Numerical analysis: Project 1

Instructor: Anil Damle
Due: May 1, 2024

Policies

You are permitted to work in groups of up to three for this project and each group only needs to submit a single report. While it is okay to discuss the project with other groups (similar to the HW collaboration policy), every group must produce their own code and report. The report should address all of the items referred to as **goals** or **questions** in the project description. You may refer to inanimate sources (e.g., textbooks) to help you answer the questions and tackle the goals. However, your sources must be explicitly cited. For example, one of the goals requires writing pseudocode for an algorithm that exists, if you go to an external source to read more about it and help generate the pseudocoade you must cite where it came from.

Part of the purpose of this project is to provide you with an opportunity to practice writing more free form reports and carefully choosing what plots, results, etc. are needed to convince us your solution is correct. Therefore, some of the goals are leading, but do not give a concrete list of exactly what has to be included. The questions tend to be more concrete.

The report, including plots and requested output from your code, should be typeset and submitted via the Gradescope as a pdf file. This file must be self contained for grading. Additionally, please submit any code written for the assignment as zip file to the separate Gradescope assignment for code.

Preamble

For this project we are going to consider solving a simplified configuration problem. More specifically, we are going to look for minimal energy configurations of non-bonded atoms in three dimensional space using a simple model for atomic interactions. Practically, a molecular configuration problem contains many more components that we will omit for simplicity. If you are curious, I would encourage you to look further into this problem and I would be happy to point you to resources.

A simple model

For the purpose of this problem, we are going to consider N atoms in three dimensional Euclidean space and try to find energy minimizing configurations. A common model for the interaction of neutral atoms is the so-called Lennard-Jones potential. Specifically, given two atomic locations x_i and x_j in $\mathbb{R}^3$ we define $r_{ij} = \|x_i - x_j\|_2$ and the potential between atoms as

$$V_{ij} = \frac{1}{r^{12}} - \frac{2}{r^6}.$$

Note that there are several parameters in this model that define the optimal distance between two atoms, and the optimal energy. Here we have simply set those coefficients for you.

Now, given N atoms defined by their locations $\{x_i\}_{i=1}^N$ the problem we wish to solve is

$$\min_{x_1,\ldots,x_N} \sum_{i<j} V_{ij}.$$

However, since V_{ij} is invariant with respect to translation of the set of locations $\{x_i\}_{i=1}^N$ it makes sense to fix the location of one of the atoms to $(0,0,0)^T$. Therefore, we assume $x_1 = (0,0,0)^T$ and seek to find local minima (ideally the global minima) of

$$\min_{x_2,\ldots,x_N} \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} V_{ij}, \tag{1}$$

where V_{1j} represents the interactions with the fixed atom at position x_1. This is now an optimization problem in $3(N-1)$ variables.

For this project

There are two concrete tasks for this project and one open ended one. In particular, you must implement two methods for solving (1). One should be gradient descent and the other can be either Newton's method or a Quasi-Newton method. Your implementations need to include a line search using sensible conditions and reasonable convergence criteria. Using these implementations you should complete the following tasks. Your writeup should be structured as a report with narrative flow through what you have done for the project while addressing the tasks along the way—each within a separate section. A portion of your grade will come from the quality of the writeup and how you effectively convey your arguments and answer the following questions.

Question 1: Which optimization algorithms did you implement? Describe your choices for the line search and stopping criteria.

Question 2: For 2 and 3 atoms find globally optimal configurations using your implementations (discuss/illustrate what the configurations are). Argue why you believe you have found a global optima in this case. In addition, is the global minimizer you found unique? Discuss why or why not.

Question 3: Illustrate the order/rate of convergence both your algorithms achieve for 3 atoms when finding the aforementioned minimizer. Do they match what you expect?

Goal 1: Explore computing minimal configurations with more than 3 atoms (you must try and discuss experiments with at least 5 atoms, how far you go beyond that is up to you) to see what you can find and how well your implementations perform. Discuss your findings, what you observe about this problem, and where some of the difficulties arise. (This is deliberately open ended, tell us what you learn in your exploration.)