Global Minimums of LJ Clusters

Simulated Annealing Vs. Scipy Bassinhopping

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PHYS 300

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**Introduction**

Throughout the course of our computation physics class we have spent a great deal of time on local optimization of functions. We learned that optimization is an important aspect of computational physics, and that optimization differs depending on a given model you are trying to optimize. We started by being introduced to gradient decent and how this algorithm utilizes derivatives in order to find local minims of one dimensional, two dimensional, and three-dimensional curves. This then led us to discover other methods of finding local minimums like conjugate gradient and utilizing the scipy library with its minimize function.

Once we learned the concepts of minimizing functions of simple curves, we then introduced functions with multiple minima. This naturally led us to discussing the structure of atoms and introduced the Lennard-Jones potential. LJ potentials describe the ways atoms interact with one another. The true interatomic interactions are quantum mechanical in nature, and due to the complexity of quantum mechanics if very hard to find an analytical functional form. Although, we can approximate the interaction with all analytical interatomic potentials.

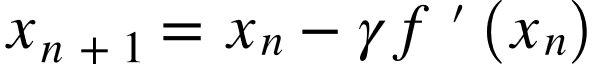
While studying Lennard-Jones potential we were introduced to the very popular optimization algorithm, simulated annealing. Simulated annealing is a very versatile algorithm and can incorporate many different types of functions such as functions that have no continuity, differentiability or dimensionality requirements, and can find the global minima and maxima. Simulated annealing mimics what happens in nature and is used in the annealing of solid metals to optimize complex systems. The term annealing refers to the heating of a solid and then cooling it down slowly. You can think of this as having an atom sitting in a minimum state that may not be the global minimum. We can then simulate the perturbing of the system by adding energy, and then seeing where the atom rests. We then repeat this process over and over to record the different energy minimums. We can then argue after many attempts which value is the global minimum.

Simulated annealing is based around a few changeable parameters. Namely the value of kT. While running simulations of LJ clusters using simulated annealing it is important to choose a good value of kT to perturb the system and look for the global minimum. For my project I decided to take away the guess work and introduce code to the simulated annealing algorithm that allows it to find local minimums, and then systematically search for other local minimums by allowing the algorithm to take more and more aggressive steps. When the code makes a small step of kT = .5 it then minimizes the function using scipy’s minimize function. If it minimizes to the same energy it was before, it will then allow the code to make a more drastic jump to get out of the current potential well it is stuck in. This way it takes a more systematic approach to finding the global minimum.

This was an exercise in my understanding of code development. It is very difficult for a novice code writer to compete with a well-known library such as scipy. The outcome will most likely be that scipy is much faster, but the exercise will test the knowledge obtained in class.

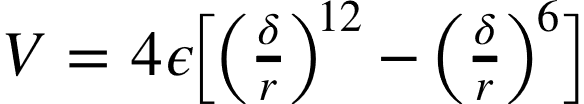
**Background Information**

While utilizing the scipy minimize function we used the default method of gradient decent. This method uses a step by step method of optimizing to the local minimum.



Here, f prime is the slope while gamma is the step length. If you can accurately calculate the value of f prime, and if gamma is very small, it is very easy to calculate the minimum value.

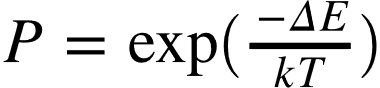
For this assignment I used the Lennard-Jones to model interatomic interactions between atoms.



In this equation epsilon is the depth of the potential well and sigma is the distance which the potential crosses zero and r is the distance between two atoms.

Here we let epsilon and sigma both equal 1. This configuration results in two atoms with the lowest potential energy.

Because simulated annealing mimics phenomena found in nature, we need some mechanism to simulate a small random displacement of atom that result in a small change of energy. For this we use an acceptance rate with a Boltzmann probability factor.



From this equation, if the energy is negative and the energy state of the new configuration is lower, the new configuration is accepted. If the energy is positive and the new configuration has a higher energy state and may not be accepted.

**Experimental Method**

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Description automatically generatedWhile comparing the basin-hopping method vs a modified simulated annealing, it is important to have an understanding of how basin-hopping works. This will better help explain the difference in my code.

This visualization shows the basics of basin-hopping. The algorithm picks an initial starting position. After generating an initial point, it then runs a minimizing function using gradient decent in order to find a local minimum. Now the algorithm uses parameters preset by the user that determines the step size. These parameters are different depending on the type of functions the user wants to find global minima of. Utilizing the parameters set in place, the algorithm takes a step. It then compares energies of the local minimum to the energy found at the step. It then uses this knowledge to meet some type of probability criteria listed above. If the step is accepted then the algorithm will move from the new position to another position in hopes of finding a new local minimum, and overtime, the global minimum.

The simulated annealing code is very similar to the basin-hopping. The biggest difference is when my code accepts it has found a local minimum, it will then take a comparably small step. If after this step the code minimizes to the same local minima (meaning it is trapped in the same potential) the code allows the algorithm to take a slightly more aggressive step calculated by the initial step kT = .5 to kT +.1. This will continue to happen until the step size is enough to leave the current local minimum and travel to another local minimum. This way the code systematically looks for local minimum and has a better chance at finding the global minimum in less attempts. From here I can print the total number of minima found and present the global minimum to the user.

1. **while** (\_iter < Max\_iteration **and** np.abs(true\_energy - obj\_now) > atol):
2. # for i in range(Max\_iteration):
3. pos\_new = neighbor(pos\_now, kT)
5. res = minimize(total\_energy, pos\_new, method='BFGS', tol=1e-3)
6. obj\_new = res.fun
7. ap = acceptance\_probability(obj\_new-obj\_now, kT)
8. **if** obj\_new - obj\_now < .0001: #first iteration we have the same obj new and obj now so it is less than .1
9. kT = kT + variable
10. **else**:
11. kT = .5
12. **if** ap > np.random.random():
13. # print('accept new energy: ', obj\_new,"\n", 'Acceptance Probability: ', ap, "\n", "Step Size: ", kT, "\n")
14. obj\_now = obj\_new
15. pos\_now = pos\_new
16. \_iter += 1

The above code shows if the energies are within .0001 it will add a kT + variable, which I have set to 0.1.

Implementations of techniques learned in class to better understand the data:

-Once I showed the algorithm can find local minimum quite easily, I then used techniques used in class to pull the positions from an online data base. I wrote code that compares the global minimum found in my runs and then compared them with the known values stored on an online data base. If it found the correct global minimum, it will then return the positions stored in the data base. This was useful to help visualize the configuration of the atoms in the nucleus and can easily be plotted using matplotlib.

1. **def** get\_true\_LJ(N):
2. url = "http://doye.chem.ox.ac.uk/jon/structures/LJ/points/"+str(N)
3. names = ['x', 'y', 'z']
4. dataset = pd.read\_csv(url, names=names, delim\_whitespace=True)
5. pos = dataset.values
6. pos = np.reshape(pos, [N\*3,1])
7. **return** total\_energy(pos)

This is the method I used to pull the positions from the online database.

-I also implement the jit function from the numba library to speed up the calculations. When comparing against a well know global minimizer such as basin-hopping, I had to use every technique at my disposal to compete with a well-established library.

**Data and Analysis**

It was easy to see from the beginning that both methods found the global minimums quite easily. Therefore, in order to properly test which technique was more useful I timed each method with similar step sizes with a total of 50 iterations each.

Timed Results

|  |  |  |
| --- | --- | --- |
| Number of Atoms | Simulated Annealing | Basin-hopping |
| N = 12 | 8.79s ± 1.43s per loop | 17.6s ± 107ms per loop |
| N = 15 | 11.1 s ± 6.71 s | 41.8s ± 3.44 s per loop |
| N = 17 | 59.5 s ± 13.6 s | 1min 2s ± 1.6s per loop |
| N = 20 | 3min 37s ± 47.2 s per loop | 1min 39s ± 3.24 s per loop |

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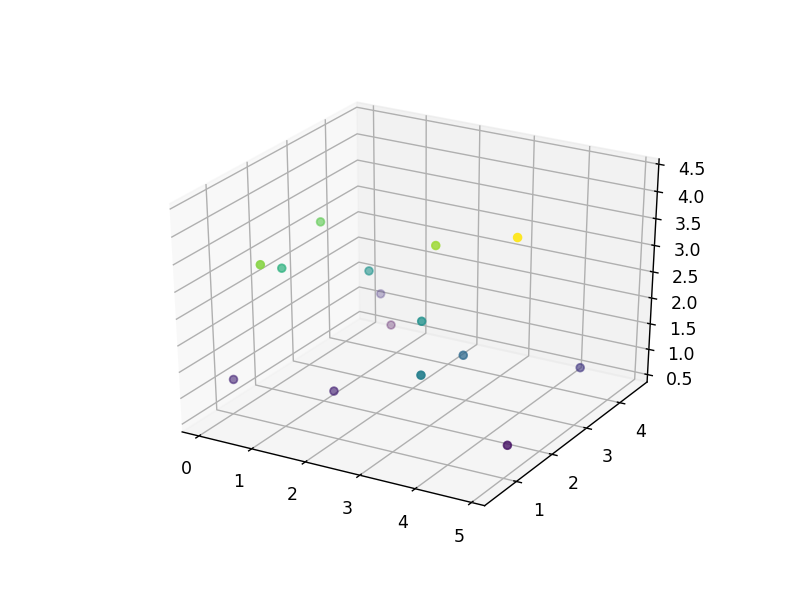
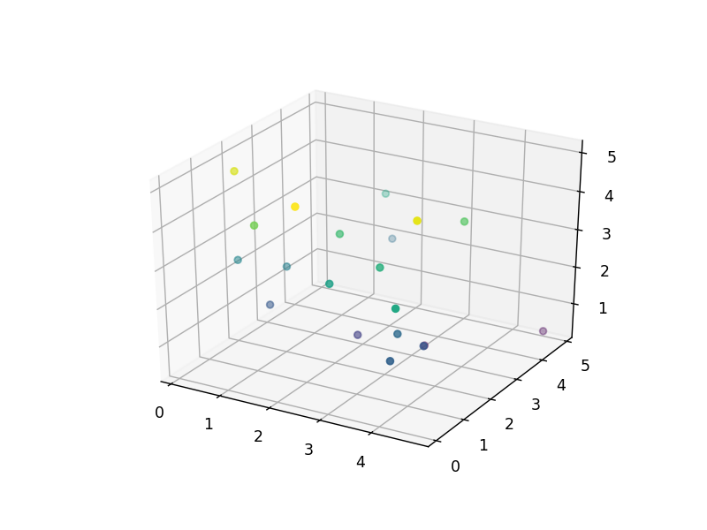
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For simpler systems the modified simulated annealing data shows that the program ran faster than the basin-hopping program. The data above also shows that as the system became more complex the basin-hopping program well out preformed the modified simulated annealing with an almost linear progression as the complexity of the simulations increased. This leads me to believe that even though my modified code did very well for simpler systems it is flawed for solving complex systems.

In addition to the basin-hopping being much faster for complex simulations the error on the time it was also much smaller. I was unable to figure out how to include error on the graph, but the number are worth stating. While basin-hopping should small variations in in error, that was also very consistent, my modified code had large spikes in timing errors even up to the point of almost plus or minus one minute in the 20-atom model.

**Position Graphs from Data**

N = 12 N=15

****

N = 17

A close up of a device

Description automatically generated

**Conclusion**

In conclusion, the point of this experiment was to see if I could take the knowledge learned in our python 300 class and write and original code that satisfied the needs of our classroom work. I successfully wrote code that implemented a modified simulated annealing. I took a systematic approach to finding the global minimum that was very successful. I was able to speed up the optimized program using techniques learned in class that utilized the features in the numba library. I also used techniques used in lecture that allowed me to utilize online databases and pull information from them in order to give visualizations of atomic structures using matplotlib. The basin-hopping code on the other hand showed a consistent trend in performance as well as the time it took to compute. This was an expected result as it is a well-established library. My interpretation of this data is that my code is very basic with minimal parameters that does very well at simple systems. My idea of taking a systematic approach was well thought out but does not compete with a more well written code. I believe the basin-hopping code is less successful at simpler systems because it has many parameters and more checks to help it find global minimums for complex systems. This shows why the time it took to compute was a near linear line as the complexity of the system also increased. In the end I tried to go head to head with well know library and lost. I did however write very good code for doing anything we needed to achieve in class.

**References**

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