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Short Communication

Distributing points uniformly on the unit sphere under a mirror reflection symmetry constraint

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ABSTRACT

Uniformly distributed point sets on the unit sphere with and without symmetry constraints have been found useful in many scientific and engineering applications. Here, a novel variant of the Thomson problem is proposed and formulated as an unconstrained optimization problem. While the goal of the Thomson problem is to find the minimum energy configuration of N electrons constrained on the surface of the unit sphere, this novel variant imposes a new symmetry constraint – mirror reflection symmetry with the x–y plane as the plane of symmetry. Qualitative features of the two-dimensional projection of the optimal configurations are briefly mentioned and compared to the ground-state configurations of the two dimensional system of charged particles laterally confined by a parabolic potential well.

1. Introduction

The essence of the Thomson problem [12,31] is to find the minimum electrostatic potential energy configuration of N electrons constrained on the surface of the unit sphere. Even though the Thomson problem has been around for more than a century now, it never ceases to inspire new developments and applications. From the aesthetic point view [30], the Thomson problem rivals some of the famous unsolved problems in number theory in terms of its aesthetic appeal such as the simplicity of the problem statement, the complexity of the general solution, the computability or tractability of some simple cases and the beauty of the minimum-energy configurations. More importantly, it is its immense practical appeal that will make it relevant well into the future. Specifically, the minimum energy configurations obtained from the Thomson problem or other uniform point sets on the unit sphere through other approaches have been found useful, and in some cases essential, in many scientific and engineering applications [1–3,6,13–20,22,24,33,34,36].

Among the many developments, we list the following research directions that have been inspired in part by the Thomson problem:

- The development of a deterministic scheme capable of generating nearly uniform points on the unit sphere, see [3,16,25,28,35].
- The development of a new variant of the Thomson problem under the antipodal symmetry constraint. The approach that deals directly with the repulsive forces was first suggested in [13] and elaborated with further details in [10]. The reformulation of the electrostatic potential energy function to account for antipodal symmetry can be found in [19,20]. A new iterative scheme based on the centroidal Voronoi tessellations [11] capable of generating large-scale uniform antipodally symmetric points on the unit sphere suitable for 3D radial MRI applications was proposed and developed in [20]. In [20], a novel pseudometric was proposed and derived from the modified Coulomb interaction term studied in [19].
- The development of a deterministic scheme capable of generating nearly uniform and antipodally symmetric points on the unit sphere [17,18]. This scheme is based on a set of equidistant latitudes under the condition that the spacing between two consecutive points on the same latitude should be approximately equal to the spacing between two consecutive latitudes for a given number of points. This type of point set has been found useful in astrophysics [14], medical imaging [7] and optical sciences[26].[1]

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[1] The author learned of the application of this type of point set in optical sciences through a private correspondence with Dr. Janaka Chamith Ranasinghesagara of University of California, Irvine.

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In this communication, we propose a novel variant of the Thomson problem under a mirror reflection symmetry constraint. The reformulation of the electrostatic potential energy function to account for the mirror reflection symmetry is similar to that of our previous work in dealing the Thomson problem under the antipodal symmetry constraint, [19,20]. We will also reformulate the Coulomb interaction term so that a new pseudometric can be gleaned from it and can be used in a similar framework to that of our pseudometrically constrained centroidal Voronoi tessellations of the unit sphere [20].

Even though our interest lies mainly on generating uniformly distributed points on the upper hemisphere for modeling and analysis purposes. The two-dimensional projections of these point sets on the x–y plane turns out to have apparent similarity to the arrangement of charged particles in a two-dimensional system confined by a potential well, which has been found useful in many atomic and condensed matter physics applications, see [4,5,21,27,29]. We should point out that the optimal configurations obtained from the proposed problem is well suited for applications in optics, especially in the modeling of spherical lenses because the boundary of the proposed uniform point sets is the equatorial great circle. Consequently, it is a simple task to map those uniformly distributed points on the upper hemisphere onto a spherical cap to facilitate the utility of this type of point set in optical and other imaging sciences. Another potentially interesting and useful application of the proposed point set that is closer to the author's interest is in making this kind of point sets as a coordinate system for mapping brain (hemispheric or left-right) asymmetry [8,32].

2. Methods

The spherical coordinate on the unit sphere can be described by, (θ, ϕ), and its transformation to Cartesian coordinate, (x, y, z), can be accomplished by the following transformations:

$$x = \sin(\theta)\cos(\phi),$$
$$y = \sin(\theta)\sin(\phi),$$
$$z = \cos(\theta).$$

The mirror reflection operation about the x–y plane is denoted by $\sigma : \mathbb{R}^3 \to \mathbb{R}^3$. For example, it maps a vector, $\mathbf{r} = [r_x, r_y, r_z]^T$, on the upper unit hemisphere to its mirror image, $\mathbf{x} = \sigma(\mathbf{r}) = [r_x, r_y, -r_z]^T$ and vice versa. Note that the vector or matrix transposition is denoted by T. The matrix representation of σ is a diagonal matrix with $\{1, 1, -1\}$ in the main diagonal.

Suppose we have a collection of $2N$ points, $\{\mathbf{r}_1, \ldots, \mathbf{r}_N, \mathbf{x}_1, \ldots, \mathbf{x}_N\}$, on the unit sphere and this collection of points is endowed with mirror reflection symmetry, i.e., $\mathbf{x}_i = \sigma(\mathbf{r}_i)$ for $i = 1, \ldots, N$. We further assume that $\mathbf{r}_i's$ are on the upper hemisphere. In general, the electrostatic potential energy of $2N$ points, say $\{\mathbf{y}_1, \ldots, \mathbf{y}_{2N}\}$, is typically expressed as a double summation of $2N$ terms

$$\sum_{i=1}^{2N}\sum_{j=i+1}^{2N}\frac{1}{||\mathbf{y}_i-\mathbf{y}_j||}.$$

Due to the mirror reflection symmetry constraint, the electrostatic potential energy of $2N$ points can now be expressed as a combination of a double sum of N terms and a single sum of N terms

$$\phi_C = 2\sum_{i=1}^{N}\sum_{j=i+1}^{N}\left(\frac{1}{||\mathbf{r}_i-\mathbf{r}_j||}+\frac{1}{||\mathbf{r}_i-\sigma(\mathbf{r}_j)||}\right)+\sum_{k=1}^{N}\frac{1}{||\mathbf{r}_k-\sigma(\mathbf{r}_k)||}. \tag{1}$$

The first term and the second term in the double sum account for the interaction between any two distinct points on the upper hemisphere and between a point on the upper hemisphere and another point in the lower hemisphere that is not its mirror image, respectively. The term in the single sum accounts for the interaction between a point on the upper hemisphere and its mirror image. The above reformulation is similar to that of the Thomson problem under the antipodal symmetry constraint [19,20] except for the appearance of the second sum in Eq. (1). The appearance of this second sum makes it harder than the case under the antipodal symmetry constraint to extract the desired pseudometric, which can then be used in a framework similar to our previous proposed pseudometrically constrained centroidal Voronoi tessellations, see Eqs. (3) and (4) in [20], to deal with large-scale problems, e.g., generating large number of uniformly distributed points in the range of tens of thousands. In order to extract the desired pseudometric, we would like the interaction term to appear within the double sum. It is not hard to see that the following expression is equivalent to Eq. (1):

$$\phi_C = \sum_{i=1}^{N}\sum_{j=1, j\neq i}^{N}\left(\frac{1}{||\mathbf{r}_i-\mathbf{r}_j||}+\frac{1}{||\mathbf{r}_i-\sigma(\mathbf{r}_j)||}+\frac{1}{2(N-1)}\left[\frac{1}{||\mathbf{r}_i-\sigma(\mathbf{r}_i)||}+\frac{1}{||\mathbf{r}_j-\sigma(\mathbf{r}_j)||}\right]\right). \tag{2}$$

The desired pseudometric, denoted by $d(\mathbf{r}_i, \mathbf{r}_j)$, is simply the reciprocal of the collective summand in Eq. (2), i.e.,

$$d(\mathbf{r}_i,\mathbf{r}_j) = \frac{1}{\frac{1}{||\mathbf{r}_i-\mathbf{r}_j||}+\frac{1}{||\mathbf{r}_i-\sigma(\mathbf{r}_j)||}+\frac{1}{2(N-1)}\left[\frac{1}{||\mathbf{r}_i-\sigma(\mathbf{r}_i)||}+\frac{1}{||\mathbf{r}_j-\sigma(\mathbf{r}_j)||}\right]}.$$

2.1. *Qualitative relationship to the 2D system of charged particles in a circular parabolic potential well.*

The potential energy of two-dimensional system of N classical charged particles confined within a circular parabolic potential well [4,5,21] is given by the following expression

$$E = \sum_{i=1}^{N}\sum_{j=i+1}^{N}\frac{1}{||\mathbf{r}_i-\mathbf{r}_j||}+\sum_{k=1}^{N}||\mathbf{r}_k||^2, \tag{3}$$

where $\mathbf{r}_i$'s are in $\mathbb{R}^2$.

Qualitatively, the effect of the second sum in Eq. (3), which comes from the the circular parabolic potential well, is to attract charged particles closer to the center of the potential well. Similarly, the effect of the second sum in Eq. (1), which comes from the mirror-symmetry constraint, is to repel charged particles that are confined to the surface of the sphere from the x–y plane, which has the same effect of pushing charged particles closer to the z-axis. Due to the qualitative effects of the potential well and the plane of symmetry on charged particles, it is not surprising that the two-dimensional projections of the optimal configurations of the proposed problem may share some qualitative features to those of a system of charged particles in the circular parabolic potential well. Shell-like structures are common features in both systems.

In the limit when the upper hemisphere reduces to a very small spherical cap centered on the z-axis, the interactions between points on the upper hemisphere become more dominant than the inter-hemispheric interactions. Further, the first non-constant and dominant term in the series expansion of the term in the second sum in Eq. (1) goes as r^2 where r is the planar distant between the position of the vertical projection of the point on the x–y plane