PHYS 331 – Introduction to Numerical Techniques in Physics

Homework 7: Gauss Elimination, LU Decomposition, Eigenmodes

Due Friday, Oct. 27, 2017, at 11:59pm.

Problem 1 – Gauss Elimination (10 points). Instead of writing new code (since you all did very well in writing `TriSolve` in the last homework set), this problem focuses on testing your understanding of the Gauss elimination method. Upload the file `HW6p1template.py` which contains a function `GaussElimin`. **Do not modify this function**; show all your work in the lines below it. In this problem, you may use built-in matrix functions (such as `np.dot`) to answer the questions.

(a) In your own words, explain what the elimination phase of the Gauss elimination does, and why.

(b) Test the code with the following example $\mathbf{A}_1\,\mathbf{x}_1=\mathbf{b}_1$ below. The solution $\mathbf{x}_1$ is provided so you can compare. Show that the output **A** and **b** matrices have the same solution as the input matrices. Explain how you are showing this using comments in your code. Two warnings: 1) Pay attention to column versus row vectors. 2) Pay attention to variable type in this problem; the function is perfectly happy to operate on variables of whatever type it is passed.

$$\mathbf{A}_1=\begin{pmatrix}4 & -2 & 1\\ -3 & -1 & 4\\ 1 & -1 & 3\end{pmatrix},\quad \mathbf{b}_1=\begin{pmatrix}15\\ 8\\ 13\end{pmatrix},\quad \mathbf{x}_1=\begin{pmatrix}2\\ -2\\ 3\end{pmatrix}$$

(c) Test the code with this example $\mathbf{A}_2\,\mathbf{x}_2=\mathbf{b}_2$. The solution $\mathbf{x}_2$ is provided so you can compare. What happens when you try to input these matrices as written, and why? Rewrite the matrices as needed so that they can be passed to `GaussElimin` without errors. (Explain what you did in your PDF file). Show that the output **A** and **b** matrices have the same solution as the input matrices.

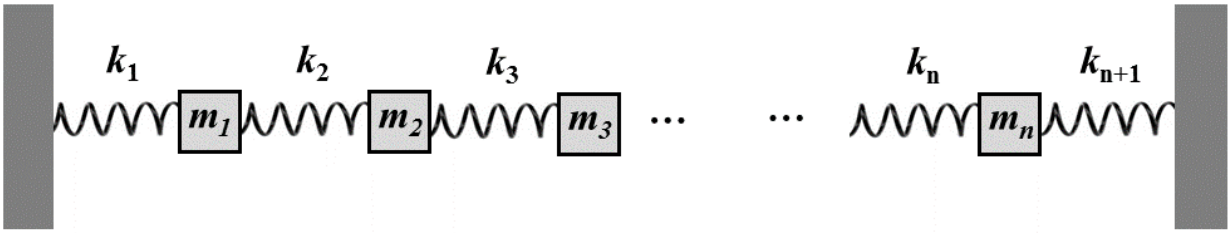
$$\mathbf{A}_2=\begin{pmatrix}0 & 2 & 0 & 1\\ 2 & 2 & 3 & 2\\ 4 & -3 & 0 & 1\\ 6 & 1 & -6 & 5\end{pmatrix},\quad \mathbf{b}_2=\begin{pmatrix}0\\ -2\\ -7\\ 6\end{pmatrix},\quad \mathbf{x}_2=\begin{pmatrix}-1/2\\ 1\\ 1/3\\ -2\end{pmatrix}$$

Problem 2 – LU Decomposition (15 points). As discussed in class, if we need to solve a linear equation system with many different right-hand sides *b*, the *LU*-decomposition is much cheaper than full Gauss elimination, because it only requires a forward- and back-substitution for each *b*, once the matrix **A** has been decomposed. With the Gauss elimination provided above, the *LU* decomposition is nearly in place.

(a) Make a copy of the `GaussElimin` function from Problem 1 into a new .py file and rename the function `LUdecomp`. Modify the function so that it now **only** inputs an n × n matrix, and only outputs its decomposition matrices `L` and `U` that are also n × n. Within this function you are **not** allowed to use any other built-in functions that perform operations on matrices; you may only perform arithmetic operations on elements of the matrices themselves. While this problem is designed to give you an easy starting point from which to build `LUdecomp`, you may, if you wish, completely rewrite the function in your own style.

(b) Show that the outputs from `LUdecomp` satisfy **A** = **LU** when inputting the arrays $\mathbf{A}_1$ and the modified $\mathbf{A}_2$ from Problem 1. Are there any differences between the input **A** and the dot product of **L** and **U**?

Problem 3 – Eigenvalue Problem (25 points). Consider the system of two coupled masses we discussed in lecture, and how we turned the equation of motion of each mass, using Newton's law, into a system of linear equations. Now I want you to consider the below system of n coupled masses m_i, connected by n+1 springs with spring constant k_i, with the displacements of each mass from equilibrium corresponding to x_i.



(a) Use the same method we used in class to write the equation of motion for each mass,

$$\sum F_1 = m_1 \ddot{x}_1 ,$$

assuming that the solution for x takes the form

$$x = A\exp(i\omega t),$$

such that

$$\ddot{x} = -\omega^2 \left(A\exp(i\omega t) \right) = -\omega^2 x .$$

Write out the equations for the first 3-4 masses to see the trend. Then, write the system as an eigenvalue problem, showing at least the first 3 rows and the last row of the $n \times n$ system matrix. (This should all be in your PDF file).

(b) Write a function, `CreateSystem(kvec,mvec)`, that inputs an $(n+1)\times 1$ vector of spring constants k, and an $n \times 1$ vector of masses, m, and outputs the $n \times n$ system matrix that you solved for in part (a).

(c) Test that your function works for the scenario explored in class, for n=2, with k_1=k_2=k_3=1, and m_1=m_2=1. Now, run the output array through `np.linalg.eig()` as we did in class on Wednesday. Are the eigenvalues and eigenvectors what you expected? Explain the physical significance of the eigenvalues. Also, explain the physical significance of the two eigenvectors in terms of the relative motion of the masses (i.e., whether they swing together or out-of-phase). Explain in your PDF file.

(d) Now use your code to determine the eigenvalues and eigenvectors for an n=3 system where all of the k's and m's equal 1 again. Draw a picture of the relative directions and amplitudes of the oscillatory motion for the 3 eigenmodes of the system (*i.e.*, the motion of the masses corresponding to the 3 eigenvalues).

(e) Now let's consider a 1D crystal lattice with atoms of alternating masses (such as sodium chloride, NaCl). Each of the bonds between the atoms can be thought of as springs with identical spring constants. Let's consider a fairly large lattice with n=1000, and set odd $m_i = m_1 = m_3 = \ldots = 1$, and even $m_i = m_2 = m_4 = \ldots = 1.5$. Use your function to create the linear system, and solve for the eigenvalues and eigenvectors.

Make a histogram plot of the eigenvalues (make the bins narrow enough to observe relevant features). What do you notice about the eigenvalues, and what does this say about the possible vibrational frequencies of the system?

Make a second histogram plot for eigenvalues when the even masses are only 1.2 times the odd masses. What changes?

The features you are observing are related to the energy *band gap* of a condensed matter system (which occurs in semiconductors and insulators).

Extra Credit (up to 3 pts): For the even masses = 1.5 case in problem 3(e) above, examine the eigenvectors corresponding to frequencies both above and below the band gap. Determine and explain what the different trends are for eigenvectors above or below the band gap – noting that we should consider the meaning of being above or below the band gap in terms of energy, which is proportional to frequency.