Project Summary Report
The Attraction of Repulsion
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A. Background/Purpose

Much of computer science is concerned with solving optimization problems which are impossible to solve with analytical methods, and must therefore be solved with computational algorithms. A classic example of such an optimization problem is *Thompson's Problem*, which is defined as follows: Given N identical point charges constrained to the surface of a unit sphere, what configuration of these charges will minimize the total Coulomb electric potential energy of the system? The total Coulomb electric potential energy of the system is equal to the sum of the Coulomb energies of each pair of particles. The simplified version of Coulomb's law used in Thompson's problem states that the Coulomb energy of a pair of particles is equal to the reciprocal of the distance between the two particles. In this project, solutions to Thompson's Problem were found for a range of N values, and a number of novel methods were used to analyze these solutions and draw conclusions from them.

The purpose of experimenting with Thompson's Problem is twofold. First, an increased understanding of any single optimization problem, such as this one, can eventually stimulate advances in the study of optimization problems in general. Historically, this occurred in the emergence of the now-widespread Simulated Annealing optimization algorithm from the rather esoteric study of how metals cool.

Second, Thompson's Problem has many direct, real-world applications. The most fascinating of these was discovered by Marzec et al [1], who successfully used a version of Thompson's Problem to predict the shapes of certain virus capsids from the ground up. Since biologists do not fully understand the specifics of how capsids form, it is reasonable to suggest that the process by which one finds solutions to Thompson's problem is similar to the process by which capsids are made, as the results of the two processes converge. Thus, the study of Thompson's Problem might have the corollary of shedding some light on the nature virus capsid formation, which could in turn lead to groundbreaking advances in biology and medicine.

B. Procedure

In Java, an original program was written to find solutions to Thompson's problem and analyze these solutions. The two independent variables which were given as input to the program each time it was run were the number of particles and the repulsion exponent. Though the importance of the number of particles is obvious, the meaning and significance of the repulsion exponent requires explanation. According to Coulomb's law, the electric force between two charged particles is proportional to the inverse square of the distance between them. This relationship was modified. Thus, in some tests, force was proportional to the simple reciprocal of the distance, while in others it was proportional to the inverse cube. It must be understood that, in varying Coulomb's law, we are not attempting to model actual physical reality. Instead it was hoped that, by comparing and contrasting characteristics of solutions to the inverse square problem with characteristics of solutions to the reciprocal and inverse cube problems, a better understanding could be attained of the original problem and of the minimization of distance functions on a sphere in general. Trials for N=2-30 were performed at $1/r^2$ repulsion, and trials for N=2-25 were performed at $1/r$ and $1/r^3$ repulsion.

To find solutions to Thompson's problem, the program employs an iterative algorithm described by Erber and Hockney [2]. In essence, the algorithm starts with a random initial configuration of particles and allows the particles to move along the sphere in the direction of the net force acting on them. The amount the particles move in a single iteration is determined by the value of a variable *Gamma*. *Gamma* begins with a very high value, but it is reduced whenever the Coulomb electric potential energy of the system increases over a step. Thus, the algorithm gradually becomes more and more precise until it arrives at a minimum. To distinguish between local and global minimum-energy configurations, each combination of a number of particles and a repulsion exponent was tested at least twenty times with a different random initial particle configuration each time. After the twenty trials, the minimum energy configuration with the lowest energy was selected as the global minimum.

For the purposes of analysis, a number of qualities of each minimum energy configuration were recorded. The two most pertinent to this report are dipole and convex hull. The dipole of a configuration of points is the magnitude of the sum of all the unit vectors going from the center of the sphere to the points on its surface. Where P_i is the unit vector to point i, dipole is $d = \left| \sum_{i=1}^{i=N} \vec{p}_i \right|$. When dipole=0, a configuration can be said to be balanced. When its value is nonzero, the configuration is unbalanced.

The program also computed the convex hull of each solution configuration. The convex hull of a set of points is defined as the minimum convex intersection of all sets containing those points and can be thought of as the smallest convex polyhedron incorporating the points. Finding a convex hull in 3-space is a nontrivial problem in itself, and a separate algorithm was implemented for this purpose.

C. Results and Discussion

The two most interesting results found in the course of this project (and the only results described in this report) dealt with the effect of a changing repulsion exponent. None of the previous studies that were examined reported these results, and none performed any tests of Thompson's problem with the repulsion exponents 1/r and $1/r^3$. Thus, it is probable that these results are new.

First, it was found that as the repulsion exponent increases, the frequency of solution configurations with nonzero dipoles also increases. When particles repel each other according to $1/r^3$, one more dipole is found than at $1/r^2$ repulsion. At 1/r repulsion, no dipoles are found. It might be speculated that increasing the complexity of the repulsion function would tend to prevent perfectly "balanced" (dipole=0) solutions in more and more cases. It is also possible that we are investigating a special case and, after $1/r^3$, no more dipoles are created by increasing the repulsion exponent. Only further research could confirm or disprove the universality of the trend we observe. Regardless of whether it continues, however, it seems apparent that at 1/r there are no dipoles at all. Assuming this continues, future work could optimize an algorithm to solve the 1/r problem by excluding all cases in which a dipole exists. Such an algorithm would be dramatically faster than the original algorithm used in this project, and so would be a great contribution to the study of Thompson's Problem and the 1/r variant of it.

The second and most interesting result deals with the convex hull of solution configurations. When the convex hull of a minimum-energy configuration was computed, a number of properties of the hull were recorded. One of these properties was the number of nearest neighbours each particle had on the hull. (In Figure 1, for example, the circled particle has five nearest neighbours.)

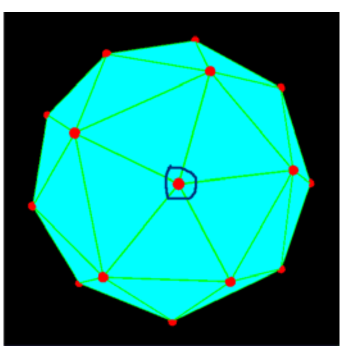

Figure 1: A convex hull. The circled particle has five nearest-neighbours.

It was found that when the repulsion exponent was varied for a given N, even though the actual configuration of particles changed, each particle's number of nearest neighbours never varied. This suggests that the general shape of the convex hull for a certain N, which the vertex nearest-neighbour counts describe, is not related specifically to any one function, but instead is related to the minimization of distance functions on a sphere in general.

If the aforementioned hypothesis is true, it has obvious applications. In order to optimize a more complex function on a sphere, one could first optimize a simpler one and record its convex hull. By ruling out all particle configurations that do not yield the recorded convex hull, one could reduce the amount of computing time required to solve the more difficult problem. One possible use of this method would be finding solutions to Thompson's problem for much higher repulsion exponents.

Further work with more computing power should first rigorously test all the observed trends at higher particle counts and higher repulsion exponents, as this project was limited by the laptop it was performed on. If the trends do continue, future researchers might create the algorithms suggested above, which would allow for vastly increased efficiency in certain situations. Researchers doing further experimentation with Thompson's problem might also find the program created for this project to be a helpful tool in their analysis. The program's ability to calculate the convex hull of a solution configuration is useful as there appears to be great potential in the convex hull approach to analysis. In addition, the program is written in object oriented style and so is easy to modify and upgrade.

Cited References

[1] Marzec, Christopher J. & Day, Loren A (1993). *Pattern Formation in Icosahedral Virus Capsids: The Papova Viruses and Nudaurelia Capensis β Virus.* Biophysical Journal, 65, 2559-2577

[2] Erber, T & Hockney, G M. (1991). *Equilibrium configurations of n equal charges on a sphere*. Journal of Physics A: Mathematics and General, 22, 1369-1377

Appendix I: Bibliography

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