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A Point Balance Algorithm for the Spherical Code Problem ⋆

HONG-XUAN HUANG[1], PANOS M. PARDALOS[2] and ZUO-JUN SHEN[2]
[1]*Department of Mathematical Sciences, Tsinghua University, Beijing 100084, P. R. China;*
[2]*Department of Industrial and Systems Engineering, University of Florida, Gainesville, FL 32611, USA (e-mail: pardalos@cao.ise.ufl.edu)*

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Abstract. The Spherical Code (SC) problem has many important applications in such fields as physics, molecular biology, signal transmission, chemistry, engineering and mathematics. This paper presents a bilevel optimization formulation of the SC problem. Based on this formulation, the concept of *balanced spherical code* is introduced and a new approach, *the Point Balance Algorithm* (PBA), is presented to search for a 1-*balanced spherical code*. Since an optimal solution of the SC problem (an extremal spherical code) must be a 1-balanced spherical code, PBA can be applied easily to search for an extremal spherical code. In addition, given a certain criterion, PBA can generate efficiently an approximate optimal spherical code on a sphere in the n-dimensional space $\Re^n$. Some implementation issues of PBA are discussed and putative global optimal solutions of the Fekete problem in 3, 4 and 5-dimensional space are also reported. Finally, an open question about the geometry of Fekete points on the unit sphere in the 3-dimensional space is posed.

Key words: Spherical Code (SC), Extremal Energy, Extremal Spherical Code, Balanced Spherical Code, Point Balance Algorithm, Global Optimization, Bilevel Optimization, Pattern Search Algorithm

1. Introduction

A spherical code is a finite collection of points on the n-dimensional unit sphere. *The Spherical Code* (SC) *problem* is referred to as how to distribute points on the unit sphere according to a certain 'generalized energy'. The SC problem has been the focus of research in various fields such as physics [1], molecular biology [9, 28], signal transmission [39], chemistry [40], engineering and mathematics [4, 23, 24, 29]. Some well-known problems, such as *the Tammes problem* (the best-packing problem), *the Fekete problem* (the minimal potential energy arrangements), *the best-covering problem*, *the maximal volume arrangements* and *the t-designs problem*, can be considered as SC problems with different objectives [5, 25]. Given a certain form of the generalized energy, a special spherical code

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can be generated via optimization to satisfy some constraints and performance measures. Hence, the SC problem has a strong connection with optimization.

The Tammes problem, which is defined as how to place N points on a sphere in the n-dimensional space so as to maximize the minimal distance (or equivalently the minimal angle) between any two points, is one of the most studied SC problems in the mathematical literature [4]. Without loss of generality, the sphere is normalized to a radius of 1. Given an integer $N \geqslant 2$, the Tammes problem is equivalent to the following optimization problem:

$$E_T = \max_{\|x_i\|=1,\, 1\leqslant i\leqslant N} \min_{1\leqslant j<k\leqslant N} \left\|x_j - x_k\right\|, \tag{1}$$

where $x_i \in \Re^n$ and the vector norm $\|\cdot\|$ is the Euclidean norm. The Tammes problem can also be stated equivalently as the best-packing problem: how to pack N non-overlapping identical circles (or spherical caps) on the sphere such that the size of the circles is as large as possible. The three-dimensional case of the Tammes problem and the related problem, whether or not the optimal packing is essentially unique, were first raised by the Dutch botanist P.M.L. Tammes in connection with the distribution of pores on pollen grains [18, 28].

In this paper, we introduce a formulation of the SC problem based on bilevel optimization. In our discussion, we adopt the following 'generalized energy' [13, 21–23]. Let $S^n = \{x | \|x\| = 1\}$ denote the unit sphere and $x = (x^1, x^2, \ldots, x^n)^T$ denote a point in the n-dimensional real space $\Re^n$. Let $N \geqslant 2$ be an integer and parameter $s \in \Re$. Let P_N^n denote a spherical code with N points on S^n, i.e., a set of unit vectors in $\Re^n$ (may require them to be mutually different for a certain value of the parameter s). The *s-energy* associated with the spherical code $P_N^n = \{x_1, x_2, \ldots, x_N\}$ can be defined by

$$\omega(s, P_N^n) = \begin{cases} \sum\limits_{i<j} \| x_i - x_j \|^{-s} & \text{if } s \neq 0 \\ \sum\limits_{i<j} \ln\left(\dfrac{1}{\| x_i - x_j \|}\right) & \text{if } s = 0. \end{cases} \tag{2}$$

The *s-extremal energy* $E_N(s)$ for N points on S^n is defined by

$$E_N^n(s) = \begin{cases} \min\limits_{P_N^n \subset S^n} \omega(s, P_N^n) & \text{if } s \geqslant 0 \\ \max\limits_{P_N^n \subset S^n} \omega(s, P_N^n) & \text{if } s < 0. \end{cases} \tag{3}$$

The spherical code $P_{s,N}^{n,*} = \{x_{s,1}^*, \ldots, x_{s,N}^*\}$ is called *the s-extremal spherical code* if it satisfies

$$\omega(s, P_{s,N}^{n,*}) = E_N^n(s).$$

The points in the 0-extremal spherical code $P_{0,N}^{n,*}$ are called *logarithmic extreme points* or *elliptic Fekete points* [33]. Clearly, the elliptic Fekete points maximize

the product of the distances between any two points in P_N^n, i.e.,

$$\max_{\|x_i\|=1,\,1\leqslant i\leqslant N} \prod_{1\leqslant j<k\leqslant N} \|x_j - x_k\|.$$

Given a large integer N, there are many saddle points and various symmetries in P_N^n, and it is very difficult to minimize the 0-energy associated with P_N^n [24]. It is one of the most challenging problems for the next century as proposed by S. Smale even to find a good approximation to the elliptic Fekete points in the 3-dimensional space for any integer $N \geqslant 2$ [26]. Reference [21] provides numerical evidence that the generalized spiral points have the following property:

$$\omega(0, P_N^n) - E_N^n(0) \leqslant 114 \log N,$$

when the number of points is $N \leqslant 12000$.

The points in the 1-extremal spherical code $P_{1,N}^{n,*}$ are called *Fekete points* [5]. Let us consider N point charges on a unit conducting sphere, interacting only through their mutual Coulomb forces. What is the configuration of the charges for which the Coulombic energy is minimized? This question was original raised by Thomson for $2 \leqslant N \leqslant 100$ [38], and has since been investigated by many researchers [1, 6–8, 21, 22]. The Fekete points in the 3-dimensional space represent the locations of N charged particles on the unit sphere that repel each other according to Coulomb's law. Hence, the Fekete problem in the 3-dimensional space is the same as *the Thomson problem*.

As $s \to +\infty$, with N fixed, the s-energy is increasingly dominated by the term involving the smallest distance. Hence, $(\omega(s, P_N))^{1/s} \to 1/\min_{i\neq j} \| x_i - x_j \|$ as $s \to +\infty$. In this sense, the s-extremal energy problem leads to the Tammes problem. In the following discussion, $s = +\infty$ is often used to indicate the Tammes problem.

There are many results about the upper, lower bounds and asymptotics for the s-extremal energy, such as the bounds of $E_N^n(s)$ for $0 < s < n-1$ and $3 \leqslant n < s+1$ [13, 21, 36, 37]; for $-2 < s < 0, n = 3$ [21, 37]; for $s = 0, n = 3$ [21, 35]; for $s = +\infty, n = 3$ [12, 15, 31, 32, 34] and asymptotics of $E_N^n(s)$ as $N \to +\infty$ for $n = s+1 \geqslant 3$ [13]; $s = -1, n = 3$ [21, 41]; $s = 1, n = 3$ [13, 21, 23]; $s = 0, n = 3$ [21, 35, 41]; $s = +\infty, n = 3$ [34]. There are also some results about the lower bounds for the separation of any pair of points in an s-extremal spherical code, such as $s = 1, n = 3$ [5]; $s \geqslant n-1, n \geqslant 3$ [13]; $s = 0, n = 3$ [22] and $-2 < s < 0, n = 3$ [27]. For the case where $s \leqslant -2$, it is known that some equilibrium points may coincide [2]. Several conjectures, concerning the asymptotic behavior of $E_N^2(s)$, have been presented for $s \in (-2, 2)$ and $s > 2$, which are based on some numerical experiments [13, 21, 23]. In addition, other types of the packing problems with equal circles have been studied. For the problem of finding the maximum diameter of N equal mutually disjoint circles inside a unit square, exact solutions exist for $N = 1, \ldots, 10, 16, 25, 36$ [10, 16].

Numerical studies on determining the extremal energy $E_N^n(s)$ and searching for the related extremal spherical code $P_{s,N}^{n,*}$ have been conducted along with the-

oretical work on bounds and asymptotic behaviors of the extremal energy. There are many methods used or proposed to allocate the points on the sphere, such as constrained global optimization based on Glauber spin flip probability and Metropolis algorithm [1], simulated annealing [6], Monte Carlo simulation [8], the gradient method and quasi-Newton method [22]. Many numerical results for the sphere in the 3-dimensional space are provided, which include more extensive and accurate putative global solutions for $s = -1, 0, 1$ [1, 6–8, 11, 22]. Some global optimization methods for the SC problem and results about the spherical code of the Tammes problem in 4 and 5 dimension can be found in [18].

In this paper, we present a new formulation for the SC problem based on bilevel optimization and introduce the concept of the balanced spherical code and a new strategy for distributing points on the *n*-dimensional unit sphere. Our strategy, *the point balance algorithm* (PBA), is based on the simple idea that every point has the same significance at the beginning of distribution.

The paper is organized as follows: In Section 2, a characterization of the *s*-extremal spherical codes is presented. The concept of *L-balanced spherical code* is introduced at the end of Section 2. In Section 3, the point balance algorithm, which is based on the necessary condition for *s*-extremal spherical code, is presented and its convergence property is established. In Section 4, implementation issues are discussed and numerical results for the Fekete problem in 3, 4 and 5-dimensional space are reported.

2. A Characterization of the *S*-Extremal Spherical Code

A *s*-extremal spherical code for N ($N \geqslant 2$) points is a globally optimal solution of the following constrained minimization problem:

$$\min \quad f_s(P_N) \triangleq f_s(x_1, x_2, \ldots, x_N) \tag{4}$$

$$\text{s.t.} \quad x_i \in S^n, \forall i = 1, \ldots, N \tag{5}$$

where

$$f_s(P_N) = \begin{cases} \omega(s, P_N) & \text{if } s \geqslant 0 \\ -\omega(s, P_N) & \text{if } s < 0. \end{cases}$$

For convenience, in the following discussion, we define $f_s(\{x\}) = 0$ for any $x \in S^n$. If we decompose the set $I = \{1, 2, \ldots, N\}$ into two disjoint subsets I^+ and I^-, and denote the sub-spherical codes $\{x_j | x_j \in P_N, j \in I^{\pm}\}$ of P_N as $P_N(I^{\pm})$, then we can decompose the objective function $f_s(P_N)$ into three parts

$$f_s(P_N) = f_s(P_N(I^+)) + f_s(P_N(I^-)) + f_s(P_N(I^+), P_N(I^-))$$

where

$$f_s(P_N(I^{\pm})) = \sum_{i<j \in I^{\pm}} f_s(\{x_i, x_j\})$$

$$f_s(P_N(I^+), P_N(I^-)) = \sum_{i\in I^+, j\in I^-} f_s(\{x_i, x_j\}).$$

Therefore, the global optimization problem (4)∼(5) can be transformed into the following equivalent one, which is a bilevel optimization problem [17, 19]:

$$\min \quad \{f_s(P_N(I^-)) + \bar{f_s}(P_N(I^-))\} \tag{6}$$
$$\text{s.t.} \quad x_i \in S^n, \forall i \in I^- \tag{7}$$

where $\bar{f_s}(P_N(I^-))$ is the global optimal value of the sub-problem:

$$\min \quad \{f_s(P_N(I^+)) + f_s(P_N(I^+), P_N(I^-))\} \tag{8}$$
$$\text{s.t.} \quad x_j \in S^n, \forall j \in I^+. \tag{9}$$

The Tammes problem (i.e., $s = +\infty$) has a similar equivalent form of bilevel optimization, but the function $f_\infty(\{x_i, x_j\})$ should be defined by $1/\| x_i - x_j \|$ and $1/0$ should be regarded as ∞. The arithmetic operation $\sum$ or $+$ should be replaced by the operation max.

Most bilevel optimization problems are NP-hard from the complexity point of view [17, 19]. In general, computing locally optimal solutions is not easier than finding globally optimal solutions. It has been shown that the problem of checking local optimality for a feasible point and the problem of checking whether a local minimum is strict, are NP-hard [20]. Whether the bilevel optimization (6)∼(9) is NP-hard or not, is still an open problem.

For the bilevel global optimization problem (6)∼(9), $P_N(I^-)$ and $P_N(I^+)$ are referred to as *the reference code* and *the active code*, respectively. Sets I^- and I^+ are called *the reference index set* and *the active index set*, respectively. The following characterization can be obtained for the s-extremal spherical code $P_{s,N}^{n,*}$ (denoted by $P_{s,N}^*$ below).

THEOREM 2.1. *A spherical code P_N is a globally optimal solution of the problem* (4)∼(5)*, if and only if, given any $I^- \subset I = \{1, \ldots, N\}$ as a reference index set, and the active index set $I^+ = I \backslash I^-$, the sub-spherical code $P_N(I^+)$ is a globally optimal solution of the problem* (8)∼(9).

Proof. The necessity holds obviously. We only prove the sufficiency.

For any spherical code $P_N \subset S^n$ of N points which satisfies the hypothesis, define a function associated with it on the set $G = \{\ P_{s,N}^* \mid P_{s,N}^*$ is the solution of problem (4)∼(5)$\}$ by

$$g(P_N, P_{s,N}^*) = \sum_{i\in I} \delta(x_i - x_{s,i}^*)$$

where $P_{s,N}^* \in G$ and the real-valued function $\delta(x)$ satisfies the condition that $\delta(0) = 1$ and $\delta(x) = 0$ if $x \neq 0$. Let $g_M = \sup_{P_{s,N}^* \in G}\ g(P_N, P_{s,N}^*)$. Obviously, $1 \leqslant g_M \leqslant N$. In particular, $g_M = N$ if and only if $P_N \in G$. Next, we prove that $g_M = N$.

Since g_M is a natural number, there exists a $P^*_{s,N} \in G$ such that $g_M = g(P_N, P^*_{s,N})$ by definition of the supremum. Let $I^- = \{i \mid \delta(x_i - x^*_{s,i}) = 1\}$. It is clear that $f_s(P_N(I^-)) = f_s(P^*_{s,N}(I^-))$. If the number of elements in I^- equals to N, then we get $g_M = N$; otherwise, let $I^+ = I \backslash I^-$ be active index set. We now consider the problem (8)∼(9) corresponding to the reference index set I^-.

According to the hypothesis that $P_N(I^+)$ is a global solution of (8)∼(9), and $P^*_{s,N} \in G$, we obtain

$$f_s(P_N(I^+)) + f_s(P_N(I^+), P_N(I^-)) \leqslant f_s(P^*_{s,N}(I^+)) + f_s(P^*_{s,N}(I^+), P^*_{s,N}(I^-) = E_N(s) - f_s(P^*_{s,N}(I^-))).$$

Thus, P_N is a solution of (4)∼(5), i.e., $P_N \in G$. Therefore $g_M = g(P_N, P_N) = N$. This indicates that the set G contains all spherical codes such as P_N satisfying the hypothesis. □

DEFINITION 2.1. *Given an integer $L \in [1, N)$, a spherical code $P_N \subset S^n$ is called the L-balanced spherical code if, for any subset $U \subset I = \{1, \ldots, N\}$ with the size L, $P_N(U)$ is a globally optimal solution of the problem* (8)∼(9) *corresponding to $U^c = I \backslash U$ as the reference index set. In particular, a spherical code $P_N \subset S^n$ is called the* 1*-balanced spherical code if, $\forall i \in I$, $x_i \in P_N$ is a globally optimal solution of the problem* (8)∼(9) *corresponding to $I_i = I \backslash \{i\}$ as the reference index set.*

COROLLARY 2.1. *If a sphere code P_N is a globally optimal solution of the problem* (4)∼(5)*, then P_N is a L-balanced spherical code for any integer $L \in [1, N)$.*

3. A Point Balance Algorithm and its Convergence

Based on Corollary 2.1, a *point balance algorithm* (PBA) is presented to search for a 1-balanced spherical code in order to solve the SC problem. A detailed description of this algorithm is first presented, followed by the proof of convergence of the point balance algorithm. Some remarks about PBA are given at the end of this section. Note that PBA can be extended to search for a L-balanced spherical code.

ALGORITHM 1. The Point Balance Algorithm (PBA)

Step 1: Set the error tolerance $\varepsilon > 0$ and the parameters N, n, s. Begin with a randomly (or otherwise) chosen initial spherical code on the unit sphere S^n, denoted by $P_N^{(0)}$. Set $k = 0$ and the strategy index $SI_k = 1$.

Step 2: At the kth iteration, choose the strategy for modifying the iterate $P_N^{(k)}$. The exploratory spherical code $\hat{P}_N^{(k)} = \{\hat{x}_1^{(k)}, \ldots, \hat{x}_N^{(k)}\}$ is set by one of the following strategies. If $SI_k = 1$, then go to Step 3; otherwise, go to Step 4.

Step 3: Strategy 1:
For every $x_i^{(k)} \in P_N^{(k)}$, compute a point $\hat{x}_i^{(k)} \in S^n$ such that

$$f_s(\{\hat{x}_i^{(k)}\}, P_N^{(k)}(I_i)) = \min_{y \in S^n} f_s(\{y\}, P_N^{(k)}(I_i)). \tag{10}$$

Go to Step 5.

Step 4: Strategy 2:
For $i = 1, \ldots, N$, let $I_i^- = \{j | j < i\}$, $I_i^+ = \{j | j > i\}$ (may be an empty set) and compute a point $\hat{x}_i^{(k)} \in S^n$ such that

$$f_s(\{\hat{x}_i^{(k)}\}, \hat{P}_N^{(k)}(I_i^-) \cup P_N^{(k)}(I_i^+)) = \min_{y \in S^n} f_s(\{y\}, \hat{P}_N^{(k)}(I_i^-) \cup P_N^{(k)}(I_i^+)).$$

Go to Step 5.

Step 5: If $f_s(\hat{P}_N^{(k)}) < f_s(P_N^{(k)})$, find the value λ^* that minimizes the function $f_s(g(\theta_N^{(k)} + \lambda(\hat{\theta}_N^{(k)} - \theta_N^{(k)})))$, where $\theta_N^{(k)}$ and $\hat{\theta}_N^{(k)}$ are the hyperspherical coordinates of the spherical codes $P_N^{(k)}$ and $\hat{P}_N^{(k)}$, respectively. $g(\bullet)$ is the transformation from the hyperspherical coordinates of some points into their Cartesian coordinates (see (13)$\sim$(14) of Section 4 later). Let $P_N^{(k+1)}$ be the spherical code $g(\theta_N^{(k)} + \lambda^*(\hat{\theta}_N^{(k)} - \theta_N^{(k)}))$ and set the strategy index $SI_{k+1} = 1$. Otherwise, let

$$i^* = \text{argmin}\{f_s(\{\hat{x}_i^{(k)}\} \cup P_N^{(k)}(I_i)) | i \in I\}.$$

Let $P_N^{(k+1)}$ be the spherical code $\{\hat{x}_{i^*}^{(k)}\} \cup P_N^{(k)}(I_{i^*})$ and set the strategy index $SI_{k+1} = 2$.

Step 6: If $f_s(P_N^{(k+1)}) > f_s(P_N^{(k)}) - \varepsilon$, terminate PBA and output the spherical code $P_N^{(k+1)}$ together with its objective function value; otherwise, set $k \leftarrow k + 1$ and go to Step 2.

We give an example to illustrate how PBA works with the SC problem. Let us consider an instance of the Fekete problem:

EXAMPLE 1.

$$\begin{aligned} \min \quad & f_1(P_3) = f_1(x_1, x_2, x_3) \\ \text{s.t.} \quad & x_i \in S^2 = \{x \,|\, x^T x = 1, x \in \Re^2\}, i = 1, 2, 3. \end{aligned}$$

Variables x_1, x_2, x_3 are coordinates of three points A, B, C, respectively. Suppose that code $P_3^{(k)} = \{x_1^{(k)}, x_2^{(k)}, x_3^{(k)}\}$ is obtained at a certain iteration, where

$$x_1^{(k)} = (-0.8, -0.6)^T, x_2^{(k)} = (0.8, -0.6)^T, x_3^{(k)} = (-0.8, 0.6)^T.$$

It corresponds to an objective function value $f_1(P_N^{(k)}) = 1.95833$.

When Strategy 1 is used to modify $P_3^{(k)}$, we have

$$\hat{x}_1^{(k)} = (-0.6, -0.8)^T, \hat{x}_2^{(k)} = (1, 0)^T, \hat{x}_3^{(k)} = (0, 1)^T$$

by minimizing $f_1(P_3)$ with respect to x_i while $x_j = x_j^{(k)}$ $(j \neq i)$ are fixed, for $i = 1, 2, 3$. These vectors correspond to an exploratory spherical code $\hat{P}_3^{(k)} = \{\hat{x}_1^{(k)}, \hat{x}_2^{(k)}, \hat{x}_3^{(k)}\}$ with objective function value $f_1(\hat{P}_3^{(k)}) = 1.79317$. The points A_1, B_1, C_1, which correspond to $\hat{P}_3^{(k)}$, are shown in Figure 1.

When Strategy 2 is used to modify $P_3^{(k)}$, we have

$$\bar{x}_1^{(k)} = (-0.6, -0.8)^T, \bar{x}_2^{(k)} = (0.98995, 0.14142)^T,$$
$$\bar{x}_3^{(k)} = (-0.50949, 0.86047)^T$$

by minimizing $f_1(P_3)$ with respect to x_i while $x_j = \bar{x}_j^{(k)}$ $(j < i)$ and $x_j = x_j^{(k)}$ $(j > i)$ are fixed, for $i = 1, 2, 3$. These vectors correspond to another exploratory spherical code $\bar{P}_3^{(k)} = \{\bar{x}_1^{(k)}, \bar{x}_2^{(k)}, \bar{x}_3^{(k)}\}$ with objective function value $f_1(\bar{P}_3^{(k)}) = 1.74389$. The points A_2, B_2, C_2, which correspond to $\bar{P}_3^{(k)}$, are shown in Figure 2.

Based on any of these exploratory codes and their equivalent forms in polar coordinates, line search can be used to search for a better code.

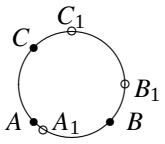

Figure 1. Example for Strategy 1.

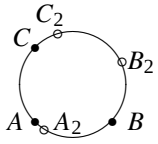

Figure 2. Example for Strategy 2.

From the point balance algorithm, we can see that $\{f_s(P_N^{(k)})\}$ is a monotonic decreasing sequence as k becomes larger and is bounded below. Therefore, PBA will terminate after certain iterations. We give the following conclusion about the convergence of the point balance algorithm as the error tolerance ε tends to zero.

THEOREM 3.1. *Let C_N be the set including all feasible spherical codes with N points on S^n (some feasible codes may have some identical points for certain value of the parameter s). Let f_s be a real-valued function defined by* (4) *on C_N. Given a code $P_N^{(0)} \in C_N$, $f_s(P_N^{(0)}) = \alpha$, define a level set*

$$L(f_s, \alpha) = \{P_N \mid P_N \in C_N, f_s(P_N) \leqslant \alpha\}.$$

Assume that f_s is continuous on $L(f_s, \alpha)$. Let $\{P_N^{(k)}\}$ be the sequence of codes generated by the point balance algorithm. For $k = 0, 1, 2, \cdots$, if the following condition holds:

$$f_s(P_N^{(k+1)}) \leqslant \min_{i \in I} f_s(\{\hat{x}_i^{(k)}\} \cup P_N^{(k)}(I_i)), \tag{11}$$

where $\hat{x}_i^{(k)}$ is defined by (10)*, $I = \{1, \ldots, N\}$ and $I_i = I \backslash \{i\}$, then every cluster point P_N^* of $\{P_N^{(k)}\}$ is a 1-balanced spherical code. In particular, for $s \in (-\infty, +\infty]$, if f_s is continuously differential at P_N^*, then $\nabla f_s(P_N^*) = 0$, where ∇f_s is calculated with respect to the spherical coordinates of points.*

Proof. If $\{P_N^{(k)} | k = 0, 1, \cdots\}$ is a finite set, then PBA terminates at $P_N^{(K)}$, where K is the number of iterates. Clearly, $P_N^{(K)}$ is a 1-balanced spherical code.

Without loss of generality, suppose that $\{P_N^{(k)} | k = 0, 1, \cdots\}$ is an infinite subset of $L(f_s, \alpha)$. Because $\{f_s(P_N^{(k)})\}$ is a monotonic decreasing sequence and is bounded below, it has a limit. In addition, S^n is a compact set and it follows from the Bolzano-Weierstrass theorem that there exists a subsequence $\{P_N^{(k_m)}\}$ of $\{P_N^{(k)}\}$ that converges to P_N^*.

If P_N^* is not a 1-balanced spherical code, then there exists a natural number p such that

$$f_s(\{\hat{x}_p^*\}, P_N^*(I_p)) = \min_{y \in S^n} f_s(\{y\}, P_N^*(I_p)) < f_s(\{x_p^*\}, P_N^*(I_p)).$$

Let $\hat{P}_{N,p}^*$ be $\{\hat{x}_p^*\} \cup P_N^*(I_p)$; then $\hat{P}_{N,p}^*$ is an interior spherical code of $L(f_s, \alpha)$ and $\epsilon = f_s(P_N^*) - f_s(\hat{P}_{N,p}^*) > 0$.

Based on continuity of f_s on $L(f_s, \alpha)$ and $\lim_{m \to +\infty} P_N^{(k_m)} = P_N^*$, we get

$$\lim_{m \to +\infty} f_s(P_N^{(k_m)}) = f_s(P_N^*)$$

$$\lim_{m \to +\infty} f_s(\{\hat{x}_p^*\} \cup P_N^{(k_m)}(I_p)) = f_s(\{\hat{x}_p^*\} \cup P_N^*(I_p)).$$

For sufficiently large k_m, the following inequality holds

$$\begin{aligned} & f_s(\{\hat{x}_p^*\} \cup P_N^{(k_m)}(I_p)) \\ & \quad \leqslant f_s(\{\hat{x}_p^*\} \cup P_N^*(I_p)) + \epsilon/2 \\ & \quad = f_s(P_N^*) - \epsilon/2. \end{aligned}$$

Since $\hat{x}_p^{(k_m)}$ is a globally optimal solution of $\min_{y \in S^n} f_s(\{y\} \cup P_N^{(k_m)}(I_p))$ and the hypothesis $f_s(P_N^{(k_m+1)}) \leqslant f_s(\{\hat{x}_p^{(k_m)}\} \cup P_N^{(k_m)}(I_p))$ holds, we have

$$f_s(P_N^*) < f_s(P_N^{(k_m+1)}) \leqslant f_s(\{\hat{x}_p^{(k_m)}\} \cup P_N^{(k_m)}(I_p)) \leqslant f_s(P_N^*) - \epsilon/2,$$

which is a contradiction from the monotonicity of the sequence $\{f_s(P_N^{(k)})\}$. Hence, P_N^* must be a 1-balanced spherical code. Based on the necessary condition of a local minimal point and the spherical coordinates of points, $\nabla f_s(P_N^*) = 0$ holds for $s \in (-\infty, +\infty]$ if f_s is continuously differential at P_N^*. □

REMARK. The conclusions in Theorem 3.1 still hold if the condition (11) is replaced by the following one: for $k = 0, 1, \cdots$, if

$$I^{(k)} = \{i \mid f_s(\{\hat{x}_i^{(k)}\}, P_N^{(k)}(I_i)) < f_s(\{x_i^{(k)}\}, P_N^{(k)}(I_i))\}$$

is not an empty set, there exists a natural number $p \in I^{(k)}$ such that

$$f_s(P_N^{(k+1)}) \leqslant f_s(\{\hat{x}_p^{(k)}\} \cup P_N^{(k)}(I_p)), \tag{12}$$

where $\hat{x}_i^{(k)}$ is defined by (10).

From Theorem 3.1 about convergence of PBA, the algorithm seems to solve N global optimization problems with respect to every $i \in I$. In order to find a 1-balanced spherical code, we do not need to get a globally minimal solution for every point due to the following reason: 'Global' and 'local' are relative concepts in the spherical code problem. When the separation of any pair of points in the s-extremal spherical code (such as $s > -2$) exists, the effect of one large change at one point is approximately equivalent to that of many small changes at multiple points simultaneously. Hence, it is sufficient to conduct a series of local optimizations for each point in order to find or approximate a 1-balanced spherical code for parameter $s > -2$. That is, we can use the following operation in place of the global optimization in Step 3 and 4 of PBA: Determine a closed neighborhood $U_i^{(k)}$ of x_i for every $i \in I$ at the kth iteration and find a local minimal solution in $U_i^{(k)}$ with respect to ith point of $\hat{P}_N^{(k)}$. For a certain value of the parameter s, it may be required that the neighborhood $U_i^{(k)}$ of x_i does not include other points. We also note that global optimization for a single point (not all points) is needed in order to assure that PBA is robust for the parameter $s \leqslant -2$.

4. Some Implementation Issues About PBA

Note that PBA can be used to distribute points on any sphere in a general n-dimensional space and determine the s-extremal energy. In the following, PBA is used to distribute points on the unit sphere in 3, 4 and 5-dimensional spaces and to determine the 1-extremal energy. Numerical experiments were conducted with an AMD K6-2/300 CPU processor, 64M memory and *MATLAB 5.3*.

Numerical results are presented in Table 1. Table 1 includes the number of points which range from 2 to 50, the dimension of space and the corresponding 1-extremal energy. In the 3-dimensional case, we have actually obtained the 1-extremal energy and the 1-extremal spherical codes (Fekete points) corresponding to the number of points ranging from 51 to 100. Our results for 51 to 100 points in the 3-dimensional space is similar to those reported in [11, 22], and thus are not listed here. It is also found that the number of equilibrium meta-stable states increases fast when N is large and all these meta-stable states have very close energies between 0.001 and 0.12 . Furthermore, we have found that the differences

of energies among these meta-stable states can not be very close (such as not less than 1.0e–6). If we can find a spherical code whose corresponding energy is close to the extremal energy at this error level, then this spherical code is very close to the extremal spherical code and can be improved to the extremal one by a powerful high precise local optimization algorithm. Given the number of points and the dimension of the space, PBA outputs the 1-extremal energy and its corresponding extremal spherical code. We let PBA be executed 20 times independently for every case and the initial code is chosen randomly before each execution. Computational times reported in Table 1 indicate the time it takes in the execution of finding the 1-extremal energy.

In the following, we discuss some implementation issues of the PBA algorithm. The constrained minimization problem (4)∼(5) can be transformed into the following unconstrained minimization problem:

$$\min f_s(P_N) \stackrel{\triangle}{=} f_s(g(\theta_1), \ldots, g(\theta_N)),$$

where $x_i = g(\theta_i) = (G_1(\theta_i), \ldots, G_{n-1}(\theta_i), \hat{G}_{n-1}(\theta_i))^T$ and θ_i is the hyperspherical coordinate of the point x_i, $i \in I = \{1, \ldots, N\}$. The transformation from the hyperspherical coordinate θ_i of a point into its Cartesian coordinate x_i is defined in [18] by

$$x_i^k = G_k(\theta_i) \stackrel{\triangle}{=} \cos(\theta_i^k) \prod_{t=1}^{k-1} \sin(\theta_i^t), \tag{13}$$

$$x_i^n = \hat{G}_{n-1}(\theta_i) \stackrel{\triangle}{=} \prod_{t=1}^{n-1} \sin(\theta_i^t), \tag{14}$$

where $k = 1, \ldots, n-1$ and $i \in I$. It is easy to see that $x_i \in S^n, \forall i \in I$. By the periodical property of the trigonometric function, $\theta_i^{n-1} \in [0, 2\pi]$ and $\theta_i^t \in [0, \pi]$, for $t = 1, \ldots, n-2$. Let us denote the domain of θ by Θ. This requirement reduces the search space, but it does not further restrict the problem.

The following strategy is also used in the implementation of PBA: The effect of one large change at one point is approximately equivalent to that of many small changes at multiple points simultaneously. We determine a closed neighborhood $U_i^{(k)} = \{\theta \mid |\theta^{n-1} - \theta_i^{n-1}| \leqslant 0.4, |\theta^t - \theta_i^t| \leqslant 0.2, t = 1, \ldots, n-2\}$ for each x_i in the hyperspherical coordinate space at the kth iteration. Certainly, the size of $U_i^{(k)}$ can be adjusted arbitrarily. Then we find a minimal solution of the function $f_s(\{g(\theta)\}, P_N(I_i))$ with respect to $\theta \in U_i^{(k)}$ by the pattern search algorithm [14, 30] and transform the solution into the domain Θ. Because the relative positions of points (i.e., structure of points) in the spherical code is more important than a single point's global minimal position or local minimal position, we can use a certain inexact algorithm to solve for the single point optimization problem in Step 3 and Step 4 of PBA, or adjust the size of neighborhood for every point, or allow the objective function value to increase a little in Step 5 of PBA.

Table 1. The Energy $E_N(1)$ and Running Time (seconds) of PBA

N	Dimension of Space 3		4		5	
	Energy	Time	Energy	Time	Energy	Time
2	0.5000000000	0.54	0.5000000000	0.86	0.5000000000	1.08
3	1.7320508076	1.22	1.7320508076	1.61	1.7320508076	3.04
4	3.6742346142	2.56	3.6742346142	2.58	3.6742346142	2.68
5	6.4746914947	2.66	6.3245553203	4.45	6.3245553204	3.22
6	9.9852813742	3.34	9.8280626463	5.26	9.6824583656	9.13
7	14.4529774142	5.17	14.0457593066	8.36	13.8915667961	11.24
8	19.6752878612	5.12	18.9705627485	7.79	18.8133440201	10.71
9	25.7599865313	7.95	24.8524723508	13.26	24.4452542432	18.88
10	32.7169494602	9.80	31.4414887344	17.54	30.7842712475	16.02
11	40.5964505082	11.50	38.8506628312	14.49	38.0803944122	23.31
12	49.1652530576	9.27	46.9772958043	13.68	46.0819991823	46.13
13	58.8532306117	12.87	56.0101273884	25.40	54.8414687111	59.68
14	69.3063632966	15.16	65.7725600449	18.07	64.3867543861	53.33
15	80.6702441143	24.00	76.3195838169	32.88	74.6446557516	59.16
16	92.9116553025	23.15	87.7825427621	41.61	85.6062329787	43.10
17	106.0504048286	26.35	100.0452496480	49.24	97.5413901586	86.65
18	120.0844674475	28.80	113.0728017807	70.90	110.2043928673	107.70
19	135.0894675567	33.11	126.9020228810	52.17	123.5951332472	96.74
20	150.8815683338	26.11	141.4633972296	68.04	137.6909394839	131.45
21	167.6416223993	45.34	156.9553620096	57.36	152.5634382327	106.42
22	185.2875361493	59.31	173.2994494671	98.21	168.4101533365	164.74
23	203.9301906629	62.27	190.4671590599	75.62	185.0042835723	149.92
24	223.3470740518	69.57	208.3373140876	94.75	202.3286626413	290.58
25	243.8127602988	68.77	227.1149670164	135.11	220.4056756676	180.71
26	265.1333263174	82.64	246.7116655734	150.11	239.2681370939	207.86
27	287.3026150330	102.27	267.1093955520	145.11	258.9793171561	281.58
28	310.4915423582	91.77	288.3353711326	175.51	279.4070088120	251.24
29	334.6344399204	136.52	310.3764656412	175.43	300.5862888064	295.40
30	359.6039459038	118.43	333.2591076218	234.00	322.5010963461	251.24
31	385.5308380634	115.93	356.9706923760	206.26	345.3071291545	395.42
32	412.2612746506	122.77	381.4576933643	158.90	368.7988169660	332.97
33	440.2040574479	127.59	406.7037565663	214.93	393.2984985854	480.10
34	468.9048532816	143.01	432.8171270786	240.99	418.5194699262	434.31
35	498.5698724907	150.86	459.9044158715	244.80	444.5351117287	526.48
36	529.1224083754	172.61	487.7461934186	298.24	471.2611700625	544.51
37	560.6188877310	189.72	516.3511306143	239.25	498.8414511878	492.23
38	593.0385035665	213.91	545.8403071907	317.29	527.1578481603	506.69
39	626.3890090168	228.73	576.1753571984	391.86	556.2545481522	675.04
40	660.6752788347	211.38	607.3059497544	358.13	586.0597565361	476.59
41	695.9167443419	218.56	639.2175331832	424.79	616.7855371793	484.78
42	732.0781075437	227.24	671.9323207345	524.31	648.2674257264	696.94
43	769.1908464594	285.10	705.4796399257	615.25	680.5772238874	802.41
44	807.1742630847	280.88	739.9028485970	446.70	713.6201171224	897.21
45	846.1884010611	325.48	775.1956954657	457.13	747.4599144210	785.83
46	886.1671136394	273.82	811.3883244928	508.79	782.1046050131	1049.13
47	927.0592706797	395.41	848.3771636310	615.39	817.5515554672	888.92
48	968.7134553438	378.05	886.1431085825	631.18	853.7564440154	1371.80
49	1011.5571826536	403.96	924.7333926864	802.29	890.7390584591	1000.52
50	1055.1823147264	330.06	964.0848033638	562.03	928.5425407307	1107.71

In order to accelerate the process of searching for the extremal spherical code, the algorithm calls the Broyden-Fletcher-Goldfarb-Shanno (BFGS) quasi-Newton algorithm at the final stage (the amount of decrease in the objective function is less than 0.1) and uses a simple quadratic/cubic interpolation algorithm for the line search [3]. This kind of accelerating strategy can be implemented by calling the subroutine *fminu.m* in *MATLAB 5.3*.

The proof of Theorem 3.1 shows that a decrease of the objective function corresponding to a certain point in a spherical code is essential in searching for a 1-balanced spherical code. Therefore, in the point balance algorithm, we should pay more attention to the significant points which result in a large decrease of the objective function. When the objective function is differential, some components in its gradient vector can be used to identify such significant points.

5. The Geometry of the 1-Extremal Spherical Code on S^3

Let $P_N = \{x_1, \ldots, x_N\}$ be a spherical code with N points on the unit sphere S^3 in the 3-dimensional space. Define

$$D_i := \{x \in S^3 \mid \|x - x_i\| \leqslant \|x - x_j\|, \ \forall j \in I\}$$

where $i \in I = \{1, \ldots, N\}$. Then D_i is called *the Dirichlet*(*Voronoi*) *cell* of x_i. The set $\{D_1, \ldots, D_N\}$ is a partition of S^3. Each D_i is a spherical polygon, i.e., its boundary consists of finitely many pieces of great circle arcs [22, 23]. It is known that the cell structure of 32 and 37-electrons resembles the C_{60} and C_{70} fullerenes, respectively [22, 23, 40]. If the centers of polygonal faces of a globally optimal configuration of 32 electrons on the sphere S^3 are linked (this process is called as *face–dual* operation [40]), a similar configuration of C_{60} molecule will be obtained. Except for C_{60}, C_{70} and C_{50}, most fullerenes from C_{20} to C_{70} with even-numbered carbon atoms have relatively low symmetries [40]. We have found that the cell structure of 14-electrons on S^3 has a similar property as above with respect to 1-energy $\omega(1, P_N^3)$ and is close to a globally optimal configuration of 24-electrons on S^3. Furthermore, we have observed an interesting phenomenon: If we pile up a globally optimal structure of 14-electrons and its face-dual structure on S^3, we will get a structure that is close to a globally optimal configuration of 38-electrons on S^3. We call this process as *structure-piling* operation.

The energy relationships among the globally optimal configurations of $N = 14, 24, 38$ are presented in the Tables 2, 3 and 4. Mass center is referred as the intersection of the sphere S^3 and a radius passing through the mass center of each polygonal face in a globally optimal configuration of $N = 14$. Dirichlet center is referred as the point in a Dirichlet cell that has equal distance to every vertex of polygonal face in a globally optimal configuration of $N = 14$. The energies corresponding to mass centers and Dirichlet centers for $N = 24, 38$ is presented in Table 2. The structures corresponding to these centers are close to globally optimal configurations. After these structures are relaxed, we get the globally min-

Table 2. The energy from face-dual and structure-piling operations

N	Optimal energy	Mass center	Dirichlet center
14	69.3063632966		
24	223.3470740518	224.9053099640	226.0894818638
38	593.0385035665	593.4042805188	593.3853109876

Table 3. The energy after relaxation of approximating configuration

N	Optimal energy	Mass center	Dirichlet center
14	69.3063632966		
24	223.3470740518	223.3470740545	223.3470740537
38	593.0385035665	593.0385035665	593.0385035666

imal energies for $N = 24, 38$ (see Table 3). The distribution of globally minimal energy for $N = 38$ is presented in Table 4. The energies corresponding to the sub-configurations for $N = 14, 24$ is slightly higher than their globally minimal energies.

An open question: Given the number of electrons N, can a globally optimal configuration for N-electrons on the unit sphere S^3 in the 3-dimensional space be obtained through a series of *face-dual* and *structure-piling* operations, i.e., is there a finite sequence $\{N_i | i = 1, \ldots, k\}$ such that $2 \leqslant N_1 < N_2 < \cdots < N_k = N$ and a globally optimal configuration of N_i electrons on S^3 can be obtained from that of N_{i-1} electrons through either *face-dual* operation or *structure-piling* operation? If yes, what is the minimal integer N_1 for the given N?

6. Concluding Remarks

The Spherical Code (SC) problem is considered in this paper using a formulation based on bilevel optimization. From this formulation, we introduce the concept

Table 4. Distribution of the globally minimal energy ($N = 38$)

N	Optimal Energy	Mass Center	Dirichlet Center
14	69.3063632966	69.3069040459	69.3069040877
24	223.3470740518	225.2370473819	225.2370506152
38	593.0385035665	593.0385035665	593.0385035666

of L-balanced spherical code and present a new approach, the Point Balance Algorithm (PBA), for searching for a 1-balanced spherical code. Since an optimal solution of the SC problem must be one of 1-balanced spherical codes, PBA can be used easily to search efficiently for an extremal spherical code of the Spherical Code problem on the unit sphere in the n-dimensional space $\Re^n$. In addition, we discuss the implementation issues of PBA. Some putative global optimal numerical results for the Fekete problem in 3, 4 and 5-dimensional spaces are also reported. Note that PBA can be extended to search for a L-balanced spherical code of the SC problem or used as a general strategy in solving other optimization problems. Finally, an open question about the geometry of Fekete points on the unit sphere in 3-dimensional space is posed.

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