Discrete Minimal Energy Problems

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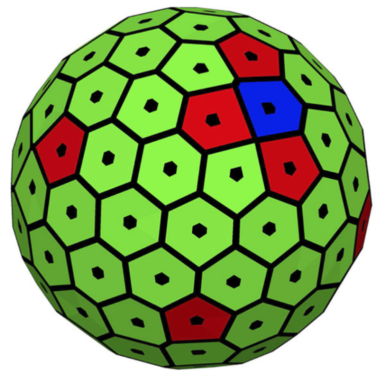
Configurations of points on the two-sphere that minimize the pairwise electrostatic energy have been the focus of considerable investigation. Computational efforts to find such energy-minimizing configurations are hampered by the presence of many locally minimal but not globally minimal, i.e. stable, configurations. This work aims to answer the question: how many stable configurations are there?

Background and Motivation

The question of finding configurations of N points distributed on $\mathbb{S}^2$ that minimize the pairwise energy $|\mathbf{x}_i - \mathbf{x}_j|^{-1}$ has its roots in Thomson's model of the atom [7]. See [1] for background and references. While there have been theoretical advances regarding asymptotic properties of such configurations [6], theoretical results for finite N have been rare. At first the problem appears amenable to computational investigation, in particular gradient descent methods. Such work goes back to at least 1977 [5]. A central challenge is that gradient descent methods often find locally minimal, i.e. stable, but not globally minimal configurations. Further, even if such a method finds a globally minimal configuration, there is no way to determine if it is globally minimal. The work described here aims to answer the question: how many stable configurations are there?

Description of Work

This work was published in [2] and consisted of three main components: The first was implementation of applicable optimization techniques, and the development of a criteria for determining if a configuration was stable. The number of free parameters is twice the number of points, and, as N increases, the dimensionality of the system can prevent optimizers from finding a stable configuration. The second was to develop a means to determine quickly if two configuration with the same energy were rotations or reflections of each other. The extremal edges in the convex hull of a configuration of points forms a planar graph that is invariant under rotations and reflections of the configuration. By using efficient techniques to find isomorphisms between two such graphs, we could find isometries between configurations of points. Finally, after months of extensive computational experiments, the rate at which new configurations occurred had not dropped to zero. In response we applied techniques developed based on the Good-Turing frequency to estimate the number of unseen configurations.

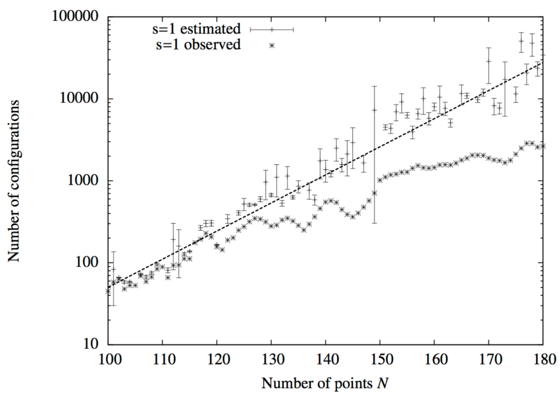


A stable configuration of 102 points on the sphere. The sphere has been partitioned into Voronoi cells associated to each point, which have been colored by the number of neighbors.

Anticipated Impact

One of the central questions about complex systems in general is whether the number of stable configurations grows exponentially with N. This work provides numerical evidence of an affirmative answer. While evidence of an affirmative answer was also provided earlier [3], the exponential factor we obtain is markedly higher than that of the earlier work, and closer to more recent explorations of the problem [4].

This work also helps provide estimates for the



The number of observed stable configurations and the estimated number of stable configurations as a function of N.

amount of computational work required to effectively sample the energy landscape.

Path Forward

Future work in this area includes understanding the fine structure of stable configurations. The broad experimental results are entirely in agreement that, as N grows, stable configurations consist of a large "hexagonal sea" punctuated by islands of defects that relieve the strain associated with wrapping a flat hexagonal lattice around a curved sphere. Stable configurations differ from each other in the location and nature of these defects, and their complete characterization would be extremely valuable.

Acknowledgements

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