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THE FEKETE PROBLEM AND CONSTRUCTION OF THE SPHERICAL COVERAGE BY CONES

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Abstract. We study whether the optimal solution of the Fekete problem (i.e. placement of n points on a unit sphere in $\mathbb{R}^d$ minimizing a certain potential function) can be used for construction of the spherical coverage by cones. The forces method (see [1]) is applied and different potentials are used for solving Fekete problem (Newtonian, logarithmic, Riesz-Fisher and Lennard-Jones). Such approach is easy for implementation and has good convergence properties. Results for $d = 3$ are compared to the referent results from [6]. A good agreement is shown (relative difference of the covering angles is less than 10% for all values of n and almost zero for some of them) which enables us to use the same methodology for higher dimensions where no referent results are available.

1. Introduction

Construction of uniformly placed points on a unit sphere $\mathcal{S}^d$ in $\mathbb{R}^d$ ($d \in \{3, 4, 5, \ldots\}$) is an important problem with various applications ranging from coding theory [2] to computational geometry and multidimensional databases [4]. There are many ways to model the criteria of "uniformity" of the points.

One of the most intuitive and mostly used approaches is to consider the minimization of the following functional

$$I(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n) = \sum_{1 \le i < j \le N} K(\mathbf{x}_i, \mathbf{x}_j), \quad \mathbf{x}_i \in \mathcal{S}^d, \quad i = 1, 2, \ldots, n$$

for a given n and d, where $K(\mathbf{x}, \mathbf{y})$ is a *kernel function*. This problem is known in literature as *Fekete problem* [5]. Usually, kernel function is given by $K(\mathbf{x}, \mathbf{y}) = \phi(\|\mathbf{x} - \mathbf{y}\|)$ where ϕ is some *potential function* and $\|\cdot\|$ is 2-norm. The potential $\phi(x) = x^s$ is known as *Riesz potential* and its special case $s = 2 - d$ corresponds to the electrostatic (or *Newtonian*) potential energy in d dimensions. The corresponding

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Fekete problem is known as Thompson problem in this special case [12]. Although this is a quite old problem, it is the subject of many recent papers (including [1, 10, 11]).

The other approach is to maximize a minimal pairwise distance between the points, i.e.

$$(\max) \quad \min_{1\le i<j\le n} \|\mathbf{x}_i - \mathbf{x}_j\|.$$

This problem is known as the Tammes problem or the optimal spherical code construction problem [7, 3]. It is known that Fekete problem with Riesz potential is reducing to the Tammes problem by taking $s \to -\infty$. So far the best solutions (for some combinations of n and d) of the Tammes problem can be found on the N.J.A. Sloane's homepage [7].

The third important approach to model a "uniformity" of points is known as *spherical coverage problem* [6]. Denote by $C(\mathbf{t}, \theta)$ the cone centered in $\mathbf{0}$, directed by $\mathbf{t} \in \mathcal{S}^d$ with the half-angle θ, defined in the following way

$$C(\mathbf{t}, \theta) = \{x \in \mathbb{R}^d \mid (\mathbf{x}, \mathbf{t})/\|\mathbf{x}\| \ge \cos\theta\}.$$

We assume that $\mathbf{0} \in C(\mathbf{t}, \theta)$ by definition. For a given n and d, the spherical coverage problem consists of finding a minimal angle θ such that there exist n cones of the half-angle θ, covering the entire space $\mathbb{R}^d$. In other words, it is needed the existence of points $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n \in \mathcal{S}^d$ satisfying

$$C(\mathbf{x}_1, \theta) \cup C(\mathbf{x}_2, \theta) \cup \ldots \cup C(\mathbf{x}_n, \theta) = \mathbb{R}^d.$$

The optimal solutions (covering angles θ as well as the corresponding points) of the spherical coverage problem for $d = 3$ and $n = 4, 5, \ldots, 130$ are available in [6]. It is recently shown in [9] that a verification variant of this problem (given the set of cones $C(\mathbf{x}_i, \theta_i)$, $i = 1, 2, \ldots, n$, with non-necessarily equal angles, find whether they cover $\mathbb{R}^d$) is an NP-hard problem.

The advantage of the Fekete problem is the fact that it enables the most easy and computationally inexpensive method for its solving, comared to the Tammes and spherical coverage problem. On the other side, spherical coverage problem seems to be the most advanced to solve. The intention of this paper is to consider whether the optimal solution of a certain Fekete problem can serve as a good approximation to the optimal solution of the spherical coverage problem. The positive answer on the previous question would enable an (both from the aspects of design and computational time) easy way to provide a good enough solution of the more difficult spherical coverage problem.

2. The Forces method for solving Fekete problem

The Forces method, introduced in [1], will be used to solve Fekete problem. It is the iterative method which starts from some given initial set of points $\mathbf{x}_1^0, \mathbf{x}_1^0, \ldots, \mathbf{x}_n^0 \in \mathcal{S}^d$

and computes the points in $k+1$-th iteration using the following scheme

$$\begin{aligned} \hat{\mathbf{x}}_i^{k+1} &= \mathbf{x}_i^k + \lambda^k \mathbf{w}_i^k \\ \mathbf{x}_i^{k+1} &= \hat{\mathbf{x}}_i^{k+1} / \|\hat{\mathbf{x}}_i^{k+1}\| \end{aligned} \tag{2.1}$$

for each $i = 1, 2, \ldots, n$ and $k \in \mathbb{N}_0$. Assume that $K(\mathbf{x}, \mathbf{y})$ is a symmetric function and that $I(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n)$ is represented in the following form

$$I(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n) = \frac{1}{2} \sum_{i=1}^{n} V_i(\mathbf{x}_i), \quad V_i(\mathbf{x}) = \sum_{j \neq i} K(\mathbf{x}, \mathbf{x}_j). \tag{2.2}$$

where $V_i(\mathbf{x})$ is total potential coming from all particles $j \neq i$ at point $\mathbf{x}$. In such case, the total force acting on particle i, denoted by $\mathbf{F}_i = -\nabla V_i(\mathbf{x}_i)$, can be written in the following form

$$\mathbf{F}_i = \sum_{j \neq i} \mathbf{F}_{ij}, \quad \mathbf{F}_{ij} = -\nabla K(\mathbf{x}, \mathbf{x}_j)\Big|_{\mathbf{x}=\mathbf{x}_i}. \tag{2.3}$$

Direction vector $\mathbf{w}_i^k$ is then computed by

$$\mathbf{w}_i^k = \mathbf{F}_i^k / \|\mathbf{F}_i^k\|. \tag{2.4}$$

Assuming that $K(\mathbf{x}, \mathbf{y}) = \phi(\|\mathbf{x} - \mathbf{y}\|)$, one can write

$$\mathbf{F}_{ij} = -\nabla K(\mathbf{x}, \mathbf{x}_j)\Big|_{\mathbf{x}=\mathbf{x}_i} = -\frac{\phi'(\|\mathbf{x}_i - \mathbf{x}_j\|)}{\|\mathbf{x}_i - \mathbf{x}_j\|}(\mathbf{x}_i - \mathbf{x}_j) \tag{2.5}$$

and find that $\mathbf{F}_{ij} = -\mathbf{F}_{ji}$ for each $i \neq j$. The magnitude of the step size λ^k is

$$\lambda^k = a \min_{1 \leq i < j \leq n} \|\mathbf{x}_i - \mathbf{x}_j\|. \tag{2.6}$$

where a is a given constant which is independent of the iteration number k. Note that the method similar to the forces method is also introduced in [10], but only for Newtonian potential.

3. Monte-Carlo method for initial points and covering angle computation

For a given cone directions $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n \in \mathcal{S}^d$, we need to compute a minimal angle θ_{min} such that $\bigcup_{i=1}^{n} C(\mathbf{x}_i, \theta_{min}) = \mathbb{R}^d$. A simple method for the accurate estimation of θ_{min} is based on the Monte-Carlo technique. Random point $\mathbf{X}_k \in \mathcal{S}^d$ is generated for each $k = 1, 2, \ldots, N$ and

$$\theta_k = \min\{\angle(\mathbf{X}_k, \mathbf{x}_i) \mid i = 1, 2, \ldots, n\}$$

is computed. Value θ_{min} is then estimated by

$$\theta_{min} \approx \bar{\theta} = \max\{\theta_1, \theta_2, \ldots, \theta_N\}.$$

In order to compute a uniformly distributed (pseudo)random point on a unit sphere $\mathcal{S}^d$, one can use the following expression (see for example [8]):

$$\mathbf{X}_k = \hat{\mathbf{X}}_k / \|\hat{\mathbf{X}}_k\|, \quad \hat{\mathbf{X}}_k = \text{randn}(d)$$

where randn(d) is d-dimensional vector of independent (pseudo)random numbers according to the zero-mean unit variance normal distribution $\mathcal{N}(0;1)$.

The same method can be used for generation of the initial set of points $\mathbf{x}_1^0, \mathbf{x}_2^0, \ldots, \mathbf{x}_n^0$, i.e. $\mathbf{x}_i^0 = \hat{\mathbf{x}}_i^0 / \|\hat{\mathbf{x}}_i^0\|$ and $\hat{\mathbf{x}}_i^0 = \text{randn}(d)$ for every $i = 1, 2, \ldots, n$.

A more accurate value of θ_{min} can be obtained using the spherical coverage verification algorithm, given in [9]. This algorithm can verify whether a given set of cones $C(\mathbf{x}_i, \theta_i)$ covers the entire space $\mathbb{R}^d$. Since obviously $\theta < \theta_{min}$, one can first compute a minimal k such that the angle $\theta_1 = \delta^k \theta$ (where $\delta = 1.05$, for example) is sufficient for covering (i.e. $\theta_{min} < \theta_1$) and then apply a binary search technique to find θ_{min}.

4. The algorithm

This section shows the complete algorithm for construction of the spherical coverage, based on the optimal solution of the Fekete problem for several given potentials. Forces method (described in section 2) is used for the optimization routine, while the covering angle is computed by methods given in the previous section.

Table 4.1 shows the list of potentials $\phi(x)$ we used for solving the corresponding Fekete problem.

Table 4.1: List of used potentials for solving the Fekete problem.

Name	$\phi(x)$	$\phi'(x)$
Newtonian	$cx^{-(d-2)}$	$-c(d-2)x^{-(d-1)}$
Riesz-Fisher	cx^s	csx^{s-1}
Logarithmic	$-c\log x$	$-c/x$
Lennard-Jones	$c\left(\left(\frac{r_m}{x}\right)^p - 2\left(\frac{r_m}{x}\right)^{2p}\right)$	$\frac{2cd}{r_m}\left(\left(\frac{r_m}{x}\right)^p - \left(\frac{r_m}{x}\right)^{2p}\right)$

Standard Lennard-Jones potential is obtained for $p = 6$ and serves as an approximation of the particle interaction in nuclear and solid-state physics. It is also called $6-12$ potential. For the purpose of numerical stability, we used a smaller value of exponent $p = 2$ and $r_m = (4\pi/n)^{1/2}$, where n is the current number of points on the sphere. These two potentials and forces are shown and compared in Figure 4.1. We found that Lennard-Jones potential is a good candidate since the value of the force is small if the distance between particles x is around r_m, and large if it is much smaller than r_m.

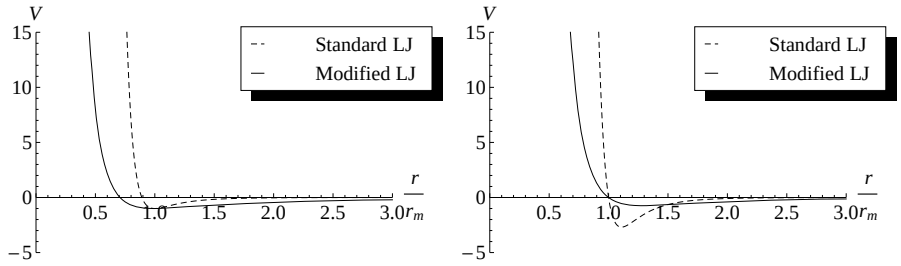

FIG. 4.1: Lennard-Jones and modified Lennard-Jones potential are shown on the left graph. The corresponding forces are shown on the right graph.

Since the force generated by all mentioned potentials tends to be very large when the particle distance x is small, a cutoff value x_0 is introduced. A modified potential is then defined by

$$\tilde{\phi}(x) = \begin{cases} \phi(x_0) + (x - x_0)\phi'(x_0), & x < x_0 \\ \phi(x), & x \geq x_0 \end{cases} \tag{4.1}$$

In such way, we the force intensity is constant and equal to $|\phi'(x_0)|$, for every $x \leq x_0$. It is worth stressing that this does not affect the actual optimizing behavior of the algorithm, it just ensures that no NaN-s are run into. Value of x_0 depends on which potential is used, but one way to select it is to bound $\phi'(x_0)$ by some value M (for example, $M = 1000$).

Complete optimization routine can be summarized as follows:

1. Choose the initial value of a of order 1 and set $k = 0$.
2. Compute the initial set of points $\mathbf{x}_1^0, \mathbf{x}_2^0, \ldots, \mathbf{x}_n^0 \in \mathcal{S}^d$.
3. Compute $\mathbf{x}_i^{k+1}$, $i = 1, 2, \ldots, n$ using (2.1) together with (2.4), (2.6), (2.5) and (2.3).
4. Compute total energy difference $\Delta I^k = I^k - I^{k+1}$ where I^k is the total energy in step k, i.e. $I^k = I(\mathbf{x}_1^k, \mathbf{x}_2^k, \ldots, \mathbf{x}_n^k)$. If $\Delta I^k < \Delta I^{min} = \ldots$, set $a := \delta' a$ where $0 < \delta' < 1$. Value $\delta' = 0.8$ turned out to be a good choice.
5. If $a > a^{min}$, where a^{min} is a constant of small order (10^{-6} is used), set $k := k + 1$ and go to step 3.
6. Compute the minimal covering angle.

Since we require the results for different values of n (i.e. $n = 3, 4, \ldots, 130$), the initial set of points for some value of n, can be chosen by adding additional

(randomly generated) point to the optimal solution for $n-1$. This strategy is applied in the step 2 of the previous routine.

Computation of the covering angle was done by Monte-Carlo method (described in section 3) and verified by spherical coverage verification algorithm from [9]. It is shown that by taking total $N = 10^9$ points, Monte-Carlo method produces the covering angle which differs by no more than 1% from the exact value (obtained by spherical coverage verification algorithm). It shows that Monte-Carlo method, which is much simpler for implementation, obtains a satisfactory good results for covering angle.

5. Numerical results

This section provides concrete numerical results for potentials given in the previous section. Results obtained for $d = 3$ are compared to those available in [6] (which will be referred as referent results).

5.1. Results in the case $d = 3$

Using the Newtonian potential $\phi(x) = x^{-1}$ iterations (2.1) converged fast and results could be easily obtained in real time. Covering angles are given on Figure 5.1 (left), together with the referent results from [6].

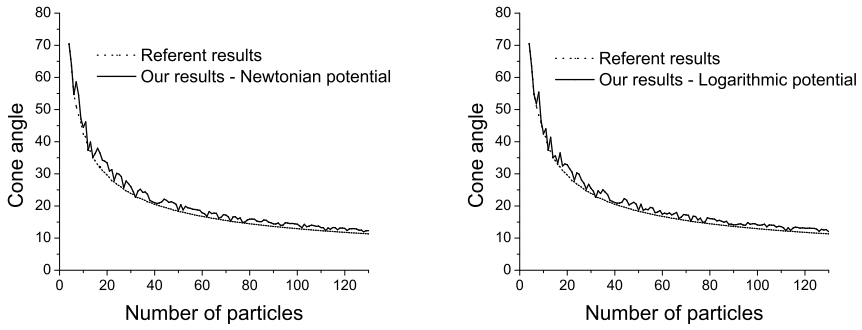

FIG. 5.1: Results (solid line) obtained using Newtonian potential (left graph) and logarithmic potential (right graph), compared to the referent results from [6].

It can be seen that the obtained covering angles are in most cases worse, but close to the ones obtained from the much harder problem of the optimal spherical covering construction. However, this difference is negligible small for the certain values of n (for example, $n = 4, 5, 6, 7, 12, 23...$). This phenomenon can rise a question

about the characterization of such values of n. It can be also noticed that for these values of n holds an additional property: covering angle is larger for $n+1$ points than for n points. That behavior is not intuitive.

It is also shown that Riesz-Fisher potential produces the best results for $s = -1$, hence we omit the results for other values of s.

The results obtained when using logarithmic potential $\phi(x) = -\log x$ are shown and compared to referent results on Figure 5.1 (right). As expected, no significant difference is found in comparison to Newtonian potential. Again, there are very good results for some values of n, and results that are up to 10% worse than referent results from [6].

The results obtained in the case of Lennard-Jones potential are shown and compared to the referent results on Figure 5.2. As one can see, this solution behaves in a very similar manner to previous two.

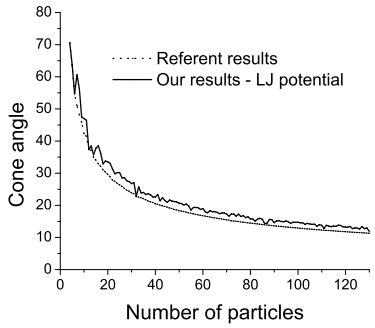

FIG. 5.2: Results (solid line) obtained using Lennard-Jones potential compared to the referent results from [6].

Finally, we compare our best obtained covering angles for all values of n (combining results from the three potentials) to the referent results. Comparison is given on Figure 5.3.

It can be seen that our covering angles are not more that 10% larger than the referent results from [6]. This encourages us to use the same methodology in higher dimensions and to expect satisfactory results. Those results are given in the following subsection.

5.2. Results in higher dimensions

As it turned out from the results presented in the previous section, no significant differences in covering angles are expected for all considered potentials. Hence, we only give the results for Newtonian potential $\phi(x) = x^{-(d-2)}$.

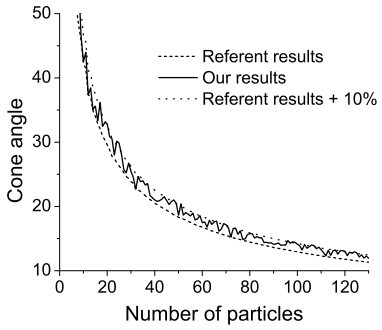

FIG. 5.3: Our combined results (solid line) compared to referent results from [6] (dotted line).

Figures 5.4, 5.5 and 5.6 show these results compactly. Note that there are no referent results which can be used for comparison in this general case. Analyzing these graphs, we see that there is a similar behavior as in the $d = 3$ case.

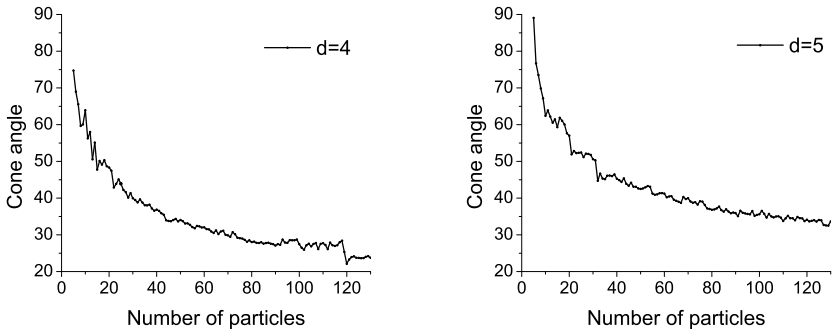

FIG. 5.4: Results for $d = 4, 5$.

Using the same methodology, one can easily obtain satisfactory results for an arbitrary dimension d.

6. Conclusion

According to experiments made for $d = 3$, we can conclude that by solving the Fekete problem with the forces method, one provides a good approximation of the optimal solution of spherical coverage construction problem. Moreover, this is achieved for all well-known potential functions, including Newtonian, logarithmic

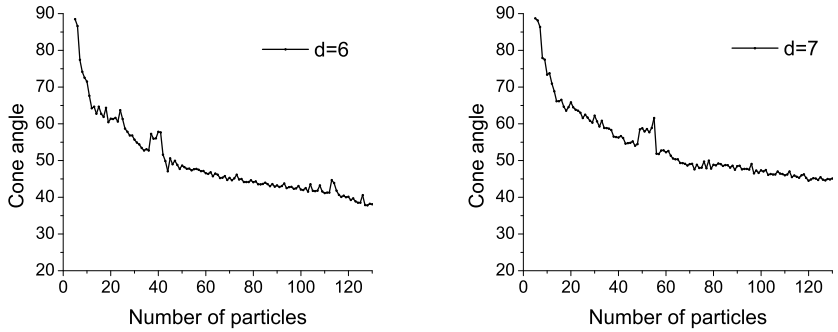

FIG. 5.5: Results for $d = 6, 7$.

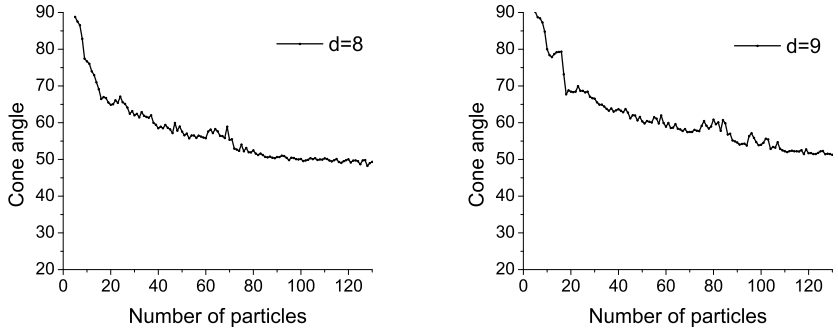

FIG. 5.6: Results for $d = 8, 9$.

and also (modified) Lennard-Jones potential. The fact that the time complexity is linear function of d encourages us to use the proposed scheme even for higher values of d. Moreover, the advantages of proposed method are ease of implementation and good convergence properties.

The choice of potential still remains an open question, since one may expect even better results by choosing some other function for the potential. The idea for using the potentials we used, comes from different physical models (Coulomb law, molecular forces, etc.), and these are given (together with their derivatives) by nice analytical expressions. However, the only required criterion is the ability to easily compute the derivatives (and the forces themselves).

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