CS 4220 / MATH 4260: Project 2

Instructor: Anil Damle
Due: April 26, 2019

Policies

For this project, each individual will be turning in their own write up and code. However, you may work in groups of up to three on the project, this includes helping each other write and debug code, and reading and editing each others reports. This is a bit beyond the level of collaboration allowed on the HW. Within a group you can look at "solutions" and discuss them in detail. However, you cannot simply copy each others reports and code. Furthermore, please clearly list your collaborators (if any) in your project report. 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 given below are deliberately open ended and do not give a concrete list of exactly what has to be included. Please submit your code along with the typeset report via CMS.

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. **Clearly describe what you have implemented, including your choices for the line search and stopping criteria, in your writeup.** Using these implementations you should complete the following tasks. In your report please make each of the below separate sections and make sure your report is visually clean and easy to follow.

- For 2 and 3 atoms find the 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.

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

- 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.)

While these are itemized, 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. A portion of your grade will come from the quality of the writeup and how you effectively convey your arguments and answer the above questions.