Algorithms for Two Dimensional Geometry Optimisation

A discussion of alternate approaches for solving the two dimensional geometric optimisation problem using arbitrary bond lengths.

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***Abstract*—This is a big yeet**

I. Introduction

Molecular model optimisation is the process of minimising the potential energy of a molecule with a given number of atoms, each constrained linearly using unit length bonds. In the field of computational chemistry, this process is also referred to as geometry optimisation. The potential energy of such a system, 'V' is given by the scaled pairwise addition of Lennard-Jones potentials. The purpose of this investigation is to develop an algorithm for optimising the geometry of a two dimensional linear bonded molecule of a given size 'N' and investigate new, efficient approaches for solving this problem that take advantage of the features of this problem which separate it from other global optimisation problems. While this problem operates on an extremely simple representation of an atom in a two dimensional space, the investigation is useful for developing molecular structure optimisation algorithms as most algorithms for solving the two dimensional problem can be translated to higher dimensions without undue complexity.

II. Literature Review

A molecule can be defined as "the simplest unit of a chemical substance, usually a group of two or more atoms.""(Dictionary,2018). An atom is defined as "the smallest unit of any chemical element, consisting of a positive nucleus surrounded by negative electrons." (Dictionary, 2018). Understanding the stable configurations of a molecule is important because it enables us to understand its properties and behaviour with respect to its structure. When a molecule is constructed using computational chemistry software it may not be given a stable initial state. This means that if the same molecule were to be constructed in reaslity, it may be unstable and behave unexpectedly. In order to prevent this, geometry optimisation is performed to find a stable state for the molecule.

A number of studies have been performed on solving this problem using randomised global search algorithms such as genetic algorithms or simulated annealing. In some investigations, these higher-level global search algorithms are accompanied by a local optimisation algorithm, such as the Limited Memory Broyden Fletcher Goldfarb Shanno algorithm, or L-BFGS. An example of such a study was published in 1996 by author Wayne Pullan, who developed an in-depth report of numerous algorithms applied to geometry optimisation for both two and three dimensional problems.

Based upon previous research, for this investigation it was decided that an interesting and under explored approach for solving this problem was to optimise each angle individually, one at a time in order rather than trying to optimise the entire population at each step. There are several different approaches using this method which were investigated, and these will be elaborated upon in the following sections of the report.

III. Algorithm Description

A. Section Introduction

The following section will describe the algorithms which were implemented for testing different approaches for solving this problem. The algorithms implemented are relatively similar in function and implementation, and serve the purpose of comparing the efficiency of solving the same problem using fundamentally similar methods but approach the order of operations differently.

1) Data Structures:

a) Matrix: The following data structure is a simplified matrix class which was developed to store the $r(i, j)$ components for each molecule object so they could be referred to when calculating the Molecule system energy rather than recalculating each time the same $r(i, j)$ is required.

Matrix (template <class T>)
x: int y: int data: T *
Matrix(x: int, y: int): ~Matrix(): set(i: int, j: int, v: T): void get(i: int, j: int): T

b) Point: The following data structure is a simple point data structure developed for storing the calculated coordinates for each atom in a Molecule object.

Point
x : double y : double
=(a : Point) : Point +(a : Point) : Point -(a : Point) : Point ==(a : Point) : bool absolute() : Point

c) Molecule: A Molecule class object was implemented for encapsulating all of the data structures necessary for defining a molecule with respect to geometry optimisation. a class diagram of the molecule object is outlined below.

Molecule
distance : Matrix<double> alphas : Eigen::VectorXd real : Eigen::VectorXd coords: std::vector<Point> n: int
getRealAngleList(void) :void getCoords(distance : double, angle : double) : Point getSystemCoordinates(void) : void getR(x : double, y : double) : double getEulerianDistanceMatrix(void) : void getSystemEnergy(void) : double Molecule(n : int): updateSystem(void) : double operator()(x : const VectorXd& , grad : VectorXd&) : double

d) Molecule Function Descriptions: A number of functions utilised within the Molecule class object are fundamental to the operation of the overarching algorithms, and their function will be demonstrated in this section.

B. Ordered Single Pass α Optimisation

1) Discussion: This algorithm follows the application of an extremely strict annealing algorithm, which randomly optimises α_m in order α_0 ... α_{n-1}. This search is performed by iteratively assigning each α a value in the range of -180°...180° until a maximum number of iterations have been performed. Once the maximum is reached the algorithm performs the same steps on the next α variable.

2) Pseudocode:

C. Standard Annealing α Optimisation

1) Discussion:

2) Pseudocode:

D. Brute Force α Optimisation

1) Discussion:

2) Pseudocode:

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