N Points on a Sphere
Introduction

1 Problem Statement

Consider n points confined to a unit sphere with its center at o and let C be the set $\{\hat{r}_{io}\}|_{i=1}^{n}$ of position vectors associated with those n points. Each represents an electron and thus experiences a force described by Coulomb's Law:

$$\vec{F}_i = \sum_{\substack{k=1 \\ k\neq i}}^{n} \vec{F}_{ik} = \sum_{\substack{k=1 \\ k\neq i}}^{n} r_{ik}^{-3}\vec{r}_{ik}$$

Where $r_{ik} = ||\vec{r}_{ik}||$, and in general a vector without its hat is to be interpreted as its magnitude. Because the points are confined to the sphere, the radial component of each force vector $\vec{F}_i^R = \hat{r}_{io}\left(\hat{r}_{io}\cdot\vec{F}_i\right)$ can be ignored. The goal is to find every equilibrium distribution, that is, every arrangement for which the tangential component $\vec{F}_i^{\perp} = \vec{F}_i - \vec{F}_i^R$ of every point's force has zero magnitude. To that end, we define the "Cross Sum" (so named because it was initially formulated using a cross-product) as the average of the magnitudes of these tangential components:

$$CS(C) = \frac{1}{n}\sum_{i=1}^{n} F_i^{\perp}$$

The challenge is now to create an algorithm that takes just a single value, n, and returns every distribution C for which $CS(C) = 0$. Such distributions will be called "solutions."

2 The Thomson Problem

The Thomson Problem is a very closely related question: what distribution of electrons within a spherical enclosure minimizes the electrostatic potential energy? And although the plum-pudding atomic model that spawned this inquiry has long-since been disproven, the question has still received attention over the last century, primarily because its nonlinearities provide a useful testing ground for minimization techniques.

It is not difficult to intuit that a distribution which satisfies the Thomson criteria must also satisfy mine (let's call it the Equilibrium criterion): a distribution cannot be at a potential energy minimum without also being in equilibrium. Thus, the Thomson Problem asks which of the solutions of the Equilibrium Problem for n points has the lowest energy.[1] In addition, it should not come as a great surprise that I have observed, with very few exceptions, that the Thomson solution is the only stable solution at any particular value of n, though that is a much harder relationship to justify mathematically. Nevertheless, the practical result of these characteristics is the somewhat ironic efficacy of an incredibly simple minimization technique: just iteratively move all points in the direction of their force.

It is, of course, more complicated than that, but the point remains that I have developed a very simple and effective means of finding solutions to the Thomson Problem. What is more interesting, however, is why this method works so well. Part of the issue of minimizing Potential energy is that the value of the minimum

[1] I would be remiss not to mention the unexpected equality that the potential energy of a distribution $U(C) = \sum\sum r^{-1}$ is equal (for the case of points on a sphere) to just the sum of the magnitudes of the radial components of the forces $\sum F^R$

is unknown and is very large relative to the difference in values between absolute and local minima.[2] When minimizing a Cross Sum, however, the minimum is always at zero, and this serves to anchor the rest of the minimization process. For instance, the primary knob that one can turn to adjust the minimizer is the step size; knowing that all distributions will trend towards the same value makes it much easier to tune this value in response to the other variables that affect the general performance: how many points there are and the nearness of the system to the minimum.

3 Difficulties

The solution-finding algorithm can be broken down into three main sections: initial position generation; minimization; classification. Practically, there is a fourth step of visualization, but the challenges therein are not generally of mathematical concern.

3.1 Minimization

The principal difficulty of the problem is ironically what makes the subset of the Thomson Problem relatively easy: the vast majority of solutions are unstable. What this means is that the minimization algorithm must be very *cautious*, as any deviation from the narrow trajectory that leads to the solution is bound to lead to minimization failure. As such, the prevailing minimization strategy has been a modification of the simple iterative model used for the Thomson Problem which incorporates an abundance of checks and countermeasures to ensure the path always moves "downhill."

For a while I thought that improvement of the minimization algorithm would be the key to identifying more different solutions, as many distributions were failing to minimize, getting stuck in valleys without any means of reaching a Cross Sum of 0. While this line of inquiry did lead to some useful insights, what I ultimately realized was that the issue laid not with the minimization algorithm, but rather with the initial positions.

3.2 Initial Positions and Classification

Something I noticed early on is that solutions are generally structured in parallel planes of polygons. For example, an icosahedron can be oriented so as to have one point on each pole and two pentagonal bands parallel to the equator, so it is given the name (1 5 5' 1), where the prime (') on the second 5 indicates that the second band has been rotated by $\pi/5$ relative to the first.

This proved a useful system and one not too difficult to generalize, but it was not without its limits. Being an observation made near the beginning of my exploration of the problem, it was made within the context of knowing only those solutions that are simple to find, which is to say those with typical geometric structure (prisms, pyramids, etc.) and thus a decent amount of symmetry. Low symmetry solutions often have no name that fits well.

Nevertheless, as it currently stands, the initial position generator still uses this theory of parallel polygons as its foundation, iterating through all valid combinations of bands to create distributions to pass on to the minimizer. However, the classification of the solutions has moved past that model to simply labeling each solution with its symmetry group.

Indeed, symmetry groups have proven to be a powerful new tool for understanding this problem, their late entry only being justified by my background in engineering as opposed to pure math. The process of incorporating symmetry groups into the initial position generator has proven very slow, however, as the sheer number of combinations of different elements among the plethora of different group structures is staggering, and the exceptions are just as numerous and confusing as the rules. For instance, there are 7 distinct starting positions for just the O_h group for just $n = 48$, and that is one of the easier examples to comprehend. But I am committed to figuring it all out and implementing it into the next update of the initial position generator, and I'm excited to see what new insights that improvement will provide.

[2] For example, if $n = 8$, the Thomson solution has a potential energy of 19.6753, whereas the second-best equilibrium is only 0.03% greater, at 19.6816; for $n = 11$, the difference is only 0.004%