimension $N = 4, 16, 64, 256, 1024$. How much time does it take? If you have access to it, try diagonalizing similar sized matrices with mathematica. Is it slower?

[**4.**] Use the subroutines provided in class to compute the eigenvalues of the matrix,

$$A = \begin{pmatrix} 4 & 1 & 0 & 0 & 0 & 1 \\ 1 & 4 & 1 & 0 & 0 & 0 \\ 0 & 1 & 4 & 1 & 0 & 0 \\ 0 & 0 & 1 & 4 & 1 & 0 \\ 0 & 0 & 0 & 1 & 4 & 1 \\ 1 & 0 & 0 & 0 & 1 & 4 \end{pmatrix}.$$

Compare with the analytic results obtained in class for the eigenvalues of such matrices.

[**5.**] Consider the coupled mass and spring system (the "one dimensional solid") discussed in class, with all masses $m_l = 1.0$ and springs k_0 connecting individual masses to their equilibrium positions ($x_l = 0$) and springs k connecting masses to their near neighbors.

a. Use the eigenvalue subroutine to compute the eigenvalues of the "dynamical matrix" for a chain with $N = 128$ masses. Take $k = 1$ and $k_0 = 1$. Check a few of the values analytically. Make a plot of the eigenvalues by showing w_n^2 on the y axis and n on the x axis. (Sort the eigenvalues from smallest to largest to make the plot look nice.)

b. Calculate the "participation ratio" for all the eigenvectors and show the normal modes are all extended.

c. Take a couple of the eigenvectors and plot the square of the components as a function of distance along the chain.

[**6.**] Now introduce a "defect spring" by setting $k_0 = 0$ for one of the springs that hook individual masses to their equilibrium positions.

a. Use the eigenvalue subroutine to compute the eigenvalues of the "dynamical matrix" for a chain with $N = 128$ masses. Make a plot of the eigenvalues as above. What is the difference from the previous problem?

b. Calculate the "participation ratio" for all the eigenvectors. Show that one of the normal modes is localized.

c. Determine the localization profile about the defect: Identify the eigenvector associated with the defect mode and plot the square of its component as a function of distance along the chain.

[**7.**] Play around with different choices of the defect k_0. What happens to the localization profile as the defect k_0 gets closer to all the other k_0?