PHY407: Lab 4

Date: October 8th. 2021

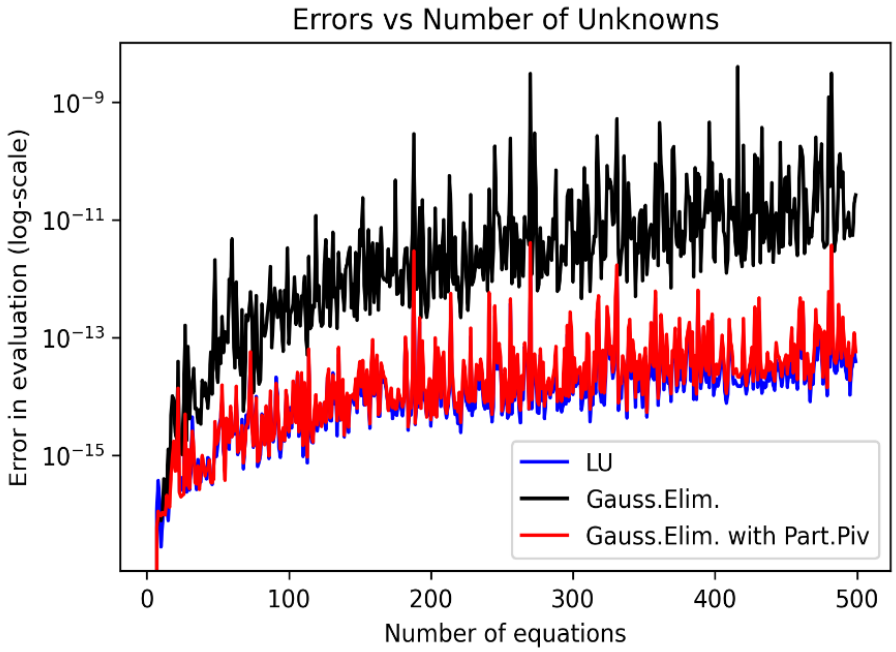
Lab Partners: Brendan Halliday and Nikolaos Rizos

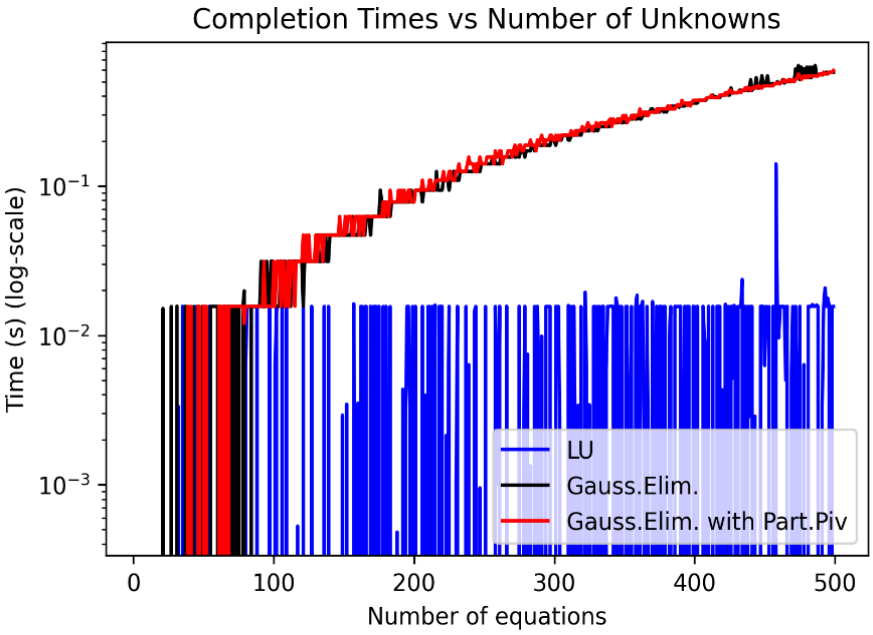
Contributions:

- Q1. Nikolaos Rizos
- Q2. Nikolaos and Brendan Halliday
- Q3. Brendan

Q1.b.

For this question, we compared the accuracy as well as the required times of completion of 3 methods of determining the solutions to random systems of N equations and N variables, for N from 5 to 500 (each time N increased by 1). The three approaches that were implemented were: Gaussian Elimination, Gaussian Elimination with Partial Pivoting on the input matrix, and LU decomposition. The first plot below is the error in the solution, resulting from each approach for each of the random systems, while the second plot below is the time required for each approach to determine the solution for each random system. (number of equations = number of unknowns).





First, regarding the errors in the two methods, we observe that the LU decomposition and the Partial Pivoting w/Gaussian Elimination methods, were almost equally accurate, with the LU decomposition method displaying slightly better accuracy for all values of N. In contrast, we observe that the Gaussian Elimination method without Partial Pivoting, seems to be less accurate than both of the other two methods, while this inaccuracy seems to increase at a slow rate when compared to the other two methods as N increases (i.e., as the system gets bigger). This slow increase in inaccuracy also seems to be displayed by the Gaussian Elimination w/Partial Pivoting approach as N increases, as we observe a slight increase in the deviation of the estimates between this method and the LU decomposition method as N gets larger. (Though the Gaussian Elimination estimates seem to deviate from the LU decomposition estimates faster than the Gaussian Elimination w/Partial Pivoting estimates do.)

Regarding the elapsed time, we observe that for small systems (up to about 80 equations with 80 variables) all 3 methods require a constant, equal time for completion. We also notice that the time required for the LU decomposition approach to determine the solution is independent of the size of the system. In contrast, both the other methods behave the exact same way, with their required completion time increasing as the system gets larger. Even though there appear to be several gaps in the time plot, it nonetheless manages to capture the trend in the elapsed time, which is what we wanted to observe.

Q1.c.

The printed output of the code for the amplitudes and the phases of the Voltages for the initial case, as well as for the case where R6 was replaced by L (represented in our calculations by replacing R6 with imaginary impedance of iR6 in the system of equations), appear below.

##

THE FOLLOWING OUTPUT IS FOR THE SYSTEM WITH THE NORMAL RESISTOR VALUES OF EX.1) (R1-R6)

##

The phases of V1, V2, and V3, correspondingly are (in degrees): -5.469094970111937 11.583418604687067 -4.164672651865924

The amplitudes of the voltages V1, V2, and V3, correspondingly are (in Volts): 1.7014390658777336 1.4806053465364062 1.8607693200562134

##

THE FOLLOWING OUTPUT IS FOR THE SYSTEM WHERE THE RESISTOR R6 TAKES IMAGINARY IMPEDANCE

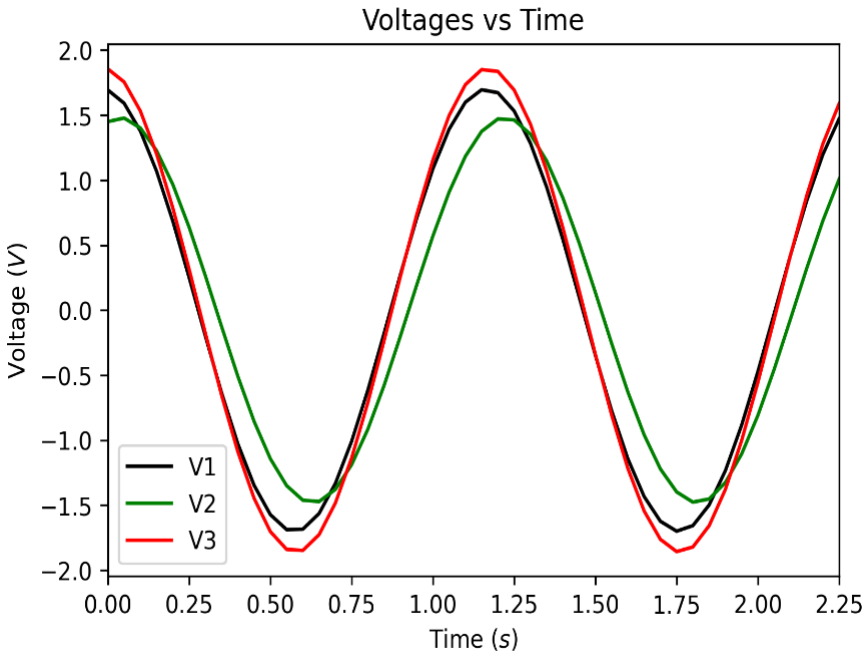
##

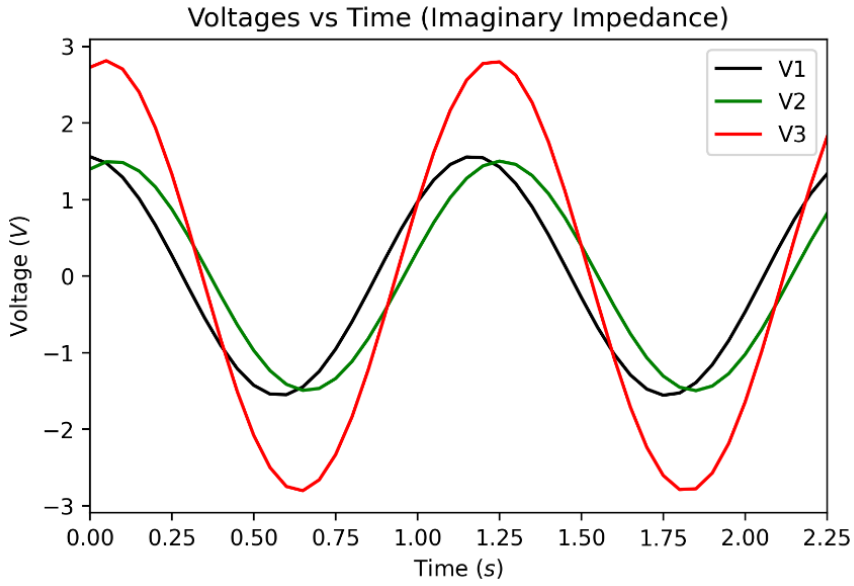
The phases of V1, V2, and V3, correspondingly are (in degrees): -4.0259088196033535 21.639282642570226 14.352479528588603

The amplitudes of the voltages V1, V2, and V3, correspondingly are (in Volts): 1.5621181940219633 1.4994286802306565 2.8112763903392537

##

The plot of the Voltages vs time for the two cases described above, appear below.





What we conclude when comparing these cases is that replacing R6 with an inductor L of 2H causes a slight increase in the phase of V1, it causes the phase of V2 to double and the phase of V3 to triple. On the other hand, this change only slightly decreases the amplitude of V1, it increases the amplitude of V3 by about 55%, and causes negligible change in the amplitude of V2. Replacing R6 with the inductor L increased the voltage at that part of the circuit, which is consistent with the premise in the Physics Background section of the lab in which it was stated that such a change will make the part of the circuit less resistive (voltage is maintained at a higher value as it goes through the inductor, compared to when it goes through the resistors).

Q2.c.

The following is the output for part c. Here, we've calculated the first 10 eigen energies:

Calculate eigen energies using a 10x10 Hamiltonian:
Ground state energy:
5.836431625798466 eV

Excited state energy number 2:
11.18116941413215 eV

Excited state energy number 3:
18.66296810182517 eV

Excited state energy number 4:
29.14427295560185 eV

Excited state energy number 5:
42.655149283739576 eV

Excited state energy number 6:
59.1853318159726 eV

Excited state energy number 7:
78.72943390895861 eV

Excited state energy number 8:
101.28555738947846 eV

Excited state energy number 9:
126.8514591868088 eV

Excited state energy number 10:
155.55540594296528 eV

Q2.d.

The following is the output for part d. Here, the eigen energies for the first 10 eigen states are calculated using the 100x100 Hamiltonian:

Now calculate eigen energies using a 100x100 Hamiltonian:
Ground state energy:
5.836431225104967 eV

Excited state energy number 2:
11.181168090823466 eV

Excited state energy number 3:
18.662966230756332 eV

Excited state energy number 4:
29.144264155690518 eV

Excited state energy number 5:
42.65514016335183 eV

Excited state energy number 6:
59.185279231411684 eV

Excited state energy number 7:
78.72938208028016 eV

Excited state energy number 8:
101.28492643929627 eV

Excited state energy number 9:
126.8506268287797 eV

Excited state energy number 10:
155.4257797026486 eV

Additionally, the relative error was calculated between the 10x10 and the 100x100 where the latter was assumed to be the expected value.

Relative error of the 10 x 10 Hamiltonian eigenvalues:
Ground state energy:
6.865385427688759e-08

Excited state energy number 2:
1.183515598026698e-07

Excited state energy number 3:
1.0025570513744426e-07

Excited state energy number 4:
3.0194316398490207e-07
Excited state energy number 5:
2.1381685090379292e-07

Excited state energy number 6:
8.884736475322082e-07

Excited state energy number 7:
6.58314305050255e-07

Excited state energy number 8:
6.229457870641502e-06

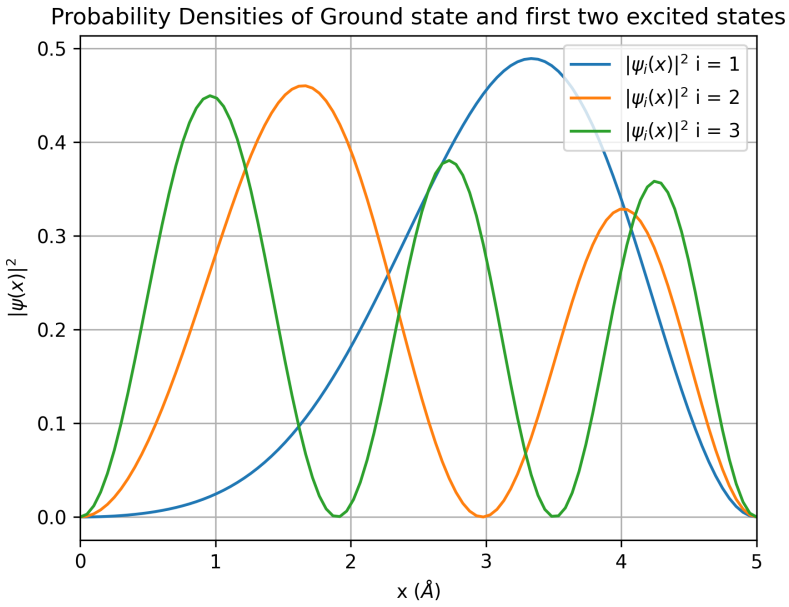
Excited state energy number 9:
6.561717903247196e-06

Excited state energy number 10:
0.0008340073349778985

The relative errors for all the eigenstates are kept reasonably small, thus even the eigenvalues generated by the 10x10 Hamiltonian are a good approximation to the true values.

Q2.e.

Here is the output plot for the probability densities of the first three eigenfunctions:

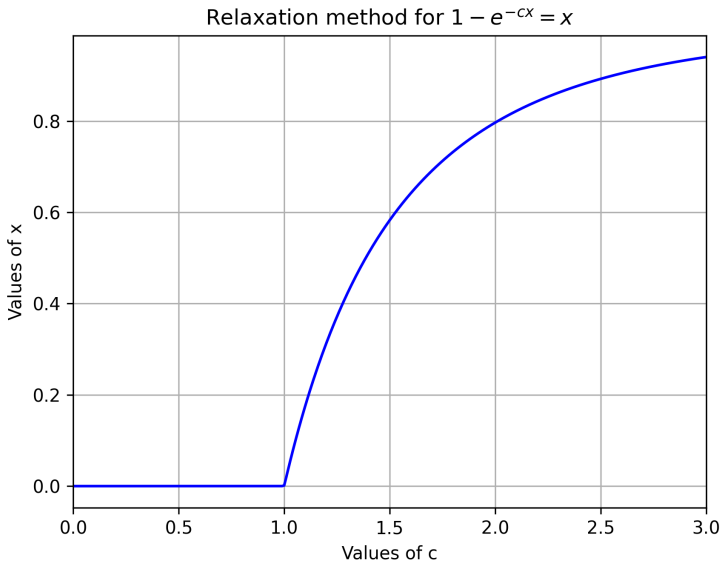


The result of the graph goes against my expectations because the potential is a positive linear function of x meaning the area of lower potential is around values of x that approach zero. The ground state function should be mirrored horizontally. I did not have enough time to investigate this any further.

Gaussian quadratures were used to evaluate A, the integral for each of the probability densities. This result was used as a normalization constant.

Q3.a.

Here is the plot for question exercise 6.10 from Newman



Q3.b.

Here is the output for the program:

> Number of iterations required for relaxation method for c = 2.0:
> 14
> Number of iterations required for over relaxation method for c =2.0:
> 5

The over relaxation method needs fewer iterations to converge within the same threshold. This is due to the fact that the overrelaxation method overshoots by omega = 0.5. This overshooting gets us closer to the true value

Part D short answer:

Suppose the initial guess is two good, and an overshooting would result in a miss.
Under-shooting with a negative value for omega would compensate for the accuracy of the guess.

Q3.c.

This is the output code for the program:

The zero is located at:

x = 4.965114414691925

Wien Displacement Constant is:

b = 0.002897771848412091

The temperature of the sun is estimated to be:

5772.453881298986 K

Here is a plot that compares the three methods. The y axis represents the number of iterations required and the x axis represents the initial guess x. This value of x is the same for each method. In the binary search method, it is the interval bound on the right hand side. We see that Newton's method dominates for each initial value of x.