Math 104A Group 6 CP1

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We are group 6. In our team, Reese is the team leader, Vidushi is the slide presentation creator, Shangcao is the math programmer who created the notebook and the graphic results, Michelle is the project designer, and Tianque is the report programmer who wrote this report.

Our group uses the van der Waals equation to highlight the performance of 2 different root finding methods: Newton's method, and secant method. The equation is used to find the actual molar volume of gas. We fix the constants in each method by fixing R = 0.0821 L * atm / (mole * K), pressure P = 50 ATM, temperature at the pressure P, T = 273 Kelvin. We retrieved the van der Waals constants a, b using the website Real Gas Problems, a = 1.355 L^2/ ATM / Mol^2 and b = 0.03201 L/Mol, number of molecules n = 5. For Newton's method we use the initial guess of $x_0 = 15$ and two initial guesses $x_0 = 10$ and $x_1 = 15$ in the secant method.

The goal behind the comparison of the methods is to see which method performs better under different conditions of initial guesses. Performance is based on the root evaluation and the number of iterations taken, as well as an extra comparison of time taken to finish the function. By using definitions and theorems we learned in class, we chose three appropriate root finding methods and wrote the code to compute the root values (the volume of the gas). By using Newton's method, the root V equals 9.986758471866345 L with 7 iterations taken, and the root equals 9.986758471866347 after 6 iterations by using secant method. With these results, we can compare the time difference by using each method to calculate the root. The volume is around 10 L which is very close to the results of both secant and Newton's method of roughly 9.98675847186635, but the convergence is quicker in the secant method. We are also able to

compare the error between true and predicted values by comparing the root we find in each method with the actual volume calculated by van der Waals equation. Moreover, we compare the sensitivity of the initial guess in each method. We note that the actual convergence of volume V ≅ 9.98675 L is smaller than the actual volume V = 10 L because of the correction needed for the a and b term due to intermolecular forces in noble gasses being weaker at higher temperatures. The actual volume of gas is really useful in many different studies like: Chemistry, thermodynamics, physics, and more. We are able to derive potential energy and distance between molecules with finding the actual volume of the gas using the van der Waals equation and our 3 methods.

Feedback from the CP1:

- What obstacles did you face and how did you overcome them?
    - The main obstacles for this project was finding proper constants to perform our methods. We needed a reliable source to find the coefficients.
- Any advice for those who want to do similar experiments?
    - To try a similar experiment, my advice would be to make sure the code is working properly on easier functions, so that implementing a more complex function, will stay the same structure in the code.
- Reflect on the whole process. What do you want to make note of to become a better program-mer/presenter/documenter/leader?
    - To become a better report programmer, it is better to understand the goal of the whole work comprehensively so that a better report can be written. Secondly, it is important to summarize the work of each group member.

- To become a better documenter, all of the important points need to be put together in slides, so making beautiful PPT slides and accurate summarization is important.
- To become a better programmer, an accurate source of information and detailed code with extensive comments is important.
- To become a better leader, the organization of the time taken of each process, the assignment of tasks and the connection to each group member is important.